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Universidad de Oviedo

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GEFES 2025

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GEFES 2025

PROGRAMME

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10:00	Invited: Alexey Nikitin (Donostia International Physics Center DIPC, Spain) *Hyperbolic Nanolight*
10:20	Invited: Andrea Mancini (Fondazione Istituto Italiano di Tecnologia, Italy) *Hyperbolic plasmon polaritons at visible frequencies in a van der Waals crystal*
10:40	Contributed: Yaiza Asensio (CIC nanoGUNE BRTA, Spain) *Chiral Hybrid Organic-Inorganic Manganese Chloride Perovskites with Circularly Polarized Photoluminescence from Bulk to Exfoliated Flakes*
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12:20	Contributed: Guadalupe Vega (University of Sevilla, Inst. Materials Science CSIC, Spain) *Extraction of effective optical constants of buried halide perovskite films for next generation optoelectronic devices*
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15:45	Invited: Miguel Romera (Complutense University of Madrid, Spain) *Reconfigurable classifier based on spin torque driven magnetization switching in electrically connected magnetic tunnel junctions*
16:05	Contributed: Manuela Garnica (*IMDEA Nanociencia, Inst. Nicolás Cabrera UAM, Spain*) *Engineering a Spin-Orbit Bandgap in Graphene-Tellurium Heterostructures*
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10:05	Invited: Amílcar Bedoya-Pinto (Institute of Molecular Science (ICMol), University of Valencia, Spain) *Topological and 2D materials grown by molecular-beam epitaxy: Synthesis and applications from the ultra-high vacuum perspective*
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Superconductivity & Low Temperatures

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16:20	Contributed: Yuriko Baba (*IFIMAC, UAM, Spain*) *Topological signatures and induced triplet pairing in proximitized quantum Hall - superconductor heterostructures*
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11:55	Keynote: Luca Giomi (Leiden University, The Netherlands) *Phase transitions in confluent epithelia*
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14:00	JUNTA GENERAL GEFES

ABSTRACTS

KEYNOTE

SPEAKERS

GEFES 2025

Optical near-field nanoscopy

Rainer Hillenbrand

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By recording the radiation scattered by a laser-illuminated atomic force microscope tip, imaging and spectroscopy with nanoscale spatial resolution can be achieved in the broad spectral range from visible to infrared to terahertz frequencies. In this talk, the basics of the technique and some applications in materials sciences and nanophotonics will be described.

Characterizing Bloch point magnetic singularities with pure experimental methods

Hierro-Rodriguez[1,2,3], J. Hermosa-Muñoz[1,2], A. Sorrentino[4], J.I. Martín[1,2], L.M. Álvarez-Prado[1,2], L. Aballe[4], E. Pereiro[4], C. Quirós[1,2], M. Vélez[1,2] and S. Ferrer[4]

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The magnetization field can be understood via the analysis of its topological characteristics as these strongly condition key properties of magnetization textures such as their stability or external stimuli responses [1,2]. Moreover, the topological properties of extended magnetic configurations condition the reversal and magnetic texture nucleation events, setting a different point of view for the understanding of these important processes in magnetic systems [3]. In this framework, a key point to get access to the topology of magnetic systems is the capability of volume resolving the three-dimensional magnetization vector field. This can be done via micromagnetic approaches for in-silico studies, but since the development of magnetic vector tomography, a purely experimental window has been open for direct characterization of the magnetization [4,5].

In this work, we characterize the full vector magnetic configuration of several magnetic systems focusing on Bloch point magnetic singularities. Specifically, we have analysed Ni80Fe20/NdCo5/Ni80Fe20 and Gd12Co88/NdCo5/Gd24Co76 ferromagnetic and ferrimagnetic heterostructures, and Ni80Fe20 microstructures. We use the unique capabilities of Soft X-ray vector tomography to access experimentally their topological characteristics [5] as well as their interactions [3]. Finally, we show how it is possible to engineer magnetic configuration of Bloch points by tuning the different magnetic interactions via multilayer design in ferrimagnetic/ferromagnetic heterostructures [6].

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Illuminating van der Waals materials with advanced TEM and machine learning

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Engineered van der Waals (vdW) materials hold tremendous promise for revolutionizing condensed matter science and driving innovation in nanoelectronics, nanophotonics, quantum communication, and sensing. These materials can be assembled into a variety of homo- and heterostructures, where strain fields, material combinations, and twist-angle manipulation generate new crystal lattice periodicities (moiré patterns), giving rise to phenomena such as exciton trapping, bandgap modulation, and unconventional superconductivity.

In this talk, I highlight recent progress in the fabrication, analysis, and interpretation of vdW materials in non-trivial configurations beyond planar structures. To achieve this, we exploit recent breakthroughs in advanced Transmission Electron Microscopy (TEM) and related techniques, such as four-dimensional (4D) Scanning Transmission Electron Microscopy (STEM) and Electron Energy Loss Spectroscopy (EELS). We deploy machine learning algorithms originally developed for high-energy particle physics for TEM data analysis, using custom-tailored open-source code developed in-house. This strategy enables to precisely control lattice reconstruction, strain- and defect-engineering, and electrostatic field distributions down to the nanoscale. I showcase key results obtained through this way, including the onset of modulated bandgaps and exciton localisation in MoS_2 nanotubes, strain-driven bandgap variations in twisted WS_2, and enhanced non-linear optical emission in large-scale arrays of Mo/MoS_2 core-shell nanopillars.

Our results illustrate how developing novel material configurations unlocks unique functionalities in vdW homo- and heterostructures, when combined with cutting-edge data processing and interpretation algorithms. This pave the way for pioneering new platforms that advance applications ranging from light sources for quantum communication to low-power electronics.

The nickel age of superconductivity

Antia S. Botana

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The physics behind high-temperature superconductivity in cuprates remains a defining problem in condensed matter physics. Among the myriad approaches to addressing this problem has been the study of alternative transition metal oxides with similar structures and electron count. After a 30-year quest, a non-cuprate compound with a cuprate-like structure that exhibits superconductivity was discovered in 2019: hole-doped $NdNiO_2$. Given that this material is one of the members of a larger series of layered nickelates, this result opened up the possibility of a new family of unconventional nickel-based superconductors. By means of first-principles calculations, we have analyzed the similarities and differences between this family of low-valence planar nickelates and the cuprates. Even though these nickel oxide materials possess a combination of traits that are widely considered as crucial ingredients for superconductivity in cuprates (a square-planar nature, combined with the appropriate 3d-electron count, and a large orbital polarization) they also exhibit some important differences (a larger p-d energy splitting, and lack of magnetism in the parent compounds). Our results show that low-valence layered nickelates offer a new way of interrogating the cuprate phase diagram and are singularly promising candidates for unconventional superconductivity.

Engineering nanoscale materials properties for optoelectronics and energy applications

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Semiconductor nanostructures, such as nanocrystals or 2D transition metal dichalcogenides are very versatile material systems offering a manifold of interesting properties ranging from size or thickness dependent electronic properties to many body interactions and plasmonic response. At the nanoscale any chemical or structural perturbation impacts their optoelectronic response. For example, their nanoscale surface is very sensitive to defects, trap states or depletion layers [1]. Precise chemical, structural and electronic design allows controlling and modulating such properties. This starts at the stage of preparation and ranges to the intentional engineering of their nanoscale properties. In this presentation I will present our efforts in modulating the properties of 2D materials by coupling them to nanocrystals with the aim of enhancing their photoresponse [2]. I will then present our recent efforts in the design of metal oxide nanocrystals through depletion layer engineering for their use in photon energy storage [3].

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Phase transitions in confluent epithelia

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In spite of the absence of gaps and interstitial structures, confluent layers of epithelial cells are able to migrate collectively and remove excess cells by extrusion. While in common with foams and other passive confluent fluids, both these phenomena crucially rely on the active remodelling of the cellular network, via topological transformations known as T1 and T2 processes. Using a combination of active hydrodynamics and Renormalization Group methods, I will show that both collective migration and cell extrusion can be thought as continuum phase transitions, with the former being in the same universality class of the Kosterlitz-Thouless transition and the latter reminiscent of sublimation in solids.

ABSTRACTS

INVITED

SPEAKERS

GEFES 2025

Hyperbolic nanolight

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Polaritons –dipole excitation in a matter coupled to electromagnetic fields– in van der Waals (vdW) crystals can enhance light-matter interactions at mid-infrared frequencies, owing to their extreme nanoscale field confinement and long lifetimes. Particularly, in some crystals the dispersion of polaritons –the relation between the momentum and energy– can take a hyperbolic shape. As a result, "hyperbolic light" can only travel along some specific directions in space, where it demonstrates highly non-intuitive "negative" reflection and refraction, negative phase and group velocities, canalization (propagation of light along very narrow sectors in space) and deeply subwavelength focusing. In this talk we outline the recent advances in the theoretical description of hyperbolic polaritons as well as interpretation of state of the art near-field experiments.

Figures

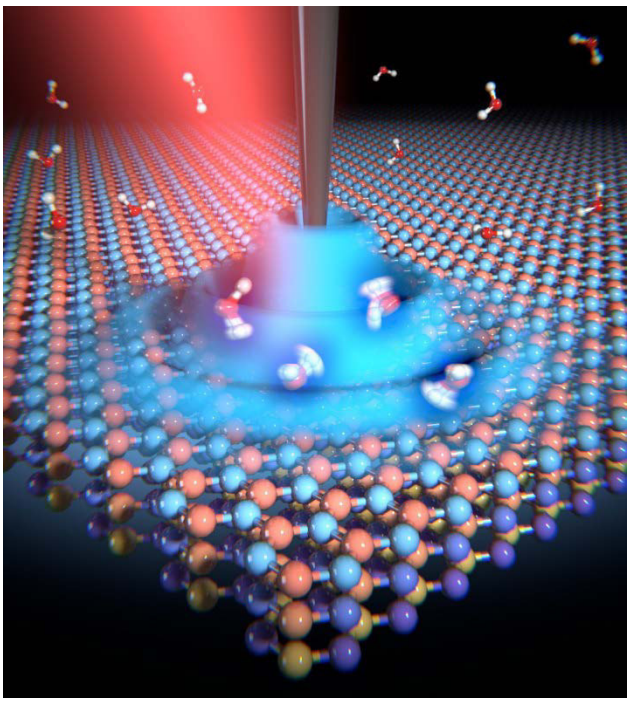

Figure 1: An artistic image of a polariton in a vdW crystal layer interacting with molecules via a near-field probe.

Hyperbolic plasmon polaritons at visible frequencies in a van der Waals crystal

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Polaritons, hybrid light-matter excitations that couple photons with quantum states of materials, have been fundamental in advancing the control of light at the nanoscale, enabling advancements in fields like heat management[1], photocatalysis[2], and nonlinear optics[3]. The nature of polariton confinement is determined by the material permittivity, with anisotropic materials capable of supporting unique wavefronts, including hyperbolic polaritons. The associated unbounded hyperbolic isofrequency contours enable deeply subwavelength confinement thanks to the high supported momenta. Van der Waals (vdW) materials hosting hyperbolic phonon polaritons, such as hBN[4] and MoO_3[5] have been largely investigated, but their utility is restricted to infrared (IR) frequencies due to the characteristic energy of optical phonons. For visible light applications, engineered metamaterials have been employed, though they are limited by fabrication challenges and ohmic losses in their metallic components[6]. We introduce molybdenum oxide dichloride ($MoOCl_2$) as a natural vdW material that supports low-loss, in-plane hyperbolic plasmon polaritons (PPs) in the visible and near-IR ranges. We present both theoretical insights and experimental validation through far field reflectivity, atomic-resolution AFM and direct near-field imaging of hyperbolic contours. Our results highlight $MoOCl_2$ potential for advanced light confinement at visible frequencies. $MoOCl_2$ air stability and natural hyperbolic response provide a unique platform for hyperbolic polaritonics without the need for protective layers or complex fabrication, overcoming the limitations of lossy metals and lithographic constraints in metamaterials.

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Terahertz Photoresponse in Graphene Moiré Superlattices

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In recent years, terahertz (THz) radiation has been shown to be extremely powerful for the accurate characterization of graphene and other two-dimensional (2D) materials [1,2]. Within this context, several THz-based techniques have emerged as efficient, rapid and (in some cases) scalable methods to quantify and map the electrical parameters of these nanomaterials such as DC conductivity, carrier density, and carrier mobility [1,2,3], as well as examine subtle electronic properties of these films, including interaction-induced phenomena [3,4]. However, little is known about the application of THz radiation to probe the electrical/electronic properties of 2D materials stacked into the so-called van der Waals (vdW) heterostructures.
In the present work, we explore the use THz radiation to unveil the electronic structure of graphene-based moiré superlattices, unique vdW systems obtained (in this case) by aligning the crystal lattices of graphene and hexagonal boron nitride (hBN) by an angle $\theta < 2^\circ$ (see Figure 1a). We demonstrate that the THz photorresponse measured in devices made from these superlattices is enhanced and exhibit features that can be directly ascribed to the specific changes occurring in graphene´s bandstructure due to the presence of the periodic moiré potentials. Such characteristics comprise miniband structures featuring a new generation of Dirac fermions, the so-called secondary or superlattice Dirac points, (sDPs, Figure 1b), as well as more precise details, including the reduced Fermi velocity of charge carriers or the presence (and size) of the energy gaps at the sDPs.
The presented level of understanding highlights THz radiation as an exceptional frequency to probe the low-energy physics of Dirac electrons in periodic nanostructures. Moreover, from a more technological perspective, the observed enhanced photorresponses prompt graphene-based superlattices as unique materials for sensitive THz photodetection.

References

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Figures

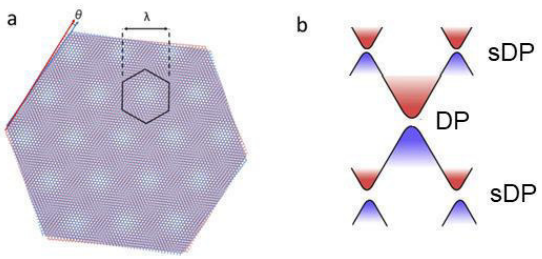

Figure 1: a, Illustration of a moiré pattern with wavelength λ, generated by aligning graphene (red) and hBN (blue) honeycomb lattices by an angle $\theta < 2^\circ$. b, Bandstructure of graphene/hBN moiré superlattices featuring a new generation of Dirac fermions (secondary or superlattice Dirac points, sDPs)

Reconfigurable classifier based on spin torque driven magnetization switching in electrically connected magnetic tunnel junctions

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A promising avenue in neuromorphic computing aims to perform cognitive operations directly in hardware, leveraging the physics of efficient, well-established nano-devices [1]. Spintronic devices, such as spin torque oscillators and superparamagnetic tunnel junctions, have emerged as promising processing units in neuromorphic networks [2-4]. However, the most mature and well-established spintronic technology is spin-transfer torque magnetic random-access memories (STT-MRAM), which relies on magnetic tunnel junctions where the spin-transfer torque effect switches the free layer magnetization between two stable states (parallel and antiparallel), characterized by a different resistance. Performing complex computing tasks with the same devices and working principles used in industrial STT-MRAM memories holds great potential for fast, large-scale integration, making it a highly attractive technological prospect. However, so far STT-MRAM devices have been investigated in neuromorphic networks only as synaptic (memory) elements [5], which require additional (software) processing units to perform classification tasks. To date, these devices have not been used experimentally as interconnected processing units capable of learning pattern recognition.

In this work, we present a reconfigurable classifier based on a network of electrically connected magnetic tunnel junctions that categorizes information encoded in the amplitude of input currents through the spin torque-driven magnetization switching output configuration [6]. The network can be trained to classify new data by adjusting additional programming currents selectively applied to the junctions. We experimentally demonstrate that a network composed of three magnetic tunnel junctions can learn to classify seven spoken vowels with a recognition rate of 96%, surpassing the performance of software neural networks with the same number of trained parameters. This first demonstration of real-time learning and pattern recognition using STT-MRAM devices and principles constitutes a significant step toward the rapid, large-scale integration of neuromorphic hardware.

References

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Transport Signatures of Altermagnetic Phases

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Spin transport phenomena in antiferromagnets have garnered significant attention due to the advantages these materials offer over ferromagnets, such as absence of stray field or faster spin dynamics. [1] However, antiferromagnets were traditionally not considered efficient sources of spin current. This perception has changed with the recent identification of a new class of compensated magnets – altermagnets. [2] The unconventional magnetic phase in these materials arises in crystals where opposite-spin sublattices are related by a rotational symmetry transformation. A key feature of this phase is an alternating spin polarization in both the real-space crystal structure and the momentum-space electronic structure.

In this presentation, I will focus on the experimental verification of the altermagnetic phase in various materials, with a particular emphasis on spin transport phenomena. One of the most significant magneto-transport effects, the anomalous Hall effect, was previously thought to be absent in collinear compensated magnets. However, since the discovery of altermagnetism, it has been observed in collinear systems such as MnTe [3], and Mn_5Si_3 [4]. Remarkably, we observe a spontaneous anomalous Hall effect, which occurs even at zero magnetic field and has a peculiar anisotropy. [5,6]

Additionally, I will discuss the observation of the anomalous Nernst effect in a compensated collinear magnet [7], along with its implications. Finally, I will explore the potential consequences for spin transport in insulating altermagnets.

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Magneto-structural intricacies at the mesoscale in van der Waals magnetic materials: challenges and opportunities

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The first van der Waals material to exhibit a sizeable spontaneous ferromagnetic hysteresis down to the monolayer was chromium triiodide (CrI_3) [1]. Strikingly, this observation was accompanied by a transition from a layered ferromagnetic to a layered antiferromagnetic order as the thickness of the crystal was reduced to the nanoscale [2]. The discovery of layered-dependent magnetism in CrI_3 posed a longstanding fundamental conundrum that lasts to date, motivating a wealth of fundamental studies seeking the origin of this phenomenon. This effect can be underpinned by the structural differences of bulk and few-layer CrI_3, where different stacking orders result in different types of spin exchange coupling [3]. However, an explanation for the layer-dependent stacking structural transition is still missing and, more interestingly, this effect might be general to other van der Waals materials with layered structures [4]. In addition, the exact crossover thickness from the bulk to the few layer regime appears to lie, surprisingly, in the mesoscale and has not been determined with accuracy. Other controversies regarding the presence of odd features in the in-plane magnetisation curve [5] and the coexistence of different structural phases in bulk single crystals of this material [6] have just kept adding layers of complexity to the problem of this archetypal magnetic 2D material. In this talk, I will portray our history of experimental insights regarding a rich coexistence and layer dependence of electronic, magnetic and crystalline phases in the archetypal magnetic van der Waals material CrI_3 beyond the reported monoclinic-rhombohedral stacking dichotomy [7]. With these results I aim to highlight a far more intricate scenario than originally thought and to discuss the challenges and opportunities provided by the family of magnetic 2D materials by also showcasing other interesting members of the rich group of the metal halides.

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Topological and 2D materials grown by molecular-beam epitaxy: Synthesis and applications from the ultra-high vacuum perspective

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In this talk, I will discuss how molecular beam epitaxy (MBE) allows the realization of fertile experimental platforms to understand and exploit exotic material systems, such as topological semimetals and two-dimensional magnets.

In the first part, I will present the long-sought thin film realization of a Weyl Semimetal [1], a recently discovered topological material class featuring a linear electronic band dispersion – known as the three-dimensional analogue of graphene. In particular, I will discuss how topology and electronic structure are linked to epitaxy-dependent parameters such as strain, doping and surface termination [2]. With a careful preparation of *in-situ* heterostructures, a practical use of topological properties will be showcased for applications in spin-orbitronics.

In the second part, I will focus on the van-der-Waals epitaxy of a two-dimensional magnet, a $CrCl_3$ monolayer grown on Graphene/6H-SiC(0001). *In-situ* X-ray magnetic circular dichroism studies reveal intrinsic ferromagnetic order with easy-plane anisotropy and a 2D-XY magnetic universality class [3] in this quasi-freestanding large-area monolayer magnet. The important role of the van der Waals substrate interaction and the underlying crystal symmetry to achieve this rather unsual magnetic behavior will be discussed, thereby highlighting routes on how to control the anisotropy of 2D magnets via growth engineering. Finally, further peculiarities of MBE-grown van der Waals magnets, such as an increase of the Curie Temperature driven by self-intercalation [4], will be shown in the prototypical high-T_c magnet Fe_5GeTe_2.

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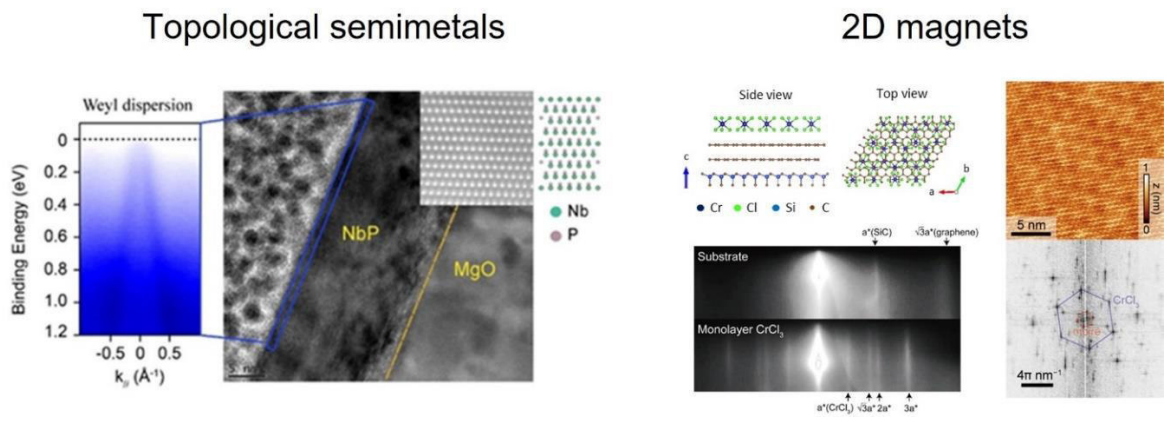

Figure 1: (left) NbP thin films (thickness: 9 nm) showing linear electronic band dispersion by ARPES. (Right) Structural properties of a $CrCl_3$ monolayer grown on a Graphene/6H-SiC (0001) substrate.

Bright single photon sources with emergent materials

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The nanoscale control of light-matter interactions allows to create new optoelectronic devices for a wide span of nonlinear and quantum photonic applications. A key part of this endeavor is the exploration of novel materials, which reveal unique properties that can be tailored to specific applications. Regarding the implementation of solid-state single photon sources, relevant emergent materials for quantum light emission are quantum dots in transition metal dichalcogenides monolayers, perovskite quantum dots, or also defects in hexagonal boron nitride nanocrystals. [1]

An optimal single-photon source should satisfy three essential criteria: (1) the emission of photons "on demand", (2) emit one photon at a time, and (3) high degree of temporal coherence and uniformity in the properties of emitted photons (spectrum, polarization, spatial mode). Achieving this ideal quantum performance relies on using a resonant cavity to enhance the emitter's spontaneous decay rate via the Purcell effect.

In the first part of this talk, we will present recent advancements in generating single photons from atomically thin WSe_2 monolayers. Local stress within these monolayers creates a confining potential that traps single excitons, resulting in single-photon emission. By embedding these quantum dots in a cryogenic Fabry-Pérot optical cavity, we achieve record emission-efficiency levels. [2] Initial quantum communication tests with these sources further demonstrate their viability for single-photon applications. [3]

In the latter part of the talk, I will discuss our experimental progress with an alternative material platform: single defects in hexagonal boron nitride. This emitter, operable at ambient conditions and integrated with a Fabry-Pérot cavity, offers a promising option for cryogenic-free quantum optical applications, including free-space quantum key distribution.

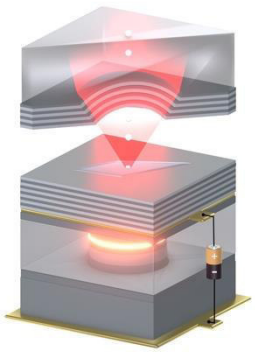

Figure 1: Schematic of the single photon device, composed by a quantum emitter in a hexagonal boron nitride monolayer, embedded in a reconfigurable Fabry-Pérot open cavity.

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Advanced Characterization of Materials by 4-Dimensional Scanning Transmission Electron Microscopy (4D-STEM)

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The scanning transmission electron microscope (STEM) has established itself as a pivotal technique for the characterization of materials, offering unparalleled capabilities for probing their structure and properties at the nano and atomic scales. Through the use of a finely focused sub-Å probe scanned over the sample, the STEM facilitates the simultaneous acquisition of multiple analytical signals with single-atom sensitivity [1]. This versatility makes it a powerful tool for the detailed characterization of materials and devices, providing profound insights into their physical, chemical, and electronic properties.

In recent years, new technologies in ultrafast and direct electron detectors have driven the development of the 4-dimensional scanning transmission electron microscopy technique (4D-STEM). This technique, which has brought about a complete revolution in the field of electron microscopy, is based on the geometry of the STEM, that allows the acquisition of a 2D image of the transmitted electron beam at the diffraction plane for each probe position as the beam is scanned over a 2D area of the material in real space. The resulting data cube exhibits a four-dimensional nature (2D in real space + 2D in diffraction space) and provides the full picture of the electron beam-specimen interaction, allowing diffraction experiments such as pattern classification, phase-orientation, or strain mapping [2]. Furthermore, the 4D-STEM technique is sensitive to the distribution of transmitted electrons in momentum space allowing the direct imaging of electric and magnetic fields in materials with atomic resolution [3].

This talk will provide an overview of the 4D-STEM technique and highlight our recent results in the advancd characterization of point defects, nanoestructures and interfaces.

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Planar Ge: spin qubits and more

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While Ge was used to realise the first transistor at Bell labs in 1947, only recently has it moved in the focus of attention for its potential for quantum information [1]. In the past few years, impressive progress has been achieved. However, there are still open challenges, such as spin misalignment due to spin-orbit interaction and long-distance spin-spin coupling. In this talk, I will report on microwave singlet-triplet qubits that allow us to characterize the misalignment between neighbouring spins. Furthermore, I will report on circuit quantum electrodynamic experiments in planar Ge. With the use of granular Aluminum as material for the realization of high-impedance resonators, charge-photon coupling with a strength of about 600MHz has been realized, paving the way towards strong spin-photon coupling.

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Coulomb screening of superconductivity in magic-angle graphene bilayers

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The origin of superconductivity in magic-angle twisted bilayer graphene has been a subject of intense debate. While some experimental evidence indicated an unconventional pairing mechanism, efforts to tune the critical temperature by screening the Coulomb interactions have been unsuccessful, possibly indicating a conventional phonon-mediated pairing. Here we study a double-layer electronic system consisting of two twisted graphene bilayers in the immediate proximity of each other but remaining electronically decoupled. By increasing the carrier density in one bilayer, we completely suppressed both the superconductivity and the correlated-insulator state in the adjacent magic-angle graphene. The observation of such a screening effect offers strong support for an unconventional mechanism of Cooper pairing in magic-angle twisted bilayer graphene, shedding new light on the underlying physics governing their properties.

Exciton topology and quantum geometry

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Topology, and more generally, quantum geometry, have emerged as a powerful tool to understand and classify states of matter. The focus has mostly been on electronic topology, and examples of topological materials include topological insulators, Chern insulators, and Weyl and Dirac semimetals. While free fermion topology is now well understood, the role that interactions play on the topological properties of materials remains an open question. An example of an interacting system are the electron-hole bound states, or excitons, which form upon photoexcitation in semiconductors.

In this talk, I will describe our work on exciton topology and exciton quantum geometry. Using a combination of phenomenological theory and first principles calculations, I will discuss the interplay between individual electron and hole topologies and the resulting exciton topology. I will also describe some physical consequences of the underlying exciton topology and geometry, with a focus on exciton transport. Finally, I will present a family of organic semiconductors which host the proposed exciton topology and discuss the wider implications of our findings for optoelectronics devices such as solar cells.

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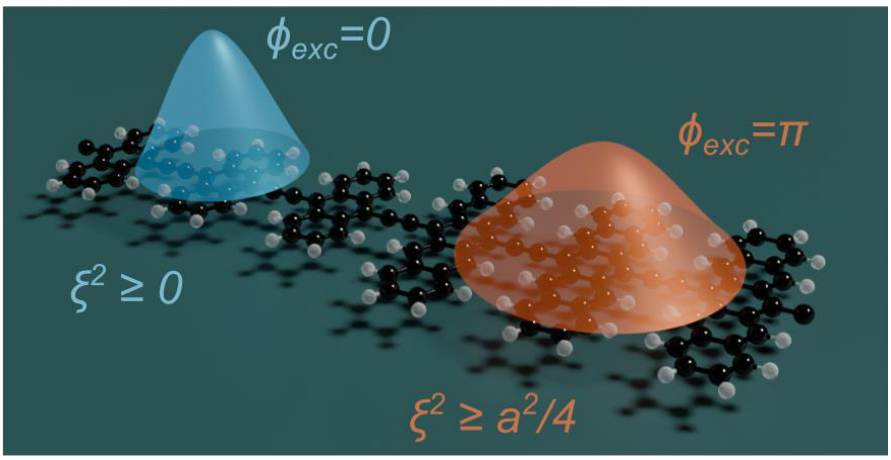

Figure 1: Schematic representation of trivial (blue) and topological (orange) excitons in a polyacene chain. The spread ξ of topological excitons necessarily exceeds the size of the unit cell.

Molecular transport in lipid mesophases: a challenge at multiple scales

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Lipid mesophases are aggregates formed by lipid-water mixtures in various contexts, appearing for instance in vivo during digestion and in various applications for drug delivery, protein crystallization and cryo-enzymatic reactions. These objects are characterized by peculiar topological and geometrical features at the nanoscale [1], which regulate the diffusion of molecules therein and have therefore a major impact on the applications based on mass transport. In this talk, I will illustrate our efforts to understand how the nanoscopic properties of lipid mesophases [2] and of the water nanoconfined in their channels [3,4] determine transport at the macroscopic scales [2,5,6] relevant for the practical applications of these fascinating systems.

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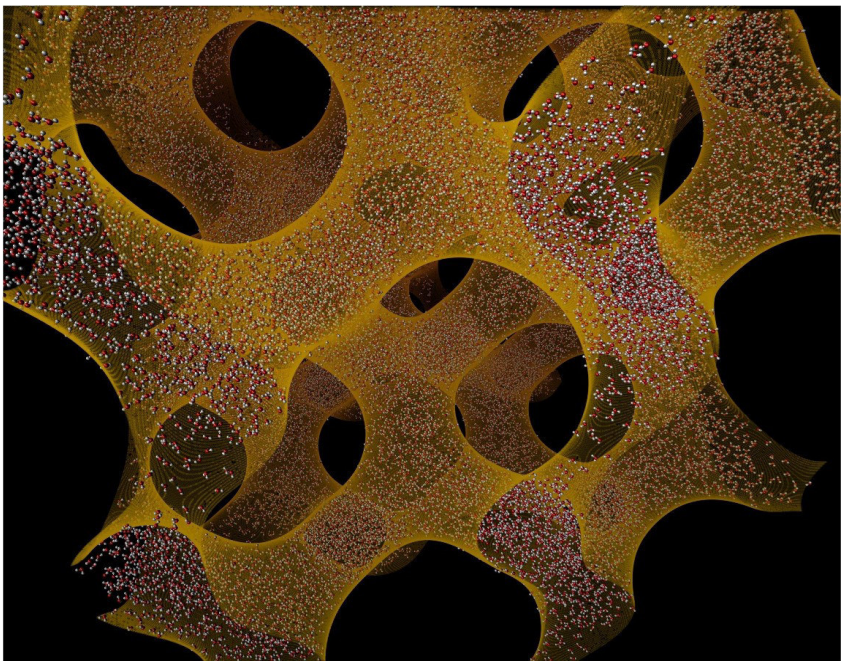

ABSTRACTS
CONTRIBUTED
SPEAKERS

GEFES 2025

Chiral Hybrid Organic-Inorganic Manganese Chloride Perovskites with Circularly Polarized Photoluminescence from Bulk to Exfoliated Flakes

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In recent years, layered (2D) hybrid organic–inorganic metal-halide perovskites (HOIPs) have attracted increasing attention due to their ability to acquire chirality through the incorporation of chiral organic molecules, presenting promising potential for applications in optoelectronics and spintronics [1,2]. However, most studies to date have focused on bulk compounds, specifically on the unstable and toxic Pb-based HOIPs. Here, we report the chiroptical properties of antiferromagnetic R- and S-***β***-methylphenethylammonium Mn chloride HOIPs [3] in both bulk and mechanically-exfoliated flakes. These compounds exhibit red photoluminescence (PL) emission originating from the octahedrally coordinated Mn^{2+}, with a PL redshift as they transition from bulk to flake form. Circular dichroism (CD) and circularly polarized luminescence (CPL) mirrored signals confirm the chirality transfer from the organic cations to the inorganic perovskite framework in bulk materials, presenting g_{lum} values among the highest reported for chiral hybrid Mn halides. This chirality is preserved in the exfoliated flakes, reaching degrees of circularly polarized PL (P) of up to 17% at 80K, which systematically decrease with increasing temperature as previously observed in 2D Pb-based HOIP microplates [4]. Additionally, angle-resolved PL measurements show that the PL emission and P are isotropic. Therefore, our results demonstrate that these 2D Mn-based HOIPs are highly valuable, as they can compete with their Pb analogs and offer additional functionalities for spin-optoelectronic applications, thanks to the magnetic behavior associated with Mn^{2+} [5].

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Extraction of effective optical constants of buried halide perovskite films for next generation optoelectronic devices

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Halide perovskites are considered prime candidates for next-generation solar cells, LEDs, and detectors, among others, due to their exceptional optoelectronic properties, such as tuneable bandgaps and narrow emission lines. It is well-known that the morphological, structural, and optoelectronic properties of perovskite thin films are strongly influenced by the deposition methods used and the surrounding layers. [1] However, how these heterogeneities correlate with the effective optical constants of perovskite materials is still unexplored, hampering the design of realistic optimised devices.

In this talk, we will discuss how the optical behaviour of perovskite thin films is strongly influenced by the surrounding materials such as hole and electron transporting layers. This observation represents a challenge when modelling light-matter interactions in perovskite devices where optical constants have been extracted from naked perovskite films. To overcome this issue, we present methodology to extract the optical constants of buried perovskite films by employing a transfer matrix-based model enhanced with genetic algorithms. [2] This approach resolves discrepancies often seen between theoretical simulations and experimental data, offering accurate, realistic designs to be implemented in ultimate devices. We will show the applicability of our work for LEDs with angular response on demand, [3] narrow band photodetectors, [4] and multijunction devices. [5]

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Figures

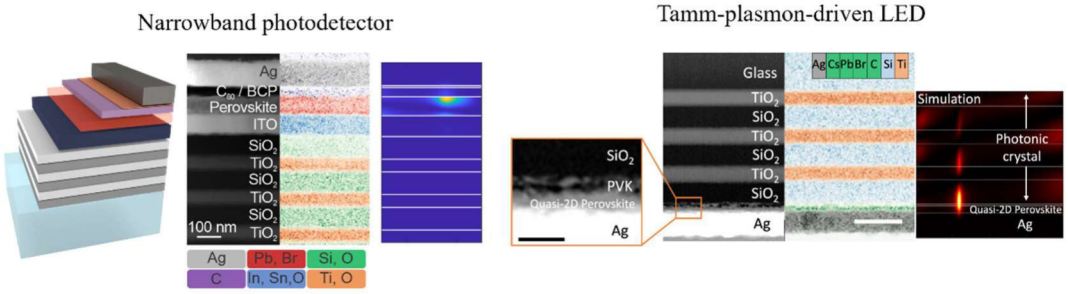

Figure 1: Scheme of halide perovskite optoelectronic devices: narrowband perovskite and tamm-plasmon-driven LED.

Photoinduced ferroelectric control of Second-Harmonic Generation in monolayer MoS_2

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The association of ferroelectrics and Transition Metal Dichalcogenides (TMDs) has recently emerged as a promising approach for controlling the optoelectronic properties of 2D materials [1]. However, previous studies have primarily focused on the electrical and linear optical properties of TMDs, while the influence of ferroelectric substrates on the nonlinear optical properties of TMDs remains largely unexplored [2].

In this work, we exploit light-induced ferroelectric control of electronic doping in monolayer MoS_2 [3] to experimentally demonstrate the spatial modulation of quadratic Second Harmonic Generation (SHG) in MoS_2 deposited on a periodically poled $LiNbO_3$ substrate. As shown in Figure 1, a pronounced contrast in SHG intensity is observed between signals collected from MoS_2 on ferroelectric domains of opposite polarities, with maximum values occurring on the P_{down} domains. The influence of the fundamental beam's intensity, polarization, and photon energy on the SHG response modulation is systematically analyzed. The spectral response of the SHG modulation reveals a clear resonance with the C band of MoS_2. In agreement with calculations, the SHG enhancement is correlated to electron doping, which originates from domain-oriented photoinduced charge-transfer processes at the ferroelectric/MoS_2 interfaces.

The obtained results contribute to the fundamental understanding of nonlinear processes in TMD/ferroelectric heterostructures under external optical stimuli, and open new routes to their application into the fabrication of 2D photonic and optoelectronic devices.

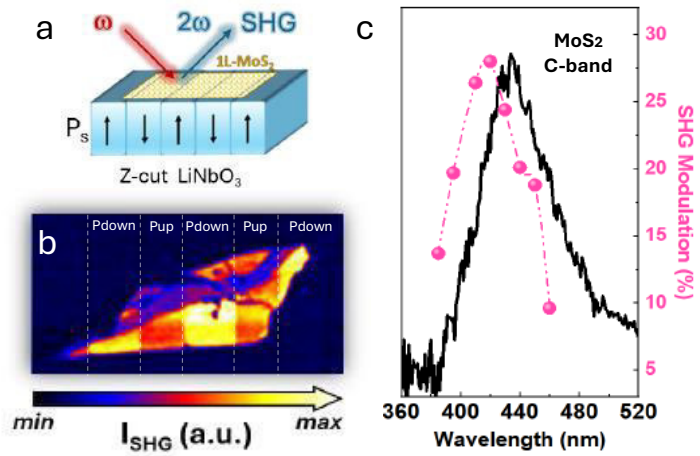

Figure 1: a) Schematics of SHG from a $MoS_2/LiNbO_3$ heterostructure. b) SHG spatial modulation of monolayer MoS_2 deposited on a periodically poled $LiNbO_3$ crystal. c) Spectral response of the SHG modulation (red) in the C band spectral region (black) of MoS_2.

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Thermal radiation propulsion and lateral force on asymmetric nanostructures

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The thermal and quantum fluctuations of the electromagnetic field produce forces that significantly influence the movement of material structures. This is exemplified by the thermal radiation drag, which decelerates objects moving with respect to a thermal radiation bath [1-2]. Such force arises from the different rates of absorption of photons propagating with and against the object, which are red or blueshifted in the reference frame comoving with the object.

Because of its counterintuitive concept and its interesting prospects, the thermal radiation drag has received increasing attention in recent years. However, previous works on thermal radiation forces have focused on the study of isotropic and homogeneous objects. Such approach simplifies the study at the expense of neglecting phenomena arising from the symmetry of the object.

Here, we show that nanostructures with an anisotropic optical response are subject to a thermal radiation lateral force and torque when moving through a thermal radiation bath, as depicted in Figure 1(a) [3]. In particular, the lateral force is of the same order of magnitude as the drag force for structures with a high degree of anisotropy, as illustrated in Figure 1(b). As a result, the trajectory of the object is strongly modified and tends to align with the direction in which the polarizability of the nanostructure is maximum. Furthermore, we observe interesting similarities between the movement of the nanostructure in the thermal radiation bath with that of a wing in a viscous fluid.

The anisotropy of the nanostructure allows us to gain control over its trajectory. However, such motion is still limited by the thermal drag. We further show that, by engineering a bilayer structure combining an absorbing and a reflecting material, the system spontaneously accelerates when placed in a thermal environment at a different temperature [4]. This propulsion is fueled by the thermal energy stored in the system, thus effectively working as a thermal engine.

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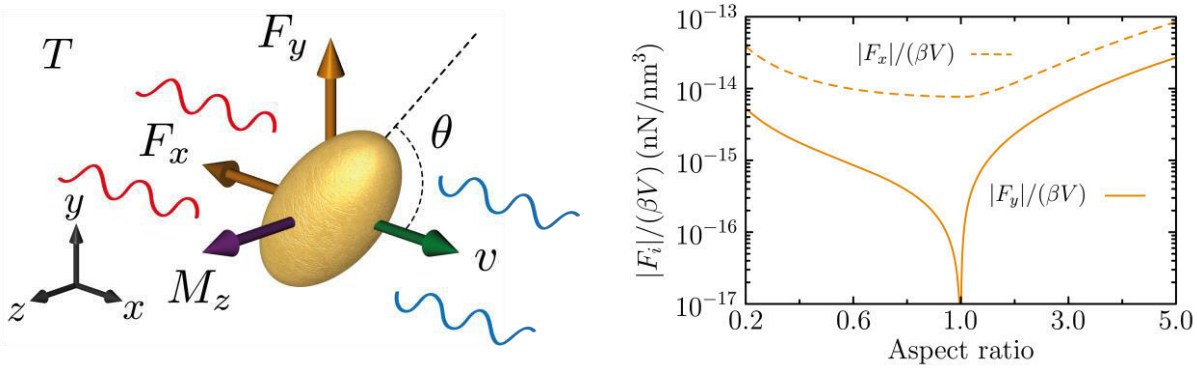

Figure 1: Schematics of the system (left) and components of the force as a function of the aspect ratio (right).

Engineering a Spin-Orbit Bandgap in Graphene-Tellurium Heterostructures

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The spin-orbit interaction (SOI) is fundamental in shaping the electronic properties of graphene-based heterostructures, making it essential for the development of novel electronic and spintronic devices. In these systems, the interaction between intrinsic SOI and external influences - such as heavy elements or intercalated species - can be carefully manipulated to induce and control unique electronic phenomena. Fine-tuning the SOI enables the creation of customized bandgaps at the Dirac point, paving the way for the emergence of quantum spin Hall phases.

In this work, we report on a combined scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and angle resolved photoemission spectroscopy (ARPES) study on a new superstructure when Te is evaporated on graphene over Ir(111) [1]. Notably, a significant bandgap at the Dirac point is revealed at room temperature, rendering graphene nearly charge-neutral and allowing for the tuning of the Fermi level into the gap as a function of the Te coverage. The origin of the bandgap has been attributed to a substantial intrinsic SOI, which suggest the potential of this system as a platform for realizing spin-dependent transport phenomena, such as the quantum spin Hall (QSH) effect. Indeed, an increase in the dI/dV signal, compatible with an edge state, is reported at the position of the gap by STS. Our work suggests then the possibility that in this system the transport properties near the Dirac point are dominated by charge carriers of a single spin component, indicating the potential of this system as a platform for realizing spin-dependent transport phenomena.

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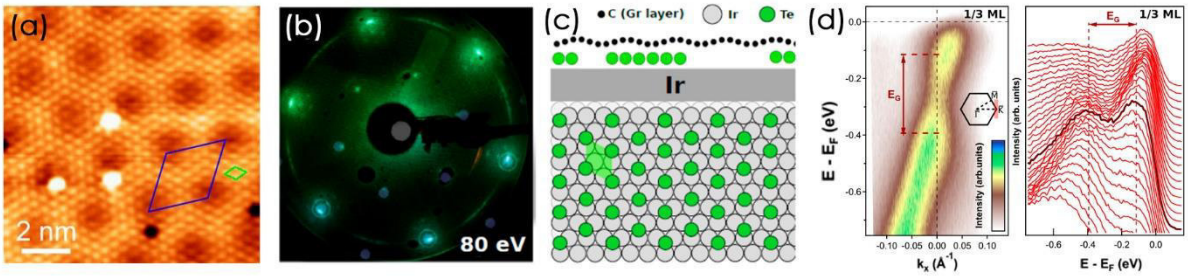

Figure 1: (a) High resolved STM image (V_b=2 V, I_t=0.35 nA). The moiré pattern unit cell of gr/Ir(111) and the one created by the intercalated Te are depicted in blue and green, respectively. (b) LEED pattern showing a pure (√3×√3)R30º reconstruction, described by the real space model in (c). (d) ARPES spectrum at K point of the Gr/Te/Ir(111) heterostructure and the corresponding Energy Distribution Curves evidence the gap opening at the Dirac point.

Emergent moiré topological skyrmion phases in twisted multiferroics

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Layered van der Waals materials are one of the most promising platforms for engineering emergent phenomena in condensed matter physics. The weak van der Waals bonding between their layers allows to easily reach the single-layer limit, offering intrinsic degrees of freedom to artificially design new materials. For instance, monolayers of different compounds can be stacked together, and even a specific twist angle between stacked layers can be fixed, creating a moiré pattern that leads to novel heterostructures with emergent properties. Recently, the first purely two-dimensional multiferroic material, NiI_2, was isolated and characterized at the atomic scale [1,2], establishing a novel building block to create functional van der Waals heterostructures.

In this presentation, we reveal the emergence of electrically tunable topological moiré magnetic textures in twisted bilayers of the spin-spiral multiferroic NiI_2 [3]. In this work, we uncover a detailed phase diagram that includes uniform spiral phases, various kπ-skyrmion lattice structures, and nematic spin alignments organized at the moiré scale. These phases arise due to local stacking interactions and moiré-modulated frustration. Specifically, when the spin-spiral wavelength is commensurate with the moiré scale as an integer multiple k, multiwalled skyrmions are anchored to the moiré pattern. The pronounced magnetoelectric coupling found in the moiré multiferroic permits electrical adjustment of kπ-skyrmion lattices using an out-of-plane electric field. Our findings introduce a highly tunable platform for skyrmionics based on twisted van der Waals multiferroics, paving the way for a new era of topologically spintronic devices. These have the potential to be easily integrated with other van der Waals materials or within optical setups in the pursue of novel quantum technologies.

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Ising domain wall networks from intertwined charge density waves in single-layer $TiSe_2$

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When the period of an incommensurate charge density wave (ICDW) approaches an integer multiple of a lattice vector, the energy gain obtained from locking the period to the lattice can lead to a fascinating transition into a commensurate state. This transition occurs through an intermediate near-commensurate (NC) phase, with locally commensurate regions separated by an ordered array of phase slips of a complex CDW order parameter. $TiSe_2$ is a paradigmatic CDW system where incommensuration is believed to be induced by carrier doping, yet its putative NC state has never been imaged or its nature established. Here we report the observation of a striking NC state in ultraclean, slightly doped monolayers of $TiSe_2$, displaying an intricate network of coherent, unidirectional CDW domain walls over hundreds of nanometers [1]. Detailed analysis reveals these are not phase slips of a complex CDW, but rather sign-changing Ising-type domain walls of two coupled real CDWs of previously known symmetry, consistent with the period doubling nature of the parent commensurate state. In addition, we observe an unexpected nematic modulation at the original lattice Bragg peaks which couples to the CDW order parameters. A Ginzburg-Landau analysis naturally explains the couplings and relative modulations of all order parameters, unveiling $TiSe_2$ as a rare example of an NC-CDW of two intertwined real modulations and emergent nematicity.

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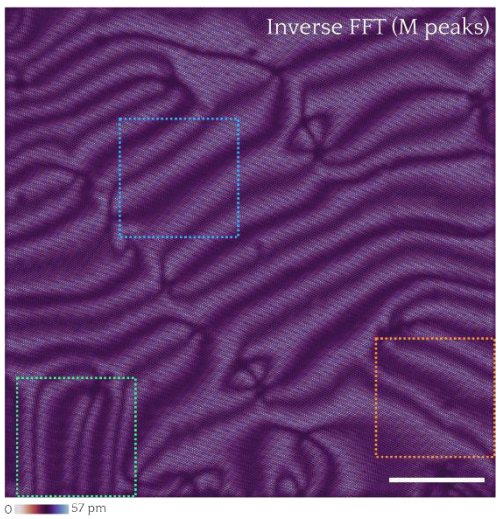

Figure 1: Near-commensurate CDW state in monolayer $TiSe_2$. Inverse Fourier transform of the amplitude of the CDW **M** points. An intricate network of one-dimensional trains of domains (high amplitude) separated by domain walls (low amplitude) is observed.

Unveiling intrinsic bulk photovoltaic effect in atomically thin ReS_2

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The bulk photovoltaic effect (BPVE) is a nonlinear photocurrent that arises in non-centrosymmetric crystals when exposed to light [1]. It is an intrinsic property of the material, distinct from extrinsic effects like interfacial pn junctions or Schottky barriers. The BPVE manifests as a quadratic response to the incoming electric field or light polarization, offering a promising avenue for surpassing the efficiency limitations of conventional solar cells [2].

A key challenge in studying the BPVE lies in isolating the real intrinsic signal from other extrinsic, first-order photocurrents that can arise at different interfaces within a device. These extrinsic contributions can mask the intrinsic BPVE, making it difficult to accurately assess its performance.

To address this challenge, we fabricate high-quality, lateral ReS_2 devices with minimal contact resistance, providing an optimal platform for isolation of the intrinsic BPVE signal [3]. Our devices exhibit large bulk photovoltaic performance with intrinsic responsivities of ~1 mA/W in the visible range, without the need for external tuning knobs such as strain engineering. Our experimental findings are supported by theoretical calculations. Furthermore, our approach can be extrapolated to investigate the intrinsic BPVE in other non-centrosymmetric van der Waals materials, paving the way for a new generation of efficient light-harvesting devices.

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Figures

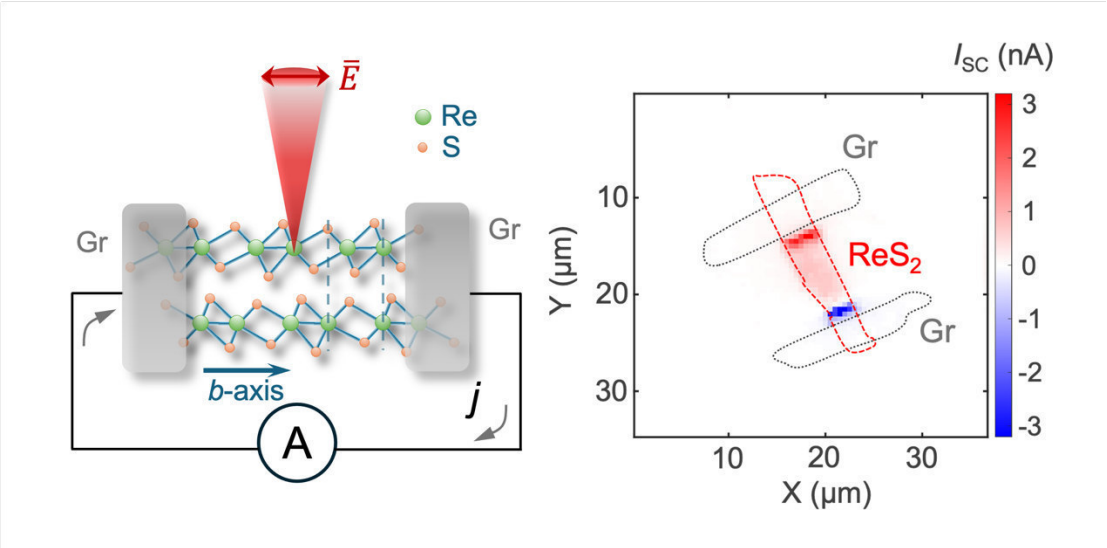

Figure 1. Left: Sketch of the device, where a directional photo-generated current arises at zero applied external bias along ReS_2 as a response to an incident electric field or light polarization. Right: Scanning photocurrent map of a representative device at zero applied bias. Here, a photovoltaic contribution with opposite signs coming from the Schottky barriers can be observed. In addition, the map also reveals a photovoltaic effect along the active ReS_2 channel, which is attributed to an intrinsic bulk photovoltaic response.

Strong magnon-spin coupling between layered van der Waals antiferromagnet CrSBr and paramagnetic ion crystal GdW10

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Cavity Quantum Electrodynamics (C-QED) is used to manipulate and interrogate qubits or to engineer hybrid light-matter states. However, cavity photons impose severe restrictions on the maximum coupling strengths, thus limiting the accessible regimes and the physics that can be explored in C-QED platforms. Beyond light, the solid state offers a variety of quantized bosonic excitations. One particularly appealing candidate is the magnon, the quantum of spin waves in magnetic solids. The rich physics of light-matter hybrids is, in principle, also applicable to magnon-matter states, which come with additional advantages such as reduced size and enhanced coupling strengths.

Here we report on magnon-spin interaction between the layered van der Waals antiferromagnet CrSBr [1,2] and paramagnetic ion crystal GdW10 [3], measured via microwave absorption spectroscopy at millikelvin temperatures. This experiment and further characterizations, performed with macroscopic samples, show a rich spectrum of resonances from CrSBr which, based on our theoretical model, we attribute to phase differences among the many layers of the material. The avoided crossing seen at low probing power indicates we achieve the strong coupling regime of interaction between both systems, while higher probing power saturates the paramagnet, thus losing the anticrossing. This result opens a path for the use of CrSBr and similar layered materials as magnonic platforms in hybrid quantum systems, both for fundamental physics and device-oriented experiments.

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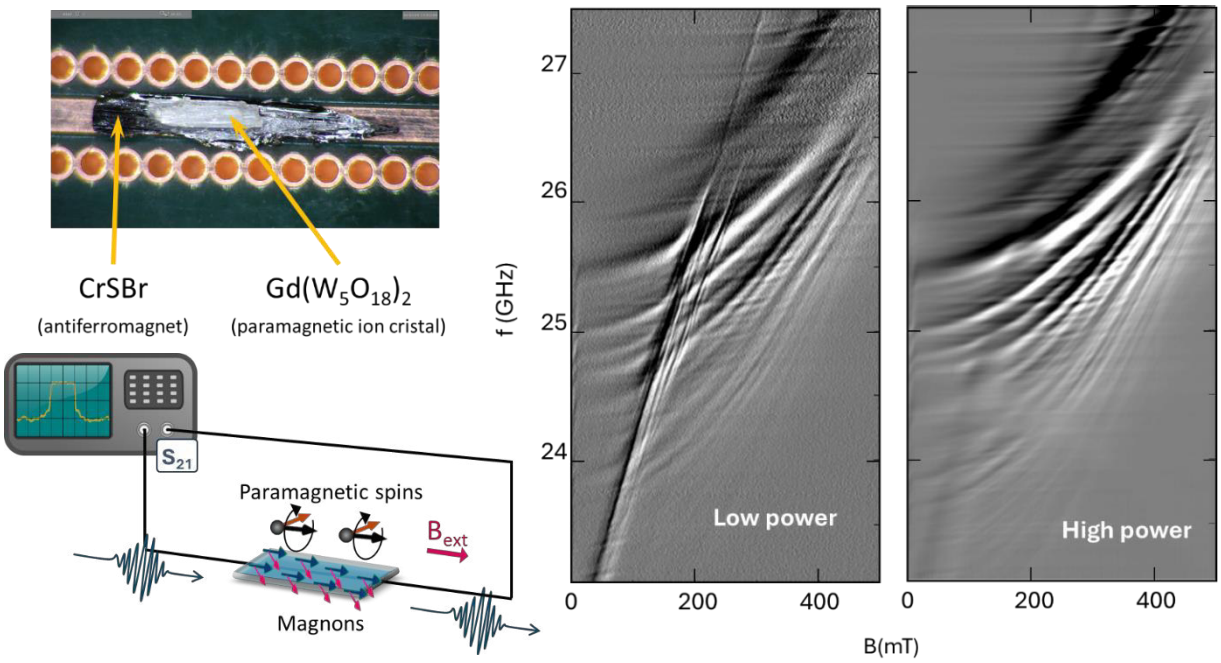

Figure 1: (Top left) Picture of the samples measured. Both materials lie on top of a coplanar waveguide connected to a VNA. (Bottom left) Scheme of the measurement setup. (Right) Derivative of the transmission coefficient S21 in two measurements at different power, where white (black) indicates positive (negative) value.

Polarization-dependent photocurrent spectra and nanoscale characterization of 2D ReS_2 field effect transistors.

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Transition metal dichalcogenides (TMDCs) are a class of bidimensional semiconductors that have attracted a lot of attention in the last decade for their integration in optoelectronic devices due to their unique electronic and optical properties [1]. In particular, lots of efforts are focused on Rhenium disulphide (ReS_2) due to its low crystal symmetry, that leads to the emergence of dichroic optical and optoelectronic response [2,3]. To unravel the full potential of ReS_2, studies on its optoelectronic response as well as in the impact of the morphology of the layers on its electrical and electrostatic properties must be done. In this work we perform a thorough study, characterizing the morphological and electrostatic characteristics of single and multi-layer ReS_2 samples and extracting the polarization-dependent photocurrent spectra of few-layer ReS_2 photodetectors, both in room conditions and at cryogenic temperature (14 K). By measuring the polarization-resolved photocurrent spectra [4], we obtain a clear linear dichroic behaviour of the photocurrent and the modulation as function of the light polarization angle of three different excitonic transitions, X^1, X^2 and X^3, matching the photoluminescence measurement. Moreover, Kelvin Probe Force Microscopy (KPFM) measurements were performed in few-layer thick samples and working devices, obtaining the work function dependence with the number of layers. Surface potential images of few-layer flakes reveal striking contrasts, not reported before. Differently shaped areas are clearly visible on ReS_2 flakes on SiO_2 and Au substrates. We have performed Temperature dependent KPFM measurements, revealing modified local work function upon higher substrate temperature.

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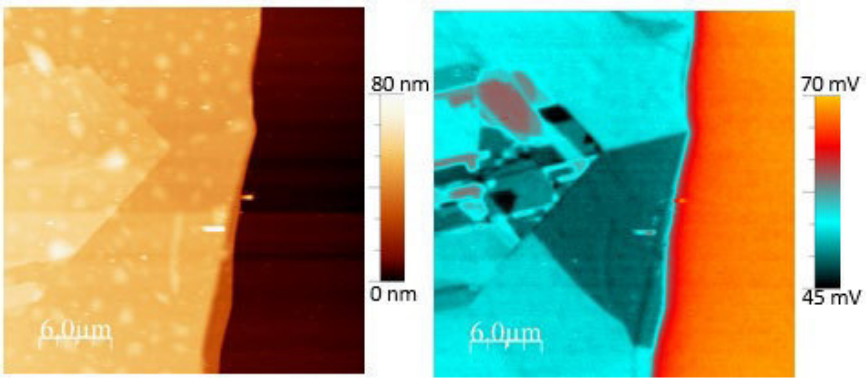

Figure 1: Topographical (left) and Surface potential image (right) of a ≈20nm thick ReS_2 flake.

Single molecules as thermometers for cryogenic temperature

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Measuring cryogenic temperatures with high sensitivity and spatial resolution in the nanoscale is a challenging task, being portability and non-invasivity desirable qualities for the thermometers. Moreover, the characterization of thermal properties at low temperatures and in complex environments has become essential for understanding phenomena such as non-Fourier thermal transport, which have recently attracted great interest both for the challenging fundamental questions it poses [1] and for the potentially relevant technological implications in nanotechnology [2, 3].
Herein we propose a molecular thermometer composed by dibenzoterrylene molecules embedded in anthracene nanocrystals, a quantum two level system in which the broadening of the zero-phonon line with temperature allows for measuring temperatures in the range 3 – 32 K. Thanks to the extreme sensitivity of quantum probes to the environmental temperature effects together with the small size of nanocrystals, our thermometer presents outstanding sensitivity, submicrometric spatial resolution, and high temperature resolution, which set it among the best reported thermometers in the nanoscale for this range of temperatures [4]. The portability of our thermometers allows for depositing them on a wide variety of surfaces, including nanostructured samples, in contrast to other thermometry techniques which require a specifically designed sample. Furthermore, the low-operating power (around 5 nW) of the thermometric technique proposed here, ensures non-invasitivy of the sample. We validate our molecular thermometer by measuring and, comparing with literature, the thermal conductivity of silicon phononic crystals, exemplary samples to dig into the study of non-Fourier heat transport. Finally, as a direct application, we show the temperature mapping with submicrometric spatial resolution in the cryogenic temperature range, collecting information from different points simultaneously from areas of tens of microns wide. Our results show that our molecular thermometer is an excellent candidate for studying fundamental phenomena such as non-Fourier heat transport at cryogenic temperatures thanks to its outstanding figures of merit as a thermometer at cryogenic temperatures, whereas it can be used practically for non-invasive high-resolution temperature mapping at cryogenic temperatures over a wide range of surfaces, including samples with nanostructuration, being potentially relevant for technological implications in nanotechnology.

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GEFES 2025

Side groups functionalization and charge transport properties of graphene-curcuminoids single-molecule junctions: experimental and theoretical study.

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The ability to control charge transport in a single-molecule junction is indispensable to analyze fundamental aspects of quantum transport through a molecule, as well as for designing advanced functional molecular electronic devices.

In this context, interface engineering plays a key role in regulating the transport mechanism in single-molecule transistors [1]. Unlike standard metals, graphene-based electrodes offer the possibility of using both covalent bonding and π-π stacking to couple molecules with electrodes. Supramolecular functionalization via π-π stacking through small polycyclic aromatic carbon is generally preferred over covalent bonding which could result detrimental for the extended π conjugation intrinsic to both components.

In this work, we investigate the charge transport properties of single-molecule junctions obtained by coupling linear diarylheptanoids (CCMoids) embedded between graphene nanogap electrodes fabricated by feedback-controlled electroburning. We explored two different backbone functionalization strategies: adding anthracene anchoring groups [2] and introducing a spacer amide bond between the conjugate chain and the chosen anchoring group [3] (i.e.pyrene). In all cases, we demonstrated gate-dependent transport at room and cryogenic temperatures. Contrary to our intuition, we found higher conductance values for the longest system studied, which we attribute, according to DFT calculations, to the fully planar configuration of the molecule within the junctions, facilitated by the presence of the amide bond.

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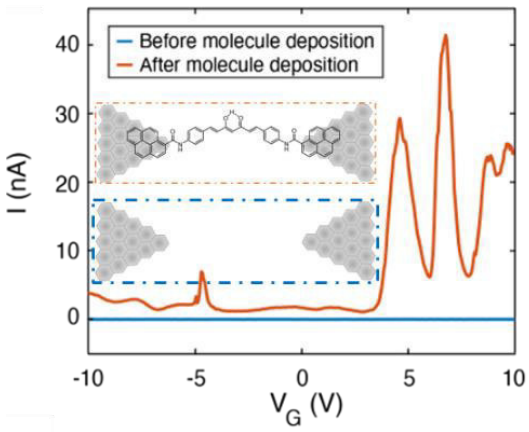

Figure 1: Current vs gate voltage before and after molecules deposition.

Achieving superconductivity in infinite-layer nickelate thin films by aluminum sputtering deposition

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After decades of research, a cuprate analog displaying superconductivity was finally found within the nickelate family. It was in 2019 when superconductivity was discovered in infinite-layer (ABO_2) nickelates with a critical temperature (T_C) around 10-15 K [1]. This discovery has sparked a new realm of research, whose progress is slowed by challenges in materials synthesis and the limited number of research groups capable of producing high quality superconducting samples. The main difficulty lies in the topotactic reduction process required to selectively remove all the apical oxygens from the initial precursor perovskite phase to achieve the superconducting infinite-layer phase, which is typically achieved by an *ex situ* complex chemical process using CaH_2 as the reducing agent. Two alternative *in situ* reduction methods —metal overlayer deposition via molecular beam epitaxy and atomic hydrogen bombardment— have recently improved this aspect, but their limited accessibility underscores the need for simpler and more reliable methods to facilitate the synthesis of superconducting infinite-layer nickelates.

In this work, we demonstrate the possibility to synthesize high quality superconducting infinite-layer $Pr_{0.8}Sr_{0.2}NiO_2$ thin films by aluminum deposition, using a more accessible technique such as direct current magnetron sputtering [2]. The sputtered aluminum on the parent perovskite thin films pumps the apical oxygen atoms through a redox reaction, transforming the films into the superconducting infinite-layer phase. We systematically optimized the aluminum deposition parameters and compared the superconducting properties of samples reduced through *in situ* Al deposition with those exposed to air prior to Al reduction (*ex situ*). *In situ* Al reduction enhances the quality of the SC $Pr_{0.8}Sr_{0.2}NiO_2$ thin films, with a maximum superconducting transition temperature T_c^{onset} of 17 K. This simplified synthesis route, much more accessible than existing methods, offers better control and reproducibility over the topotactic transformation, providing new opportunities to gain insights into the physics of superconductivity in nickelates.

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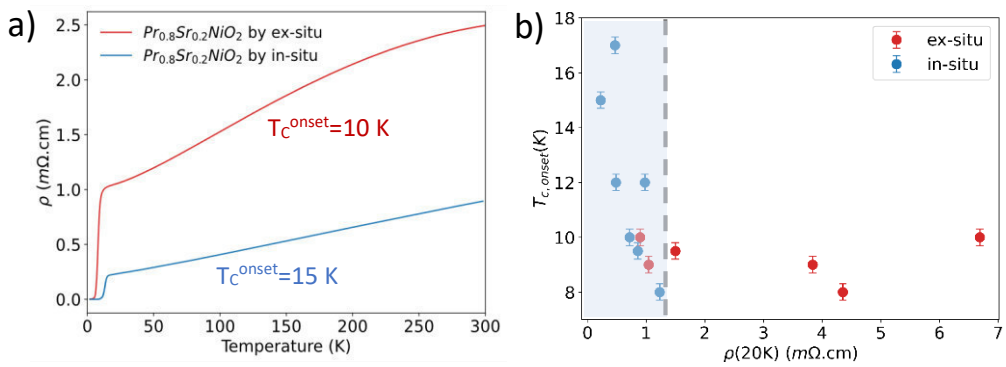

Figure 1: a) Resistivity (ρ) as a function of the temperature for infinite-layer phase after *ex situ* (red line) and *in situ* (blue line) aluminum reduction, showing critical temperature onset (T_C^{onset}) of 10 K and T_C^{onset} = 15 K, respectively. b) T_C^{onset} as a function of the resistivity (ρ) at 20 K for *ex situ* (red circles) and *in situ* (blue circles) samples. Blue shaded area is a guide to the eye indicating the most common values for *in situ* reduced samples.

Topological signatures and induced triplet pairing in proximitized quantum Hall - superconductor heterostructures

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A two-dimensional electron gas (2DEG) in the presence of a strong magnetic field exhibits the quantum Hall (QH) effect, which supports chiral 1D conducting states at the edges. Proximity to a superconductor (SC) leads to the formation of chiral Andreev edge states (CAES)[1-3], see Figure 1: hybridized electron-hole states with promising potential applications in quantum metrology and topologically protected quantum computing. Although the strong magnetic fields required for the QH effect are detrimental to superconductivity, recent experiments have achieved QH-SC hybrid junctions based on InAs 2DEGs [4], graphene [5], and magnetic topological insulators [6]. Although these experiments involve conventional SCs, where Cooper pairs are formed by electrons with opposite spins, experimental evidence for emerging CAES has been found even in the lowest QH edge states, where spins are polarized by ultra-strong Zeeman coupling.
In this work, we theoretically study the formation of CAES in QH-SC hybrid junctions on a 2DEG. Using numerical simulations in Kwant [7], we study the formation of spin-polarized triplet Cooper pairs by considering the effect of Rashba spin-orbit coupling and Zeeman splitting [3], which may be important in the case of 2DEG devices. We also consider the effect of the geometry of nanodevices in planar junctions [8], see Figure 1(b), and in a narrow-finger configuration, see Figure 1(c). In these geometries, the coupling of CAES can induce a topological band inversion and trivial localized states, both of which show particular signatures in non-local electron transport.

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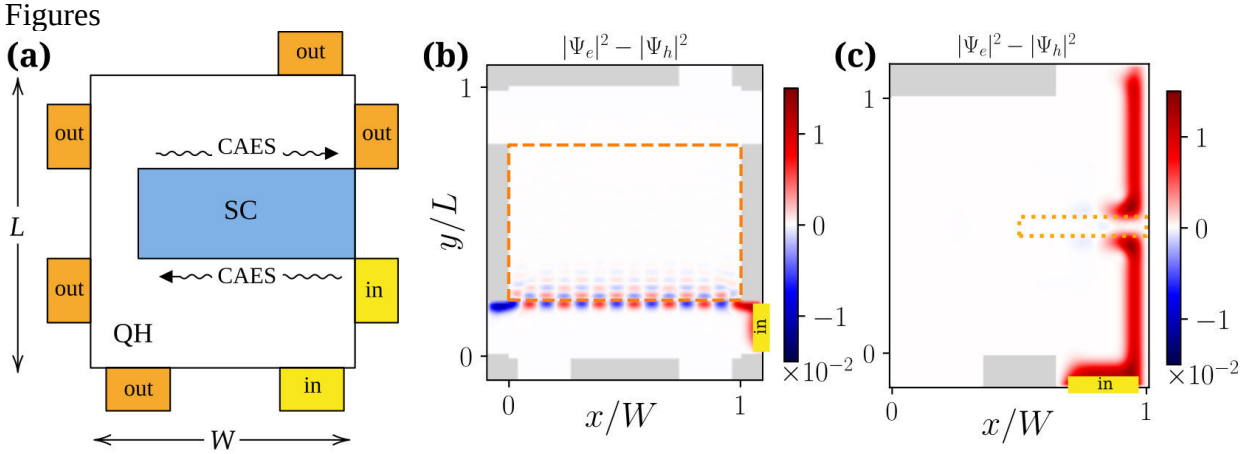

Figure 1: (a) Sketch of the QH-SC junction showing the CAES (wavy lines) formed near the SC interface. (b) Electron and hole probabilities of the scattering wavefunction in a planar geometry in the QH regime with filling factor v=2. (c) Same quantity as in (b) in a narrow finger geometry with v=1 and band inversion.

Proximity-induced superconductivity in the flatbands of Magic Angle Twisted Bilayer Graphene

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The distinct electronic band structure of twisted bilayer graphene, marked by flat bands at specific twist angles, presents a unique platform for investigating the interplay between superconductivity and electron correlated states through the Josephson effect. This study investigates the proximity-induced superconductivity in a Josephson junction (JJ) made from a magic-angle twisted bilayer graphene (MATBG) weak link coupled to superconducting electrodes. This geometry, compared to previous works on gate-defined JJs [1-3], enables us to study all the phase diagram of MATBG under an induced superconducting proximity effect.
While the Josephson effect is stronger when the junction is tuned into the high-energy dispersive bands, finite critical currents are still found inside the flat bands despite their small Fermi velocity (Figure 1). In fact, calculations of the pairing amplitude of the injected Cooper pairs show good agreement with the experiment, but only when multiband processes and quantum geometry contributions of the flat bands are considered, revealing the importance of these mechanisms into the formation of superconducting phases in MATBG.
Finally, at the hole (electron) side of positive (negative) half-filling, we observe unconventional interference patterns with broken inversion and preserved time reversal symmetries, enabling us to engineer a reversible Josephson diode between opposite magnetic fields. Our experiment imposes constraints on the ground state symmetries of the flat bands at these fillings.

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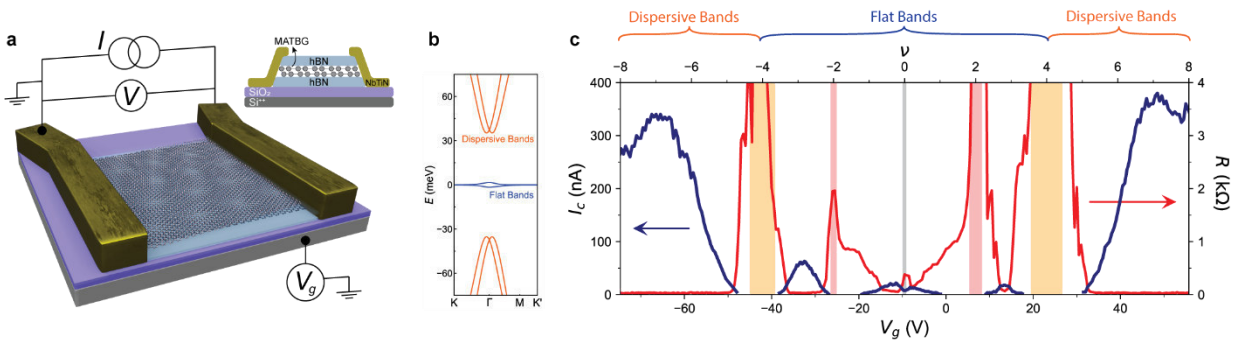

Figure 1: a, Device schematic of a MATBG sheet acting as the weak link of a JJ. The voltage V across the junction is recorded as a current bias I is applied through the superconducting electrodes in a two-probe measurement. The carrier density is tuned by a gate voltage V_g to the doped Si. **b,** Bandstructure of MATBG for a twist angle $\theta = 1.00°$. **c,** Resistance R in red (right axis) at zero current bias, as a function of V_g (bottom) and the corresponding moiré filling factor ν (top). Color-shade stripes indicate peaks at integer fillings of the moiré unit cell $\nu = 0, \pm2, \pm4$, characteristic of samples near the first magic angle θ_m=1.1°. Regions with low resistance have a finite critical current I_c (blue, left axis), extracted from the non-linear characteristics. These indicate where the superconducting proximity effect takes place.

A twist for tunable electronic and thermal transport properties of nanodevices

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Twisted graphene-layered materials with nonzero interlayer twist angles (θ) have recently become appealing, as they exhibit a range of attractive physical properties, which include a Mott insulating phase and superconductivity. In this study, we consider nanodevices constructed from zigzag graphene nanoribbons with a top rectangular benzenoid [6,3]-flake. Using density functional theory and a non-equilibrium Green's function approach, we explore how the electronic and thermal transport properties in such nanodevices can be tuned through a twist of the top flake by an angle $0° \leq \theta \leq 8.8°$ for different stacking configurations. We found a strong dependency of the electronic structure on the stacking type, as well as on the twisting regime, specifically in AA-stacking devices. Electron and hole van Hove singularities (vHSs), which originate, respectively, from the flatness of the top of the valence band for the minor-spin component and the bottom of the conduction band for the major-spin component, are found very close to the Fermi level in the density of states and electronic transmission spectra of AA-stacking devices with a twist angle of 1.1°. We establish that these vHSs in AA-1.1° devices are stable at higher temperatures and, with the increased number of available states, lead to larger values of electron thermal conductivity and finally total thermal conductivity in AA-1.1°. Our work highlights the essential role of twisting and stacking for the fabrication of nanoscale charge and heat switches and spurs future studies of twisted layered structures.[1]

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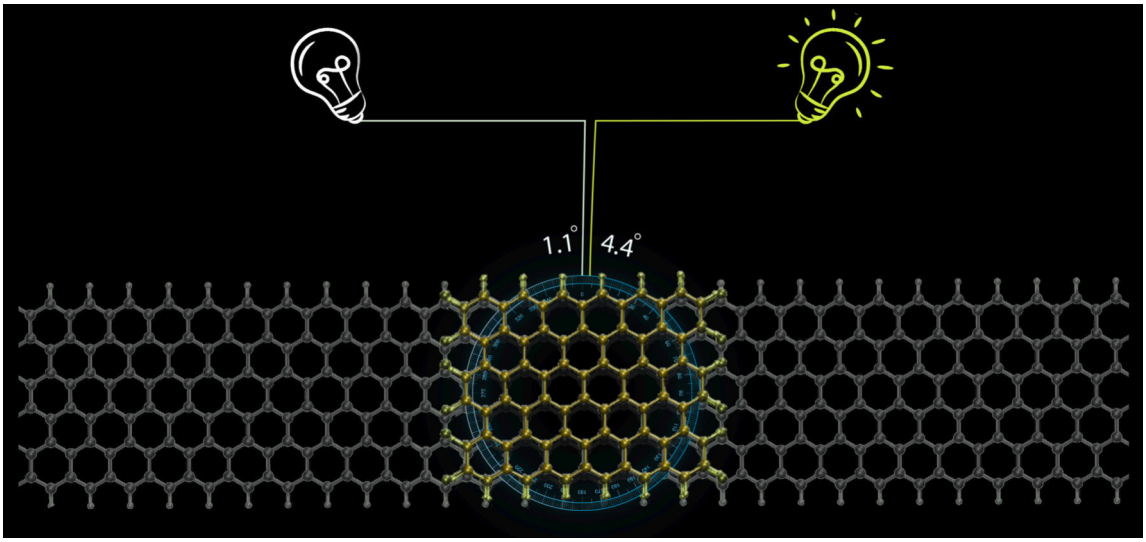

Charge-Transfer Complexes for organic semiconductor thin film devices

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Charge-transfer complexes (CTCs), arising from an ordered mixed assembly of small conjugated molecules, typically an electron donor and acceptor, have emerged as a materials design strategy for developing organic semiconductors with novel electrical and optical properties far beyond the performance of single materials, avoiding more complicated synthesis procedures [1-3]. Here, we study the formation of a thin film co-crystal made of 2,7-bis(octyloxy)[1]benzothieno[3,2-b]-benzothiophene (C8OBTBTOC8) and 1,3,4,5,7,8-hexafluoro-tetracyanonaphthoquinodimethane (F6TCNNQ) and demonstrate their absorption in the near-infrared (NIR). Obtained from molecular beam deposition in UHV, the co-crystal formation is revealed and characterized by combining Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS), Atomic Force Microscopy (AFM), Kelvin Probe Force Microscopy (KPFM) and UV-vis spectroscopy.

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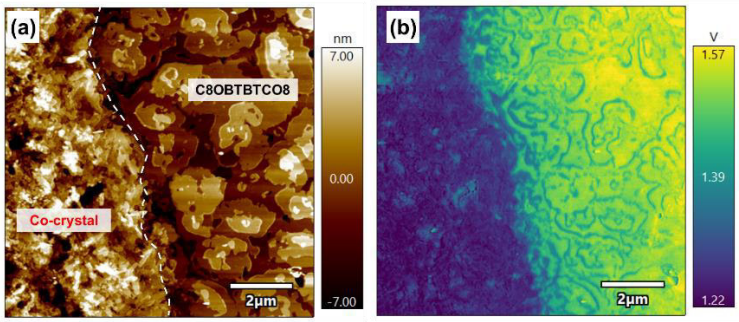

Figure 1: *(a-b) Topography and KPFM image of a co-crystal region next to C8OBTBTOC8 region. In the C8OBTBTOC8 region, the step edges are decorated by a single layer co-crystal rim.*

Heterostructure properties from tight-binding models made with Graph Neural Networks (GNN)

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When heterostructure unit-cell surpasses a few dozen atoms, effective mass (envelope function) approximation fails to grasp short-range potential features, and density function theory (DFT) becomes computationally too demanding. At this scale, tight-binding (TB) models are the best tools to calculate material properties. Despite the abundance of models for Graphene, Si/Ge, III-V semiconductors, and a few others; constructing a semi-empirical model for novel materials could be very time-consuming, or even impractical. Here we present an equivariant graph neural network [1] (GNN) model able to infer hopping parameters of big unit cells and multi-material heterostructures learned from a few examples with small unit cells employing LCAO-DFT. We show examples of heterostructures like Pb(Sn)O and Ga(In)S(Se,Te) where TB models did not exist so far, discuss the importance of gauge and symmetry for the learning process, and finally, compare some of the properties e.g. density of states (DOS), absorption and conductivity calculated with these GNNs with the ones calculated with others methods.

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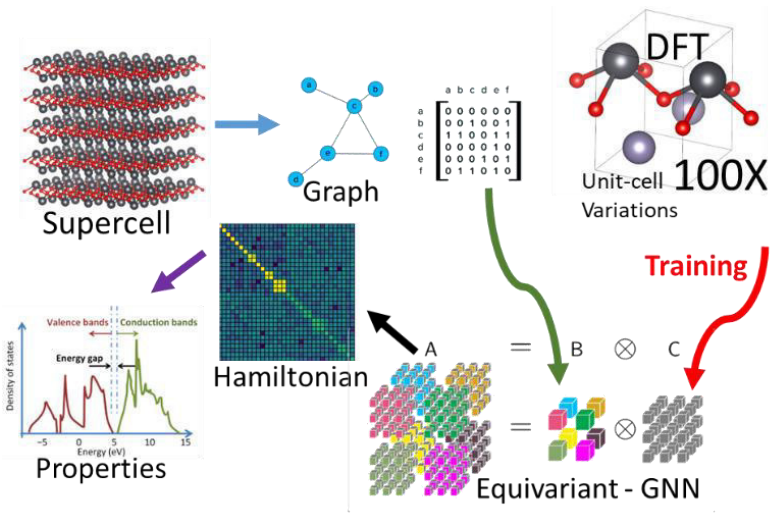

Figure 1: Diagram of heterostructure properties calculation by tight-binding model using equivariant graph neural network.

An atomistically informed stochastic continuum model for small scale plasticity

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Progress towards fulfilling the promises of multiscale simulations and nanoscale solutions to engineering problems hinges not only on the development of computational and characterization techniques for an adequate assessment of the materials but also on the integration of information across the length-scales and time-scales involved. In such direction, we present a stochastic discrete slip approach to model plastic deformation in submicron domains [1]. The integration of an atomistically-informed dislocation mobility law and a surface nucleation model into a kinetic Monte Carlo selection process results in a novel method that incorporates several aspects of utmost importance to small-scale plasticity, i.e. source truncation effects, surface nucleation effects, starvation effects, slip localization and an inherently stochastic response. The model is implemented in an efficient FFT-based solver [2] and applied to the study of submicron pillar compression experiments on tungsten (W), a prototypical metal for applications under extreme conditions. The results are thoroughly compared with experimental literature [3] with significant agreement.

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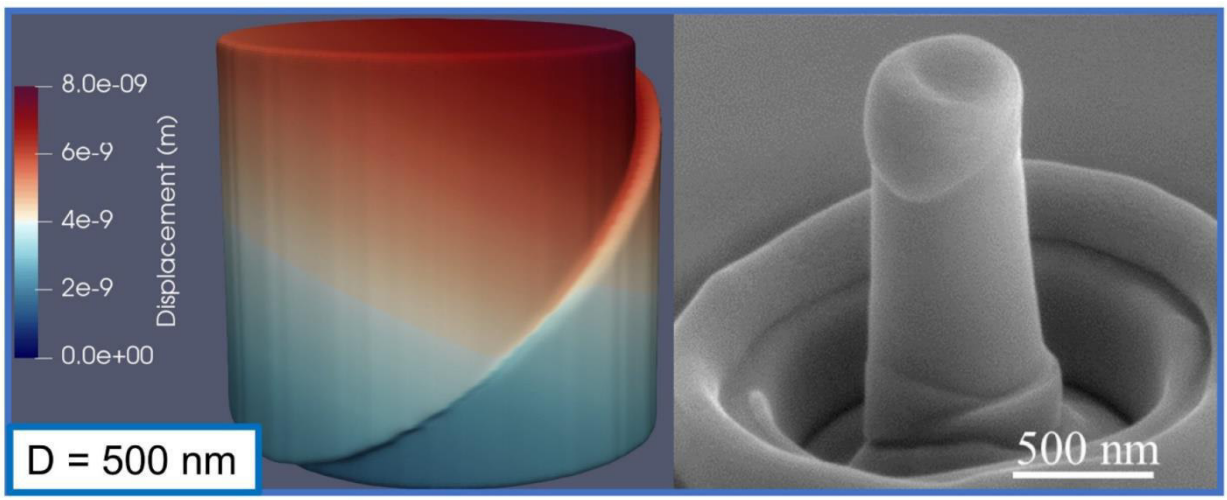

Figure 1: Residual deformation patterns for a 500 nm diameter W pillar [1] compared to SEM experimental observations [3].

Soft network materials immersed in viscous fluid media

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Many soft network materials consist of polymer strands connected by crosslinkers. This is the idealized version of hydrogels, where the network typically exhibits a disordered structure characterized by flexible polymer strands of different lengths, giving rise to a wide mesh size distribution. Additionally, since hydrogels are immersed in water, they are coupled mechanically to the fluid resulting in poroelastic behavior [1,2]. As a result, the speed of deformation could influence the mechanical response by allowing or preventing the solvent from equilibrating inside and outside the hydrogel. Explicitly accounting for the solvent is thus essential to accurately capture the behavior of real polymer gels.

In this work, we try to unravel the microscopic aspects that induce the mechanical coupling between the solvent and the disordered polymer network under uniaxial deformation. Experimentally, we generate chitosan hydrogels and study their mechanical response as a function of strain amplitude and straining speed. Our results show that the effective elastic modulus in the rapid-straining regime increases while the volume of the gel does not change. We then perform Molecular Dynamics simulations of soft polymer networks [3] immersed in an explicit solvent. We find that different compression speeds lead to different mechanical response. Specifically, low-speed deformations allow the hydrogel to compress without resistance, expelling the solvent. In contrast, speeds higher than the relaxation time of the polymer network prevent expelling solvent, rendering the network incompressible. This behavior qualitatively agree with the experiments.

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Ionic Conductivity in Engineered Protein Thin Films

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Protein-based conductive materials are promising for next-generation bioelectronics due to their versatility, biocompatibility, and biodegradability. Protein films composed of engineered consensus tetratricopeptide repeat (CTPR)[1] – proteins with a high content of negatively charged amino acids – have been demonstrated to be ionic conductors [2], with the dominant mechanism being protonic conduction. Proton transport within proteins is of interest for designing biocompatible energy storage devices or intelligent devices such as biosensors; raising the interest on improving protein film conductivities that can make them suitable for applications. In this work, we present an electrical characterization of thin films (≈ 100-200 nm thickness) prepared using engineered CTPR protein variants modified by different rates of glutamic acid substitution. From impedance spectroscopy measurements of CTPR films drop-casted on interdigitated electrodes, we find an increase of ionic conductivity with increasing the substitution rate, which suggests an increase in protonic carrier concentration. Additionally, we investigate the impact of NaCl doping on the ionic transport of the films, finding also an improved conduction performance of engineered variants. Finally, we explore the variations of the mechanical properties of the films with the amino acid substitution. Our results suggest that engineered proteins, such as modified CTPR scaffolds, can generate appropriate materials for bioelectronics applications.

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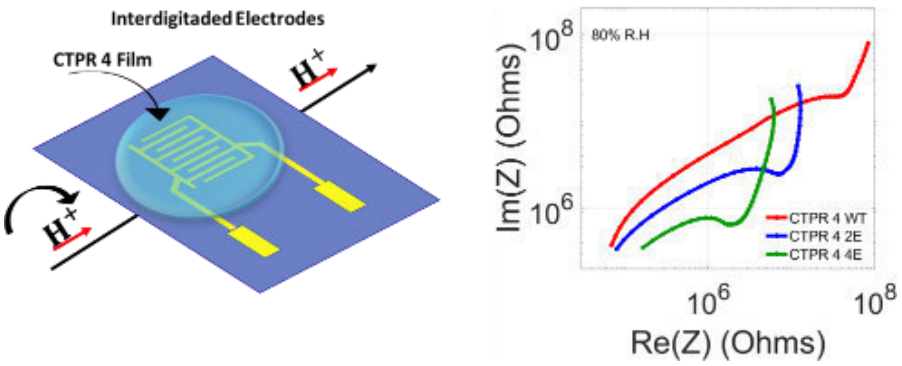

Figure 1: a) Schematic representation of a CTPR4 film deposited on interdigitated electrodes for electrical impedance spectroscopy characterization. b) Nyquist plots from EIS measurements of CTPR4 films prepared from different variants (WT, 2E, and 4E) at 80% relative humidity.

ABSTRACTS

POSTERS

GEFES 2025

On-surface synthesis and characterization of [19]-starphene

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Starphenes are appealing compounds formed by symmetric trimerization of acenes. The potential electronic conjugation of acene arms offers starphenes distinctive physiochemical properties, thus being promising candidates for future organic optoelectronic applications. However, due to the low solubility and instability that large starphenes present, their synthesis has been challenging. To date, the largest starphene obtained by solution-phase synthesis is [16]-starphene [1]. Herein, we propose new strategies using different molecules as precursors, obtaining a larger [19]-starphene by on-surface synthesis on Au(111) [2]. Bond-resolving STM images unambiguously confirmed its chemical structure, and the density of states (DOS) of frontier molecular orbitals were resolved by dI/dV maps, further supported by density functional theory (DFT) calculations. Its multi-radical character is discussed [2].

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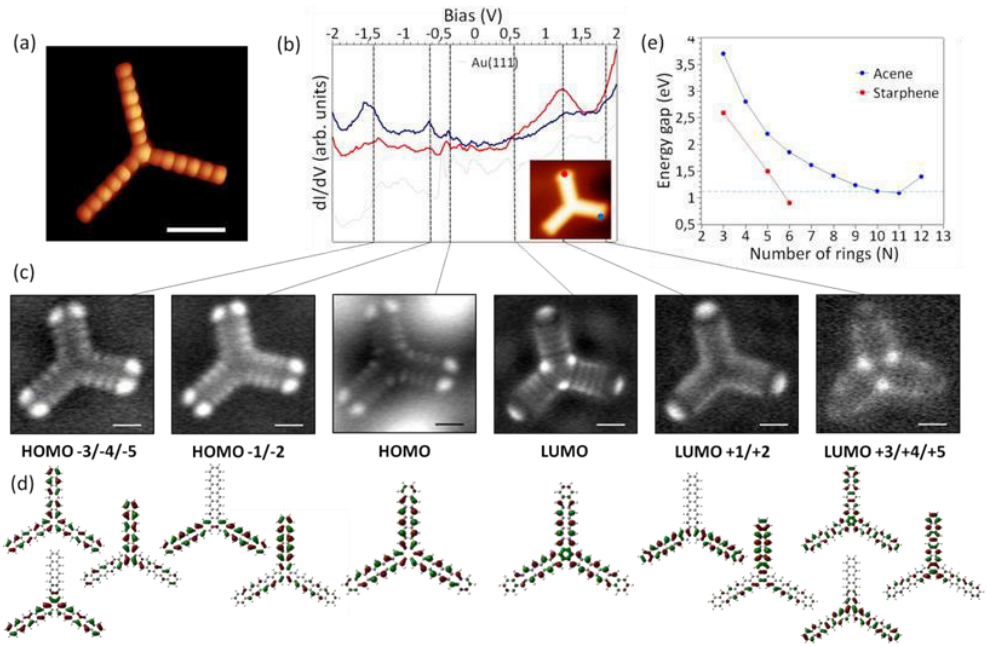

Figure 1: a) BR-STM image of [19]-starphene. b) Differential conductance point spectra acquired on the molecule at the positions marked in the inset and on the bare surface. c) Conductance maps acquired at −1.42 eV, −0.64 eV, −0.36 eV, 0.54 eV, 1.2 eV and 1.85 eV. d) Wavefunctions of the orbitals associated with each of the measured resonances and conduction maps in previous panels. e) HOMO-LUMO gap as determined by scanning tunneling spectroscopy for starphenes and acenes of varying size. For a better comparison, the starphene size is given by the number of rings on each of its arms, the currently analyzed [19]-starphene thus corresponding to N = 6. The dashed horizontal line marks the smallest acene gap reported to date, observed on undecacene.

Building altermagnets on graphene by H atom manipulation

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Engineering all fundamental magnetic phases within a single material may well be a significant milestone in materials science and spintronics. In this poster, we demonstrate that graphene can act as a platform to host all non-relativistic magnetic phases -namely, diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism, fully compensated ferrimagnetism, and altermagnetism- by utilizing adsorbed single hydrogen atoms as building blocks. Through precise manipulation of these atoms using scanning tunneling microscopy (STM), we have experimentally constructed all these magnetic phases. Their different electronic character is revealed by our density functional theory (DFT) and mean-field Hubbard calculations. Specifically, we show that the new magnetic paradigm known as altermagnetism can be realized, exhibiting directional spin-split energy bands without net magnetization due to protecting spatial symmetries. Furthermore, fully compensated ferrimagnets, lacking these symmetries, can also be realized, displaying full spin splitting of the bands. Our findings establish hydrogen-functionalized graphene as a versatile platform for exploring and controlling magnetic phases at the atomic scale, paving the way for spintronic applications without the need for ferromagnetic materials or heavy elements.

Next-generation X-ray Detectors Based on Metal-Organic Frameworks

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Next-generation X-ray detector materials are increasingly requested for high-resolution, high-throughput applications, particularly in medical imaging [1]. Metal-organic frameworks (MOFs), self-assembled structures composed of metal nodes linked by organic ligands, exhibit an intrinsic porosity and unique tuneable properties making them promising candidates for indirect detection and in vivo applications [2-3]. In this talk, we explore the potential of MOFs as scintillators using a high-throughput screening approach to identify optimal candidates with enhanced radioluminescence properties. Using the Cambridge Structural Database, we screen a wide range of MOFs and identify [Eu2(NDC)3(4,4′–bpy)0.5(H2O)3]·(4,4′–bpy) as the most promising candidate due to the inclusion of 4,4′-bipyridine (bipy), a ligand known for enhancing photoluminescence [4]. Through steady-state and time-resolved spectroscopic characterization, we demonstrate that the incorporation of bipy also translates into a significant improvement of radioluminescence performance, leading to a bright emission at 637 nm. This emission is driven by two distinct recombination mechanisms: an initial fast process with a characteristic decay of 0.9 ns, followed by a secondary slower relaxation in the ms regime. To complete the time-domain analysis, we perform stability tests using a laboratory X-ray source at 60 kV and synchrotron-based X-ray irradiation experiments. The MOF was exposed to doses of 5 Gy and 23 kGy, which are equivalent to 50,000 and 225 million radiographic cycles, respectively. The integrity of the Eu-MOF structure is maintained after exposure to the synchrotron radiation dose rate, as demonstrated by WAXS and SAXS analysis, underscoring its stability and potential for use in X-ray detector applications. These findings highlight the significance of selecting and combining ligands, such as bipy and NDC, to optimize the performance of MOFs.

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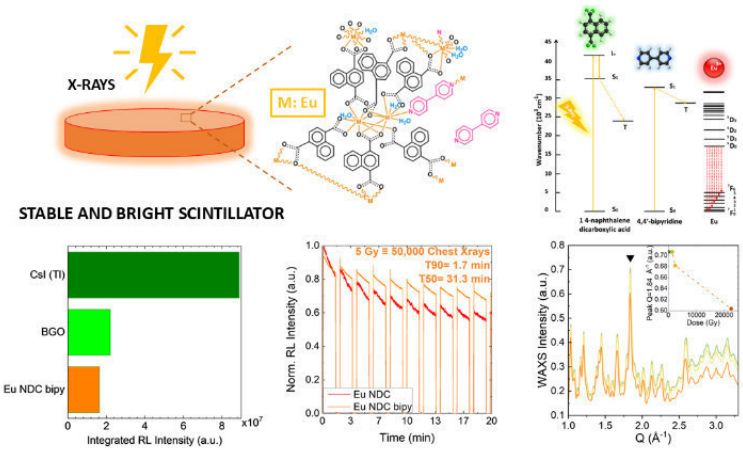

Figure 1: Structure of the Eu NDC bipy MOF and its energy levels. Results of RL intensity vs. commercial scintillators, RL stability under lab X-ray source, and structure stability (WAXs) under synchrotron radiation.

Photoinduced ferroelectric control of Second-Harmonic Generation in monolayer MoS_2

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The association of ferroelectrics and Transition Metal Dichalcogenides (TMDs) has recently emerged as a promising approach for controlling the optoelectronic properties of 2D materials [1]. However, previous studies have primarily focused on the electrical and linear optical properties of TMDs, while the influence of ferroelectric substrates on the nonlinear optical properties of TMDs remains largely unexplored [2].

In this work, we exploit light-induced ferroelectric control of electronic doping in monolayer MoS_2 [3] to experimentally demonstrate the spatial modulation of quadratic Second Harmonic Generation (SHG) in MoS_2 deposited on a periodically poled $LiNbO_3$ substrate. As shown in Figure 1, a pronounced contrast in SHG intensity is observed between signals collected from MoS_2 on ferroelectric domains of opposite polarities, with maximum values occurring on the P_{down} domains. The influence of the fundamental beam's intensity, polarization, and photon energy on the SHG response modulation is systematically analyzed. The spectral response of the SHG modulation reveals a clear resonance with the C band of MoS_2. In agreement with calculations, the SHG enhancement is correlated to electron doping, which originates from domain-oriented photoinduced charge-transfer processes at the ferroelectric/MoS_2 interfaces.

The obtained results contribute to the fundamental understanding of nonlinear processes in TMD/ferroelectric heterostructures under external optical stimuli, and open new routes to their application into the fabrication of 2D photonic and optoelectronic devices.

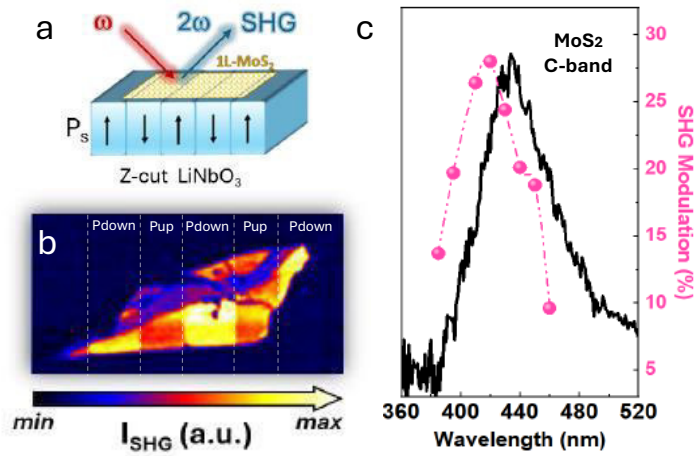

Figure 1: a) Schematics of SHG from a $MoS_2/LiNbO_3$ heterostructure. b) SHG spatial modulation of monolayer MoS_2 deposited on a periodically poled $LiNbO_3$ crystal. c) Spectral response of the SHG modulation (red) in the C band spectral region (black) of MoS_2.

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Cooper pair diode in Coulomb blockade Pb islands on graphene

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Non-reciprocity, essential for current rectification in electronics, is challenging to achieve in superconducting devices without external magnetic fields. Current methods rely on non-centrosymmetric materials or magneto-chiral effects, limiting their versatility.

We investigate small Pb islands on graphene where Coulomb and superconducting correlations coexist. The quasiparticle excitations at edge of the superconducting gap are modified by the Coulomb blockade and rationalized by a double tunneling junction model.

Approaching the scanning tunneling microscope (STM) tip to Josephson regimes, we observe Resonant Cooper Pair Tunneling (RCT) peaks in the current voltage characteristics. The RCT energy values change with gating, that we can control with STM tip pulses. We test this in a current-biased STM junction [1] and find a CP current asymmetric with polarity. This is a realization of non-reciprocal transport of CP, tunable with a gate.

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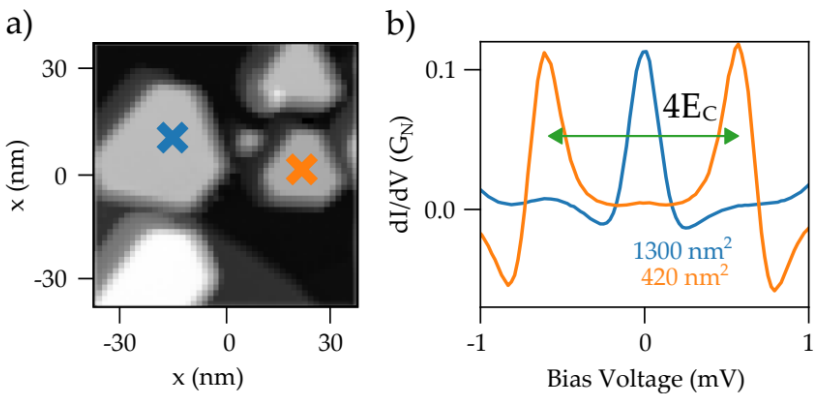

Figure 1: (a) Topographic image of Pb islands on graphene. (b) dI/dV spectra of the Josephson peak at R=25kOms of the islands in (a) of lateral area 1300 nm^2 and 420 nm^2. The larger island shows a conventional Josephson peak, while the smaller islands shows a split Josephson peak (RCT).

Mirror-induced effects in cavity polaritonics: Influence on edge states

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Optical cavities are widely used to induce strong light-matter coupling and thereby enable the presence of polaritons [1]. While polaritons are at the source of most of the observed physics, identifying effects resulting strictly from the polaritonic nature of the excitation may be difficult. Indeed, the mirrors forming the cavity may themselves be responsible for a number of phenomena, leading to recent discussions on cavity-induced nonpolaritonic effects [2,3].
Motivated by these debates, we use here a toy model of a chain of dipolar emitters embedded in a cuboidal multimode cavity to unveil direct effects originating solely from the boundary conditions that such a cavity imposes on the electromagnetic field, independently of the presence of polaritons [4]. We demonstrate that mirrors in the direction transverse to the chain may act as effective defects, leading to the emergence of Tamm edge states. In a topological chain, such transverse mirrors may also protect edge states against the effects of the strong light-matter coupling. Moreover, mirrors parallel to the chain, by the image charges they involve, may induce topological phase transitions even in the case of highly off-resonant photons.

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Use of graphdiyne as active element inphotoelectrochemical cells for hydrogen generation

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It has been recently demonstrated that hydrogen substitution of acetylenic groups in graphdiyne is an effective strategy to tune the electronic band gap of this material [1,2]. A "bottom-up" method for H-substitution of GDY enables to adjust adequately the bandgap for optimal interface charge carriers' separations, electron transfer from H-GDY to TiO_2, higher H_2 generation and visible light photosensitization. H-substituted GDY has a bandgap of 2.4 eV as estimated by Density Functional Theory (DFT) calculations, and confirmed by experimental analysis (2.5 eV), with well-disposed valence and conduction band edges that promote the electron/hole transfer between H-GDY and TiO_2, and then its photosensitization. The results are promising, since under visible light irradiation H-GDY photosensitizes TiO_2 leading to impressive photocatalytic hydrogen generations, for a metal free- photocatalyst.

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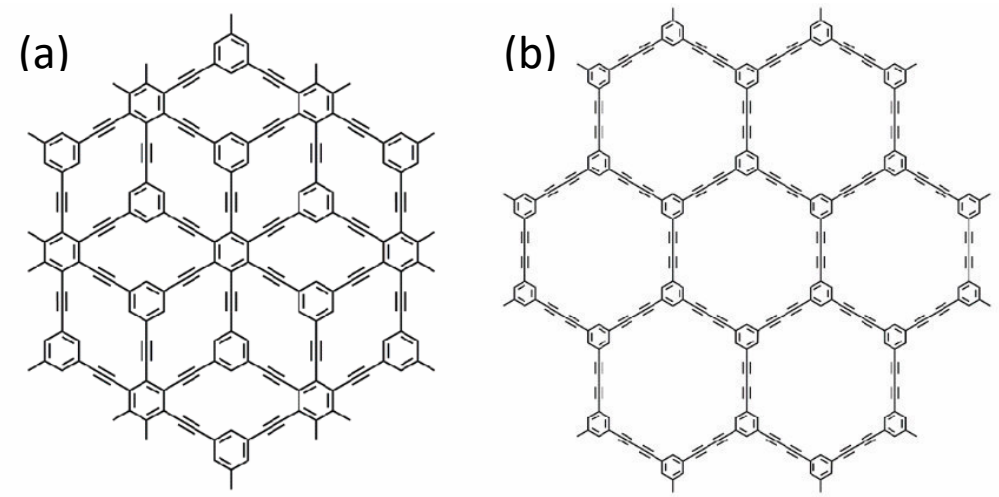

Figure 1: Structure of graphdiyne (a) and hydrogen-substituted graphdiyne (b).

Technology demonstration of a superconducting Kinetic Inductance Detectors (KIDs) camera for Dark Matter axion detection

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Kinetic Inductance Detectors (KIDs) play a crucial role as ultrasensitive detectors in many fields due to their high sensitivity and simple multiplexed readout. Being made of low critical temperature superconductors, which enable the detection of low energy excitations, microwave KIDs may pose an advantage against coherent detectors thanks to their simplicity, compactness, and large detection bandwidth [1, 2]. In the Canfranc Axion Detection Experiment (CADEx), KIDs will be used to search for the axion in the unexplored mass range of 330-460 μeV. Operating in the W-band (75-110 GHz), CADEx will be installed with a dilution cryostat at the Canfranc Underground Laboratory (LSC), combining, for the first time, a cavity haloscope in a strong magnetic field with a Lumped Element Kinetic Inductance Detectors (LEKIDs) camera [3]. This novel combination is designed to detect the polarization signature of the axion in contrast to the usual spectrometer configuration.

Achieving the necessary sensitivity requires reaching the ultimate sensitivity of the LEKID-based detection system in the W-band. In this work, we present the initial results concerning the bandwidth and noise obtained from a 3-by-3-pixel prototype camera of Ti/Al superconducting LEKIDs. Our characterization, performed in a dilution refrigerator at 10 mK, confirms W-band sensitivity and raises a Noise Equivalent Power (NEP) value in the order of 10^{-19} W/√Hz. These results are a promising indication of the camera's performance, marking an essential step towards realizing the full potential of CADEx's search for distinct signals of the dark photon or axions in the W-band.

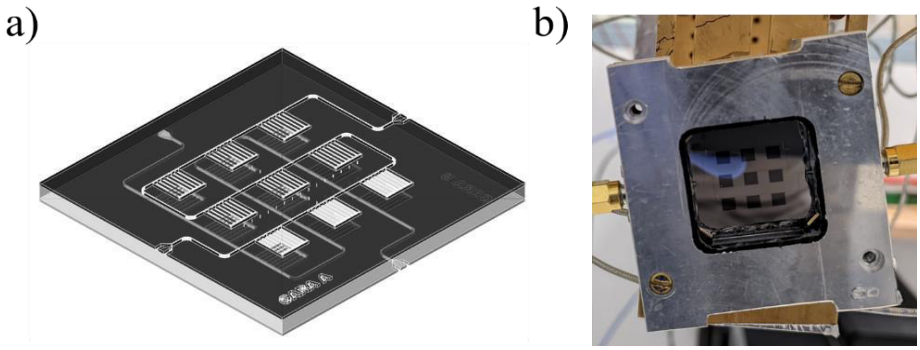

Figure 1: a) Design 3D schematics of the 3-by-3 LEKID array prototype camara. **b)** Picture of the prototype camera mounted in the measurement holder in the dilution refrigerator prior to RF characterization.

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Partons and non-abelian anyons in twisted 2D materials for quantum computation

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Parton states beyond the Abelian Laughlin and Jain models are being explored as candidates to describe fractional quantum Hall effect (FQHE) states in higher Landau levels in monolayer and multilayer graphene. Theoretical and experimental work is investigating spin polarization in graphene's lowest and first Landau levels, with a focus on whether the states are Abelian or non-Abelian. In gapped and twisted bilayer graphene, recent research shows that tuning the external magnetic field can induce topological quantum phase transitions, transforming an Abelian composite fermion state into a non-Abelian parton state. These states host exotic anyons that could serve as the building blocks for fault-tolerant topological quantum computers. Non-Abelian anyons have topological properties that protect quantum information from local errors, making them ideal for robust quantum computation. By exploiting the stability of parton states and the braiding statistics of anyons, parton-based systems could perform quantum operations that are less susceptible to decoherence, addressing a key challenge in building scalable quantum computers. Additionally, studies of real-space entanglement spectra of parton states in FQHE systems offer insights into new methods for stable quantum information processing. Non-Abelian topological order, which allows quasiparticles to retain the order of their exchanges, is a sought-after state of matter. Though challenging to achieve, recent progress has demonstrated non-Abelian topological order in wavefunctions generated by trapped quantum processors, with precise control over anyons. Using non-Abelian anyons in graphene-based heterostructures could transfer this approach from trapped-ion systems to solid-state devices. Given that the quantum Hall effect in graphene persists at room temperature, it is feasible to manipulate fractional states at temperatures above the millikelvin regime. Experiments with hBN-graphene-hBN heterostructures are advancing the study of fractional filling FQHE states and their potential use in topological quantum computing [1].

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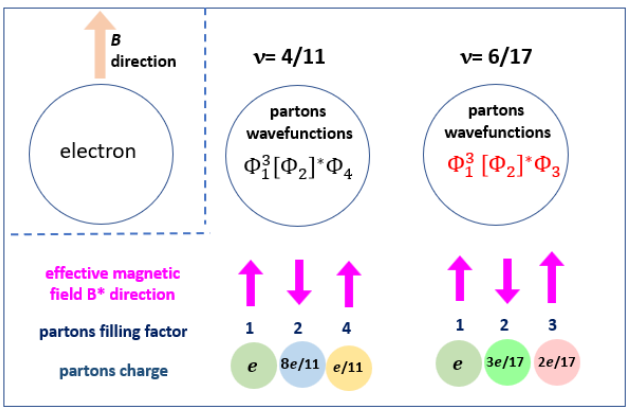

Figure 1: a) Representation of two fractional quantum Hall states of composite fermions, along with the corresponding parton states, which could serve as foundational elements for fault-tolerant topological quantum computers.

Spin-Magnon Coupling in GdW_{10} and CrSBr: Theoretical Models with Experimental Validation.

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We investigate the spin-magnon interactions between two promising magnetic materials: GdW_{10}, a single-ion magnet (SIM), and the two-dimensional antiferromagnetic semiconductor CrSBr. GdW_{10}, a polyoxometalate-based SIM with a simple Hamiltonian, exemplifies the intriguing single-molecule magnetic properties of lanthanide encapsulation. CrSBr, in contrast, exhibits A-type antiferromagnetic order (T_n = 132 K) and strong electronic-magnetic coupling in both bulk and monolayer forms, making it an exciting candidate for spintronic applications. Our derived Hamiltonians for both materials yield theoretical plots in excellent agreement with experimental data, supporting further exploration of SIMs and 2D antiferromagnetic systems.

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Figures

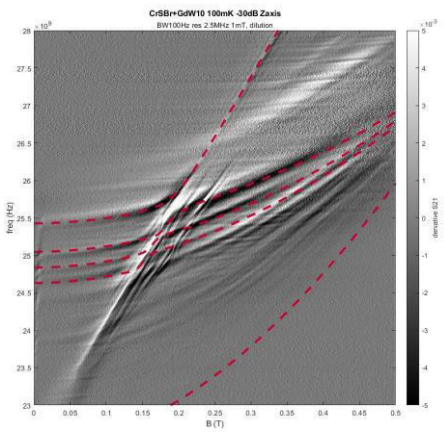

Figure 1: Anticrossings due to the interaction between **GdW_{10}** and **CrSBr**

Enhancement of heat transfer induced by polaritonic topological transitions in twisted van der Waals crystals

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Twisted stacks composed of thin α-MoO_3 layers offer the possibility to tailor electromagnetic waves at the nanoscale by the excitation of directional phonon polaritons -light coupled to lattice vibrations-, giving rise to the field of twistoptics. Although emergent in nano-optics, the application of twistoptics to heat transfer has lagged behind, particularly regarding near-field radiative heat transfer (NFRHT), which despite its importance for thermal management in nanodevices remains insufficiently explored. Here, we report a theoretical study on the role of twistoptics in NFRHT, demonstrating that the heat flux between two twisted α-MoO_3 bilayers can be monotonically increased/decreased by simply increasing/decreasing the twist angle. Interestingly, this modulation is explained by the emergence of topological transitions from open (hyperbolic) to closed (elliptical) polaritonic dispersions. This phenomenon is further demonstrated by considering α-MoO_3 trilayers, which show greater flexibility to regulate NFRHT since they support a larger number of topological transitions. Based on these findings, we finally propose an experimental scenario in which the heat flux between a nanoparticle and a twisted α-MoO_3 bilayer can be modulated by a factor of three by simply adjusting the twist angle. This work provides theoretical guidance for the modulation of NFRHT using twistoptics, making an important step toward the development of twisted thermotics.

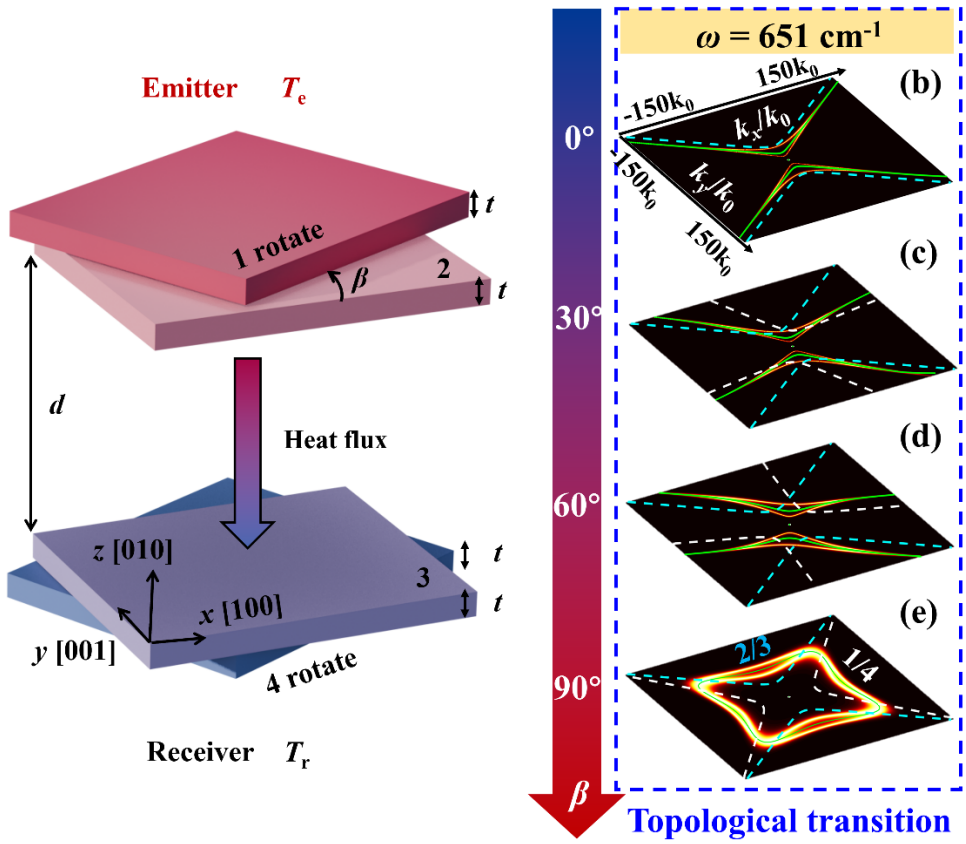

Figure 1: Topology-mediated enhancement of heat transfer in twisted van der Waals crystals

Layer thickness and substrate effects on superconductivity in epitaxial FeSe films on BLG/SiC(0001)

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The layered nature and simple structure of FeSe reveal this iron-based superconductor as a unique building block for the design of artificial heterostructure materials. However, while superconductivity develops in single-layer FeSe on $SrTiO_3$ substrates, it remains unclear whether single- and few-layer FeSe can develop superconductivity on more chemically inert, van der Waals materials such as graphene. Here, we report on the characterization of the structural, chemical and electronic properties of few-layer FeSe epitaxially grown on bilayer graphene (BLG) on SiC(0001) using low-temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS) and X-ray photoelectron spectroscopy (XPS). STM imaging of our FeSe films with thicknesses up to three layers exhibit the tetragonal crystal structure of bulk FeSe, which is corroborated by XPS measurements by contrasting the binding energy of the Fe-2p and Se-3d core levels with the bulk counterpart. While our high-resolution STS measurements at 340 mK reveal a metallic character for few-layer FeSe on BLG/SiC(0001), they show an absence of superconductivity, as the electronic structure around the Fermi level exhibits a spatially anisotropic dip-like feature robust against magnetic fields. Superconductivity in FeSe on BLG/SiC(0001), however, emerges for thicker films (on average > 20 layers), with a superconducting transition temperature of 6 K. Our results underscore the significance of the substrate as key factor driving the suppression superconductivity in FeSe in the 2D limit.

Towards a Standardised Methodology of Radiation Damage Defect Distributions for Microstructure Evolution Models

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In the context of material irradiation simulations, we have developed a model that combines results from Molecular Dynamics (MD) and the Binary Collision Approximation (BCA) to reconstruct the damage produced by irradiated ions of energies of the order of MeV. Our tool, which will be available for the community, is aimed to provide a standardised way of introducing defects in large scale models. Our code takes the energy and position of the primary knock-on atoms (PKAs) along the ion track from SRIM [1] and combines it with a database of MD cascade debris (CascadesDB [2]) of single PKA calculations to obtain the total damage produced. For the lowest energies, the full energy range arc-dpa model [3] is used to compute the number of Frenkel pairs generated. Thereafter, the results can be used as an input for microstructure evolution models. In addition, the model could be extended to simulate neutron irradiation.

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Figures

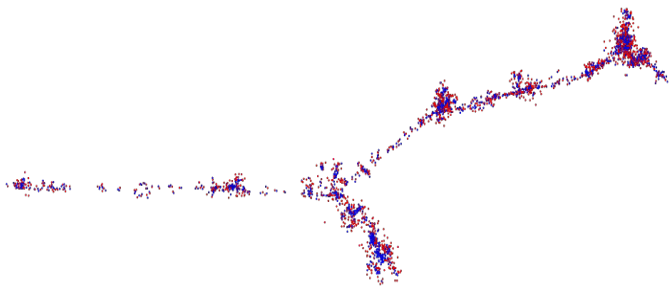

Figure 1: Defects produced by a 1 MeV ion of Fe irradiated into Fe. Self-interstitals and vacancies are represented as red and blue spheres, respectively.

Strain-induced exciton transfer among quantum emitters in two-dimensional materials

A. Martínez-Suárez[2,4,*], G. Ronco[1], D. Tedeschi[3], M. Savaresi[1], A. Hierro-Rodríguez[2,5], S. McVitie[5], S. Stroj[6], J. Aberl[7], M. Brehm[7], V. M. García-Suárez[2,4], M. B. Rota[1], P. Alonso Gonzáles[2,4], J. Martín-Sánchez[2,4], and R. Trotta[1]

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The discovery of quantum emitters (QEs) in two-dimensional (2D) materials [1] has spurred considerable research into their potential for quantum photonics. While the microscopic origin of these QEs remains under active investigation, position-controlled QEs are typically fabricated using static strain gradients to direct excitons toward localized regions of the crystal, where quantum light emission occurs [2]. However, the dynamic use of strain to modulate the brightness of single-photon sources in 2D materials has not yet been explored.

In this work, we address this gap by introducing a hybrid semiconductor-piezoelectric device, where WSe_2 monolayers are integrated onto piezoelectric pillars that generate both static and dynamic strains [3]. The static strain induces QE formation, with photon anti-bunching observed in their emission. Applying voltages to the piezoelectric pillars allows control over the QEs' energy and brightness. Numerical simulations, combined with drift-diffusion equations, reveal that these effects arise from strain-induced modifications to the confining potential landscape, resulting in exciton redistribution among the QEs. Additionally, simulations demonstrate that embedding these QEs within optical cavities significantly enhances their emission brightness and efficiency.

This work offers a method for dynamically controlling the brightness of single-photon sources in 2D materials, advancing their potential for quantum photonics applications.

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Figures

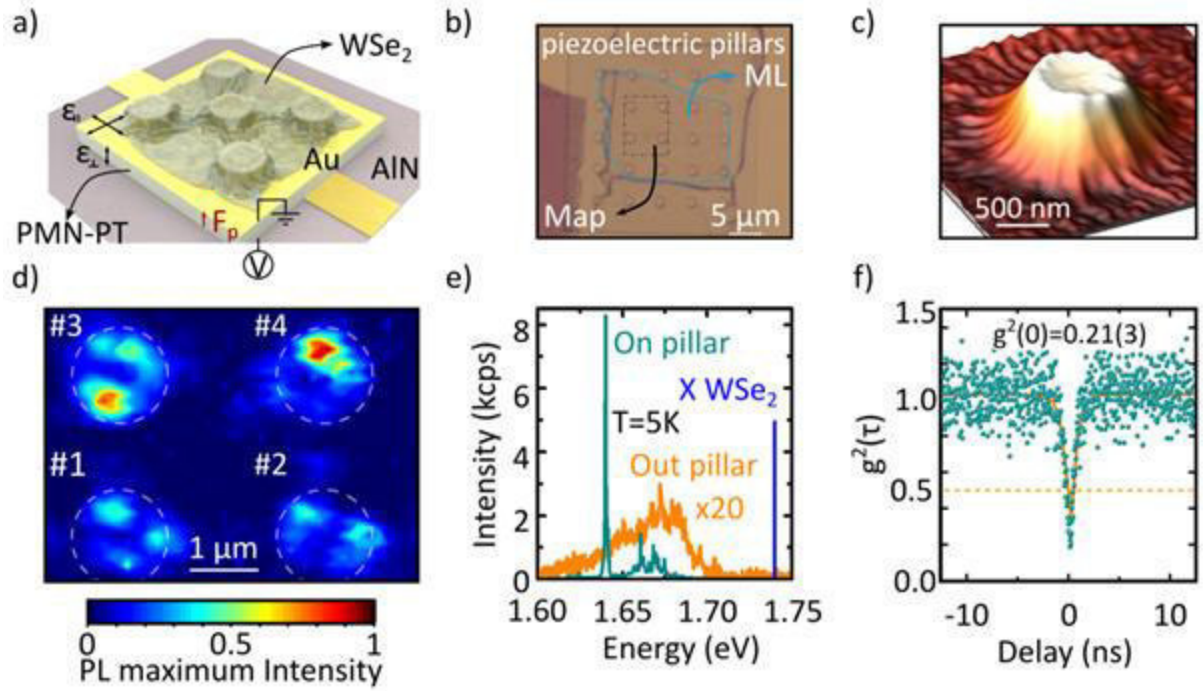

Figure 1: a) Schematic illustration of the device, showing a PMN-PT piezoelectric plate with pillars, onto which a WSe_2 monolayer (ML) is transferred. The top and bottom surfaces of the plate are coated with gold. Applying a voltage (electric field F_p along the poling direction) through an AlN chip-carrier induces out-of-plane (ε_∞) and in-plane ($\varepsilon_\%$) deformations in the piezoelectric plate, which are transferred to the attached monolayer. b) Optical microscopy image of a WSe_2 ML (appearing as a transparent brownish region outlined by a dashed white line) placed atop the piezoelectric pillars. c) 3D AFM image of a representative piezoelectric pillar (height ~115 nm, diameter ~1400 nm) covered by the WSe_2 ML. d) Micro-PL map of the WSe_2 ML over the piezoelectric pillars, focusing on the region outlined by the point-dashed black box in panel b. Each pixel shows the normalized maximum intensity of the PL spectrum, with dashed white circles indicating the positions of four pillars. e) Micro-PL spectra measured outside a pillar (orange line) and at the edge of a pillar (dark-cyan line). The blue vertical line marks the emission energy of the 2D neutral exciton in the WSe_2 ML. f) Second-order autocorrelation function measured for a single QE, demonstrating single-photon emission with $g^{(2)}(0)=0.21$. The solid orange line represents the fit to the experimental data.

A Novel Hybrid 3D-Printed Compliant Mechanism Device for High Strain Fields in 2D Materials

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The physical properties of materials can be controlled by the deliberate introduction of elastic deformation fields (elastic strain engineering). In the field of nanophotonics, the introduction of reversible strain fields can be used to efficiently tune the optical emission properties in a reversible manner in optically active nanomaterials. In this regard, atomically-thin and bright semiconductor van der Waals materials (or two-dimensional materials, 2D) are particularly interesting, as they can withstand large elastic deformations (up to values of 10%). Therefore, the development of novel platforms that allow the introduction of elastic deformation fields with control in their sign (tensile/compressive) and magnitude is particularly interesting.

In this work, we present a device based on flexible mechanisms capable of introducing uniaxial elastic deformation fields (Compliant Mechanisms): an innovative solution that take advantage of the elasticity of the material to achieve a highly directional movement, without relying on traditional mechanical joints. As a proof-of-concept, we demonstrate the capabilities of this device to tune the optical emission energy in WSe2 monolayers (~30 meV) and quantum emitters present in two-dimensional hexagonal boron nitride (h-BN) crystals (~50 meV). As future work, we intend to scale these devices to the nanoscale for integration into compact platforms capable of operating in systems with reduced dimensionality and at cryogenic temperatures.

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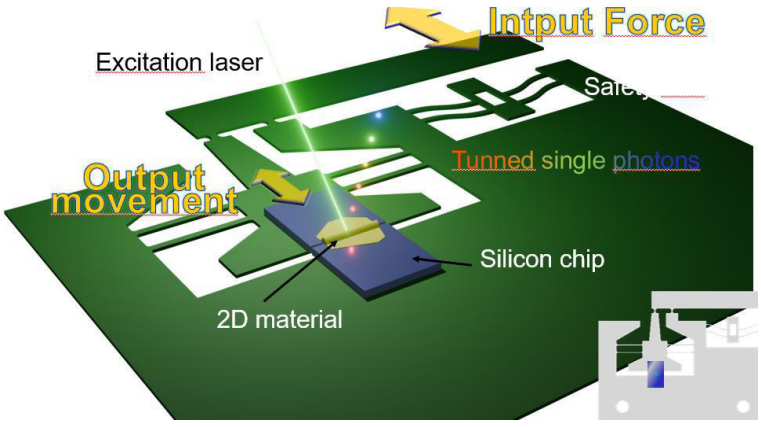

Figure 1.- A novel customized hybrid 3D-printed compliant mechanism device to introduce large strain fields in nanomaterials [1].

Real-space criteria for non-crystalline fractional Chern insulators

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Predicting which single-particle bands favor, many-body states with a fractional quantum Hall conductivity, known as fractional Chern insulator ground states, usually relies on momentum-space criteria. These criteria single out bands that closely resemble Landau levels, with small dispersion, flat Berry curvature and a saturated trace inequality for the quantum metric. However, for systems without translation invariance these criteria seem inapplicable due to the lack of a well defined momentum. Here we introduce an analogue set of criteria for ideal Chern bands based on real-space quantities. The criteria of small fluctuations of the Berry curvature in momentum space translates into small fluctuations of the local Chern marker in real-space. We formulate the trace inequality in terms of the real-space vortexability, which measures the degree to which many-body states admit a vortex attachment, in terms of the local Chern marker. We then compute these criteria for several disordered Chern insulating models, including amorphous systems. We end up by discussing the potential of these criteria to signal many-body fractional Chern insulator groundstates upon adding strong electron-electron interactions

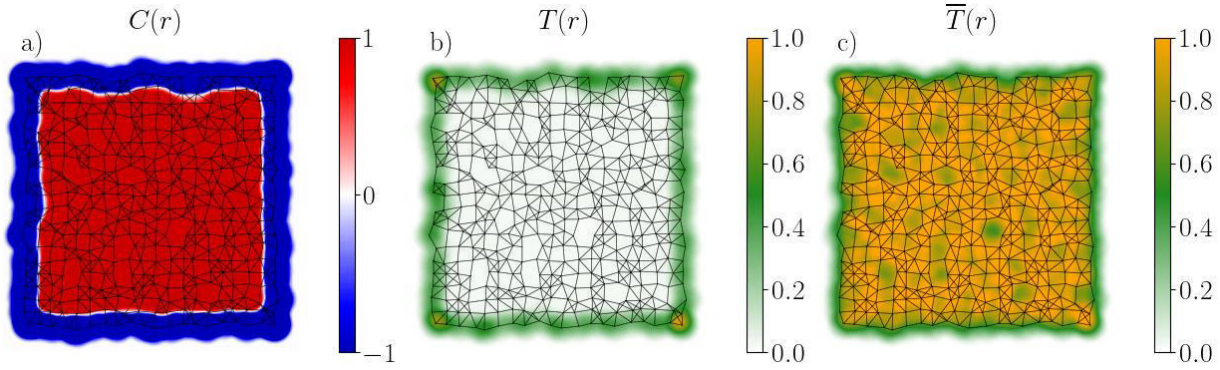

Figure 1: Real-space dependence of the (a) local Chern marker, (b) vortexability and (c) anti-vortexability for an amorphous Chern insulator.

THE ODD WEIGHT OF GRANULAR PACKINGS

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German engineer Janssen showed that pressure in granular columns does not increase linearly with added mass as it does in liquids [1,2]. Instead, it reaches saturation due to internal friction and supportive force chains, which are curves of highly stressed particles. Here, we revisit the traditional experiment by Janssen using grains of different shapes—spherical, oblate (lentils), and prolate (mung beans)—within cylindrical containers of varying diameters under the influence of gravity.

For all grain types, we recover the classical saturation behavior but, interestingly, we also find that in narrow containers there is an overshoot in the mass of the granular column before reaching saturation. This is hypothesized to be caused by compressive force chains. This overshoot is more pronounced in narrower containers and decreases as the container diameter increases [3]. However, this decrease seems different for different grain geometry, suggesting that this aspect could influence packing efficiency, frictional forces with the walls and force-chain distribution.

We are also performing work with birefringent grains in 2D cells to directly visualize force chains. These grains "glow" between crossed polarizers when deformed, allowing identifying the force-chain structure. Preliminary results indicate that indeed compressive chains are responsible for the overshoot observed experimentally.

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Probing the dynamics of microgel suspensions with respect to concentration using 3D-DLS

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The dynamics of a microgel suspension is highly dependent on its particle concentration, as well as particle size and softness. We perform 3D dynamic light scattering [1,2] (3DDLS) experiments with a system consisting of NIPAM and AAc (crosslinked with pEG-d) at a temperature and pH range to analyze its swelling behaviour. Next, we focus on its relaxation time dependence with concentration. At higher concentrations, two different time scales show up, associated to a diffusive and a structural relaxation regimes. This shows up as a two step decay, the second of which is modeled through a stretched exponential [3]. We analyze the dependence of the structural relaxation time, τ_α, as the particle concentration increases above the glass transition.

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Interplay Between Crystal and Magnetic Textures in Iron Oxide Nanoflowers

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Magnetic iron oxide Nanoflowers (IONF) have been drawing much attention because of their superior magnetic performance compared to single-core magnetic nanoparticles [1]. Despite the large sizes of IONF, these aggregates show almost zero remanences and nearly vanishing coercivities, while preserving high saturation magnetization [2]. This seemingly effective superparamagnetic behavior has motivated their use in biomedical and environmental applications since the net magnetization can be controlled at will by an external magnetic field so that the particle agglomeration is effectively reduced. Some authors have attributed this phenomenology to the existence of some exchange coupling among the cores, leading to a super ferromagnetic state of the whole aggregate [3]. However, the effect of the crystal texture on the nearly demagnetized remnant state of these systems is still unclear. This study reports on how the local magnetic texture, originating from crystalline correlations among the cores, governs the unique magnetic properties of individual IONF in sizes ranging from 40 to 400 nm [4]. Despite size variations, all samples exhibit consistent crystalline correlations extending beyond the IONF cores. A nearly zero remnant magnetization, a persistently blocked state, and temperature-independent magnetization support the existence of a 3D magnetic texture throughout IONF. Magnetic transmission X-ray microscopy confirms nearly demagnetized states caused by magnetic texture vorticity. Moreover, micromagnetic simulations show vortex-like spin configurations with partial topological protection, stabilized by inter-core exchange coupling and demagnetizing fields at low magnetic fields (see Fig. 1). Overall, this study provides valuable insights into the impact of crystalline texture on the magnetic properties of IONF over a wide size range.

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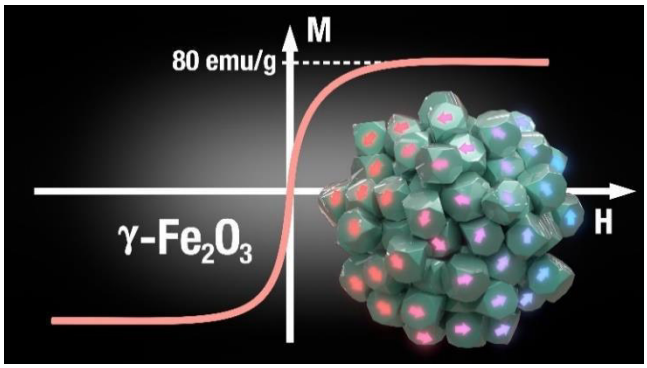

Figure 1: Effective super ferromagnetic behaviour in IONF caused by the near demagnetized state driven by the high vorticity of the core moment texture at low magnetic fields.

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Quest for subsurface amorphization in topological Bi–Sb materials by MeV ion implantation

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Approximately 70 years ago, it was observed that amorphous bismuth —a strongly diamagnetic semimetal with unconventional properties— and some of its alloys, particularly those with antimony (Bi–Sb), exhibit superconductivity with a critical temperature of about 6 K [1], unlike their crystalline counterparts, which do not display such behavior.
More recently, Bi–Sb alloys have gained renewed interest due to their behavior as topological insulators [2]. The possibility of combining this feature with the superconducting properties renders amorphous Bi–Sb alloys promising candidates for topological superconductivity [3]. However, a significant challenge arises as both pure Bi and Bi–Sb alloys tend to crystallize when exposed to temperatures above 20 K [1,4].
In this study, we aimed to address this limitation by creating controlled structural disorder in crystalline Bi–Sb alloys using MeV ion irradiation. We fabricated various polycrystalline $Bi_{100-x}Sb_x$ films (x = 0, 5, 10, 15) using thermal evaporation and melt–spinning techniques, and then exposed these films to ion beam irradiation with swift heavy ions (Bi and I ions in the 10–40 MeV range) to induce localized amorphization in a deeper region.
To evaluate the effects of irradiation, we performed multiple characterizations before and after the process, including X–ray Diffraction, Scanning Electron Microscopy, and low-temperature electrical resistivity measurements spanning from room temperature down to nearly 2 K. We assessed the impact of both preparation method and degree of disorder when trying to modify the properties of these materials for superconducting and thermoelectric technologies [5].

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Force profiles for penetrating colloidal particles inside dipolar brush polymers

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Via Langevin Dynamics simulations we have studied the interaction of a large colloidal particle (the penetrating particle) with a dipolar brush consisting of polymers chains grafted to a surface whose monomers bears a point dipole. The forces exerted by the dipolar brush onto the penetrating particle has been recorded as a function of the particle-surface distance (the force profiles).

As expected, in the absence of an external field dipolar brushes exhibit rather monotonous force profiles which is a reflection of the steric hindrance created by the compactness of the brushes. Nonetheless, a radical change is observed when an external field is applied to the brush. In addition to the expected extension of the chains that translates into an extended range of the force profiles, a force barrier at large distances from the surface appears. Another important feature that emerges is the existence of an intermediate range of surface-particle distances in which repulsion forces are drastically reduced. For bad solvent and intermediate field strengths, the forces in this intermediate regime of distances can turn even from repulsive to attractive and lead to the existence of a stationary point in which penetrating particles with tend to remain entrapped inside the brush. This unexpected attraction between the brush and the penetrating particle can be reasoned, as the result of an equilibrium between two opposite forces: the entropic or steric repulsive force due to the high density of monomers near the grafting surface, and an attractive force emerging from the mismatch between the dipolar media created by the monomers of the brush, and the non-dipolar media existing inside the particle and inside the grafting wall that holds the chains. As the strength of both forces depends on the external field applied, it is possible by tuning the strength of the external field to induce larger or smaller attractive forces onto the penetrating particle in that region of the brush. It is observed that for a given grafting density of chains, there exist an optimal value of the external field that maximizes the attraction between the brush and the penetrating particle: if the field strength is too low or too high, only repulsive forces are observed.

The possibility to induce via external fields force profiles with stationary points can be used to favor applications in which the entrapping and retention of colloidal particles for a later release is required. On the other hand, the possibility to create and control the strength of force barriers at a certain distance of the grafting surface can also be used, among other applications, to control the rate of adsorption and reactivity of catalytic surfaces. The results obtained in this work also envisage the potential of dipolar brushes in the field of self-assembly, the fabrication of materials based on self-organized colloidal structures, protein crystallization assistance, shape and size selection of colloidal particles, among other uses.

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Nanometer scale studies of thermal stability and orbital currents in Bi-Cu nanowires

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Bi-doped Cu nanowires (CuBi NWs) hold significant potential for spintronic applications due to their ability to exhibit a giant spin Hall effect (SHE).[1, 2] In this study, CuBi NWs with different Bi content (0%, 2%, 4%, and 7%) and crystallite sizes were synthesized using template-assisted electrodeposition. Structural properties and thermal stability were examined using scanning transmission electron microscopy (STEM) and X-ray scattering, revealing the influence of synthesis conditions on Bi distribution, grain boundaries, and lattice distortions. Larger crystalline domains allowed uniform Bi incorporation into the Cu lattice, whereas smaller domains led to Bi accumulation at grain boundaries. Thermal stability studies using *in-situ* variable-temperature STEM and electron energy-loss spectroscopy (EELS) demonstrated Bi diffusion out of the Cu lattice upon heating, followed by recrystallization into rhombohedral metallic Bi or atomic terraces of Bi on the NW surface. Density-functional theory provided insights into these processes, crucial for understanding nanosystem behavior under operational conditions in future SHE-based devices.

Further exploration of the CuBi NW system involved *in-situ* current experiments (up to 1 µA) to study the orbital Hall effect (OHE), analogous to SHE but involving orbital angular momentum. Using energy-loss magnetic chiral dichroism (EMCD) combined with EELS,[3] nanoscale observations potentially related to orbital currents were achieved. These results are essential for advancing fundamental physics and enables novel technologies such as spintronics.

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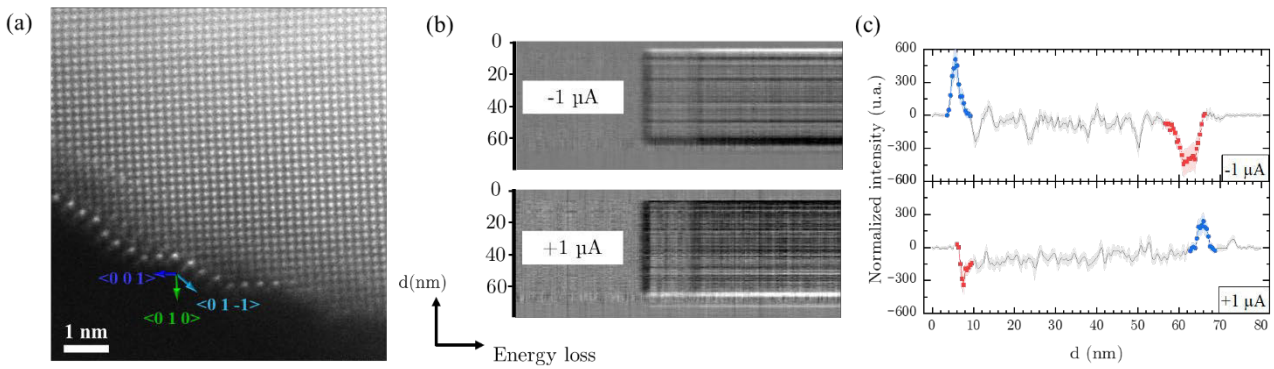

Figure 1: (a) High resolution HAADF-STEM image of the surface of a NW showing Bi segregation after heating at 400ºC and subsequent Bi recrystallisation at the edge of the CuBi NW. (b) EMCD mapping showing the difference in Cu $L_{2,3}$ edges for two-beam polarizations of the CuBi NW, for ±1 µA. (c) Normalized intensity values, averaged for each EEL spectrum along the energy dispersive direction, from the corresponding EMCD map on the left.

Topological invariants in space-time photonic systems with travelling wave modulation

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Imparting a travelling wave modulation to the optical parameters of a photonic system breaks time reversal symmetry, which results in non-reciprocal band structures, unidirectional propagation, or broadband amplification of light [1]. In this work, we study the topological properties of these band structures and the associated edge-states [2]. More precisely, we discuss how to define the topological invariant of one-dimensional systems, the Zak phase, in these spatiotemporal media, as well as examining the bulk-boundary correspondence with a semi analytical calculation of the interface states between topologically distinct materials. Finally, we discuss the differences between spatial and spatiotemporal interfaces and how these differences translate into the edge-states.

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Figures

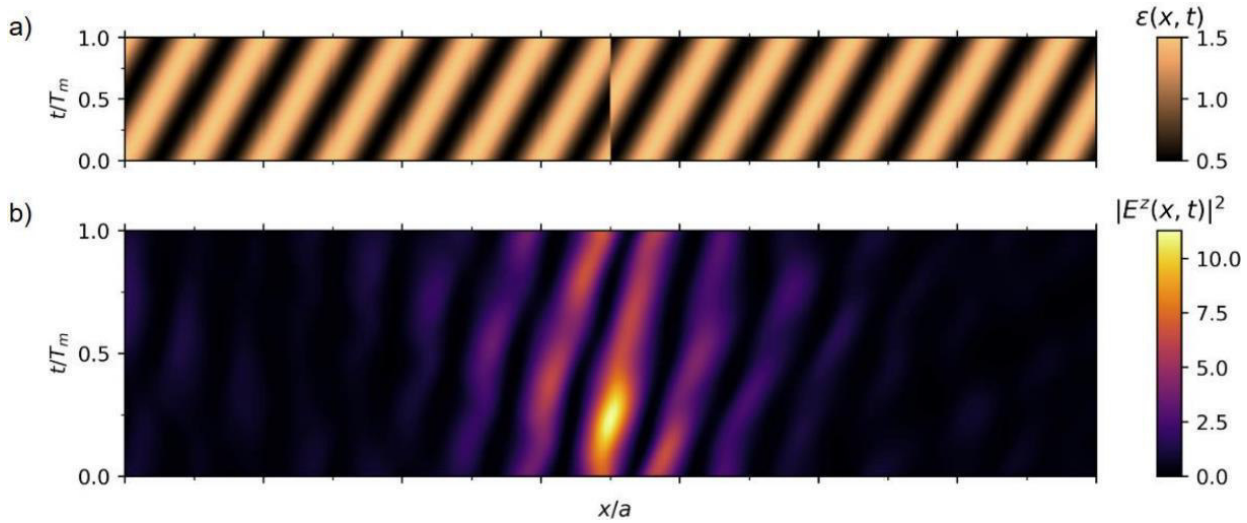

Figure 1: a) Permittivity distribution of two spatiotemporal metamaterials slabs as a function of space and time. The spatial modulation period is a, and the temporal modulation period is T_m. b) Distribution of the field intensity inside the slabs for a single frequency excitation. When excited at the characteristic frequency inside the gap, an interface state is clearly observed.

Chiral Light-Matter Interactions with Thermal Magnetoplasmons in Arrays of Graphene Disks

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The exceptionally strong and tunable plasmonic response of doped graphene structures makes them a promising platform for photonics. When arranged in a periodic configuration, the plasmon resonances of individual structures can interact and, under the appropriate conditions, form a collective mode known as lattice resonance. In the first part of this talk [1], we will conduct an in-depth analysis of the response of periodic graphene disk arrays, identifying the specific conditions that enable the system to support lattice resonances. To that end, we will present a semi-analytical theoretical framework and use it to derive closed expressions for the strength, the wavelength, and the width of the optical resonance of the arrays.

In the presence of an external static magnetic field directed normally to a graphene sheet, the optical conductivity of this material exhibits off-diagonal Hall components that result in an extraordinary magneto-optical response. As a consequence, graphene structures can sustain intense magnetoplasmon excitations, whose characteristics are largely determined by the doping level of the structure and the strength of the static magnetic field. However, the linear band structure and two-dimensional nature of graphene, together with its low electronic heat capacity, makes the temperature a significant factor in the optical response of graphene nanostructures, which is often overlooked.

In the second part of this talk [2], we will extend our theoretical approach to describe novel thermal magnetoplasmon excitations that originate from the hybridization of transitions between thermally populated Landau levels and the localized magnetoplasmon resonances of graphene nanodisks. We will show that, due to the quantized nature of the Landau levels, these excitations are enhanced rather than suppressed by temperature. Furthermore, as an illustration of their capabilities, we demonstrate that the thermal magnetoplasmons supported by an array of graphene nanodisks enable chiral perfect absorption and chiral thermal emission.

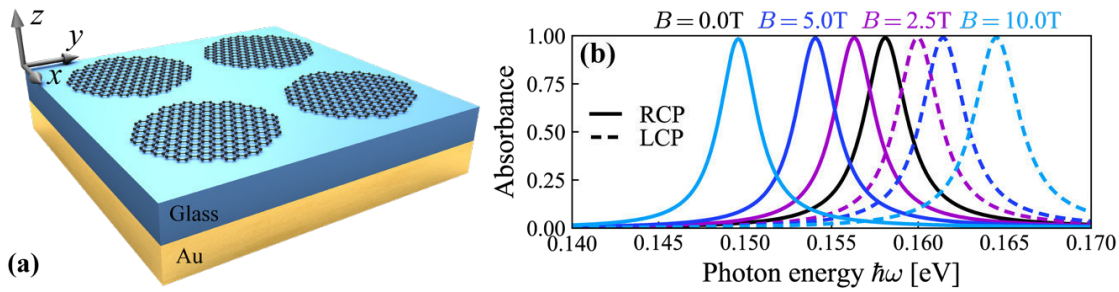

Figure 1: Array of graphene nanodisks on a dielectric/metal substrate. (b) Chiral absorbance of the system of (a) for different magnetic field strengths.

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Excitonic coherence phenomena in monolayer transition metal dichalcogenides

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In recent years, the study of coherent states has received much attention due to their fundamental role in quantum information. Regarding the optical properties in semiconductors, coherent excitons allow new pathways for exploring light-matter interactions. Their ability to maintain the phase over extended timescales enables phenomena like Rabi oscillations or exciton condensation. Materials with large exciton binding energies like Transition Metal Dichalcogenides (TMDs) or bulk semiconductors as BiI_3 are the ideal candidates for these processes to take place.

From a theoretical point of view, the use of *ab-initio* approaches to study femtosecond exciton dynamics is still at the early stage. A promising approach is the solution of the equation of motion for the time-dependent density matrix, accounting the excitonic effects within the Bethe-Salpeter formalism and describing the pump and probe fields at the same foot. This approach allows a detailed modelling of ultrafast pump and probe experiments during the overlapping pump-probe regime and is a promising tool for investigating coherent excitonic states.

We apply our theoretical framework to model pump and probe experiments under selected conditions to describe coherent excitonic states in layered materials. First, we study the case in BiI_3, where employing a quasi-resonant pump we identify the creation of a coherent excitonic population, further supported by experimental measurements. In addition, we analyse the case in a WS_2 monolayer. Given the spin and vallely physics of WS_2, a suitable pump, with same detuning between the A and B excitonic resonances, will produce ultrafast oscillations due to the coherent coupling of the two excitonic states. Our results proves that *ab-initio* modelling of pump and probe experiments as an ideal theoretical tool for characterizing exciton coherent states.

Magnons in CrI3 single and double layers from TDDFT and the BSE

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Magnons are the quasiparticles from the quantization of spin waves, which are collective-spin excitations in a magnetic system. In their study, linear spin wave theory is often applied to extensions of the Heisenberg Hamiltonian, provided some previous knowledge of its parameters. In general, they are obtained by fittings to experimental data or to first-principles calculations. In this sense, we present a spinorial formulation based in linear-response time-dependent density functional theory (LR-TDDFT) and the Bethe-Salpeter equation, that we have recently implemented in the Yambo code. Both LR-TDDFT and BSE approaches are applied to single and double layers of Chromium triiodine, CrI3, a semiconducting magnet. Our approach permits the direct study of the magnon wavefunctions, their dispersion relation and an *ad-hoc* obtention of the Heisenberg exchange constants. In particular, we observe a gap in the magnon dispersion of the single layer, opened by spin-orbit coupling. We also study the reciprocal and real-space projections of the magnon states to find wide-energy contributions from the band structures and a wide Brillouin-zone delocalisation. By fitting the obtained magnon dispersion to a three-neighbors Heisenber model, we extract the isotropical exchange values and obtain a good agreement between both LR-TDDFT and BSE methods. All in all, our work expands the applications of first-principles techniques to the study of magnons in two-dimensional materials and allows the extension to couplings with other interactions in a pure *ab initio* scenario.

Self-assembled Multifunctional Photonic Foams

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Abstract

Self-assembled photonic materials, such as photonic crystals or photonic glasses, are at the lead of light-matter interaction studies, offering different opportunities to control and enhance optical phenomena [1]. Self-assembly is an inexpensive and scalable method for creating complex photonic architectures [2,3]. Here, we show a straightforward colloidal self-assembly method to fabricate sub-monolayer macrofoams composed of monodisperse spherical particles (**Figure 1**). By leveraging a simple foaming process followed by ambient drying, ridge-trough networks are formed on unpatterned flat substrates, yielding dual-scale optical functionalities. At the macrocellular scale, random lasing is demonstrated, while the plateau borders exhibit Bragg scattering in crystalline domains or Mie resonances in disordered domains, spanning the visible and near-infrared spectral regions. The optical properties of these photonic glasses align with Mie calculations for individual spheres, validating the feasibility of designing portable optical devices. Furthermore, the use of silica-based disordered arrays showcases potential as refractive index sensors with enhanced sensitivity. These findings highlight the versatility of colloidal foaming techniques in advancing photonic applications through simple, scalable processes [4].

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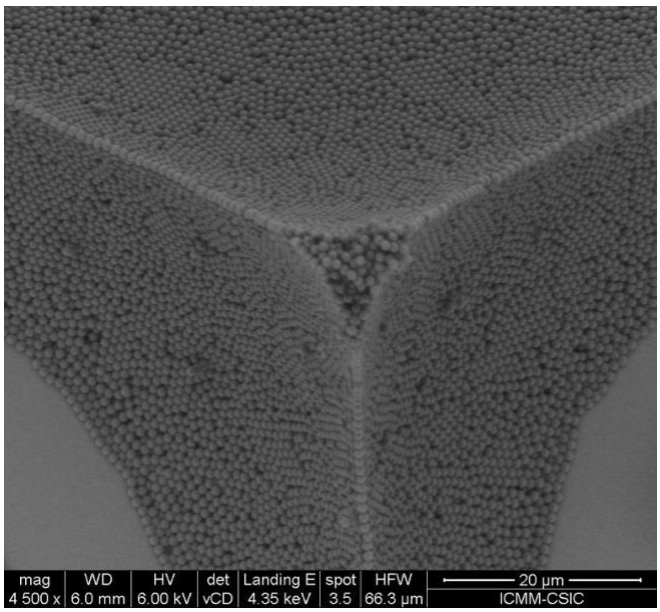

Figure 1: Scanning Electron Microscopy (SEM) image of a plateau border formed by self-assembly of monodisperse polysterine spheres of 1 micron.

Magneto-transport properties in ferromagnet/superconductor heterostructures

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Ferromagnetism and superconductivity are topics of significant interest within the condensed matter physics community, not only because of the diverse physical phenomena but also due to their promising potential for applications in areas such as memories, sensors, and quantum devices. Although traditionally seen as antagonistic effects, their interaction can give rise 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].

In this work, we investigate magneto-transport properties of a ferromagnetic (FM) multilayer with perpendicular magnetic anisotropy (PMA) in contact with a superconductor (SC). We observe clear changes in the magneto-resistance and Hall resistance of the FM at temperatures below the transition temperature of the SC. The symmetry of the Hall response indicates that these changes are likely not due to topological effects but possibly due to proximity effects or caused by modifications in FM multilayer domains by the supercurrents.

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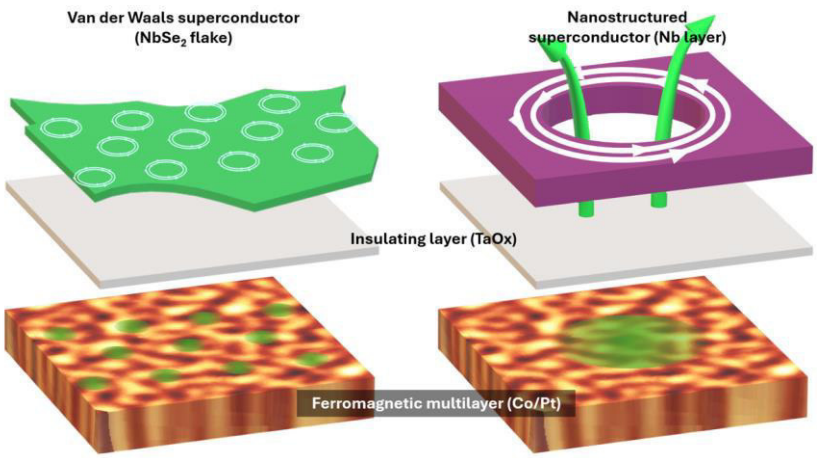

Figure 1: Ferromagnetic/Superconductor hybrid systems.

Enhanced Biaxial Compressive Strain Tuning of the Optical Absorption Properties of Single-Layer WS_2 via Hot Transfer on Polymer Substrates

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Strain is an effective method for tuning the electronic and optical properties of two-dimensional (2D) semiconductors [1,2]. However, few methodologies efficiently modulate these properties by applying large levels of compressive strain, particularly at very low temperatures.

In this study, we induce biaxial strain by controlling the heating or cooling of samples consisting of a single-layer 2H-WS_2 deposited on thermoplastic substrates. Specifically, the effect of strain is tracked in the energy shift in the differential reflectance resonances associated with exciton formation. We propose a hot transfer method, based on a dry transfer technique developed by Castellanos et al [3]., which enables us to achieve approximately 0.5% biaxial compressive strain at room temperature by depositing the 2D semiconductor on polycarbonate. Upon cooling the samples to 5 K, the strain surpasses levels reported in the literature for conventional dry transfer methods, reaching an unprecedented compression of approximately 1.7%. This results in a significant modulation of exciton energies, exceeding previous results by approximately 40 meV. The strain transfer efficiency was notably high at low temperatures, as shown by the substantial gauge factor values that matched theoretical predictions, demonstrating the approach's effectiveness. Furthermore, comparison between polycarbonate and polyamide 12 results reveal that the Young's modulus of the thermoplastic substrate plays a more critical role than the thermal expansion coefficient in facilitating strain transfer from the polymer to the 2D material.

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ELECTRON DELOCALIZATION IN A 2D MOTT INSULATOR

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When a magnetic impurity is placed in a metallic host, the screening of the magnetic moment by the conduction electrons is known as Kondo effect [1-3]. The presence of several localized magnetic moments (as opposed to just one) in a metallic host can further modify the physics of the system.
Theoretical predictions of the possible existence of Kondo lattices and the physics behind this phenomenon date from as early as the 1980s [4,5]. In Kondo lattices, at temperatures below a characteristic value, T_{KL}, the Kondo clouds of the individual impurities are coherently superimposed and acquire the periodicity of the crystal. Bloch's theorem ensures the formation of a renormalized flat band of width of the order of T_{KL}. The electrons originally localized at the magnetic impurities are thus delocalized becoming part of the new Fermi surface, while at the same time the conduction electrons of the crystal acquire very large effective masses due to the hybridization of the new flat band with the existing conduction bands [6].
We follow by means of low temperature Scanning Tunneling Microscopy and Spectroscopy, the buildup of a 2D Kondo lattice in a system composed by a Mott insulator, a single 1T-TaS_2 layer, stacked on the surface of a metallic crystal, 2H-TaS_2. We unambiguously demonstrate the existence of the resulting collective quantum coherent phase by measuring the characteristics of the Kondo-lattice gap that develops within the Kondo resonance at the Fermi level. When the sample temperature is lower than 27K, the magnetic moments present in the Mott insulator experience the Kondo screening by the conduction electrons of the metal, leading to the appearance of a Kondo resonance at the Fermi level. Below 11 K, a gap opens within the Kondo resonance, which is the signature of the formation of a coherent quantum state that extends all over the sample, i.e., a Kondo lattice [7,8]. This state results from the overlap between the Kondo clouds associated with the local magnetic moments in the Mott insulator layer. The observed modifications in the LDOS are well explained by state-of-the-art Density Functional Theory calculations

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Machine Learning prediction of magnetic exchange parameters in transition metal alloys

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Magnetic Exchange coupling (J) provides a powerful description for atomic interactions in magnetic alloys under the Heisenberg model. These parameters can be computed *ab initio* from density functional theory (DFT) calculations and subsequently used in a micromagnetic simulator to determine, for example, the Curie temperature of the material. This computational workflow is relatively efficient for pure elements or simple alloys but becomes considerably time-consuming for multicomponent systems such as high-entropy alloys (HEAs). Machine learning (ML) techniques have already proven successful in addressing other challenges in the HEA field, particularly in predicting phase formation and mechanical properties. In this work, we present an ML-driven approach for predicting J values, using a graph neural network model trained on approximately 100 BCC and FCC binary alloys. The Graph2Mat framework is employed to enhance the data efficiency of the model by leveraging the equivariance of the magnetic exchange tensor [1]. This simple J predictor model is enabled by the so-called *"regular solution model"* initially introduced for calculating HEA mixing enthalpies [2], which we test if also holds true for the magnetic exchange parameters.

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Figures

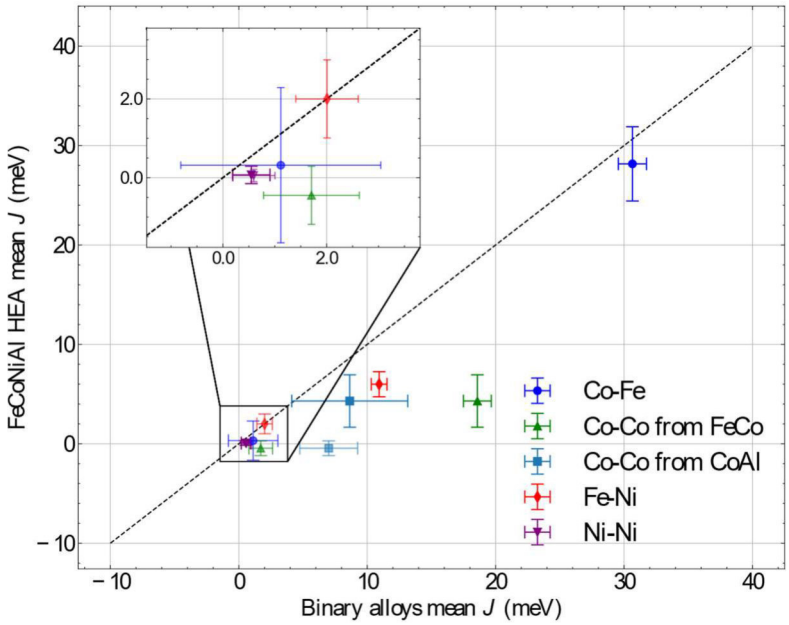

Figure 1: Preliminary validation of the binary regular solution model in FeCoNiAl HEA from first-principle calculations.

Exchange Bias Effect of Ni@(NiO, Ni(OH)$_2$) Core/Shell Nanowires Electrodeposited in Nanoporous Alumina Membranes

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The development of groundbreaking technologies increasingly depends on our ability to precisely control the magnetic properties of materials at the nanoscale. In addition to refining alloy compositions, crystalline structures, and nanomaterial geometries, magnetic heterostructures are being explored to fine-tune functional magnetic properties. Specifically, the combination of ferromagnetic (FM) and antiferromagnetic (AFM) layers has gained attention for generating one-way magnetic anisotropies, particularly in the design of novel read heads for magnetic recording media based on giant magnetoresistance [1]. Although the magnetic properties and exchange bias effect have been examined in stacked thin films and core/shell nanoparticles, core (FM)/shell (AFM) cylindrical nanowires have not been the primary focus of research [2]. In this work, we used a purely electrochemical method to create arrays of core (FM)/shell (AFM) Ni@(NiO, Ni(OH)$_2$) nanowires, avoiding thermal oxidation processes incompatible with integrated semiconductor technologies. We conducted morphological and compositional analyses using SEM, HR-TEM, and XPS, as well as temperature-dependent magnetic hysteresis loops, thermomagnetic curves, and FORC analysis to investigate the impact of electrochemical surface modification on the magnetic properties of Ni nanowires. Magnetic hardening of the FM/AFM nanowires along the easy magnetization axis was found to be about 17% (43%) at 300K (50K). On the other hand, as the temperature drops below 100K while field cooling the nanowires under a 3T applied magnetic field along their easy magnetization axis, an increasing exchange bias effect becomes evident.

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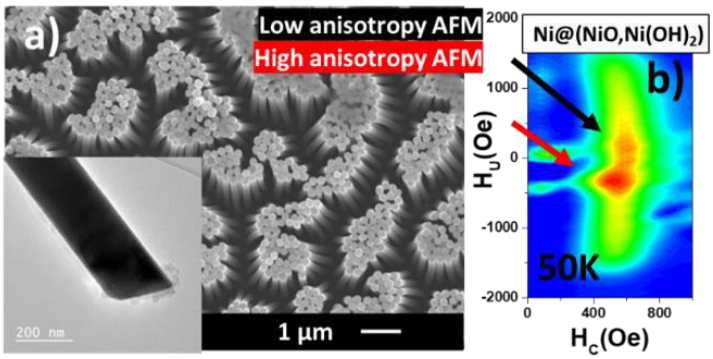

Figure 1: a) SEM image of electrochemically modified Ni@(NiO, Ni(OH)$_2$) nanowires. The inset shows a high-magnification HRTEM image of a single nanowire. b) FORC distribution at 50K showing two distinct magnetic behaviors attributed to the different interactions between the core and shell of the Ni@(NiO, Ni(OH)$_2$) nanowires.

Co_2FeIn Heusler Nanowires – Magnetic and Structural Properties

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The relentless pursuit of advancing information storage technologies has fueled interest in three-dimensional network nanostructures as a potential alternative to conventional microelectronics. Particularly, arrays of nanowires (NWs) exhibit unique magnetic properties suitable for enhanced high-density magnetic data storage and novel spintronic devices. Hereby, we present our recent study on Co_2FeIn Heusler alloy NWs, which exhibit high spin polarization, making them ideal for spintronic applications [1]. Magnetic NWs of Co_2FeIn full Heusler alloy were fabricated by pulsed electrochemical deposition (PED) method, employing nanoporous alumina membranes (NAMs) as patterned templates. Their morphology, composition, and structure were thoroughly characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques. These analyses revealed highly uniform NWs with an average diameter of (165±11) nm, about 12 μm in length, an average composition of $Co_{49}Fe_{28}In_{23}$, and an A2 crystallographic phase. Magnetic characterization using vibrating sample magnetometry (VSM) of the NWs within the array, showed a coercive field of (H_C = 72±10) Oe, while first-order reversal curve (FORC) analysis, carried out at different temperatures for the parallel configuration, displayed magnetostatic interactions with a narrow switching field distribution. Furthermore, magneto-optic Kerr effect (MOKE) microscopy analysis of single isolated NWs revealed a Lorentzian-like switching field distribution with a mean value of (H_{SW} = 70±5) Oe, consistent with the VSM results. Finally, the thermomagnetic, M(T), curves for these Co_2FeIn NWs array measured with the VSM, showed a high Curie temperature (T_C) over 1000 K, which is in good agreement with the values reported in literature for similar Heusler compounds.

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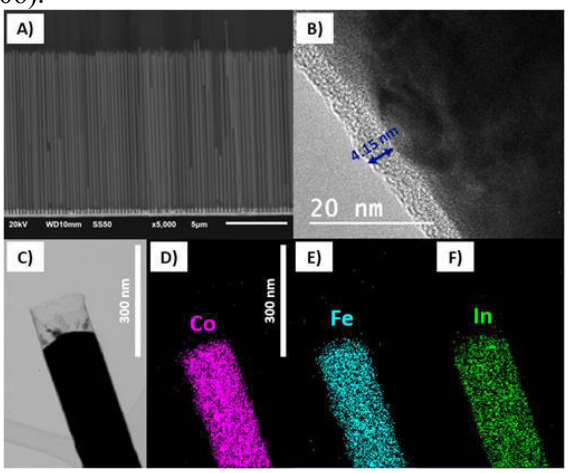

Figure 1:A) SEM micrograph of the cross-section of an array of Co2FeIn NWs. B) Amplified TEM image of a single NW where the 4 nm thick SiO2 layer can be appreciated. C) TEM micrograph of a single isolated Co2FeIn NW and EDX chemical composition mapping for the Co D), Fe E) and In F) atomic elements.

Exploring the charge density wave in monolayer $NbSe_2$ with angle resolved photoemission spectroscopy

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$NbSe_2$ is a prototypical system for studying the interplay between charge density wave (CDW) and superconductivity phases. Understanding how these phases evolve as the crystal dimensions are reduced to the monolayer (ML) limit is of great interest. While CDW in ML-$NbSe_2$ has been documented using STM [1], transport measurements and Raman spectroscopy [2], direct spectroscopic evidence of the CDW gap via angle-resolved photoemission spectroscopy (ARPES) has been lacking. Moreover, there is a notable discrepancy in the reported CDW transition temperatures: STM/STS studies of ML-$NbSe_2$ on bilayer graphene (BLG) suggest $T_{CDW} < 45$ K [1], while Raman spectroscopy of $NbSe_2$ on sapphire report $T_{CDW} \sim 140$ K [2]. In this work, I present the first ARPES observation of the CDW gap in ML-$NbSe_2$ grown on BLG/SiC. Using a helium lamp-based lab setup, the measured gap aligns with prior findings in bulk $NbSe_2$ and complements established transport and STM results, providing a critical benchmark for future spectroscopic studies of 2D CDW systems.

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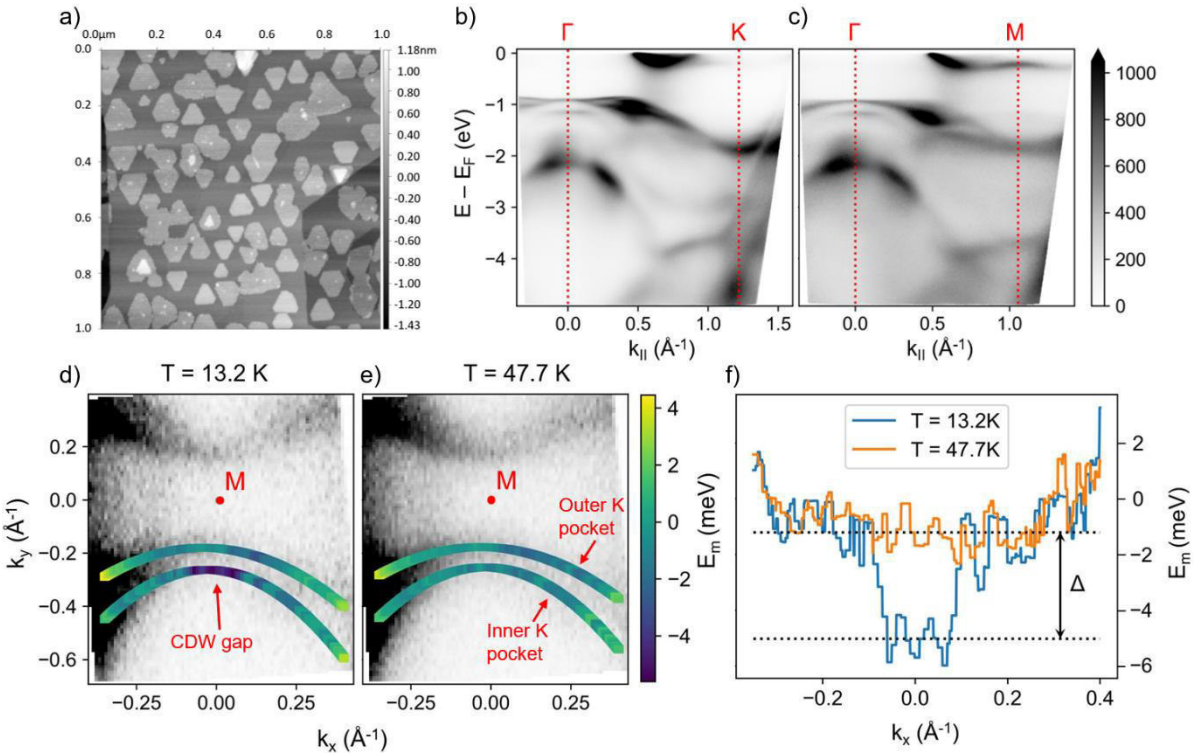

Figure 1: a) Topographic image of ML-$NbSe_2$ on a BLG/SiC substrate, measured with atomic force microscopy (AFM), showing the quality of the fabricated $NbSe_2$ film; b,c) ARPES spectra along ΓK (b) and ΓM (c) directions in the $NbSe_2$ Brillouin zone; d,e) Fermi surface map around the M point, measured at 13.2K (d) and 47.7K (e), with the leading edge midpoint values (E_m) overlapped over the spectra; f) Values of E_m along the inner K pocket for T = 13.2 K (blue) and T = 47.7 K (orange).

Mechanosensitivity in dithia-helicenes trough thermopower and conductance calculations

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Helicenes are chiral carbon-based molecules of interest in many fields, including electron transport in molecular junctions. Recently, our research in dithiahelicenes molecular junctions has revealed that electronic conduction is based on the off-resonant mechanisms of transport [1]. In the off-resonant regime conductance decays exponentially with the misalignment between the HOMO/LUMO level of the molecule and the work function of the metals, and the HOMO level of dithiahelicenes is misaligned less than 1eV from gold's work function.

Further research on other helicenes have shown that their electronic properties can be mechanically tuned [2]. Break-junctions experiments can apply a force to either compress or stretch a single helicene, giving us a experiment to mechanically tune the conductance and thermopower of the junction. With that thought in mind the group of Nicolas Agraït measured thermopower in endo/exo-dithia[10]helicenes and endo/exo-dithia[11]helicenes, and we have perform DFT transport calculations with the Non-Equilibrium Green's Functions (NEGF) method to characterize the change in thermopower under mechanical deformation of these helicenes. The conductance and thermopower allow us to characterize the alignment of the metal's work function and the HOMO level for the elastic conformations of the helicene.

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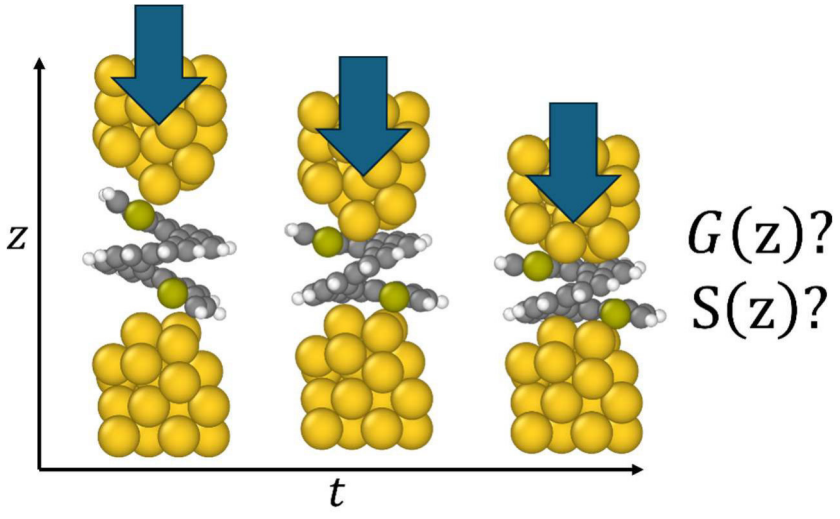

Figure 1: Schematic representation of a endo-dithia[10]helicene in a junction being compress.

Torsional mechanical modes in coupled acousto-plasmonic antennas

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Metallic nanoantennas have been studied as efficient coherent phonon generators and detectors, harnessing their characteristic optical absorption and polarization dependence of the optical modes [1-2]. The ability to control the excitation of phononic modes depends on the properties of the multiple optical resonances of the system. Lately, it has been made possible to optimally excite and detect phonon modes via plasmon resonances at the same optical frequency using chiral nanostructures and circularly polarized light [3]. However, torsional modes remain elusive in nanophononic studies. In this work we present a simple system composed of two coupled bars, where torsional mechanical modes can be excited using light with null angular momentum. The twisting of the phononic mode (Fig. 1) is provided by the peculiar symmetry of the mechanical eigenmode due to the interaction of the bars via either the substrate or a central connector.
We will present a complete theoretical analysis of the phononic and plasmonic modes, their surface deformation field and electromagnetic field profiles. [4].

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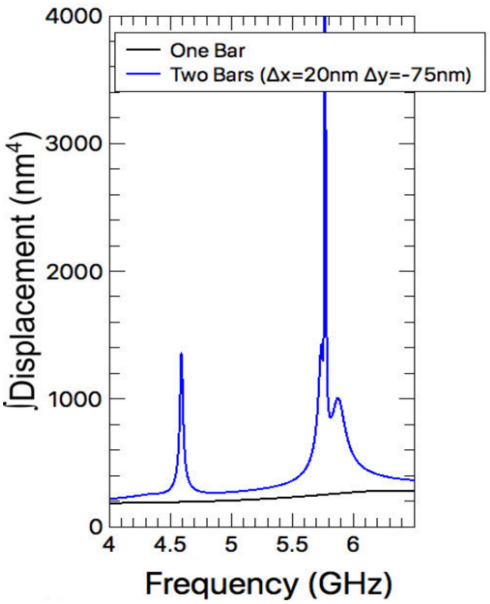
Figures



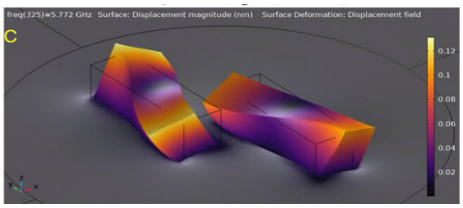


Figure 1: Left: Integral of the displacement, showing the resonances occurring for interacting bars. Right. Deformation profile depicting the torsional nature of the mechanical modes.

Machine Learning Interatomic Potential for Fe-C Systems: Fusion Oriented Materials

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In recent years, significant advancements have been made in the development of Interatomic Potentials (IP) using Machine Learning (ML) techniques. They predict with low error the results obtained via Density Functional Theory (DFT) and have a great capacity to predict new geometries not included in the training. Another important characteristic of MLIPs is the capability of treating multiple atomic species without loss in precision. One of the most promising models at the time is the Message Atomic Cluster Expansion model or MACE [1].

In particular, interfaces are systems that require a great amount of computational resources to avoid strain due to misfit while, at the same time, are difficult to fit to classical potentials for Molecular Dynamics due to its chemical and structural complexity. This creates a situation where DFT is needed to compute accurate results, but usually impossible to employ due to technical or time limitations.

In this work, we train a MACE model for carbon defects in ferrite and cementite structures that are commonly found in structural steels employed in fusion. In Fig.1 we show the formation energies obtained with the trained potential for several carbon defects in bcc-Fe and compare them with DFT results. Using this training, it is possible to compute the interface energy of various ferrite-cementite systems, proving the transferability of the potential. We obtain similar values to DFT while saving time and computational resources.

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Figures:

Computational time (s)		
SIA	VASP [2] 128 cores	MACE GPU
<110>	70200	1.58
<111>	63120	1.02
Tetrahedral	68628	1.59
<100>	45000	1.23
Octahedral	44180	0.94

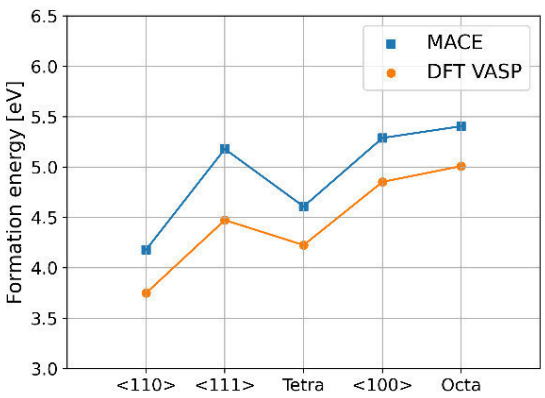

Figure 1: Left: Prediction of Self Interstitial Atoms SIAs formation energy. Right: Computational user time for the relaxation of the defects shown in Fig 1.

Geometric Antibunching and Directional Shaping of Photons Anticorrelations

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Although the study of temporal photon statistics has been a cornerstone since the beginning of the field of quantum optics, the second order spatial coherence has been greatly overlooked. In this work [1], we investigate the directional characteristics of photon statistics in dimers of quantum emitters. For their analysis, we construct a two-point second-order correlation function that allows us to find a new mechanism for photon anticorrelation, termed as *geometric antibunching*. This phenomenon is completely agnostic to the quantum state of the emitters and emerges from quantum interference effects due to the indistinguishability of different two-photon optical pathways. Finally, we explore its occurrence in emitters placed in the vicinity of a flat substrate and a nanosphere, demonstrating that these *geometrical zeros* are not a coincidence of free-space [2, 3] but a general property of the photonic environment where the emitters are placed. We also demonstrate its tunnability through the different material and geometric parameters of these structures.

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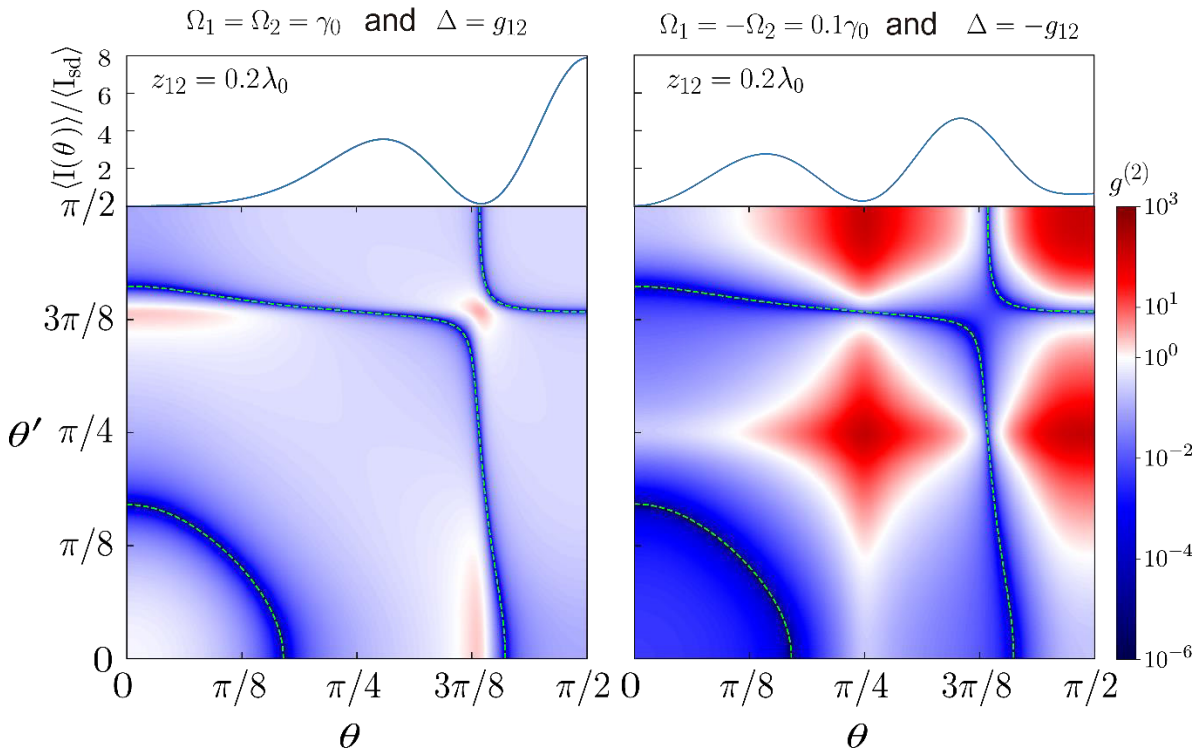

Figure 1: Maps of directional correlations, $g^{(2)}(\theta, \theta')$, for a vertically oriented QE dimer placed above a perfect mirror ($z_1 = 0.6\lambda_0$ and $z_1 = 0.8\lambda_0$). The polar angles θ, θ' represent the directions in the far-field where light is detected. The laser drivings are set to target the Bell symmetric (left) and antisymmetric (right) states of the QE dimer. The upper panels show directional intensity plots in both scenarios, normalized to $\langle I_{sd}\rangle$ (the emission of a single emitter in free space at $\theta = \pi/2$). Green dashed curves indicate geometric antibunching zeros, where $g^{(2)}(\theta, \theta')$ vanishes independently of the quantum state of the emitters.

Atomically Precise Control of Topological State Hybridization in Conjugated Polymers

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Topological quantum states in carbon nanostructures show promise for coherent, controllable quantum dot spin qubits, though their manipulation remains challenging. We report [1] atomically precise control over the hybridization of topologically protected edge states in π-conjugated polymers, achieved through selective dehydrogenation of pentacene-based polymer units. Using low-temperature scanning tunneling microscopy and spectroscopy with high-resolution atomic force microscopy, we demonstrated reversible modulation of edge state interactions. Density functional theory, tight-binding, and Hubbard model calculations show that orbital overlap between edge states can be finely tuned via geometry and bandgap of the interconnecting region, highlighting topological edge states' potential for complex quantum device design.

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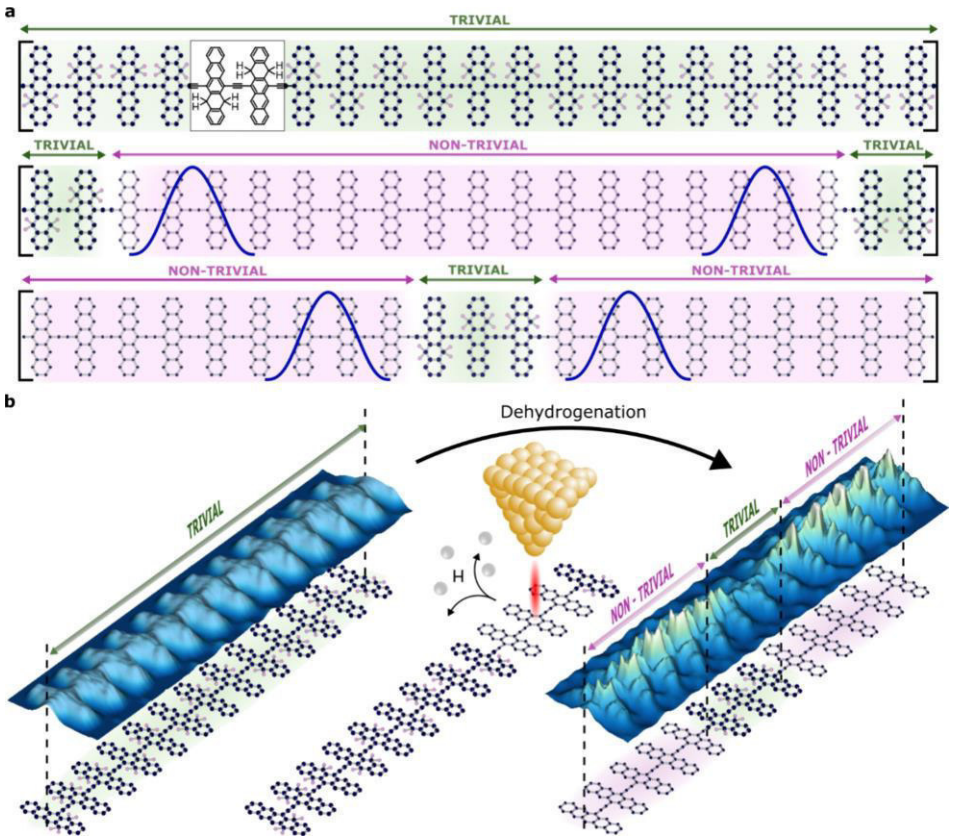

Figure 1: (a) Schematic representation of different configurations for the hydrogenated pentacene polymer and two different topological heterostructures after the dehydrogenation process. (b) Tip-induced dehydrogenation setup for the formation of the nontrivial region inside the pentacene polymer from the hydrogenated trivial phase. Note for chemical representation: Atoms in pink represent hydrogen, while atoms in black represent carbon.

Understanding the origin of single photon emission in h-BN crystals

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The development of novel ultra-compact two-dimensional photonic technologies for their application in quantum information processing relies on our ability to fabricate single photon sources in 2D van der Waals materials preferably working at room temperature, whose optical emission properties can be controlled. Recently, the possibility of obtaining room temperature single photon emission from 2D hexagonal boron nitride (h-BN) crystals has been demonstrated. The emission has been attributed to the presence of defect states within its wide bandgap [1], which has triggered an intense research activity in the last years [2]. Most recent theoretical works have focused on the study of VB-, VN and VNNB vacancies as the origin of single photon emission in h-BN crystals [3,4].

We reproduce in this study the structures and the symmetry of the wavefunctions associated with those defects using the DFT code SIESTA. We have further calculated the transition dipole for our structures in order to gain a better understanding of the photoluminescence of the transition [5]. Our theoretical findings are compared with the optical emission obtained by micro-photoluminescence on h-BN thin crystals fabricated by mechanical exfoliation.

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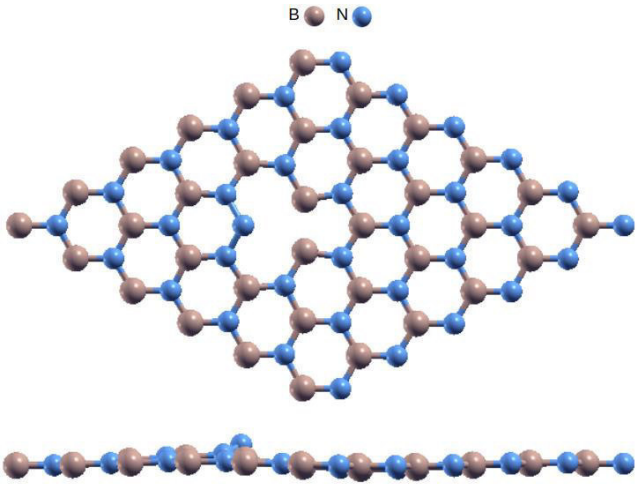

Figure 1.- Representation of the V_NN_B defect on a monolayer hBN. The relaxation of the structure on SIESTA gave us this little *displacement, appreciated* clearly on the side view, meaning that we could be working with different states due to symmetry than the ones expected on the lattice in [1].

SUPERCONDUCTING LEVITATION SYSTEM DESIGNED FOR SUB-MILLIKELVIN TEMPERATURES EXPERIMENTS

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We present the performance of a magnetic levitation system capable of levitating a type I superconducting sphere at ultralow temperatures [1]. The system enables precise control of the sphere's motion and incorporates a low-energy detection system to monitor its position [2]. We have characterized experiments involving uniform linear motion, free oscillations, and sustained near-uniform circular motion at superfluid 4He temperatures, down to 1.5 K, in the presence of He gas. The system is specifically designed to operate at ultralow temperatures, minimizing dissipation across all subsystems. Only pure materials with low background radiation were employed.

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Figure 1: Levitation system and Pb levitating sphere

In-situ SAXS and WAXS to monitor the formation of monolithic MOFs for X-ray detection applications

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X-ray detection has a wide range of applications; however, still offer significant room for improvement, particularly, in reducing the time of exposure in medical applications. Despite its porosity (which negatively affects their density), MOFs are getting attraction as X-ray detectors due to their high versatility and the possibility of functionalizing pores with the incorporation of molecules, allowing optimization based on the different metal-ligand and guest molecule combinations. In general, this combination must maximize the absorption of high-energy radiation and the ability to generate signals in the form of lower-energy emitted photons or in the form of electric current. In particular, our group has developed a methodology for synthesizing highly robust, stable, and dense monolithic MOFs, making them ideal for this application [1,2]. However, understanding how these compounds form is still unclear, hampering the identification of routes towards optimized properties.

In this talk, we present a methodology to understand the mechanisms that govern nucleation and crystalline growth in monolithic MOFs, and how these impact their final bulk properties [3]. We will discuss how we have implemented this synthesis method to simultaneously measure SAXS, WAXS, and radioluminescence at the B21 beamline of the Diamond Light Source synchrotron (UK) (**Fig 1a**). Using a continuous flow of the reaction medium over time allows us to link their structural and morphological properties and their radioluminescence spectrum and efficiency while the growth and nucleation regimes take place. We analyze three monolithic MOFs based on Zn (ZIF-8), Zr (UIO-66) and Pb (which we name Pb-MOF). As for radioluminescence, Pb-MOF presents more potential for radiation detection as a result of a more dense and optimized particle shape. Interestingly, after 3 minutes of particle growth, the radioluminescence does not change, indicating an optimum reaction time (**Fig 1b**). In addition, our results also show that these monolithic MOFs maintain 55% of their luminescence efficiency after a dose of 7.5 kGy, equivalent to 75 million chest radiographs, surpassing standard MOF powder scintillators.

The fundamental understanding of the nature of the particles and the monolith provided by this work enables the design of materials with skeletal and bulk properties on demand, with optimal porosity, density, crystallinity and detection capabilities.

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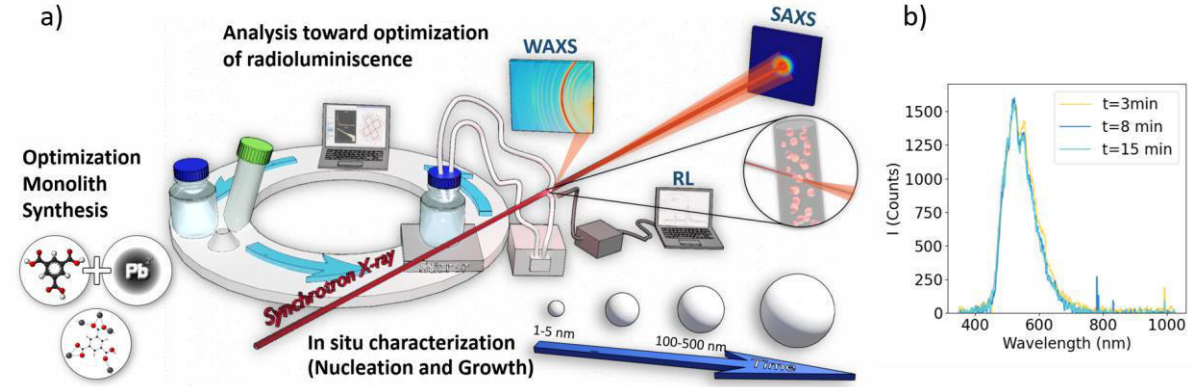

Figure 1: a) Process and setup for the in-situ flow experiment; b) Radioluminescence according to reaction time

Quantum-scale electronic properties of graphene nanoarchitectures

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On-surface reactions, via programmed interactions of molecular building blocks, has recently emerged as a promising route to synthesize atomically precise materials from the 'bottom-up'. This approach ensures exquisite atomic-scale control of the structural and chemical functionalization, allowing to design a vast number of carbon-based nanoarchitectures not available by traditional solution chemistry nor with the 'top-down' methodologies.

In this talk, I will discuss our recent results to synthetize atomically precise nanoporous graphene [1], graphene nanoribbons and their chemical functionalization and how to organize them into atomically-sharp heterojunctions [2-4], and the molecular bridge engineering (fig.1) for tuning quantum electronic transport and anisotropy in nanoporous graphene [5].

At the end of the day, this talk will demonstrate the full path to synthetize a semiconducting graphene material with a bandgap similar to that of silicon, its atomic-scale characterization, and its implementation in a three-terminal electronic device, as well, its implementation as atomically-thin membrane for gas filtration and integrated into photonic biosensors.

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Figures

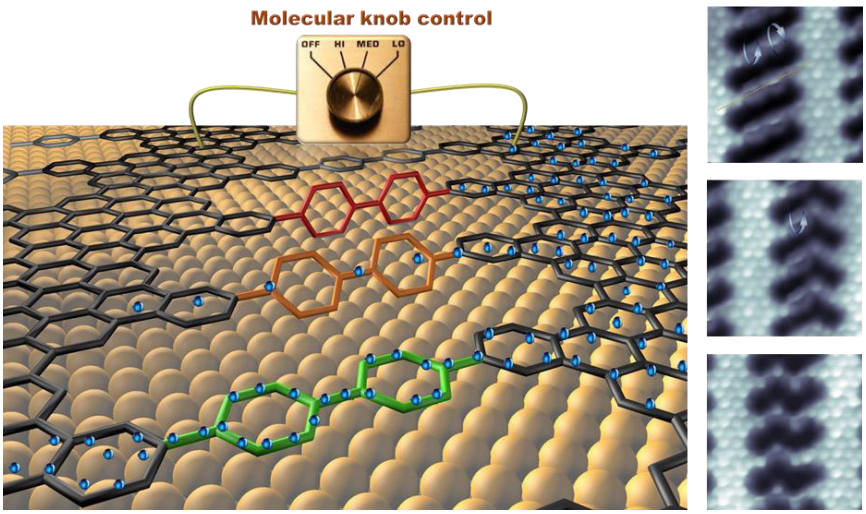

Figure 1: Concept sketch of molecular bridge engineering for tuning quantum electronic transport and anisotropy in nanoporous graphene, and (right) STM images displaying its experimental realization.

Canalization-based super-resolution imaging using an individual van der Waals thin layer

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Canalization is an optical phenomenon that enables unidirectional light propagation without predefined waveguiding designs. Recently demonstrated using phonon polaritons in twisted van der Waals (vdW) layers of α-MoO_3 [1,2], it offers unprecedented possibilities for controlling light-matter interactions at the nanoscale. However, practical applications have been hindered by the complex sample fabrication of twisted stacks. In this work, we introduce a previously unexplored canalization phenomenon in a single thin vdW layer (α-MoO_3) [3] interfaced with a substrate exhibiting a given negative permittivity. This enables a proof-of-concept application of polariton canalization: super-resolution nanoimaging (~λ_0/220) [4]. Canalization-based imaging transcends conventional projection constraints, allowing the super-resolution images to be obtained at any desired location in the image plane. This versatility stems from the synergetic manipulation of three key parameters: incident frequency, rotation angle of the thin vdW layer, and thickness. Our results provide new insights into the properties of canalization and constitute a seminal step towards multifaceted photonic applications, including imaging, data transmission, and ultra-compact photonic integration.

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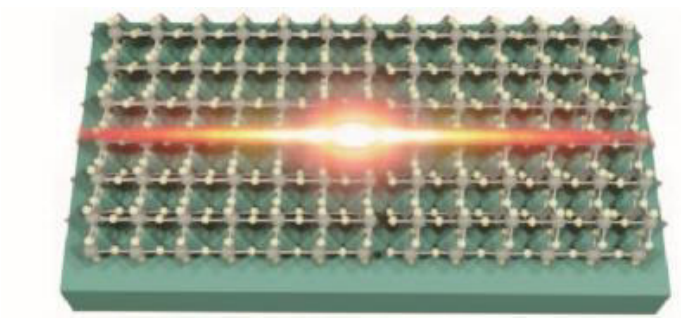

Figure 1: Schematics of phonon polariton canalization in α-MoO_3/SiC heterostructures.

Intercalation of van der Waals materials with photochromic molecules

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Intercalation of guest species in vdW materials is an effective processing technique for customizing their properties [1-2]. Compared to metal ions, often used as guest species [3], organic molecules provide an impressive versatility with multiple options to vary their size, charge, dipolar moment, magnetic spin and optical properties [4]. Moreover, functional molecules can be intercalated to provide unique capabilities to layered materials. For instance, photochromic molecules possess a unique light response, as they can be switched between two metastable isomers with different sizes through light irradiation at different wavelengths. Their intercalation in a van der Waals material may enable a controllable modification in the interlayer distance through light irradiation. However, this possibility has not been explored.

In this work, we explore the intercalation of a photochromic azobenzene derivative in the layered van der Waals magnets $RuCl_3$ and MnPS3. Preliminary data indicates that different interlayer distances can be obtained by intercalating one isomer or the other, as obtained by irradiating with UV or visible light during the intercalation process. These data indicate the potential of the intercalation of photochromic molecules to tune the physical properties of layered compounds through light irradiation.

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Figures

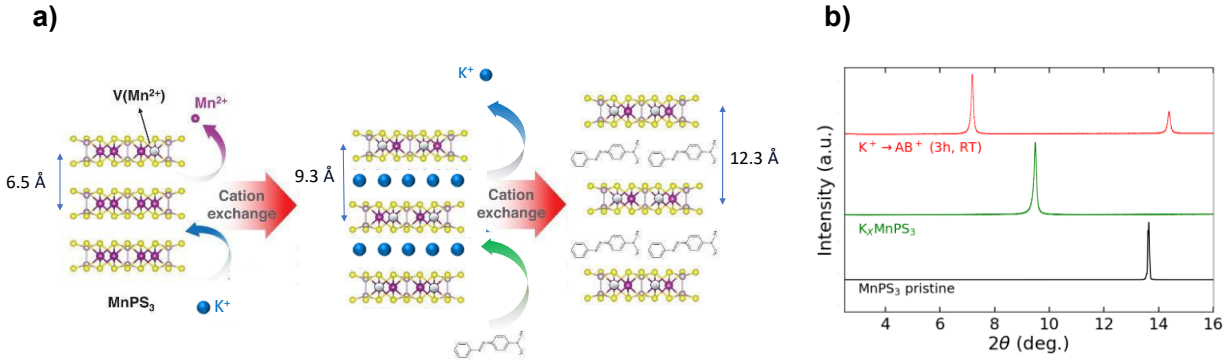

Figure 1: a) Scheme of the intercalation of $MnPS_3$ with the molecule Azo-AB by a two-step cation exchange. b) X-ray diffraction patterns of $MnPS_3$ pristine (black line) and AB_XMnPS_3 before and after cation exchange with K (green and red lines, respectively).

Thermodynamics of Non-Hermitian Josephson junctions with exceptional points

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We present an analytical formulation of the thermodynamics, free energy and entropy, of any generic Bogoliubov de Genes model which develops exceptional point (EP) bifurcations in its complex spectrum when coupled to reservoirs. We apply our formalism to a non-Hermitian Josephson junction where, despite recent claims, the supercurrent does not exhibit any divergences at EPs. The entropy, on the contrary, shows a universal jump of 1/2log2 which can be linked to the emergence of Majorana zero modes (MZMs) at EPs. Our method allows us to obtain precise analytical boundaries for the temperatures at which such Majorana entropy steps appear. We propose a generalized Maxwell relation linking supercurrents and entropy which could pave the way towards the direct experimental observation of such steps in e.g. quantum-dot-based minimal Kitaev chains.

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Figures

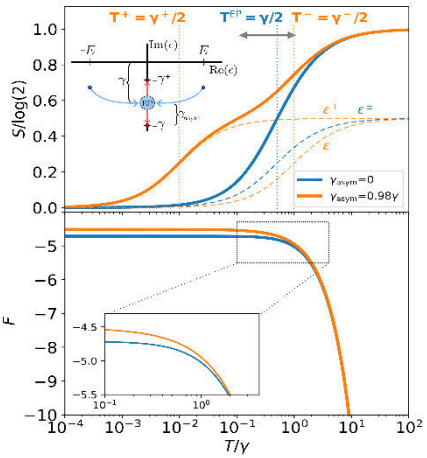

Figure 1: Top (inset): Formation of an exceptional point. Top (main): Entropy development after an exceptional point. Bottom: Free energy dependence of the temperature.

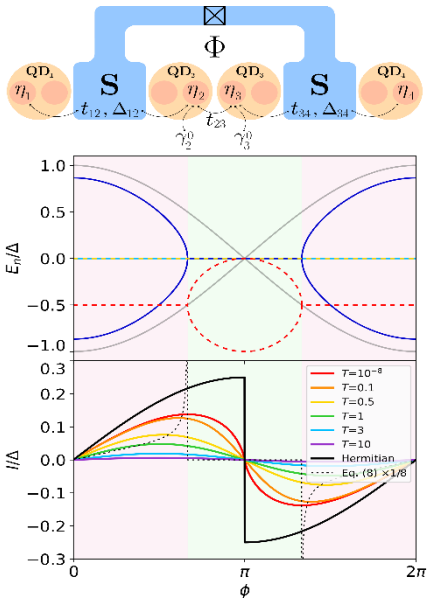

Figure 2: Top: Illustration of the four-Majorana Josephson junction device. Center: Energy spectrum of the junction. Bottom: Phase dependence of supercurrent.

Polarization dependent excitonic features in ReS_2 revealed by low temperature photocurrent spectroscopy

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The low crystal symmetry of ReS_2 leads to the emergence of dichroic optical and optoelectronic response [1, 2], absent in other layered transition metal dichalcogenides, which is appealing for device applications requiring polarization resolution. To date, spectroscopy studies on the optical response of ReS_2 have relied exclusively in characterization techniques involving optical detection, such as photoluminescence, absorbance, or reflectance spectroscopy [3]. However, to realize the full potential of this material, it is necessary to develop knowledge on its optoelectronic response with spectral resolution. In this work, we study the polarization-dependent photocurrent spectra of few-layer ReS_2 photodetectors, both in room conditions and at cryogenic temperature. Our spectral measurements reveal two main exciton lines at energies matching those reported for optical spectroscopy measurements, as well as their excited states. Moreover, we observe an additional exciton-like spectral feature with a photoresponse intensity comparable to the two main excitons. We attribute this feature, not observed in earlier photoluminescence measurements, to a non-radiative exciton transition. The three main excitons, as well as their excited states, modulate with linear polarization of light, each one acquiring maximal strength at a different polarization angle. Our results bring new perspectives for the development of ReS_2-based nanodevices.

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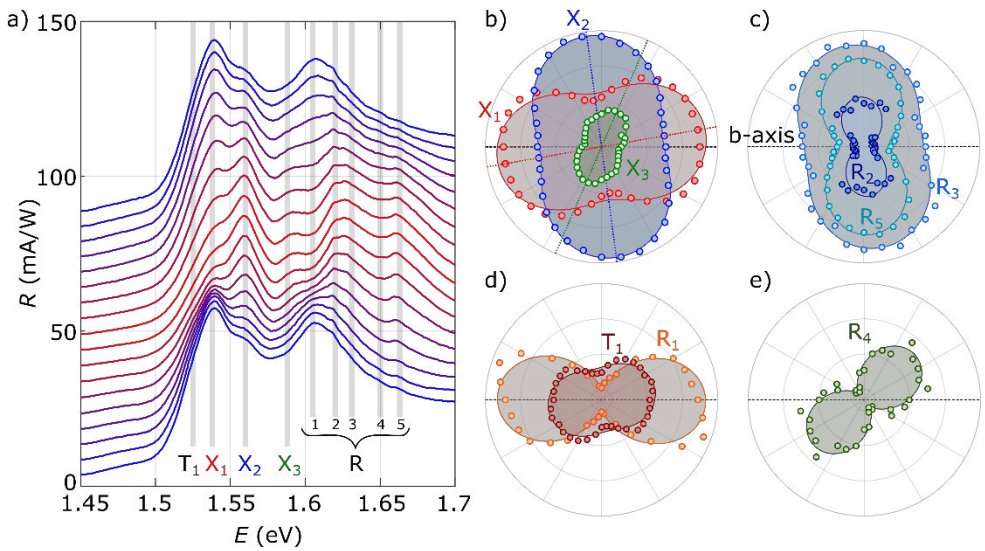

Figure: (a) Photocurrent spectra acquired for different angles of light polarization, from 0 to 170º relative to the b crystalline axis, with V_{ds} = 5 V, V_g = 45 V and a power density of 500 W/m^2. Consecutive spectra have been shifted vertically in steps of 5 mA/W for easier visualization. (b)–(e) Polar plots showing the modulation of the different spectral features as a function of the polarization direction, extracted from fittings to multi-Lorentzian curves.

Tunable Ising Superconductivity in organically intercalated transition metal dichalgoneides.

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Layered transition-metal dichalcogenides (TMDs) host remarkable electronic phenomena, including charge-density wave (CDW) and superconducting orders in their metallic phases. These properties are strongly influenced by dimensionality[1] and electronic doping[2]. The former leads to intriguing behaviors in atomically thin samples, such as Ising superconductivity or two-band superconductivity, while susceptibility to electronic doping arises from the hole pockets in the transition metal bands. The intercalation of molecular species between the layers of van der Waals (vdW) compounds has recently emerged as a powerful approach to combine the unique properties of vdW materials with the chemical flexibility of organic molecules[3,-5].

Here, we investigate NbSe2 and TaS2, two prototype TMD superconductors with contrasting thickness-dependent superconducting orders,[6] intercalated with a range of organic cationic spacers, including non-centrosymmetric chiral molecules. A novel *in-situ* galvanic intercalation method[7] facilitates spontaneous molecular insertion, enabling the creation of diverse thin hybrid heterostructures and advancing circuit integration. Our comprehensive analysis reveals several appealing findings: *(i)* **Tailored Superconductivity**: a significant tunability of the superconducting order, surpassing the monolayer limit in TaS2, while decreasing in NbSe2 in the inversely symmetric heterostructures. *(ii)* **2D superconductivity:** Enhanced Ising protection in both systems mimicking monolayer behaviour and *(iii)* **Carrier polarity reconfiguration**: large electronic doping combined with the decoupling of interlayer interactions leads into a reconfiguration of charge carriers from p-type to n-type and suppression or modification of the CDW order.

These findings pave the way for the functionalization of vdW superconductors with Ising protection and their circuit-integration in next-generation quantum devices

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Evaluating Ion Beam Techniques and Optical Methods (IBM-OM) to trace H-sorption processes: the magnesium-hydrogen case

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Magnesium (Mg) is a plentiful, widely distributed and cost-effective element that can absorb substantial quantities of hydrogen (7.6% wt.). This characteristic renders it a promising candidate for applications in the hydrogen sector [1]. However, certain aspects regarding the thermodynamics and kinetics of the hydrogenation mechanism remain unresolved. To overcome those problems, a precise characterization of the hydrogenation process is needed. In this context, the metal-insulator transition under hydrogen, resulting in significant alterations of its optical properties, makes it suitable for hydrogen optical-sensing in thin films and offers a straightforward way to characterize the hydrogenation process in situ. On the other hand, ion beam techniques present a robust suite of tools for characterization [2], capable of providing detailed depth profiles of hydrogen concentration [3], thus making them ideal for investigating hydrogenation reactions.

In this work, we compared the capabilities of both techniques on tracing the hydrogenation of Pd-capped Mg films under low temperatures (140ºC) and hydrogen pressures (1 bar). Whereas IBT revealed the growth of the MgH_2 layer from surface to substrate, OM scarcely detected any changes up until the end of the hydrogenation process. Results provide the reaction mechanism and the H-diffusion coefficient. Finally, the advantages/disadvantages of both techniques (IBT-OM) during H-absorption/desorption reactions will be discussed.

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Figures

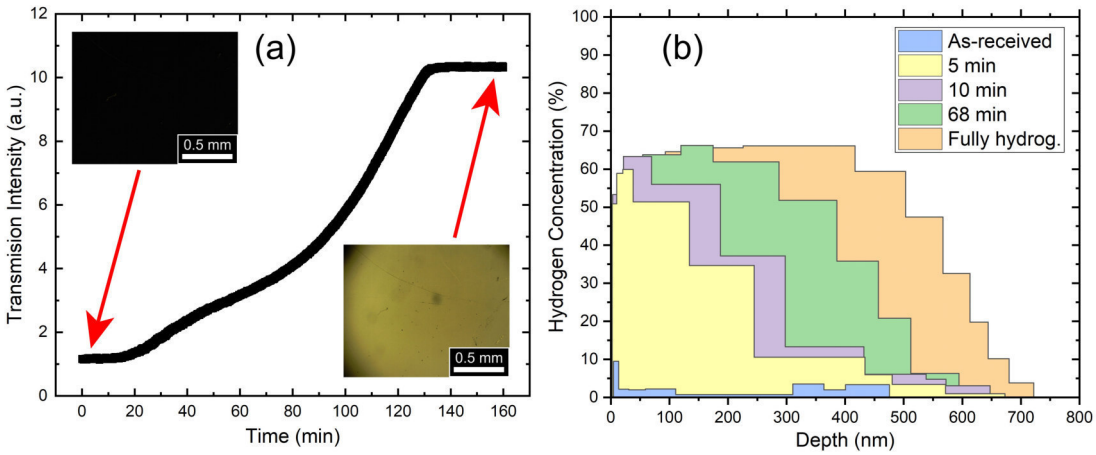

Figure 1: (a) Evolution of optical transmittance upon hydrogenation (b) Hydrogen distribution in the films at different hydrogenation times

GEFES 2025

Micrometric neural network using the Metal-Insulator Transition of VO_2

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Nowadays standard von Neuman computers are starting to find a bottleneck regarding their enormous energy consumption, struggling to keep up with an upgoing use of huge amounts of data. This problem has impulsed the development of more efficient alternatives, one of them being the denominated "neuromorphic computing", a novel computing paradigm that seeks hardware-based implementation of neural networks, that is, it searches for devices that have intrinsic properties like those of neurons and synapses, coined as "neuristors" and "synaptors", respectively [1].

We present a project to build a neural network based on materials with MIT (Metal-Insluator Transition). Here, we propose the implementation of VO_2 thin films, with a well-studied MIT near room temperature and an associated hysterisis behavior that can be tailored locally with FIB (Focused Ion Beam). We expect to achieve a complete neural network on the microscale and over a single VO_2 platform by exploding its voltage-triggered transition [2], for neuristors in pristine zones, and also a domain wall motion driven by Peltier effect at the nanoscale [3-4], for synaptors in FIB radiated zones, where a working temperature in the middle of their transition hysteresis would permit the coexistence of both metal an insulator domains.

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Figures

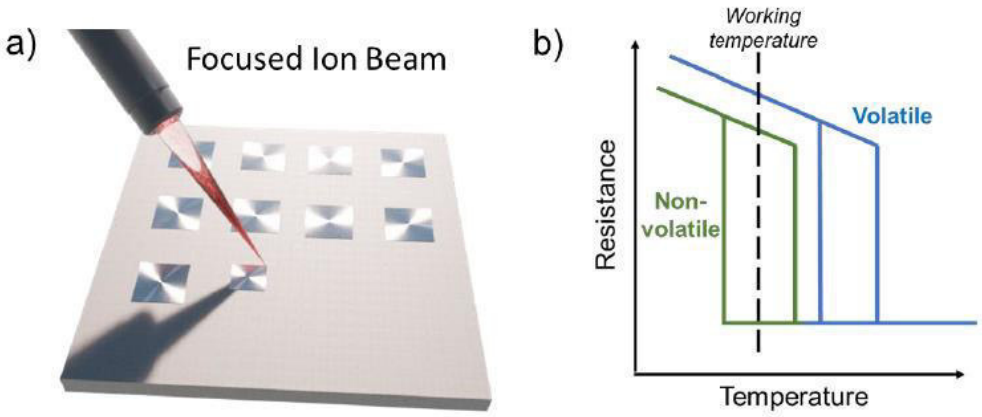

Figure 1: Key scheme for our single platform micrometric neural network based on VO_2. a) FIB to locally tailor the MIT of VO_2 thin films. b) Representation of the hysteresis behavior of pristine (blue) and FBI radiated (green) zones, indicating the working temperature that will enable a volatile and nonvolatile transition for their implementation as neuristors and synaptors, respectively.

Smart Magnetic Microrobots Learn to Roll with Deep Reinforcement Learning

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Accurate control of micron-scale robots, or microrobots, requires addressing unique challenges, including the difficulties associated with achieving motion in a non-inertial fluid dynamics regime, the development of real-time control strategies, and the presence of complex and dynamic environments. Unlike their macroscopic counterparts, microrobots are subject to Brownian motion, which randomizes their position and orientation. Deep reinforcement learning is a promising method for autonomously developing robust controllers to create smart microrobots, providing them with the capability to adapt their behavior to operate in uncharacterized environments without the need to model system dynamics. In this work, we report the development of smart magnetic-driven spherical particles that harness lubrication forces to facilitate rolling on a substrate. We use real-time control of these rollers to train a reinforcement learning model that generates an actuation policy to direct their motion in a simple standard navigation problem whose optimal solution can be derived from the underlying physics. The model's performance is analyzed under different sets of physically-informed system states. As a hallmark of the microscopic world, we characterize the influence of Brownian motion on the learning process by comparing learning rates under different Peclet numbers. Although the field of microrobotics has not yet reached the evolutionarily honed refinement of microscopic living organisms, deep reinforcement learning is a promising approach that is likely to enhance the capabilities of the next generation of microrobots.

Figures

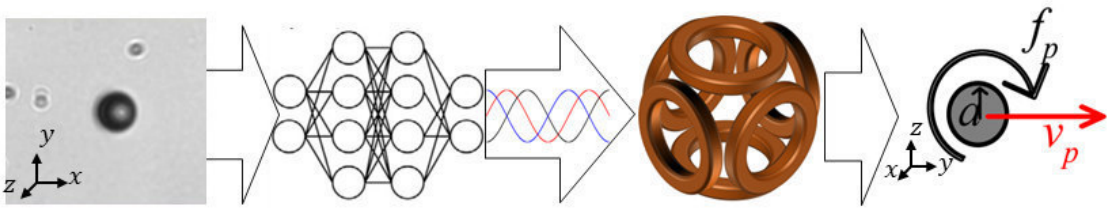

Figure 1: Schematic representation of the microrobot control process using deep reinforcement learning. From left to right: microscope image input, deep neural network for policy learning, rotating magnetic field actuation, and resulting roller motion.

Surface Roughness and Epsilon-Near-Zero SiC Substrates

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Epsilon-near-zero (ENZ) materials, i.e., those with a near-zero permittivity, give rise to a qualitatively different optical phenomena [1]–[4]. However, similar to plasmonics the quality of the ENZ response is limited by surface roughness [5]. Interestingly, theoretical studies provide confronting views on how roughness influences the behavior of ENZ materials [6]–[7], highlighting the need for further experimental investigation.

In this work, three samples with different surface root mean square (RMS) roughness values and the commercial one without etching are the object of study. The roughness was induced via Reactive Ion Etching (RIE). The characterization of the surface morphology was made with Atomic Force Microscopy (AFM), and the reflectivity response measured with used Fourier Transform Infrared Spectroscopy (FTIR). Our results reveal a significant change in the material's response as the surface roughness increases. Two different regimes can be roughly differentiated. Low RMS levels will lead to coupling with longitudinal ENZ modes and resonances with surface phonon polaritons (SPhPs). As the roughness becomes more pronounced, localized SPhP resonances will emerge. This is because the roughness scale becomes comparable to the size of pillar resonators reported in previous works [8], causing a noticeable drop in reflectivity, particularly in the Reststrahlen band, but also in dielectric bands. Consequently, the reflectivity spectrum shifts to a two-peak structure: one at the ENZ wavelength and another at the TO wavelength. Additionally, large-scale surface roughness enhances coupling to zone-folded phonons (ZFLO), which manifests as a peak at $\lambda = 11.92\ \mu m$.

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Remote spin-spin interactions mediated by superconducting circuits for quantum applications.

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Hybrid platforms combining molecular spins and superconducting circuits allow scaling up quantum computational resources by either exploiting the chemical design of molecules behaving as multiple qubits or qudits or via a proper engineering of the superconducting circuit [1-3].

In this work, we address experimentally this second option. We focus on circuits based on lumped element LC resonators. Their relevant properties, resonance frequency ω_r and quality factor Q, can be widely tuned without affecting the transmission through the readout line. Here, we realize resonator pairs able to introduce communication channels between remote spin qubit ensembles (Fig. 1). A superconducting chip consisting of seven LC resonator couples has been designed and fabricated. Resonators have ω_r ranging from 1.7 GHz to 3.0 GHz, which makes them individually addressable. Couplings between resonators in each pair have been engineered by the design of the two capacitors and their mutual distances. We explore their coupling to free radicals, model S=1/2 spin qubits, deposited onto either one or the two inductors of each pair (Fig.2). In the first case, we observe strong coupling of the spin ensemble to "its local" resonator and, besides, to photon modes in its remote companion. In resonator pairs hosting two different organic radicals we have observed evidence for the coherent coupling between the polaritonic light-matter states of both resonators. These experiments provide a method for performing spin resonance on a given specimen at two resonances simultaneously and pave the way for introducing coherent communication channels between two remote spin qubit ensembles, thus for scaling up this hybrid platform.

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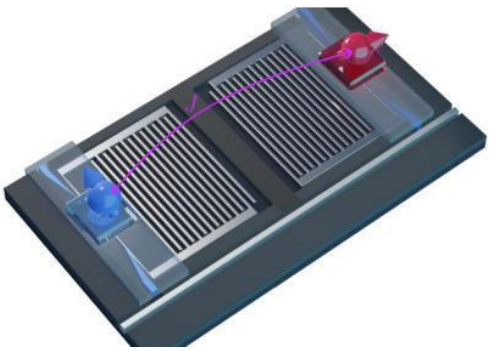

Figure 1: Sketch of two coupled resonators hosting two different molecular spin ensembles.

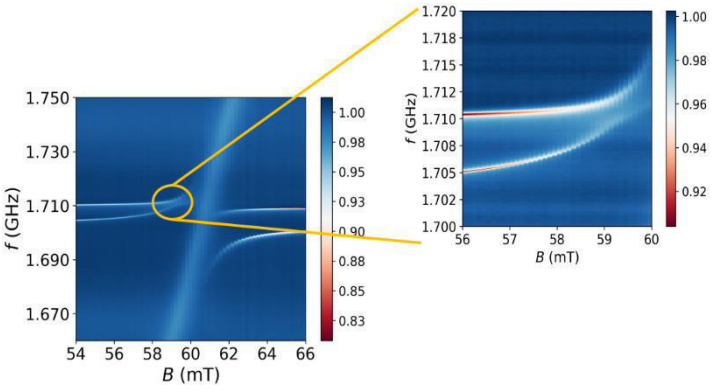

Figure 2: Microwave transmission data showing an additional anticrossing between two polaritons, which bears evidence of coherent communication between the spin ensembles.

Magnetic Field Screening of 2D Materials Revealed by Magnetic Force Microscopy

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2D materials possess exceptional mechanical properties making them promising candidates for protecting nanostructures. However, the magnetic field screening properties of 2D materials are largely unexplored.[1] Here, Magnetic Force Microscopy (MFM) is used to unveil the effects on the magnetic field of magnetic nanostructures when 2D materials are placed on top of them. It is demonstrated that while graphene and few layer graphene (FLG) exhibits a weak diamagnetic response due to its unique electronic structure around the Dirac point, the overall screening effect remains minimal (~0.5% per layer). Conversely, graphene oxide (GO) and MoS_2 show negligible response to the magnetic field, making them ideal for applications where preserving the original magnetic properties is crucial. These findings suggest that 2D materials can offer effective protection while minimally affecting the underlying magnetic functionalities, important for data storage technologies and spintronics.

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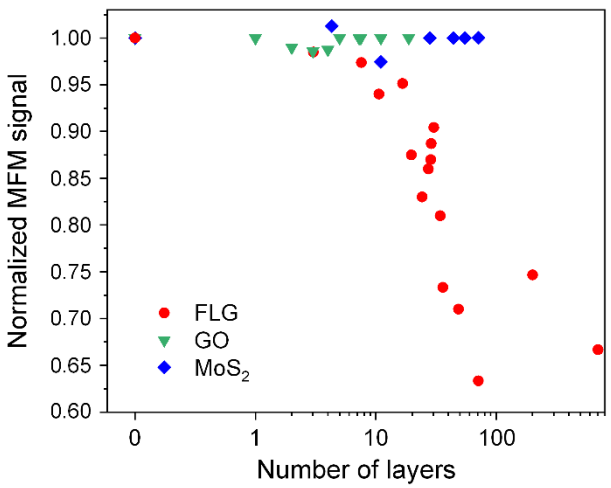

Figure 1: Magnetic field screening quantified by the decrease of the MFM signal for regions covered by FLG, GO, and MoS_2 as a function of the number of layers.

Standing Spin waves in Permalloy-NiO bilayers as a probe for the exchange coupling

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Ferromagnetic/Antiferromagnetic (FM/AFM) bilayers dynamics have been a recent topic of interest due to the interaction occurring at the interface, where the magnetic moments of the AFM can be imprinted into the FM [1], and the exchange bias field can affect these dynamics. Here, we investigate Permalloy (Py) and NiO films (Py/NiO) and control Py films of various thicknesses using both an experimental broadband VNA-FMR setup and micromagnetic simulations. Our experiments cover films with Py thicknesses up to 73 nm, while our simulations consider thicknesses up to 200 nm. We see a clear enhancement of the perpendicular standing waves (PSSWs) modes frequencies upon adding the NiO both in our experiments and in our simulations. We attribute this effect to a reduction of the effective thickness of the Py film when pinning of the magnetic moments at the interface takes place due to the exchange bias. This enhancement of the frequency becomes less pronounced as the thickness of the film increases, a similar trend is followed by the evolution of the exchange bias and therefore the coupling between the FM and AFM layers. Thus, the detected PSSWs may serve as probes of the interface exchange strength between the FM and the AFM. Additionally, through micromagnetic simulations, we explore the mixing and changes in the shape of the n=0, 1 and 2 PSSWs modes. As the thickness is increased, there is a hybridization of the PSSWs modes with the fundamental FMR mode, resulting in asymmetric modes. Our study opens a new pathway to the interfacial exchange characterization with high frequency responses in FM/AFM heterostructures [2].

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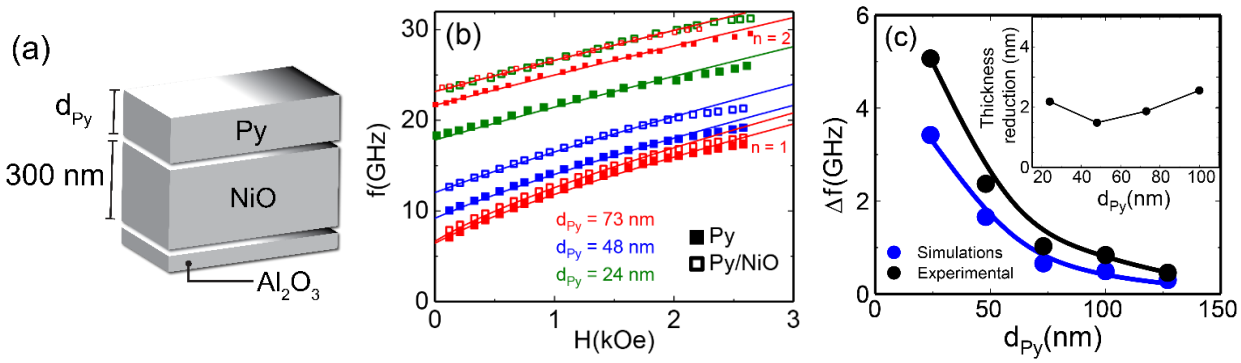

Figure 1: (a) Sketch of the Py/NiO samples. (b) PSSWs on the Py and Py/NiO for 73, 48 and 24 nm thick Py against frequency and bias field. (c) Frequency shift of the first order PSSW in our films upon the addition of the NiO layer at an applied magnetic field of 2 kOe and simulated frequency shift at the same thicknesses and field for a Py film with an antiferromagnetic interface. Inset in (c) is the effective thickness reduction of the Py films against its thickness upon the addition of NiO due to the pinning of the magnetic moments at the interface.

Tuning the electronic properties of graphene nanoribbons through the incorporation of pores and changes in the dimensionality

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Graphene nanoribbons (GNRs) are versatile structures interesting for applications because their electronic properties can be tuned by changes in their width, their edge topology or by doping with heteroatoms or functional side-groups. Insertion of holes is another promising strategy to obtain new materials with different electronic properties and functionalities. Moreover porous GNRs can be laterally fused to obtain a diverse family of nanoporous graphene (NPG) structures with atomically precise pore size, shape and density. Here, we show selected examples on the synthesis and characterization of porous graphene nanoribbons, on their lateral fusion, and the electronic changes that this change in dimensionality brings about (Fig. 1).

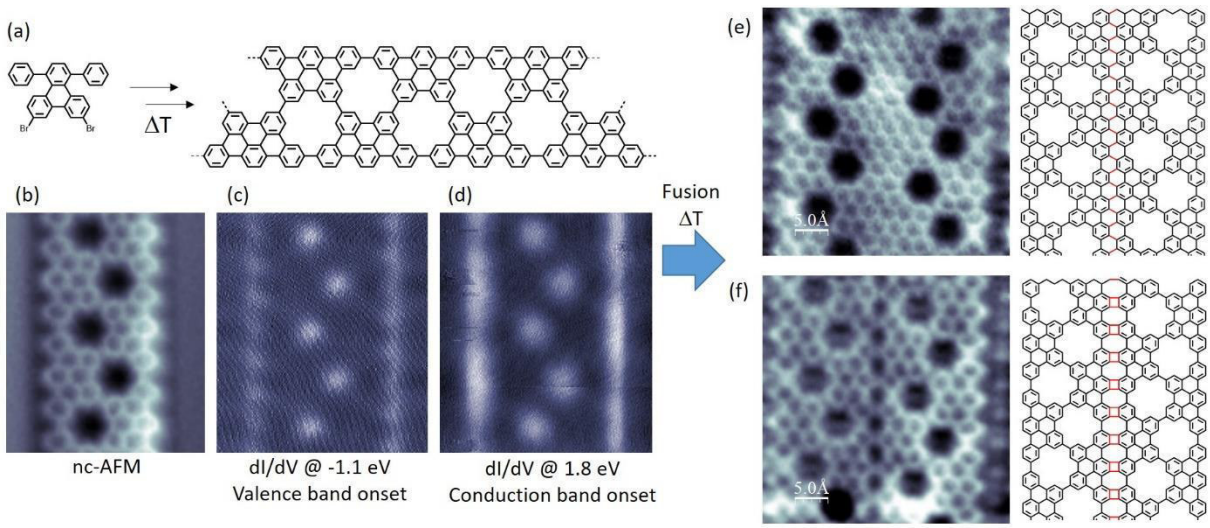

Figure 1: (a) Chemical structure of the reactant and product (porous GNR). (b) nc-AFM image of the product, along with conductance maps acquired at the (c) valence band onset and (d) conduction band onset. (e,f) nc-AFM and chemical structure drawings of representative products upon GNR fusion at higher temperatures.

The Essential Role of Water in Screening the Effects of Sodium Carboxymethylcellulose on Carbon Nanotubes

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The search for suitable materials safe for applications in biosensors is crucial for reducing waste in biomedical device manufacturing. Sodium carboxymethylcellulose (NaCMC) is well known for its ability to enhance dispersion of single walled carbon nanotubes (SWNTs) in aqueous solutions [1], addressing one of the main challenges in processing carbon nanotubes (CNTs). Its biocompatibility and environmental safety make NaCMC/CNTs composites suitable for applications such as biosensors, where the swelling capacity or moisture absorption can be used as a sensitive response to environmental changes. So far, the precise atomic scale interactions between NaCMC and carbon nanotubes remain unexplained and it is unclear whether NaCMC/CNT composites can maintain their structure in the absence of water [2].
In this study, we conducted density functional theory (DFT) calculations, along with tight-binding based on DFT (DFTB), molecular dynamics (MD) simulations, and electronic transport calculations using the non-equilibrium Green's function (NEGF) method. These computational approaches were conducted alongside experimental work on NaCMC/CNTs composites, providing a comprehensive analysis that integrates both theoretical and experimental perspectives.
The results show that NaCMC without the presence of water molecules has a tendency to form a collapsed structure where the sodium atoms form clusters. The preferential position of the polymer is perpendicular to CNT and there is no helical wrapping due to the rigidity of the cellulose chain, which is consistent with previous studies[3]. Preliminary DFTB calculations show that the absence of water in the system has a negative impact on pristine CNT transmission and water is needed to screen the effect of polymer on CNTs. However, in CNT junctions, the findings differ: in metallic–metallic one, there is a decrease in transmission, while in semiconducting–metallic and semiconducting–semiconducting junctions, the presence of polymers with water leads to an improvement in transmission. MD calculations show deformation in SWNT structures from the polymer, but the effect on thicker CNTs is less pronounced. This study provides evidence that NaCMC/CNTs composites cannot exist without an aqueous medium and only in this environment can sodium carboxymethylcellulose preserve the intrinsic properties of the carbon nanotubes.

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Figures

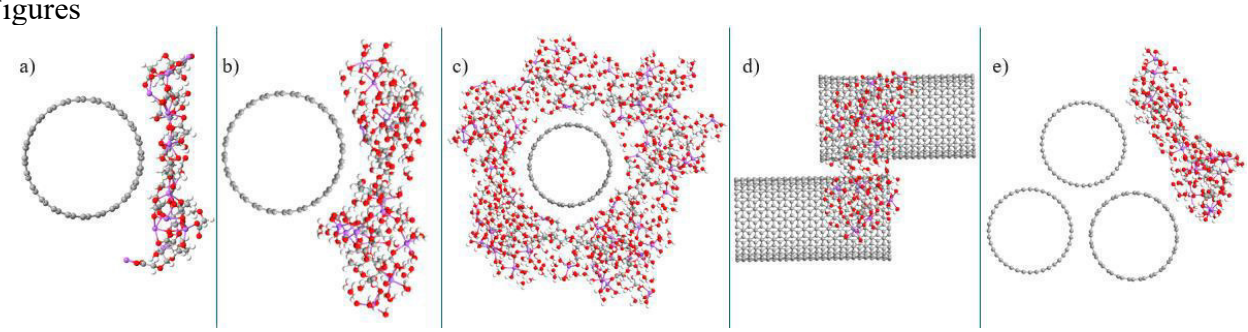

Figure 1: NaCMC/SWNT with and without water (a,b), NaCMC surrounding SWNT (c), junction (d), bundle (e)

Magnetism of Multifunctional Metal-Organic Frameworks Incorporating Tailored Combinations of Multiple Lanthanides

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Metal-Organic Frameworks (MOFs), constructed from organic linkers and metal ions arranged in crystalline, porous structures, have gained widespread attention due to their versatility in applications such as catalysis, gas storage, and sensing. Lanthanide-based MOFs, in particular, stand out for their unique magnetic, electronic, and optical properties, making them attractive molecular materials for advanced technologies including information storage and processing, magnetic refrigeration, luminescence etc. Recently, we achieved the unprecedented synthesis of multivariate MOFs using bulky, acidic carborane linkers, enabling the incorporation of customizable combinations of multiple lanthanides (Ln) in different ratios [1]. This breakthrough offers a versatile playground for investigating "complex magnetic materials" and designing new materials with tailored functionalities [2, 3]. Here, we demonstrate the remarkable potential of our strategy showing selected examples of multifunctional MOFs, prepared by combining strategically chosen Ln ions: {Gd_xY_{1-x}} "quMOFs" for quantum computing; {GdLn} (Ln=Tb, Eu, Tb/Eu) MOFs exhibiting magnetocaloric effect (MCE), Single-Molecule Magnet (SMM) behavior and luminescent properties [4]; {Nd/Yb} and {Ce/Er} magnetic and NIR emissive MOFs; and the first-ever MOF containing eight different rare earth ions (Dy, Tb, Gd, Ce, Yb, Eu, La, Y) [3]. Magneto-thermal properties were investigated using dc/ac magnetometry, heat capacity down to mK, and XAS-XMCD. This synchrotron, element-selective technique was essential to characterize the spectroscopic, magnetocaloric and magnetic properties of individual Ln ions in these multivariate MOFs (Figure 1).

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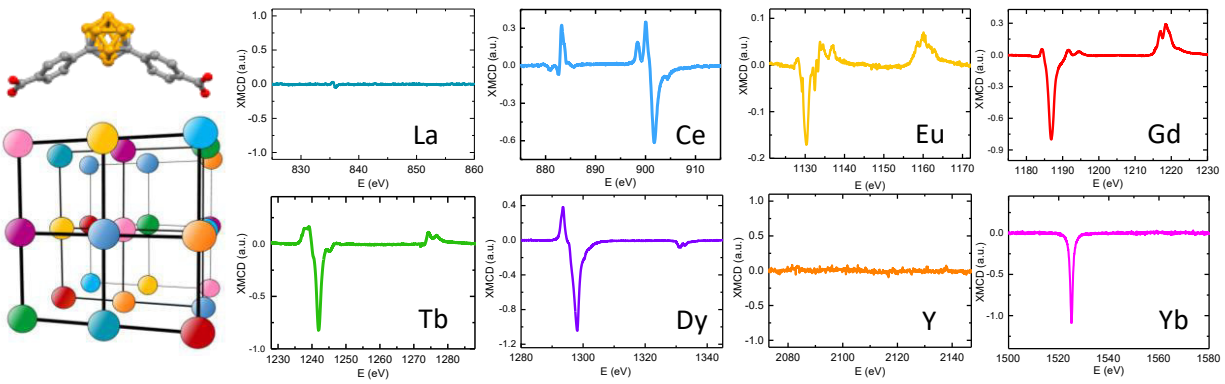

Figure 1. XMCD spectra at the $L_{2,3}$ edges of Y, and $M_{4,5}$ edges of La, Ce, Eu, Gd, Tb, Dy and Yb in a multivariate carborane-based MOF at 3.4 K, 6 T.

Reconfigurable Nanophotonic Devices by Spin-State Modulation

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The development of reconfigurable nanophotonic devices fundamentally relies on phase-change materials (PCMs) due to their ability to undergo significant alterations in optical properties when subjected to thermal or electrical stimuli. This work introduces a novel PCM nanomaterial that exhibits spin-crossover (SCO) behavior, demonstrating both reconfigurability and optical bistability at room temperature. This unique characteristic stems from the material's capability to transition between two distinct spin states when exposed to external triggers such as temperature, pressure, light, or voltage. Moreover, these transitions are accompanied by variations in structural (volume), magnetic, optical, electrical properties, and color [2]. Utilizing these distinctive optical properties and the ability to modulate spin states at the nanoscale, we investigate the creation of adaptable platforms for modulating, steering, and controlling light within reconfigurable metasurfaces. Furthermore, SCO materials show immense promise for developing non-volatile, low-power nanophotonic switches operating in the infrared (IR) regime. This breakthrough enables dynamic, on-demand control of optical signals in real-time, facilitating a wide range of applications, from ultrafast data processing to adaptive optical systems.

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YBCO thin films for broad-band nanoSQUID operation

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We present the fabrication, characterization and optimization of Yttrium Barium Copper Oxide ($YBa_2Cu_3O_7$, YBCO) thin films grow through pulsed laser deposition (PLD) on two different bi-crystal substrates. First, strontium titanate ($SrTiO_3$, STO), one of the most widely used materials with optimal lattice matching to YBCO. Second, magnesium oxide (MgO), due to its suitability for transport measurements at microwave frequencies, enabled by its excellent low-loss properties and minimal parasitic capacitance. Both bi-crystals have a 24° grain-boundary misorientation, which translates into a structural grain boundary in the YBCO layer, behaving as a Josephson junction. NanoSQUIDs will then be patterned using focused ion beam (FIB) milling with Ga ions to create a nano-loop interrupted by two Josephson junctions. The design will be optimized to ensure maximum microwave transmission, enabling the nanoSQUID response to be read at frequencies reaching several GHz. The resulting devices will be employed to investigate the dynamic properties of magnetic textures in the quantum regime at very low temperatures.

Real-space visualization of Canalized Ray Polaritons in a single van der Waals Thin Slab

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Polaritons [1] are central to the development of nanophotonics, as they provide mechanisms for manipulating light at the nanoscale. A key advancement has been the demonstration of polariton canalization [2-4] in which the energy flow is directed along a single direction. An intriguing case is the canalization of ray polaritons [5], characterized by an enhanced density of optical states. Experimental demonstrations of ray polaritons are scarce and their observation in single crystal slabs remains elusive. Here [6], we propose a novel polaritonic platform based on single thin slabs allowing for the excitation of canalized ray polaritons. By performing near-field nanoimaging, we demonstrate that the necessary conditions for their observation (a synergistic combination of large material permittivity modulus and dielectric environment) are fulfilled for phonon-polaritons at mid-IR frequencies in thin α-MoO_3 slabs on SiO_2 substrates. Our real-space images reveal the propagation of unidirectional phonon-polaritons exhibiting a constant propagating phase. These results might impact the development of compact, low-loss optical nanodevices for applications requiring strong light directionality.

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Figures

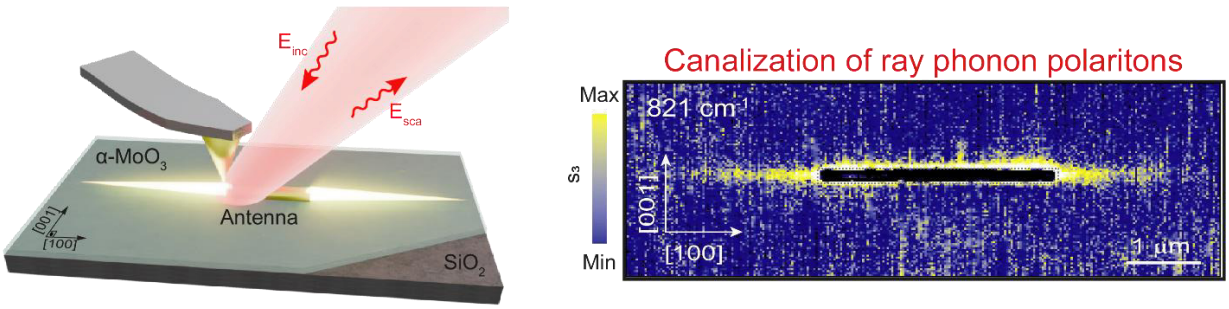

Figure 1: Near-field real-space visualization of canalized ray phonon polaritons launched by an Au rod nanoantenna in a single thin slab of α-MoO_3 placed on top of a SiO_2 substrate.

Improving the output signal at the spin-orbit module of MESO devices

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The MagnetoElectric Spin-Orbit (MESO) device architecture is a promising energy-efficient solution for integrating spin logic into the existing electronics industry [1]. The information of the logic state is stored in the magnetization $\vec{M}$ of a nanoscale ferromagnetic (FM) element, that can be reversed (i.e. write the logic state) via ME coupling. To read the logic state, a spin-polarized current is created by flowing a charge current through the ferromagnet into a material with spin-orbit coupling (SO), where it is converted by the inverse spin Hall effect (ISHE) into a transverse voltage with two well-defined states depending on $\vec{M}$, being ΔV_{ISHE} the difference between those two states. The spin to charge conversion in such devices must be efficient enough so that ΔV_{ISHE} can switch the writing module of another cascaded MESO unit and perform logic operations. In this regard, there have been demonstrations of a scaling law for ΔV_{ISHE} in FM/SO ohmic interface devices, that prove the importance of using SO materials with high spin Hall efficiency while also highlighting the current shunt across FM and spin backflow in the interface as limiting factors for the growth of ΔV_{ISHE} [2].

In this work, we explore how using an insulating MgO barrier as a spin injection layer in CoFeB/MgO/Ta nanostructures can improve the scaling law for ΔV_{ISHE} in comparison to ohmic FM/SO interfaces. At the same time, we investigate Bi as SO material, which reportedly shows a high spin Hall angle θ_{SH}, a high spin diffusion length λ_s, and high resistivity ρ_{Bi}, parameters that should improve the output signal.

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Figures

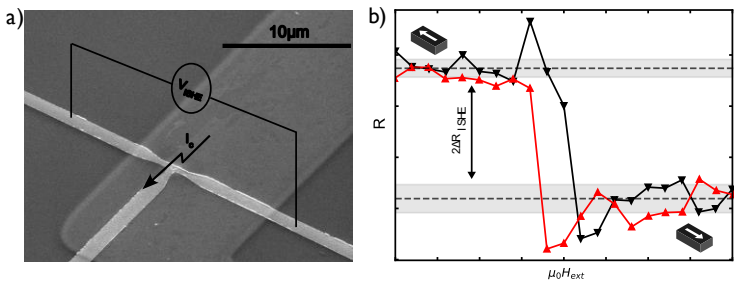

Figure 1: a) SEM image of a local spin valve, indicating the configuration used to measure ΔV_{ISHE}. b) Transverse resistance $\Delta R_{ISHE} = \Delta V_{ISHE}/I_C$ as a function of applied magnetic field, showing two different values at saturation.

Computational Thermodynamics Made Simple Using Quasiparticle Theory

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The computational prediction of thermodynamic properties under extreme conditions, i.e, high pressures and temperatures is fundamental in many fields, e.g., in the discovery of novel materials, and in Earth and planetary sciences. For example, a proper description of the thermodynamic properties of the minerals that form the Earth mantle is fundamental to understand its composition and dynamics. Nevertheless, experimentally replication of these conditions is expensive and complicated. For these reasons the computational predictions based on the quasi-harmonic approximation (QHA) are very popular as it provides a good balance between accuracy and computational cost, with excellent results in most of the cases[1]. However, due to the intrinsic assumptions in QHA, this approximation breaks down at sufficiently high temperature, as well as when describing second-order phase transitions.

Our method starts with the calculation of the n-th order force constants of the system, which is accomplished by computing the DFT forces on a set of structures with randomly displaced atoms, followed by a regularized regression. Next, the temperature-dependent effective frequencies $\omega(V,T)$ are obtained, and QP theory is used to derive the entropy $S(V, T)$[2]. A simple Debye model is used to fit the calculated QP entropies and obtain the other thermodynamic properties. We showcase the new methodology with two examples for which QHA fails at high temperature (MgO and CaO) and demonstrate that the new method prevents the QHA blowout, yielding thermodynamic properties in much better agreement with experiment and with a similar computational complexity.

Acknowledgements: We thank the Spanish MICIU/AEI/10.13039/501100011033, FEDER, UE, and by European Union: Next Generation EU/PRTR, the European Regional Development Fund (grants PID2022-138063OBB-I00, TED2021-130874B-I00 and PID2021-122585NB-C21(2)).

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Computational Thermodynamics Made Simple Using Quasiparticle Theory

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Biaxial Compressive Strain Tuning of Quantum Properties in 2D Materials

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Strain engineering is a powerful tool for tuning the properties of 2D materials. While the effects of tensile strain have been widely studied, compressive strain remains less explored, particularly at cryogenic temperatures, where conventional methods are limited. Biaxial compressive strain is expected to induce significant changes in the quantum phenomena of two-dimensional materials, such as tuning magnetic or superconducting phase transitions [1]. However, experimental validations of its impact remain limited, highlighting the need for further research in this area.

In this work, we demonstrate the effects of large, uniform biaxial compressive strain on 2D materials at low temperatures, namely, tuning the optical properties of single-layer transition metal dichalcogenides (TMDs) and modulating the superconducting phase transition of multilayered $NbSe_2$ deposited on polycarbonate (PC) substrates. First, as the temperature drops to cryogenic levels, the thermal expansion mismatch between the polymer and TMDs, combined with the PC substrate's contraction (up to 1.2%), induces biaxial compressive strain in the flakes. Furthermore, we demonstrate efficient transfer of this strain to single-layer TMD semiconductors [2]. Our findings show strain-induced shifts in exciton energy and gauge factor values that exceed previous compressive strain results. The improved spectroscopic resolution at low temperatures allows us to distinguish the effects of strain on both neutral and charged exciton energies. Next, we demonstrate the modulation of the superconducting transition in $NbSe_2$ flakes deposited on PC substrates [3]. Specifically, we observe a consistent decrease in the superconducting critical temperature compared to similar devices prepared on SiO_2/Si substrates (which induce negligible strain). This effect is more pronounced for thinner flakes (10 nm), with shifts in T_c of up to 1.5 K, although it remains noticeable for flakes as thick as 86 nm (see Fig. 1).

In conclusion, our findings show that strain can be efficiently transferred to single-layer and across several layers in van der Waals materials. Furthermore, our results provide an affordable method to tune phase transitions and other quantum properties at cryogenic temperatures.

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Figures

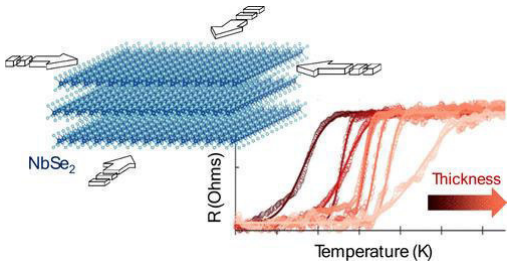

Figure 1: Left: Sketch of $NbSe_2$ multilayer flake under biaxial compressive strain. Right: Two-terminal resistance as a function of temperature for $NbSe_2$ flakes of varying thickness, deposited on PC.

Deep Reinforcement Learning for Radiative Heat Transfer Optimization Problems

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Reinforcement learning is a subfield of machine learning that is having a huge impact in the different conventional disciplines, including physical sciences. Here, we show how reinforcement learning methods can be applied to solve optimization problems in the context of radiative heat transfer. We illustrate their use with the optimization of the near-field radiative heat transfer between multilayer hyperbolic metamaterials. Specifically, we show how this problem can be formulated in the language of reinforcement learning and tackled with a variety of algorithms. We show that these algorithms allow us to find solutions that outperform those obtained using physical intuition. Overall, our work shows the power and potential of reinforcement learning methods for the investigation of a wide variety of problems in the context of radiative heat transfer and related topics.

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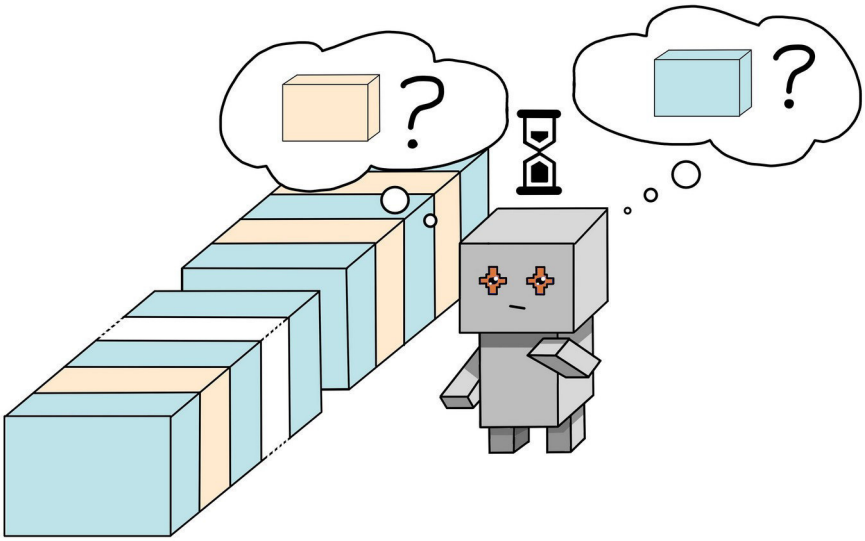

Figure 1: Reinforcement Learning schema for the enhancement of near-field radiative heat transfer through the design of a multilayer system.

Doping induced Nematic Charge Density Waves in bulk $TiSe_2$

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Despite decades of study, the nature of the Charge Density Wave (CDW) transition in $TiSe_2$ remains a source of controversy, in particular regarding the existence of more than one transition and the breaking of inversion symmetry, often associated to chirality, or threefold rotation symmetry. In this talk, I will review the experimental evidence with an emphasis on symmetry analysis, and argue how rotation symmetry may be broken with the standard CDW order parameter, while breaking inversion necessarily involves extra order parameters for which experimental evidence is not sufficiently established. Then I will present a general model to show how the breaking of threefold symmetry emerges naturally in a second transition within the CDW dome as a function of conduction band population, a variable often uncontrolled in experiments. Finally, I will argue how this theory reconciles previous claims and propose further experiments to test it.

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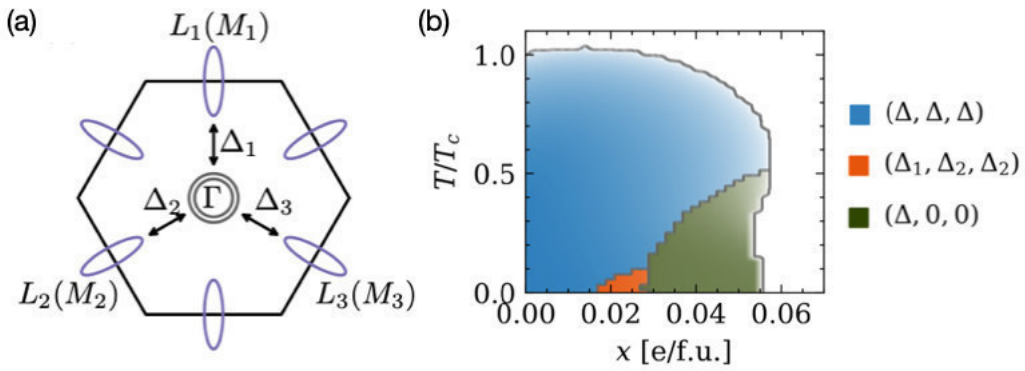

Figure 1: (a) Schematic band structure of TiSe2. The three-component order parameter Δ couples different electron and hole pockets. (b) Phase diagram of effective tight binding model. The isotropic CDW (blue) transitions to a nematic one (orange) and then to a stripe (green) as a function of carrier density.

A Kitaev quantum spin liquid candidate isolated in a two-dimensional $Co^{II}Rh^{III}$ bimetallic oxalate network

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A quantum spin liquid (QSL) is an elusive state of matter characterized by the absence of long-range magnetic order, even at zero temperature, and by the presence of exotic quasiparticle excitations [1,2]. In spite of their relevance for quantum technologies and for the understanding of strongly correlated systems, like high-T superconductors, the unequivocal experimental identification of materials behaving as QSLs remains challenging. Here, we present a novel 2D heterometallic oxalate complex formed by high-spin Co(II) ions alternating with diamagnetic Rh(III) in a honeycomb lattice (Fig. 1, left). This complex meets the key requirements to realize a Kitaev QSL [3,4]: a spin ½ ground state for Co(II), a strong spin-orbit coupling, a magnetically-frustrated triangular lattice, and strongly suppressed direct exchange and super-exchange interactions between Co centres. A combination of electronic paramagnetic resonance, 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 [5] (Fig. 1 right). These results show that bimetallic oxalates are versatile systems to realize and chemically tune key aspects of a QSL, like magnetic frustration and superexchange path geometries.

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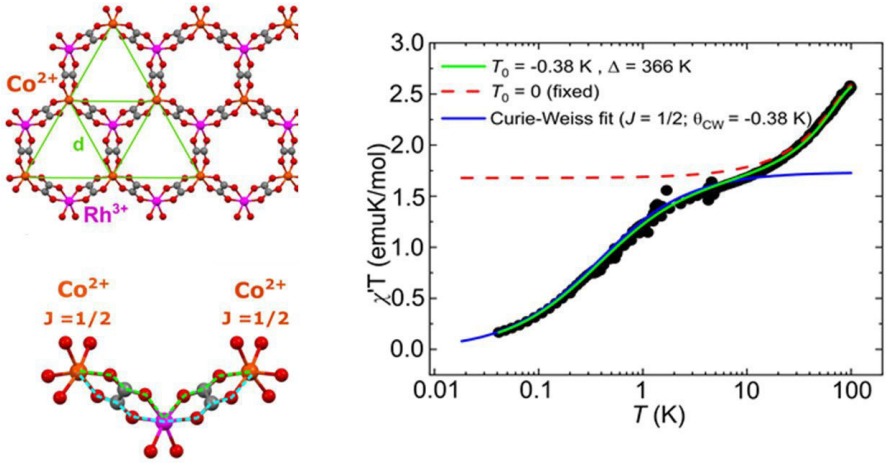

Figure 1: Oxalate honeycomb lattice (left) and temperature dependence of the χT product (right). From [5].

A Kitaev quantum spin liquid candidate isolated in a two-dimensional $Co^{II}Rh^{III}$ bimetallic oxalate network

Enrique Burzurí,*[a,b] María José Martínez-Pérez,[c,d] Carlos Martí-Gastaldo,[e] Marco Evangelisti,[c] Samuel Mañas-Valero,[e] Eugenio Coronado,[e] Jesús I. Martínez,[c] Jose Ramón Galán-Mascarós[f,g] and Fernando Luis *[c]

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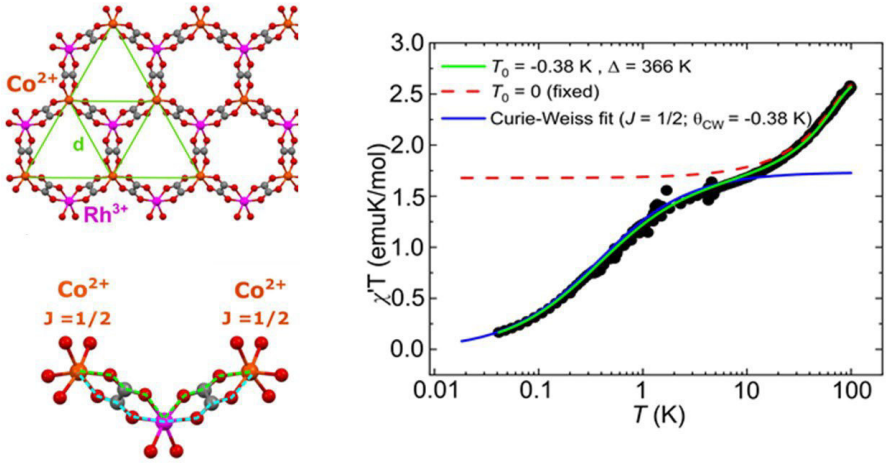

Figure 1: Oxalate honeycomb lattice (left) and temperature dependence of the χT product (right). From [5].

Photocurrents as a correlated phase indicators in twisted bilayer graphene

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The competition between many correlated phases within a narrow energy range in magic angle twisted bilayer graphene (TBG) makes the task of diagnosing the ground state as a function of filling challenging. Photogalvanic effects that access the geometrical properties of the band structure, can be a promising tool to experimentally distinguish symmetry broken phases. In this work, by using a heavy fermion description for TBG [1], we perform self-consistent calculations for the second order optical responses associated to the spontaneous symmetry-broken states mainly arising from the local interaction between the heavy electrons. These optical responses can be used to obtain a wealth of information about the correlated ground states in TBG as a function of filing. We conclude that the comparison of our predictions with experiments can serve to constrain the theoretical modelling of correlated phenomena in TBG.

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Thin layer interference effects on optical properties of layered BiI_3

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When precise measurement of optical properties in very thin systems, such as 2D materials, is required, thin layer interference effects play a crucial role [1,2]. This is particularly important when a thickness dependent characterization is needed [3]. Contrary to intuition, these kind of effects can take place even when the investigated thicknesses are well below the probing wavelength scale. In our work we have studied the layer-dependent optical properties of the archetypal 2D semiconductor BiI_3 [4], with thicknesses varying from the monolayer to the mesoscale. This material is of high interest for possible applications in optoelectronics, photovoltaics and X-Ray detection systems [5]. This study, based on transmission and photoluminescence measurements, allowed us to estimate how a strongly bound exciton in the material causes a giant stokes shift. A parallel thin layer interference analysis allowed us to disentangle the intrinsic material properties from simple optical effects in the measured phenomena.

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Engineering spin configurations in aza-triangulene architectures

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Graphene nanostructures with designer shapes can exhibit non-conventional paramagnetism associated with open-shell states of their conjugated π-electron lattice. Triangulene molecules are one of the most paradigmatic platforms for π-paramagnetism, with total spin increasing with its size [1]. This spin builds up from several radicals delocalized along the periphery and it is highly entangled by electronic correlations and hybridization.

A desirable step towards utilizing graphene platforms for quantum computing applications is the localization of spins at distant sites with tunable interactions. Here, we demonstrate an on-surface synthesis [2] strategy to transform the S = 1/2 state of an aza-triangulene unit [3] into a triradical platform by connecting anthracene units. Combining scanning probe microscopy techniques at low temperature with quantum chemistry simulations, we confirm the increasing polyradical character with the length of the anthracene extensions. This is reflected by the bunching of active molecular states into a narrow energy window and a competition between Jahn-Teller distortion and topology. The result is that anthracene extensions quickly transform the triangulene doublet into a weakly entangled spin trimer that can be potentially employed as a three-qubit registry. In addition, tweaking the shape of the extensions, we tune the exchange interaction between spins.

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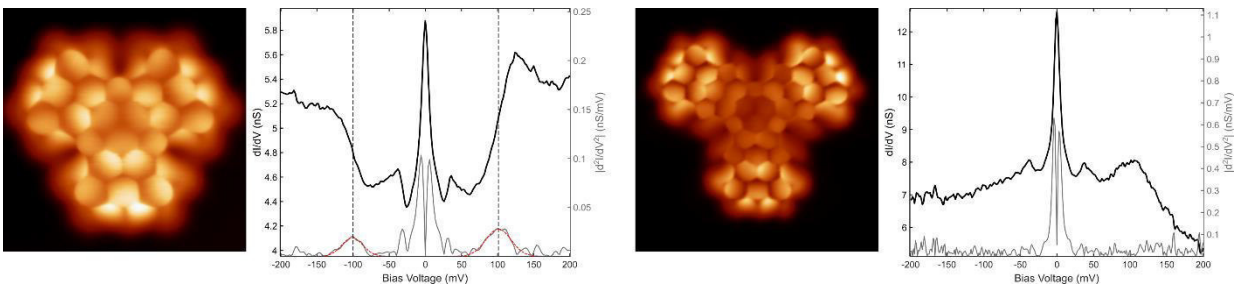

Figure: Bond-resolved scanning tunneling microscopy image and tunneling conductance spectrum of a single (left) and doubled (right) anthracene extended aza-triangulene.

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Electronic transport in α-Sn in atomic-sized contacts

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Tin has two allotropic crystalline forms, below 13°C changes its structure into the white form (***α***-Sn). Under tensile or compressive strain it behaves as a topological insulator or Dirac semimetal respectively[1][2].
In this work, we studied atomic-sized contacts through electronic transport in ***α***-Sn, using STM-BJ under cryogenic vacuum. In the process of stretching a ***α***-Sn wire, we have recorded the traces of conductance as a function of relative displacement between the electrodes. We found that these would be distributed in three different groups when they are sorted by a clustering-machine learning tool[3].
Conductance spectroscopic curves were obtained at the last stages of rupture of the wire, showing different behaviors depending on the trace. These preliminary results show the richness of scenarios of the electronic transport properties of tin at the atomic scale that could indicate a strong dependence on directionality and local-crystal orientation.

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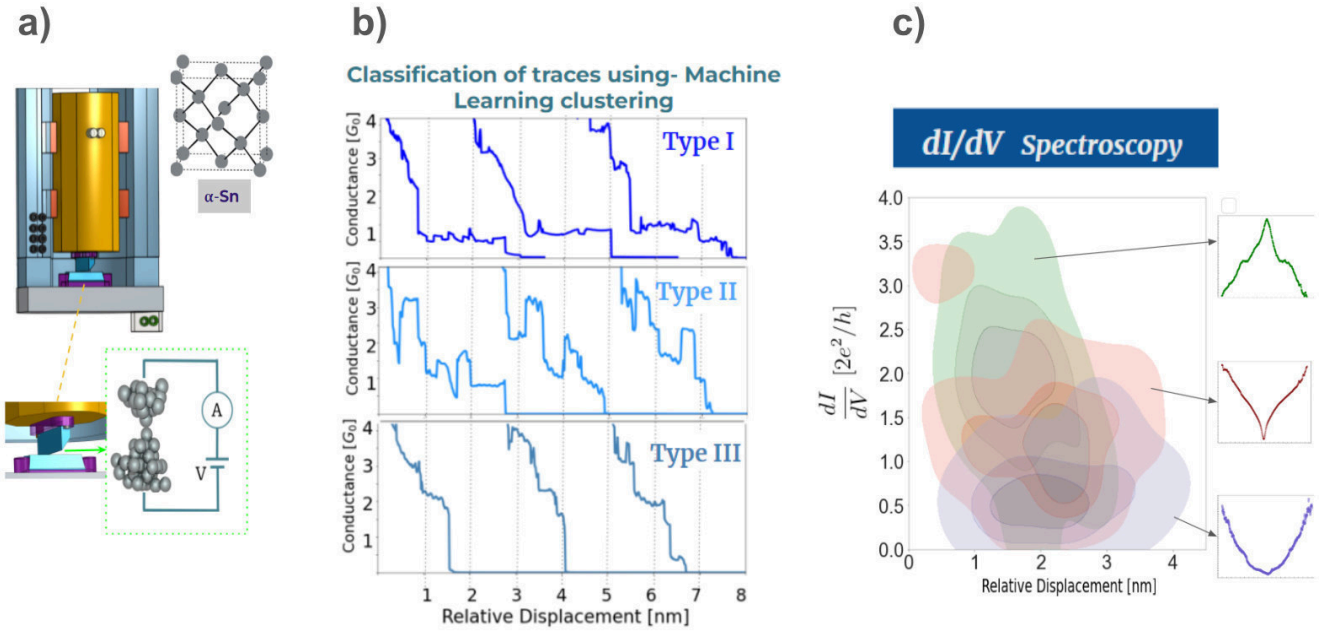

Figure 1: a) Schematic representation STM-BJ the zoom shows the sized atomic contact in ***α***-Sn at 4K, at the top the diamond structure in ***α***-Sn. b) Classification of quantum conductance rupture traces using Machine Learning Clustering. c) 2D differential conductance histogram for the values of the spectroscopy dI/dV(Bias=0) in relationship with his ubication in relative displacement, for each kind of curve spectroscopy obtained: 'peak shape' (green color), 'v shape' (red color), 'parabolic shape' (purple); in different rupture traces in atomic-sized contacts.

Oxygen vacancy imaging in strongly correlated oxides

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The interplay between spin, charge, orbital and lattice degrees of freedom in strongly correlated oxides gives rise to a wide range of emergent phenomena such as high temperature superconductivity, colossal magnetoresistance, or metal-insulator transitions, to name a few [1]. Lattice defects, ubiquitous to any crystal system, offer a promising path towards modulating such interactions. In transition metal oxides (TMOs), the macroscopic response is ultimately determined by the coupling between the oxygen and transition metal electrons, putting oxygen vacancies in the spotlight. Their microscopic distribution is of special interest, as small variations in their concentration and spatial structurization can lead to substantial changes in the functional properties of the system [2]. Thus, the in-depth comprehension of said phenomena relies on being able to detect the presence of very reduced densities of oxygen vacancies, highlighting the need for tools capable of detecting single oxygen vacancies in real space with atomic resolution. Techniques like scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) have provided a unique insight into the nanoscale nature of this problem [3], but the direct detection of single oxygen vacancies has remained a challenge.

In this work, we propose a new method for the detection of point-like defects such as single-oxygen vacancies using the capabilities of 4D-scanning transmission electron microscopy (4D-STEM) [3]. This technique combines a sub-angstrom electron beam with position-resolved diffraction measurements, capturing a multidimensional diffraction signal at each scanning position. As a result, we have direct access to the scattered distribution derived from the interaction between the beam and our material. Through 4D-STEM experiments and simulations, we have identified the characteristic variations in the scattered intensity distribution caused by individual oxygen vacancies. Harnessing such variations, we have developed an imaging mode that enhances the contrast between fully oxygenated and vacancy-containing columns. We illustrate the application of the technique in SrTiO3, showing a significant improvement in detectability of oxygen vacancies and enabling the experimental identification of single oxygen vacancy sites and possible nucleation of vacancy clusters. This method provides a new path in the field of advanced materials characterization by electron probes, showcasing the potential of 4D-STEM to probe atomic-scale defects. By providing new opportunities to study oxygen vacancies, our work highlights the implications of this technique in understanding and tailoring the properties of complex oxide materials.

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Generalized Epsilon-Near-Zero Polaritons on Silicon Carbide Hyperbolic Metasurfaces

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Ultrathin films of near-zero negative permittivity sustain volume-confined polaritons known as Epsilon-Near-Zero (ENZ) polaritons. These exhibit negative phase velocity, strong dispersion and high field confinement, making them ideal for tailored absorbers, non-linear devices and thermal emitters [1]. However, these polaritons have only been described in isotropic materials. In this study, we overcome this limitation by investigating laterally nanostructured Silicon Carbide (SiC) thin films —a polar material supporting phonon-polaritons (PhP) in the Mid-IR—. This nanostructuring enables precise modulation of the anisotropic effective permittivity of SiC over a wide range of parameters [2].

By systematically analyzing the optical response of the metasurface as a function of wavelength and filling factor (SiC ribbon density), we map out its photonic phase diagram. This diagram reveals the emergence of topologically distinct polaritonic regimes [3], characterized by different combinations of open and closed modes and differing phase velocity signs. We derive the analytical conditions delineating these distinct regions, demonstrating the existence of previously unreported ENZ modes with topologies beyond those found in isotropic thin films. We introduce new expressions for the asymptotes and vertices of the metasurface-supported modes and analyze their modal field distributions and exotic near-field patterns. Notably, we demonstrate that at the boundaries between different optical phases, the local density of states (LDOS) varies by orders of magnitude.

Our work broadens the scope of ENZ polaritons by extending them to anisotropic metasurfaces, unveiling a rich landscape of polaritonic behaviors not accessible in isotropic materials. The ability to engineer ultraconfined ENZ modes with unique dispersion properties, strong field confinement and tunable LDOS in SiC metasurfaces holds promise for devices requiring intense light-matter interactions, such as tailored thermal emission and absorption, and non-linear optics. This theoretical generalization lays the foundation for studying ENZ modes in new materials, such as biaxial, shear and moirè metasurfaces and multilayers.

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WHICH IS THE CHEMICAL BONDING IN PHASE CHANGE MATERIALS?

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Phase change materials (PCMs) are mostly chalcogens related to IV-VI and V_2-VI_3 families, which bear a strong relationship with electron-rich elements, such as pnictogens (group V or 15) and chalcogens (group VI or 16). The exceptional property portfolio and technological applications of PCMs, such as in re-writable data storage in DVDs and Blue-rays, phase change RAM memories, highly efficient thermoelectric systems, and also as topological materials, have sparked interest in the nature of the unconventional chemical bonding present in the crystalline phases of PCMs.

Two bonding models for PCMs rival to explain their properties in the last decade: the metavalent (electron-deficient) bonding model [1,2] and the electron-rich multicenter bonding (ERMB) model, also known as the hypervalent model [3,4]. In this work, we present a third model to explain properties of PCMs, the electron-deficient multicenter bonding (EDMB) model [5,6,7]. This model can be considered a reconciliation of the previous two models [8] and that it is part of new unified theory of multicenter bonding, which explains the formation of both [7].

We show that PCMs are characterized by electron-deficient multicenter bonds (EDMBs) by theoretically studying the simplest materials that could show this unconventional bonding at high pressure, i. e. pnictogens and chalcogens. These elements show a multicenter interaction at low pressures that leads to the formation of multicenter bonds (EDMBs) at their octahedrally-coordinated phases at high pressure. Our work suggests a change of paradigm since it proves that EDMBs can be observed in electron-rich elements (pnictogens, chalcogens, and halogens) unlike previously assumed [9]. Unexpectedly, the understanding of EDMB formation in electron-rich elements allows understanding the structure and properties of many materials even at room pressure, like polyiodides [10].

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Volatile and non-volatile resistive switching in three-terminal memtransistor based on mechanically exfoliated MoS_2

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Memristive behaviour has been widely demonstrated in 2-terminal MIM-based (Metal-Insulator-Metal) systems.Two-dimensional materials have become core active materials for novel electronic, optoelectronic and sensing applications. Transition metal dichalcogenides (TMDs) and other low-dimensional materials, such as hexagonal boron nitride (hBN), exhibit memristive behaviour [1] making them attractive candidates as building blocks for resistive memories and neuromorphic computing devices [2].

Here, we study the memristive behaviour on 3-terminal devices based on few layer MoS_2 [3]. The devices exhibit either volatile or non-volatile resistive switching depending on the fabrication process and operating conditions. A gate voltage is used as an extra knob to modulate the resistance switching window. We investigate the influence of contact pad geometry and symmetry in current-voltage (IV) characteristic curves.

The devices were fabricated by a mechanical exfoliation process, from natural bulk MoS_2, using the scotch tape method and transferring few-layer MoS_2 flakes onto a Si commercial substrate with a 290 nm thick SiO_2 layer on top.The memristive behaviour has been studied in freshly exfoliated devices as a function of temperature, under atmospheric and high vacuum conditions. A gate voltage (V_G) pulse was used to modulate the resistance change window, i.e. the ratio I_{LRS}/I_{HRS} (where I_{LRS} and I_{HRS} are the currents in the low and high resistance states, correspondingly), by few orders of magnitude. The influence of pad geometry and symmetry in the memristive behaviour was studied by using the electrodes defined by electron-beam lithography with varying contact areas.

Temperature dependent IV characteristics were used to determine the transport mechanisms and the Schottky barrier height in our devices. The experimental results are supported by simulations of the device conductance based on Schottky diode-like model [4].

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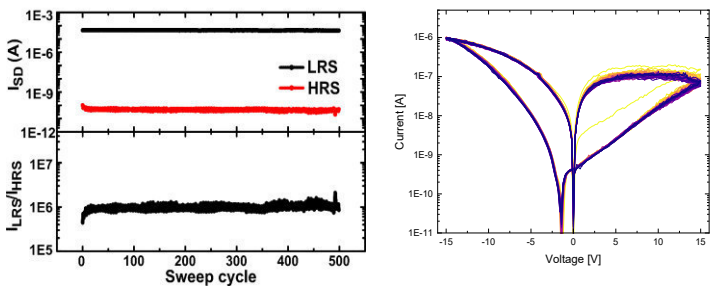
a) b)



a) Endurance of high (HRS) and low (LRS) resistance states (top) and I_{LRS}/I_{HRS} at voltage bias of 7.5 V (bottom) of a 3-terminal MoS2 device.
b) IV characteristics of a non-volatile device during 50 voltage sweep cycles.

Tuning magnetic exchange interactions in 2D magnets: the case of $CrGeX_3$ (X= Se,Te) and Janus $Cr_2Ge_2(Se,Te)_3$ monolayers

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We present a computational study to explore the potential of different experimental approaches to tune the magnetic interactions in two-dimensional van der Waals magnets. We selected $CrGeSe_3$, $CrGeTe_3$, and Janus $Cr_2Ge_2(Se,Te)_3$ monolayers as case studies and calculated the full exchange tensors among all relevant atomic pairs and analyze their dependence on different external parameters, such as biaxial and uniaxial strain, as well as gate voltage. We focus particularly on interactions that emerge or vanish due to changes in the system's symmetry, especially under uniaxial strain and gate voltage. We find that biaxial and uniaxial strains significantly modify isotropic exchange couplings, which can lead to a transition from a ferromagnetic to an antiferromagnetic phase, while a gate voltage induces Dzyaloshinskii–Moriya interactions, forming a vortex pattern whose chirality is determined by the sign of the electric field. The electric dipole moment of the Janus material is large, raising the possibility of multiferroic behavior [1].

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Figures

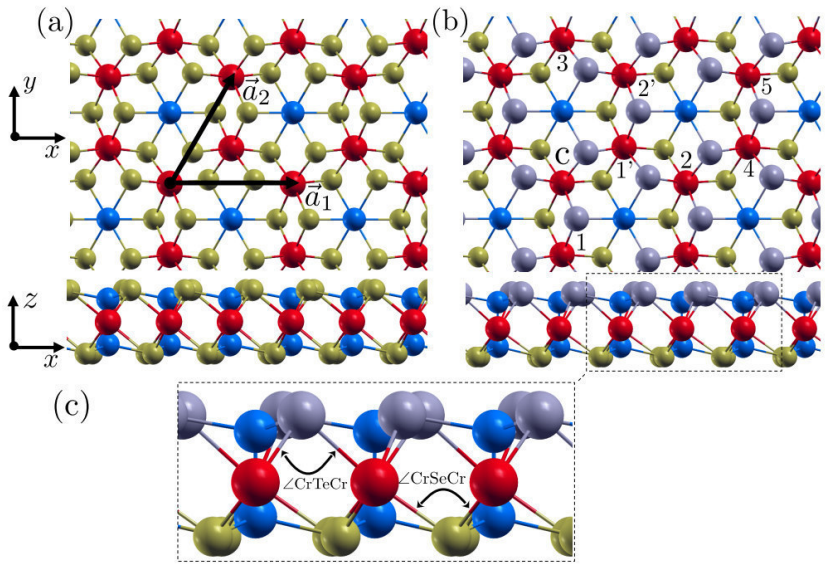

Figure 1: Top and side views of (a) the CGS and (b) the Janus CGST structures. Cr, Ge, Se and Te atoms are depicted in red, blue, yellow and grey, respectively. Lattice vectors $\vec{a}1$ and $\vec{a}2$ are shown in (a). Labeling of the nearest Cr neighbors with respect to a reference atom c is also shown in (b). Cr-X-Cr (X = Se or Te) bond angles are shown in (c).

Excitonic insulating states in doped WTe_2 monolayers

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Due to the Coulomb interaction strength, a bandgap can be opened in the band structure of a material as a consequence of the condensation of electron-hole pairs, that is, an excitonic condensate [1]. Even though it had been proposed in the past, it has not been until the recent years that experimental evidence may support the existence of this state in transition metal dichalcogenides monolayers [2]. In particular, monolayer 1T' WTe_2 has shown a plethora of promising correlated quantum states, from quantum spin hall insulting to unconventional superconductivity [3]. Without interactions, monolayer 1T' WTe_2 is semimetallic, therefore electron and hole Coulomb instabilities could drive the pairing mechanism for the observed experimental behaviors. Moreover, a repulsive on-site interaction mechanism has been proposed theoretically as the origin of unconventional superconductivity that appears at low-density electron doping [4].

In this work, we employ a Hartree-Fock approach to characterize the excitonic states that arise in the system and we construct the correlated phase diagram of this material. We find a zoo of broken symmetry phases and two different excitonic states and analyze their particular spin ordering. Interestingly, each state features a different spin order, one with a spin density wave (SDW) and the other with a spin spiral (SS) state. This SS is compatible with the lack of charge modulation observed in the experimental data.

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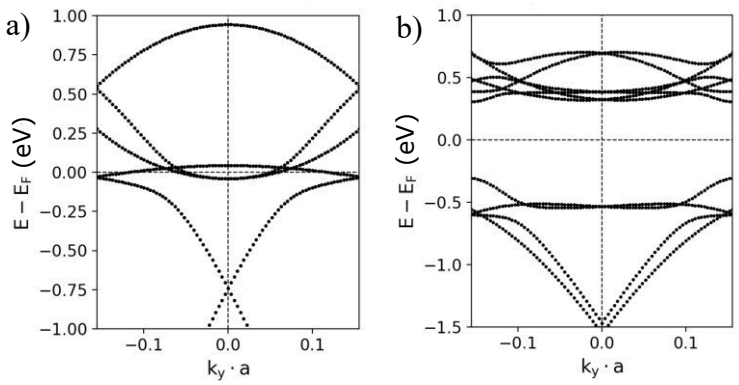

Figure 1: a) Semimetallic state prediceted by DFT. b) Renormalized bands where interactions opens a gap by condensation of an excitonic condensate.

Coexistence of spatially decoupled unconventional superconducting condensates in $4H_b$-TaSSe

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Materials exhibiting multiple superconducting phases are exceptionally rare in nature. The few known examples of multiphase superconductors display complex phase diagrams, where distinct phases can be independently induced by means of external stimuli such as pressure or magnetic fields. Here we report the coexistence of two superconducting condensates with different spatial localization in the van der Waals 4Hb-TaSSe polytype. Its layered structure consisting of alternating layers of the T-type and H-type polymorphs enables the development of two effectively decoupled superconducting phases with marked distinct microscopic properties. Using high-resolution quasiparticle tunneling and Andreev reflection spectroscopy in the two polymorph layers, we identify two different superconducting gaps in size in each layer, with signatures compatible with weakly coupled condensates, potentially of different pairing symmetry. The coexistence of these condensates is further corroborated by our measured critical temperatures and upper critical magnetic fields, which significantly differ in each polymorph layer. We explore the possible superconducting ground states using a minimal model based on ab initio calculations that captures many of the experimental features. Our results challenge the current understanding of superconductivity in low-dimensional superconductors and open new pathways for customizable superconducting devices that could independently operate several superconducting states.

Origin of step-edge states in NiS_2 in terms obstructed Wannier charges

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In recent years, the pyrite compound NiS_2 has attracted intensive attention as a platform to investigate the metal-to-insulator transition controlled via pressure or chemical substitution. While the material is a charge-transfer type Mott insulator in the bulk, its surface exhibits metallic conduction. Recent observations suggest that this surface transport might be related to metallic one-dimensional states located on step-edge dislocations. However, the origin of these metallic states remains elusive. In this work, we employ a combination of first-principle calculations and scanning tunneling microscopy to elucidate the origin of the metallic step-edge states. Our analysis indicates a relation between the obstructed-atomic charges in the bulk and the 1D metallic step-edge states. We also present a precise characterization of the low-temperature magnetic structures based on state-of-the-art neutron scattering measurements.

Carrier density and disorder effects on the Quantum Hall Plateau widths in epitaxial graphene

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Since its discovery, graphene has been one of the most prominent 2D materials due to its unique properties and broad range of possible applications. In particular, the relativistic nature of the electrons near the Dirac points and the electron-hole symmetry are responsible for the half-integer Quantum Hall Effect (HI-QHE). This phenomenon, characterized by the quantization of Hall resistivity, offers opportunities for advancements in quantum metrology and the understanding of topological quantum states. While the role of disorder in stabilizing Quantum Hall Plateaus (QHPs) is widely acknowledged, the precise interplay between their width and disorder, mobility and carrier density remain unresolved.

In this work, we investigate the width of the $\nu = 6$ QHP in epitaxial graphene Hall bar, focusing on two distinct regions of the device with markedly different electronic mobilities**.** We observe that depending on the storage conditions, it is possible to modify the carrier density of graphene QHE devices and consequently increase or reduce the mobility of the sample. Our experiments reveal mobility variations of up to 200% of their initial value. Notably, the sample storage time and conditions cause also noticeable changes in the positions and extension of the QHPs. Our results show that the QHP extension for $\nu = 6$ differs significantly between regions, influenced by both mobility and disorder, rather than solely by carrier density. Transport simulations based on the Landauer-Büttiker formalism with Anderson disorder in a scaled model reveal the critical role of impurities in shaping transport properties and the width of the QHPs. This study provides valuable insights into the interplay between mobility, disorder, and quantum transport in graphene systems.

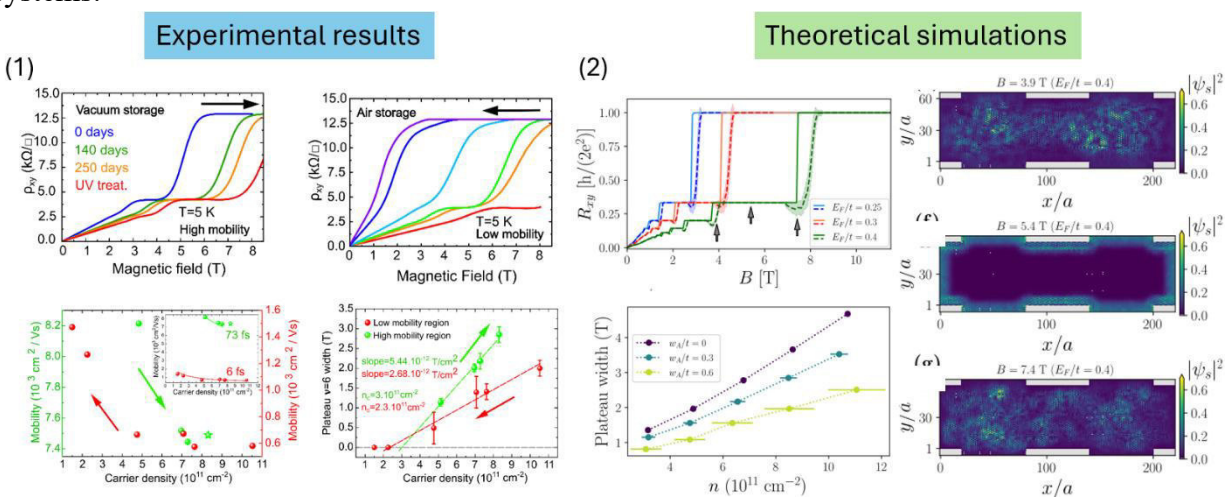

Figure 1: Panel (1): QHE experimental results for the longitudinal and transversal resistances as a function of the applied magnetic field for two mobility regions. Panel (2): Kwant transport simulations for different disorder strengths and the evolution of plateau width as a function of chemical potential and disorder strength.

[*] To be published

Ferroelectric hafnia: an opportunity for next-gen memory devices

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Electronics industry is demanding for more and more energy-efficient devices. Specifically, the advent of the artificial intelligence era makes necessary the development of new computing platforms able to dramatically reduce the power processing costs. In this regard, new architectures are being conceptualized. However, their efficient implementation makes indispensable the integration of new materials. Ferroelectrics keep non-volatile memory states, but their use in commercial applications is very limited due to the complexity of the ferroelectric perovskites, which hinders the miniaturization of the devices.

During the last years there is a renaissance on the interest of the scientific community and industry on the use of ferroelectric materials for memory applications. The reason is the discovery of ferroelectricity in a simple binary and fully CMOS compatible oxide, HfO_2. Most of the work related to ferroelectric hafnia is based on the characterization of polycrystalline samples, because of their CMOS compatibility. However, the understanding of the functional properties of polycrystalline films is challenged by the presence of multiple phases/orientations and blurry interfaces. In this regard, epitaxial films are an excellent platform for better understanding [1]. Epitaxial films present several interesting properties, such as their atomically flat surface, the absence of wake-up effect and the large polarization/endurance of ultrathin samples. We will show some of our recent results on epitaxial ferroelectric hafnia films, which include the achievement of excellent endurance (up to 10^{10} cycles) [2], and the proposal of novel HfO_2-based light [3] and magnetic field [4] responsive memory devices.

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Polar vortices in twisted $SrTiO_3$ bilayers

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The mechanical assembly of freestanding oxide membranes in twisted bilayers has led to the recent discovery of polar topologies in twisted $BaTiO_3$ homojunctions [1]. A ferroelectric vortex array is generated by the pattern of non-homogeneous shear-strains via flexoelectric coupling of polarization to strain gradients. Since flexoelectricity has been demonstrated to induce polar features in a wide set of materials, an important question is whether polar topologies can be induced in twisted bilayers of non-ferroelectric materials. In this communication we explore the effect of non-homogeneous moiré strains in twisted bilayers made of $SrTiO_3$. $SrTiO_3$ is a quantum paraelectric developing polar response at very low temperatures. Yet, it has been reported that in thin films ferroelectricity is induced by epitaxial strain. We have found that twisted $SrTiO_3$ bilayers display an array of polarization vortices. While fingerprints of ferroelectricity are found in individual $SrTiO_3$ freestanding layers of low thickness (6 nm), thicker layers (10-15 nm) used in the twisted junctions do not show measurable ferroelectricity. Inhomogeneous strain patterns with the periodicity of the moiré lattice measured from high resolution electron microscopy images have been used to set initial conditions for first principles simulations. Full structural relaxation shows polar vortex arrays in close agreement with experimental results. The results of DFT simulations, apart from confirming the stability of the polar vortex state, indicate that the origin of the polar topology is a flexoelectrically induced polar state driven by a highly anomalous negative flexoelectric coefficient. Future studies will be devoted to highlighting its origin.

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Plasmonically Enhanced Perovskite Solar Cells and LEDs

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In the past decade, halide perovskite based optoelectronic devices such as solar cells (SCs) and light emitting diodes (LEDs) have experienced a rapid increase in their performance.
Nevertheless, despite the remarkable optoelectronic properties of perovskites, these devices efficiencies still lag behind their theoretical ceilings. Dealing with light matter interactions cannot only be used to push toward these limits, but also to open new avenues. In this context, some promising strategies have emerged that take advantage of the localized electric field enhancement provided by plasmonic nanoparticles (NPs), demonstrating substantial potential for improving the performance of these devices [1]. This approach has been previously studied for absorption enhancement and thickness reduction in materials used in single junction solar cells [2], but never employed in a full tandem device, and neither in the emitting layer of a perovskite LED.
In this talk, we provide a simulation-based guideline to show how both near- and far-field plasmonic effects of randomly distributed metallic NPs address the inherent absorption limitations in the narrow bandgap (NBG) rear subcell in all-perovskite tandem solar cells. 3-dimensional (3D) Finite-Difference Time-Domain (FDTD) simulations demonstrate that embedding plasmonic NPs within NBG perovskite layers significantly enhances light harvesting, allowing for reduced film thickness, and thus an improved charge extraction, leading to increased power conversion efficiencies. Our results show up to a 2% absolute increase in efficiency with optimized plasmonic NP metal type, size and concentration [3].
Building on the concepts we applied to solar cells, we present the first rigorous theoretical analysis of the previously unexplored impact of metal NPs on the emission properties of blue, green and red emitting perovskite-based LEDs. By incorporating these nanoparticles, we can effectively control both the brightness and directionality of the emitted light. Herein, we leverage plasmonic effects to increase the optical density of states and thus enhance the radiative recombination rates, resulting in boosted effective Quantum Yields. Furthermore, our findings reveal that plasmonic effects allow for emission directivity control, guiding photons for optimized outcoupled light [4].

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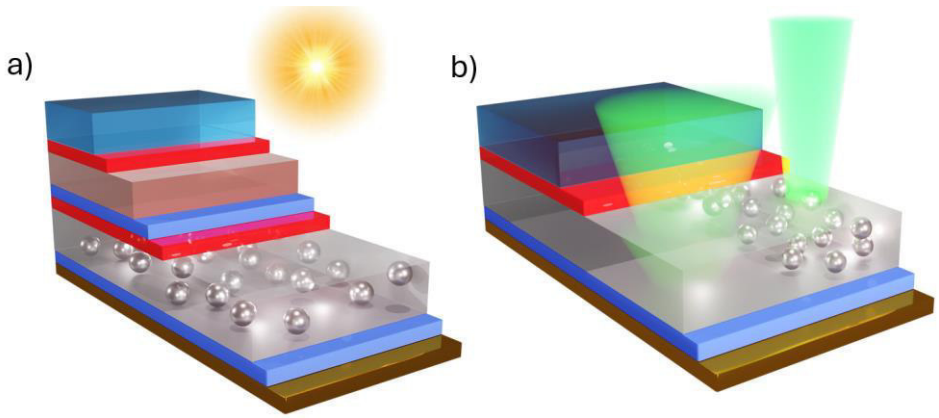

Figure 1: Schematic of the calculated plasmonically enhanced SC (a) and LED (b) model.

Quantum Theory of Photon Pair Creation in Photonic Time Crystals

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In this work, we study the generation of photon pairs in a photonic time crystal (PTC), the temporal counterpart of a spatial photonic crystal. In a PTC, the optical properties (either ε or μ or both) vary periodically in time under the action of an external mechanism [1]. We assume an instantaneous change in the refractive index between two values, namely, a temporal interface, (see Fig. 1a) and follow a transfer matrix approach to describe the classical and quantum electromagnetic fields. On a classical level, temporal interfaces result in the amplification of electromagnetic waves, but a backward wave (propagating opposite to the incoming one) is created due to momentum conservation. The quantum counterpart of the latter is the spontaneous generation of entangled photons with correlated momenta. In this work, we prove how the classical amplification of waves, whose strength is quantified by the reflectivity of the PTC, can be directly related to the probability of creating photon pairs from the vacuum (see Fig. 1 b-g). We also show how the classical reflectivity of the PTC coincides with the average photon number extracted from the vacuum, thus demonstrating how a classical quantity completely determines a quantum mechanical one [2].

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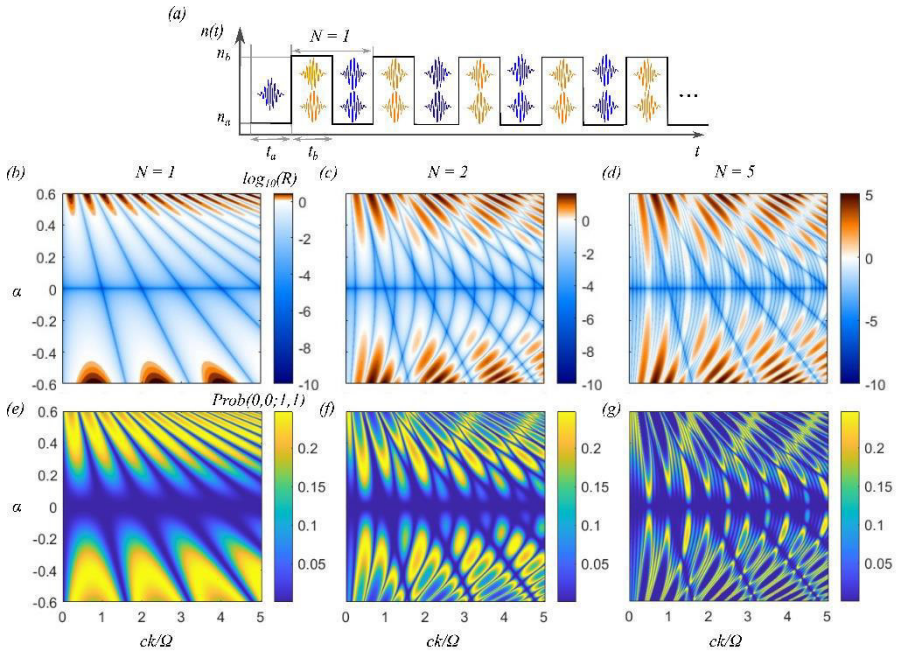

Figure 1: (a) Sketch of the PTC. (b-d) Classical reflectivity of the PTC for N=1, 2 and 5 periods of the temporal modulation. (e-g) Probability of single pair creation, once again for N=1, 2 and 5 periods.

Rotating reduced size STM for high magnetic fields experiments

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Cryogenic Scanning Tunneling Microscopy (STM) has been instrumental in the development of scanning probe microscopies. The addition of a magnetic field opens new prospects, such as the observation of vortex lattices in superconductors or of Landau quantization. For the latter, it is of particular importance to decrease as far as possible the size of the STM. Although efforts made during past years have led to some improvements, the size is still far above the typical sizes available for instruments used in high magnetic fields. Here we discuss the development of both a reduced size STM and a rotating platform meant to obtain measurements at different angles between the sample and the magnetic field. This feature will allow us to observe new exotic phases emerging at high tilted magnetic fields [1, 2], unreachable using state of the art three-axis coils [3]. Both the head and the base of the main body of the STM have been manufactured through 3D printing in grade 3 Titanium, which could turn out to be a good method to optimize the weight without modifying too much the stiffness of the microscope. Finite element calculations of the 3D printed system support the latter aspect. The STM has a diameter of 16 mm and a height of 25 mm. At the present time, we have performed successful measurements using a gold tip on a gold film at 4.2 K and applying magnetic fields up to 6 T. Namely, we have obtained topography images and observed the conductance quantization phenomenon with the STM at different tilted angles.

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Competing orders in transition metal dichalcogenides approaching the 2D limit: an ab initio study

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Transition metal dichalcogenides (TMD) have become a family of materials under intense study in recent years is that of. Their laminar structure has allowed the creation of very thin layers, down to the monolayer limit, where the community has explored all sorts of interesting physical properties: magnetism, topological properties, charge density waves, superconductivity, heavy fermions, etc. They have become central in the broader world of 2D materials as key pieces to form heterostructures. In this work, we have studied the interplay between electronic, magnetic and structural degrees of freedom in 2D TMDs from a theoretical point of view. This can be exemplified by the complex competition between structural distortion in the form of charge-density waves and magnetism in Cr-based compounds; by the appearance of strong-correlation effects caused by the star-of-David charge density wave in Ta-based monolayers; and by the rise of a ferroelectric order caused by yet a different type of charge-density wave in MoTe2. The work shows the enormous potential of TMD's as building blocks for engineering new materials on the nanoscale.

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YBCO superconductive phase transition through electrical current supply via YSZ substrate

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The superconducting critical temperature in hole-doped cuprates, like $La_{2-x}Sr_xCuO_4$, is determined by the actual concentration of holes, which can be controlled by either La^{3+}/Sr^{2+} ratio, or the oxygen content [1]. In the case of $YBa_2Cu_3O_{7-\delta}$ (YBCO), a maximum $T_c \approx 90$ K is reached at $\delta \approx 0.27$; different methods were used to achieve this optimum composition, including growth and post-annealing in atmospheres with different oxidation/reduction activity, classical electrochemical reduction, etc [2-3].

Here we present the use of solid electrolyte YSZ as a way to achieve an accurate control of the superconducting temperature of YBCO. Growing thin films of YBCO at 10 mTorr of oxygen on (001) YSZ substrates, produces non-supeconductign films with high crystalline quality. Then, applying an electric field in air, injects/removes O^{2-} ions from the YBCO film from/to the YSZ reservoir, across the YBCO/YSZ interface. We show that by controlling the charge injected to/from the film, we can accurately control the oxygen content in the sample, transforming the non-superconducting phase into a superconducting thin film.

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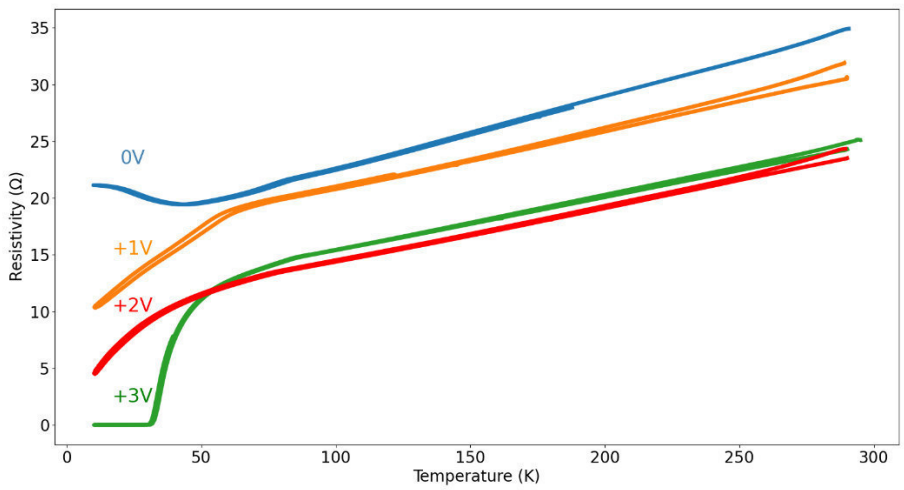

Figure 1: Resistivity measurements against temperature on YBCO films for different applied electric fields across the YBCO/YSZ interface.

What drives the metal-insulator transition in VO_2?

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Metal-Insulator transitions are among the most active topics in condensed matter physics. The electronic transition takes place concomitantly with a structural transition, making it hard to disentangle the underlying mechanism. Two scenarios are possible and are at the core of an unresolved and longstanding debate: i) the transition is driven by purely electronic interactions or ii) it is driven by electron-phonon coupling. Using VO_2 as case study, we investigated the nature of electronic and structural fluctuations within the metallic state by measuring resonant and off-resonance diffuse scattering. We found strong, pre-transitional structural fluctuations above Tc, which are closely followed by the d-electron charge distribution. Our results strongly support electron-phonon coupling as the driver of the metal-insulator transition in VO_2.

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Unveiling the Mechanism of Phonon-Polariton Damping in α-MoO_3

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Phonon polaritons (PhPs) – light coupled to lattice vibrations – in the highly anisotropic polar van der Waals material molybdenum trioxide (α-MoO_3) have recently been a subject of intense research due to their extreme subwavelength field confinement, directional propagation and unprecedented low losses [1]. However, most previous studies were focused on exploiting the squeezing and steering capabilities of α-MoO_3 PhPs for controlling light at the nanoscale, without inquiring much into the dominant microscopic mechanism that determines their long lifetimes, key for their implementation in nanophotonic applications. We explore the fundamental mechanisms of PhP damping in α-MoO_3 by combining *ab initio* density functional perturbation theory (DFPT) calculations with experimental scattering-type scanning near-field optical microscopy (s-SNOM) and conventional Fourier-transform infrared (FTIR) spectroscopy measurements over a wide temperature range (8 – 300 K). The excellent agreement between the experiment and the theory in reproducing the polaritonic lifetime, achieved without involving any adjustable parameters, allows us to identify third-order anharmonic phonon-phonon scattering as the main damping mechanism of α-MoO_3 PhPs. These results thus unveil the fundamental limits of low-loss PhPs, critical for validating their implementation into nanophotonic devices [2].

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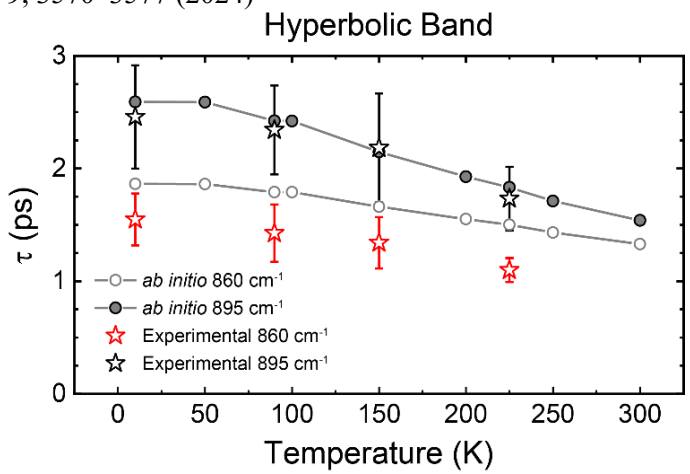

Figure 1: Temperature Dependence of the PhPs Lifetimes in α-MoO_3. Theoretical (circles) and experimental (star symbols) PhPs lifetimes for a 104nm-thick α-MoO_3 flake as a function of temperature for the hyperbolic RB (ω_0 = 860 cm^{-1} and ω_0 = 895 cm^{-1}). Gray straight lines are guides to the eye.

Spin wave stiffness constant in nanometric Fe80B20 films prepared by laser ablation

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Amorphous $Fe_{80}B_{20}$ thin films have been prepared by pulsed laser ablation under different Ar atmospheres. The morphological, chemical and magnetic properties have been studied as a function of the Ar pressure during growth. We report on the changes that the magnetic behaviour endures due to the surface nano-structuration of the films induced by the Ar-assisted growth, as demonstrated by means of AFM and XPS (Figure 1 a-b). Our study evidences that the surface nano-structuration of the films leads to an abrupt increase in coercivity and a loss of uniaxial anisotropy when compared to reference samples grown under ultra-high vacuum conditions as measured by tranverse-MOKE (Figure 1 c).

The high frequency dynamics was measured from the temperature variation of the high magnetic field magnetization ($2\ T < \mu_0 H < 7\ T$) by means of a SQUID magnetometer. The approach to saturation behavior was describable at temperatures above 50 K by means of the expression $M(H) = M(0)(1 - a/H - b/H^2) + cH$ [1] to which our data were fitted with a regression coefficient r^2 better than 0.9998. From those fits we present the temperature dependence of the spontaneous magnetization, M (0, T), which was analyzed in terms of the Bloch, spin waves excitation laws, considering both a $T^{3/2}$ term and the combination of a $T^{3/2}$ term and a $T^{5/2}$ one [2]. Also, and trying to ascertain the possible occurrence of the short-wavelength excitations known as Stoner (quasi)particles, our data for the temperature variation of the spontaneous magnetization of the amorphous $Fe_{80}B_{20}$ films was fitted to the thermal demagnetization laws predicted for a strong and a weak ferromagnet, respectively [2].

From our data we can conclude that up to ca. 140 K, the excitation of low energy, Bloch-type spin waves describes adequately the experimental results. This allowed us to evaluate [2] the spin waves stiffness constant (D) of our samples as a function of the chamber pressure during growth, obtaining larger stiffness constant and average mean square of the exchange interaction ($\langle r^2 \rangle$) values for the higher Ar pressures/rougher surfaces (Figure 1d).

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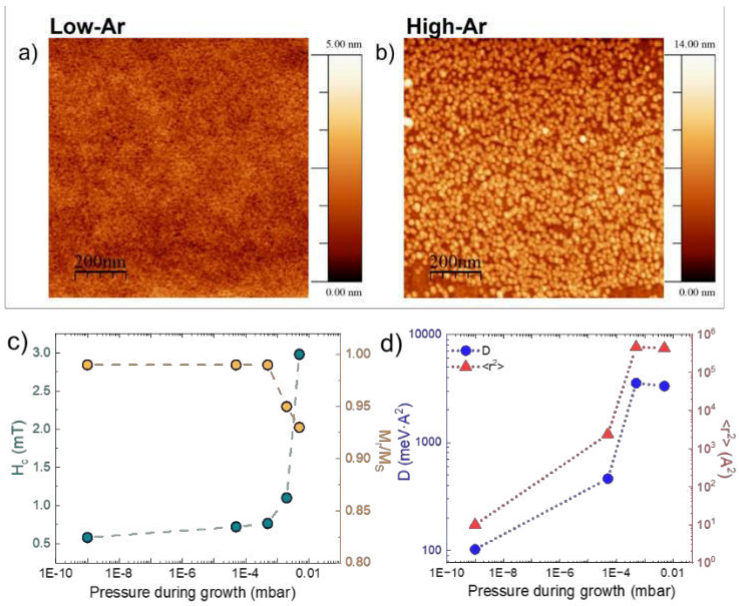

Figure 1: AFM micrographs depicting a low roughness film a) and a nanostrucutured surface b), evolution of Hc and Mr/Ms as a function of pressure during growth and d) D and $\langle r^2 \rangle$ dependency with growth pressure.

EXTENDING CONDUCTANCE MEASUREMENT RANGE IN MOLECULAR ELECTRONICS USING A CUSTOM LOGARITHMIC AMPLIFIER

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According to Landauer's formalism, the conductance G in atomic and molecular-sized contacts can be expressed as $G = G_0 \sum T$, where T represents the probability of electron transmission at the Fermi energy. In a single atomic gold contact, the transmission is typically close to one, resulting in a conductance of one quantum of conductance, $G_0 = \frac{2e^2}{h}$. However, for molecular contacts, the transmission probability is generally several orders of magnitude lower than one.

In this work, we used a Mechanically Controllable Break Junction (MCBJ) to create atomic-sized contacts under ambient conditions. To measure the current passing through these atomic junctions, we utilized a linear I-V amplifier (FEMTO DCPA 200) and a home-made logarithmic I-V amplifier.
As first result, we present the design of the logarithmic amplifier [1], as well as the external electronic circuits used to analyze the influence of the logarithmic amplifier's differential input current on the measurement range.
As second one, we compare the results from the logarithmic amplifier with those obtained from the linear amplifier. Our primary finding is that the custom logarithmic amplifier extends the measurable current range by two orders of magnitude compared to the linear amplifier (see Figure 1).
Finally, we investigated electronic transport in gold atomic and molecular junctions, including glycerin, dichloromethane (DCM), and trichloromethane (TCM).
In summary, we identified optimal differential current parameters that enable measurements in the range of [10^1–10^{-4}] G_0. Using this custom logarithmic amplifier, we characterized different molecular junctions and extended the measurable conductance range compared to a linear amplifier.
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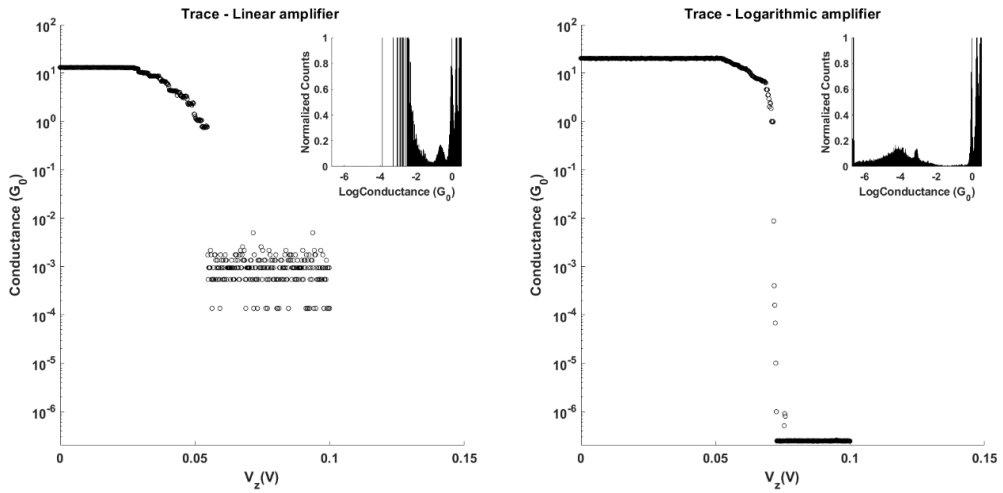

Figure 1: Traces and histograms (logarithmic scale). Comparison of the linear and logarithmic amplifiers.

Synthesis and characterization of a non-planar cyclophenylene on Au(111)

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Cyclophenylenes, i.e., macrocycles composed of linked benzene rings, have attracted intensive interest because of their appealing structures and potential applications [1] derived from their optoelectronic properties [2], their rich size-dependent supramolecular chemistry and their potential as platforms to build molecular nanobelts or carbon nanotubes.

The recently developed field of on-surface synthesis (OSS) offers unprecedented opportunities for the fabrication of various novel cyclophenylenes with intriguing physical-chemical properties. The metal surface plays a vital role in facilitating reactions of synthetic interest, including bond-forming and bond-breaking reactions, as well as stabilizing species that would otherwise be unstable. In addition, OSS alleviates synthetic limitations by eliminating the need for solubility. The two-dimensional (2D) confinement of a solid surface also impacts the OSS reactions generally promoting planar product structures.

In this work, we report the OSS of a non-planar Au-coordinated cyclophenylene, containing four meta- and two para- connections, on a Au(111) surface, by undergoing hierarchical, metal-assisted double Ullmann coupling of a 1,10-dibrominated angular phenylene, and subsequent selective C–C bond cleavage of the four-membered rings in the resulting phenylene dimer. The chemical structure was characterized by bond-resolving (BR) STM and further supported by STS and DFT. This study offers the first approach for the synthesis of non-planar cyclophenylenes on surfaces.

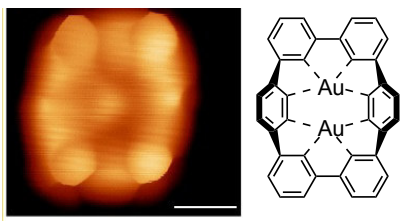

Figure 1: Bond resolving STM image (constant height, 5 mV) of the construction of a gold-complexed cyclophenylene on Au (111). Scale bar 4 Å

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Observation of the orbital Hall effect by electrical orbital injection

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Orbitronics is a new field of electronics which aims at exploiting the orbital angular momentum of the electron, similar to what spintronics does with the spin angular momentum. When an electric field is applied to a material, electrons with opposite spins are deflected to opposite directions creating a transverse spin current, an effect known as the spin Hall effect (SHE). Analogously, electrons with opposite orbital angular momentum will also be deflected to opposite directions creating a transverse orbital current, known as the orbital Hall effect (OHE). Remarkably, spin-orbit coupling (SOC) is needed for the SHE but not for the OHE. Theoretical predictions show that the generated orbital current by the OHE can be much larger than the SHE-induced spin current [1], especially in 3d transition metals such as V, Cr and Mn [2]. However, orbital current cannot directly exert a torque on ferromagnets because the orbital magnetization is usually negligible, thus requiring a conversion process from orbital current to spin current in order to manipulate the magnetization. The best ferromagnetic candidate for orbitronics seems to be Ni, which has the largest SOC among the ferromagnetic 3d transition metals and, therefore, will give the possibility to create and detect orbital currents [3]. Experimentally, OHE has been measured with spin-orbit torque [4], spin pumping [5], MOKE [6] and Hanle magnetoresistance [7].

Here, we report the observation of OHE with a different approach, by electrical orbital injection. By using lateral T-shaped devices, we electrically inject spin/orbit currents from a ferromagnet (Py and Ni) into a SHE/OHE material such as Pt and Ta, which generates a transverse current, detected as an open-circuit voltage [8]. By combining these materials, we can disentangle the spin from the orbital origin of the measured voltage: For Py, the generated and detected currents are expected to be spin currents and, thus, the SHE of the Pt and Ta will be measured; for Ni, orbital currents play a relevant role, being the OHE of the materials the origin of the experimentally measured signals. Importantly, the spin Hall conductivity can be positive (Pt) or negative (Ta) whereas the orbital Hall conductivity is predicted to be positive for all transition metals. Therefore, for Ta we expect to have a sign change on the measured voltage signals when injecting the currents with Py or with Ni (because the most efficient effect will be the SHE and the OHE, respectively), which we confirm experimentally. 3D simulations of the devices have been performed to discard the possible contributions of other effects to the measured signal, such the anomalous Hall effect of the ferromagnets. Our results introduce a new technique to study orbit currents by electrical orbital injection.

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Exploring Size-Dependent Magnetic Properties of highly pure NiO Nanoparticles

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Nickel oxide NiO nanoparticles (NP) have been drawing much attention due to their distinctive magnetic properties and p-type semiconductor behavior, which are leveraged in electronics, catalysis, and antimicrobial applications [1],[2]. From a fundamental perspective, the cause of the weakly ferrimagnetism in these systems is still not fully understood, nonetheless the difficulty entailed in obtaining a pure NiO phase further prevents meaningful advancements [3],[4]. This work sheds some light on this phenomenology by studying the influence of crystal size and Ni composition on the magnetic properties of three samples of NiO NPs with sizes of 6, 20, and 30 nm prepared by two-step chemical approaches. Structural analysis confirms the high crystalline quality of the particles, regardless of the particle size. Besides, single particle HAADF-EELS measurements show uniform composition of each sample, revealing the existence of a slight oxygen surplus due to finite-size effects. Magnetic properties are size-dependent, including weak superparamagnetism of the smallest NP, while the largest ones show features closer to the bulk counterparts, such as low values of both remnant magnetization and coercivity, with negligible shifts of the hysteresis loop and minimal coercivity after field cooling (see Figure 1). These size-dependent behavior is due to surface and structural modifications, particularly in the smallest NP. In addition, X-ray magnetic linear dichroism (XMLD) imaging and spectroscopy are being conducted to provide additional insights into the antiferromagnetic spin arrangement in these nanostructures. These findings contribute to improving our understanding of size-related phenomena in nanoscale antiferromagnetic materials.

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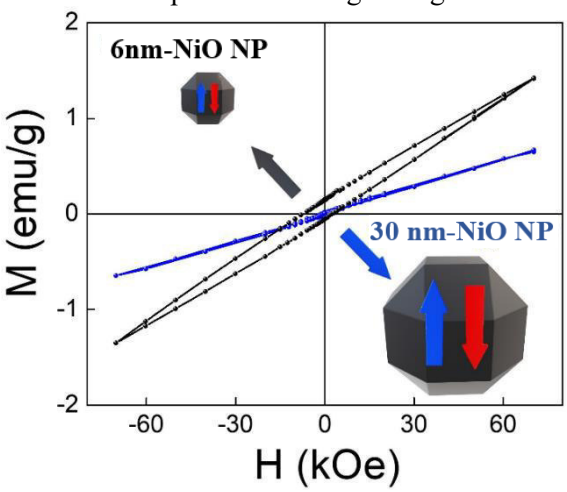

Figure 1. Comparison between hysteresis loops at 5K for NiO NP with mean sizes of 6 (gray dots) and 30 nm (blue dots) with a maximum field of H= 70 kOe.

Unveiling exciton formation at early stages in bulk BiI_3 via tr-ARPES

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Exciton physics governs the optical properties of semiconductors, so a detailed and comprehensive description of the origin of excitons as well as their relaxation pathways is vital for advancing this field. The dynamics of exciton formation and relaxation are highly dependent on the photoexcitation conditions. When the pump energy exceeds the fundamental bandgap, quasi-free charge carriers are generated in the conduction band. Consequently, these carriers bind into excitons due to the weakly screened Coulomb attraction between electrons and holes. The relaxation process that follows typically involves a cascade through numerous lower-energy excitonic states, whose intricate and ultrafast dynamics have remained challenging to resolve.

In this work, we investigate the formation of excitons and their cascade relaxation by reconstructing the time-resolved angle-resolved photoemission spectroscopy (tr-ARPES) signal. To this end, we use a DFT+GW+BSE scheme as a starting point and we compute a broad excitonic spectrum including states deep into the continuum of the electron-hole Hamiltonian, to capture the signal due to both bound and unbound excited states [1,2]. To model the tr-ARPES signal, we introduce a time-dependent distribution function, initially represented by a Gaussian wave-packet centered at the pump energy (t = 0). This evolves into a Boltzmann distribution as the system progressively relaxes toward the minimum of the exciton dispersion. For comparison with experiments, we simplify the analysis by projecting the bulk momentum dispersion onto the surface.

Using the bulk semiconductor BiI_3 as a playground, we explore the exciton dynamics at different energy ranges and compare our theoretical findings with experimental results. In such a way, combining experimental and theoretical efforts, we track the exciton formation and the subsequent relaxation process, offering crucial insights into the complete exciton relaxation dynamics and their potential applications in ultrafast semiconductor devices.

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Experimental characterization of spin-magnon interactions

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Single-molecule magnets like GdW_{10} have emerged as promising candidates for **spin qudits**, the fundamental units of quantum processors. However, their *interaction with superconducting resonators*, the standard components in quantum information systems, is often *inefficient* due to the large mode volumes of the electromagnetic fields in these cavities. To overcome this limitation, **magnons** (the quanta of spin waves) have been proposed as *alternatives to microwave photons*, acting as mediators and sensors for interactions between spin qubits.
Here, we study the spin-magnon interactions between spin transitions in GdW_{10} and magnons in the antiferromagnet CrSBr, finding evidence of strong coupling between these excitations.

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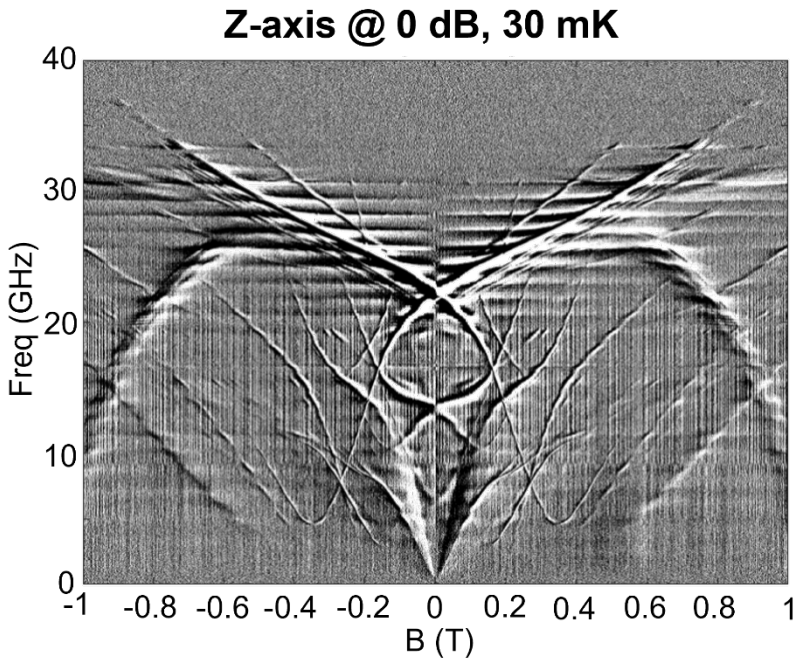

Figure 1: Experimental measurement of the GdW10 interaction with the AFM.

Unidirectional Ray Polaritons in Twisted Asymmetric Stacks

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The emergence of a vast repository of van der Waals (vdW) materials supporting polaritons – light coupled to matter excitations – offers a plethora of different possibilities to tailor electromagnetic waves at the subwavelength-scale [1]. In particular, the development of twistoptics – the study of the optical properties of twisted stacks of vdW materials – allows the directional propagation of phonon polaritons (PhPs) along a single spatial direction, which has been coined as canalization [2,3]. Here we demonstrate a complementary type of nanoscale unidirectional propagation that naturally emerges thanks to twistoptics: unidirectional ray polaritons (URPs). This natural phenomenon arises in two types of twisted hyperbolic stacks: homostructures of α-MoO_3 and heterostructures of α-MoO_3 and β-Ga_2O_3, each with very different thicknesses of its constituents. URPs are characterized by the absence of diffraction and the presence of a single phase of the propagating field. Importantly, we demonstrate that this ray behavior can be tuned by means of both relative twist angle and illumination frequency variations. Additionally, an unprecedented "pinwheel-like" propagation emerges at specific twist angles of the homostructure. We show that URPs emerge due to the twist between asymmetrically stacked biaxial slabs, while the shear effect in monoclinic β-Ga_2O_3 is of minor importance. Our findings demonstrate a natural way to excite unidirectional ray PhPs and offer a unique platform for controlling the propagation of PhPs at the nanoscale with many potential applications like nanoimaging, (bio)-sensing or polaritonic thermal management.

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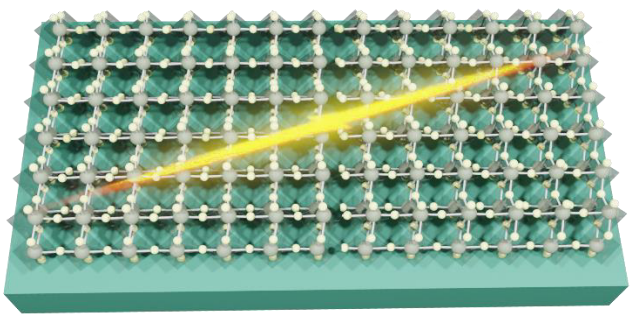

Figure 1: Schematic of the unidirectional ray propagation of polaritons in a twisted homostructure biaxial stack made of two asymmetric α-MoO_3 layers.

TaTe2: A vast landscape of structural and electronic properties

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Transition metal dichalcogenides feature a wide range of physical and electronic properties that range from semiconducting to metallic. Moreover, they can host many-body correlated states such as superconducting phases, Mott insulator phases and charge density waves (CDW) which have brought a lot of excitement to the scientific community.
The most common polymorph of group VI TMDC is the 2H since it is the most stable one. Despite that, other structures can be found in nature, and thanks to the development of new growing techniques, experimentalists can grow large samples of these structures.
Although sulphur and selenium compounds have been thoroughly studied in the past years, tellurium based have been less studied. Interestingly, group V Te-based single-layers are catching attention lately since the absence of Te-Te interlayer interactions changes the electron transfer compared to the bulk or multi-layer cases and new structures and electronic properties can be found [1,2].

In this work [3], we study the structural and electronic properties of single-layer TaTe2 using first-principles calculations [4]. We find that it presents a large number of possible structures which are very close in energy. We study in detail the formation of these structures and give a possible mechanism for their formation. Moreover, we study their electronic properties in a comprehensive way.

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Scattering theory of thermal and bipolar thermoelectric diodes

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Modern electronic devices are currently operated at the nanoscale regime, where overheating becomes a problem. Controlling the undesired heat flows in a useful manner is another less explored way of improving its performance. For this, efficient thermal diodes need to be designed [1]. We investigate the minimal requirements that induce a nonreciprocal response to temperature differences in a quantum electronic conductor. We identify two distinct mechanisms, namely inelastic scattering and screening, to locally affect the internal temperature and potential of the device, leading to thermal and thermoelectric rectification effects in the presence of an inversion symmetry breaking. We propose resonant tunnelling samples to efficiently exploit these effects, and find configurations acting as bipolar thermoelectric diodes whose currents flows in the same direction irrespective of the sign of the temperature difference, a case of antireciprocity [2].

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Morphology and dynamics of domains and domain walls through asymmetric hole density-graduated 2D-arrays

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The manipulation of magnetic domain walls (DW) opens novel strategies to design spintronic devices with potential high impact in data storage, nonvolatile logic, and magnonic applications, which may include reservoir/neuromorphic computing, data storage, and sensors among others. For the implementation of several of those applications, asymmetric DW motion controlled by electrical voltages or currents and magnetic fields is needed. The prototypical asymmetric DW motion mechanism is the so-called ratchet effect, which consists of an easier propagation of domain walls in one direction than in the other thanks to an asymmetric pinning potential.

Different mechanisms have been demonstrated to favour ratchet effect, being patterning into an asymmetric configuration one of the preferred options. 2D micropatterned arrays of asymmetric holes (2D-AAH) on magnetic thin films have been reported to show ratchet effect. In the large size regime, the DWs have been approximated as elastic lines of zero width that can distort (i.e., bend) throughout their length when pushed by a magnetic field. This bending was attributed to be the main factor determining DW propagation. However, in 2D-AAH, the optimum hole size for the occurrence of ratchet effects is twice the DW width. Therefore, when matching the hole size to the DW width of the particular magnetic thin film used, the DWs cannot be considered 1D objects and their morphologies play a very important role. Additionally, in regular arrays of asymmetric holes the very fine control of the ratchet effect can be challenging.

In order to tackle these two issues, we have fabricated 2D-AAH on $Co_{86}Zr_{14}$ with different hole shapes (triangles and arrows), sizes (from 2.5 to 6 μm), and pattern structure (regular and with different gradients in density of holes in the array) and study them combining Kerr microscopy and X-Ray PhotoEmission Electron Microscopy [1, 2]. The gradient strategy has allowed us superior control over the movement of the DWs along the array, enabling us to write various and specific magnetization states, which can be observed as a whole in the Kerr microscope due to the large field of view of this technique. A set of tools using advanced image processing techniques has been developed to analyze the KERR microscopy images, enabling fast processing of several tens of hysteresis loops across twenty arrays with varying configurations. On the other hand, zoomed-up images taken with the PEEM at ALBA synchrotron have revealed a much more complex magnetization domain and DW configuration than predicted.

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Enhancement of the thermoelectric figure of merit by combination of doping and grain boundary engineering in (Ti,Zr,Hf)Ni(Sn,Sb)

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Thermoelectric (TE) materials have garnered significant attention in recent years due to their unique ability to directly convert heat into electricity and vice versa, offering promising solutions for sustainable energy applications [1]. The performance of TE materials is commonly evaluated using the figure of merit, ZT, defined as $ZT = (\sigma S^2/\kappa)T$, where S is the Seebeck coefficient, σ is the electrical conductivity, κ is the thermal conductivity, and T is the absolute temperature [2]. The thermoelectric performance of materials is strongly influenced by their microstructure and fabrication methods. In this context, single-phase (Ti,Zr,Hf)NiSn and $ZrNiSn_{1-x}Sb_x$ (x = 0.02 and 0.05) half-Heusler alloys were synthesized via spark plasma sintering (SPS) using mechanically milled powders with varying milling times, resulting in nanometric particle sizes. High-resolution synchrotron radiation X-ray powder diffraction confirmed that all the samples exhibited the expected MgAgAs-type crystalline structure (space group $F\bar{4}3m$) and retained their powder microstructure after the SPS process. TE measurements revealed that thermal transport in the samples was dominated by phonon-phonon scattering, while the primary electrical transport mechanism was alloy scattering [3,4]. Moreover, excessive milling times (beyond 5 hours) were found to degrade thermoelectric properties instead of reducing thermal conductivity. As shown in **Fig. 1**, optimal Sb doping (x = 0.02) in 5 hours-milled alloys significantly enhanced the thermoelectric performance, achieving ZT values of approximately 0.6 at 600 K, which doubles the value obtained for undoped samples and improves that for unmilled alloys by a 50% [5].

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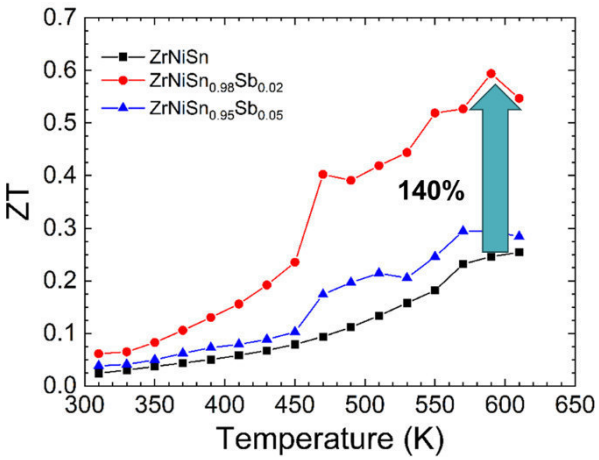

Figure 1: Temperature dependence of ZT for $ZrNiSn_{1-x}Sb_x$ (x = 0, 0.02 and 0.05) samples.

Room-Temperature Plasmon-Resonant Terahertz Graphene Photodetectors

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Frequency-selective or even frequency-tunable Terahertz (THz) photodevices are critical components for many technological applications that require nanoscale manipulation, control and confinement of light. Within this context, gate-tunable phototransistors based on plasmonic resonances are often regarded as the most promising devices for frequency-selective detection of THz fields [1]. The exploitation of constructive interference of plasma waves in such detectors not only promises frequency selectivity, but also a pronounced sensitivity enhancement at the target frequencies. However, clear signatures of plasmon-assisted resonances in THz detectors have been only revealed at cryogenic temperatures and so far, have remained unobserved at application-relevant room-temperature conditions [2]. Here [3], we demonstrate the sought-after room-temperature resonant photodetection of THz radiation (Figure 1) in short-channel gated photodetectors made from high-quality single-layer graphene. The survival of this intriguing resonant regime at room-temperature ultimately relies on the weak intrinsic electron-phonon scattering in graphene, which avoids the damping of plasma waves.

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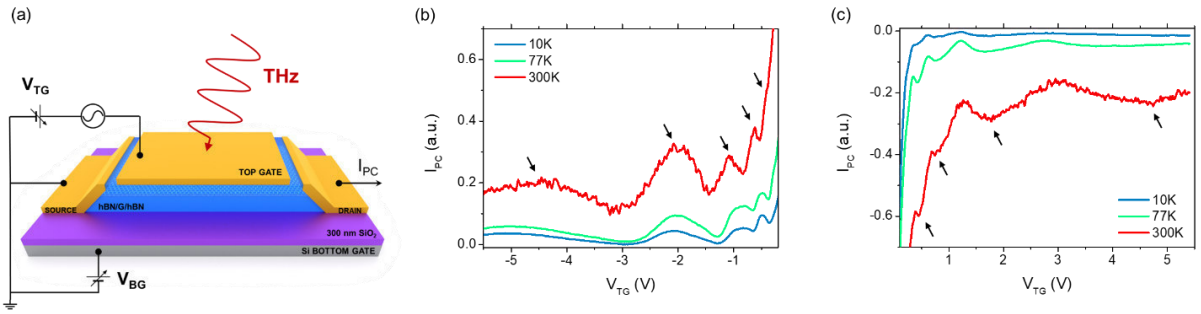

Figure 1. (a) Schematic 3D view of the zero-bias photocurrent measurements of the graphene plasmonic photodetector. Zero-bias normalized photocurrent for three selected temperatures of 10 K, 77K and 300K (room temperature) for negative **(b)** and positive **(c)** top gate potentials for an incident radiation of 2.5 THz. For easier visualization, the temperature dependence photocurrent shown in panels **(b)-(c)** are normalized with respect to the maximum near the charge neutrality point.

Exploring Electron Transport in Tryptophan Zipper-Based Peptide Assemblies

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In nature, materials like electrically conductive proteins facilitate long-range electron transfer, enabling intracellular communication in microorganisms such as the sedimentary bacterium Geobacter sulfurreducens, where this conduction occurs through its pili.[1] It has been proposed that the conductivity of these natural nanofibers depends on electronic delocalization and charge transfer between adjacent aromatic residues through π-π stacking interactions.[2] Inspired by this model, conductive nanofibers based on the self-assembly of rationally designed peptide sequences have been developed to achieve similar conductive properties.[3]

Coiled coils (CCs) are highly versatile oligomerization motifs that have demonstrated their potential for the development of de novo electroactive systems and conductive materials. Based on these precedents, modified tryptophan zipper pentamers have been designed integrating non-natural benzothiophen derivatives in place of the natural tryptophan side chains. In this study, the conductivity of self-assembled nanofibers from these Tryptophan Zipper pentapeptides was characterized. Samples were deposited on SiO_2/Si substrates with gold interdigitated electrodes, to explore their properties as biocompatible conductive materials. Electrical characterization was performed through current-voltage (I-V) and current-time (I-t) measurements under ambient conditions, followed by testing under vacuum to minimize contributions from redox processes and residual ionic conduction.

The I-V characteristics display a linear relationship between current and applied voltage, with a slight hysteresis attributed to capacitive effects at the material-electrode interface. Additionally, the increase in conductivity with temperature suggests a thermally activated transport mechanism, consistent with a hopping process facilitated by π-π stacking of aromatic residues in the structure. Steady-state I-t measurements indicated ohmic behavior, with a conductivity of 1.6×10^{-10} S/cm under vacuum. These results suggest that Tryptophan Zipper fibers exhibit enhanced electronic transport, positioning them as potential candidates for sustainable and biocompatible electronic device applications.

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Perfect Absorption by Overlapping Electric and Magnetic Lattice Resonances

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The arrangement of metallic nanoparticles in two-dimensional, periodic systems gives rise to collective modes known as lattice resonances [1]. Resulting from the coherent interaction between the constituents of the array, these resonances are distinguished by extremely narrow line profiles, making them highly suitable for various photonic applications. Fields such as photodetection and photocatalysis, which demand efficient light absorption, could benefit greatly from lattice resonances; however, 2D arrays with dipoles of a single nature face a fundamental limit, absorbing only up to half of the incident power [2]. One approach to overcome this limit is by spectrally overlapping two resonances associated with multipoles of different parity, with most past works focusing on the overlap between a collective lattice resonance and the plasmon resonance of a single particle [3]. Nevertheless, this approach results in low quality factors due to the broad profile of the plasmon mode involved, and makes it very challenging to freely modify the wavelength at which the overlap occurs.

In this work, we propose a novel method to attain perfect absorption in planar arrays of nanostructures, which solves the deficiencies of traditional approaches [4]. Our strategy consists on the overlap between two different lattice resonances, one with electric dipolar (ED-LR) and the other with magnetic dipolar (MD-LR) character. We employ a bipartite rectangular array, containing a metallic (Au) and a dielectric (Si) nanoparticle within the unit cell (Fig. 1a). Their placement is chosen to make the electric-magnetic interaction between the nanostructures vanish, allowing for independent tuning of the ED-LR and MD-LR. By properly selecting the array periods, we achieve an overlap between the electric and magnetic lattice resonances, and demonstrate that the system reaches absorbance values up to 0.998 and quality factors over 2000 (Fig. 1b). Additionally, we show how each nanoparticle contributes to the total absorbance, and illustrate that this approach is highly sensitive to the polarization of the incident electromagnetic field. Consequently, this design also serves as an ideal narrowband linear polarizer, allowing light transmission for one polarization while blocking it for the orthogonal one (Fig. 1c).

The results of this work pave the way towards the design of arrays sustaining lattice resonances that are capable of producing perfect absorption, expanding the potential of these modes towards new photonic technologies.

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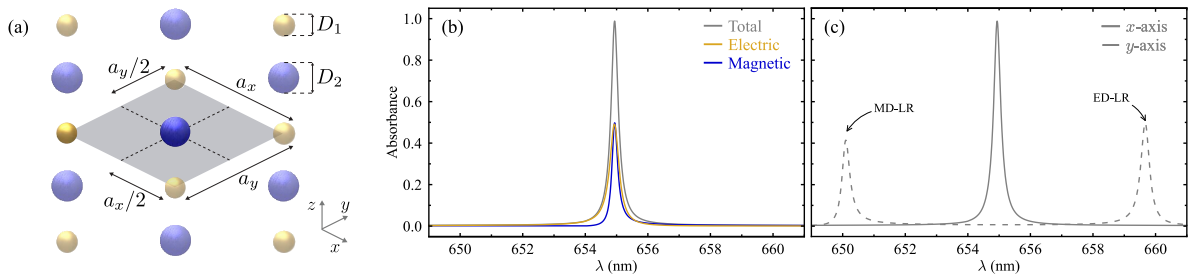

Figure 1: (a) Schematics of the bipartite rectangular array under consideration. (b) Absorbance spectra of the bipartite array (gray curve), together with the explicit contributions of the electric (yellow curve) and magnetic (blue curve) dipoles. The peak absorbance is 0.998 and the Q-factor equals 2400. (c) Absorbance spectra of the system for an x- (solid curve) or y-polarization (dashed curve) of the incident electric field.

Enantiosensitive growth dynamics of chiral molecules on magnetized substrates: diffusion and nucleation

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The recent demonstration of the existence of an intimate relationship between the chiral structure of some materials and the spin polarization of electrons transmitted through them, what has been called the chirality-induced spin selectivity (CISS) effect, is sparking interest in many related phenomena. One of the most notorious is the possibility of using magnetic materials to apply enantioselective interactions on chiral molecules and chemical reactions involving them.

In this work X ray photoelectron spectroscopy (XPS) has been used to characterize the adsorption and growth kinetics of enantiopure organic molecules on magnetic (Co) and non-magnetic (Cu) substrates. While on this latter no significant enantiosensitive effects are found, on spin-polarized, in-plane magnetized Co surfaces the two enantiomers have been found to deposit differently. [1] The observed effects have been interpreted as the result of one of the enantiomers being adsorbed in a transient, weakly-bound physisorbed-like state with higher mobility due to limited, spin-selective charge transfer between it and the substrate. The study of these phenomena can lead to broad-reaching applications from spintronics to asymmetric catalysis, as well as provide insight into the fundamental mechanisms responsible for the CISS effect.

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Figures

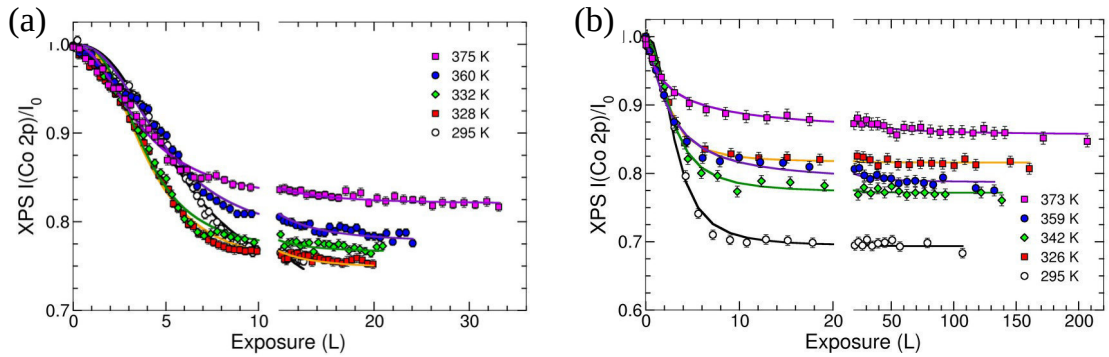

Figure 1: XPS uptake curves showing the attenuation of an in-plane magnetized Co film upon absorption of homochiral (a) (R,R)-DPEDA and (b) (S,S)-DPEDA. The solid lines are fits with Sips isotherms.

Excitons in nonlinear optical responses: shift current in MoS_2 monolayers

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It is well-known that exciton effects are determinant to understand the optical absorption spectrum of low-dimensional materials. However, the role of excitons in nonlinear optical responses has been much less investigated at an experimental level. Additionally, computational methods to calculate nonlinear conductivities in real materials are still not widespread, particularly taking into account excitonic interactions. We present a methodology to calculate the excitonic second-order optical responses in 2D materials relying on: (i) ab initio tight-binding Hamiltonians obtained by Wannier interpolation and (ii) the Bethe-Salpeter equation with effective electron-hole interactions. Here, in particular, we explore the role of excitons in the shift current of monolayer materials. Focusing on MoS_2 and GeS monolayer systems, our results show that 2p-like excitons, which are dark in the linear response regime, yield a contribution to the photocurrent comparable to that of 1s-like excitons. Under radiation with intensity ~10^4 W/cm^2, the excitonic theory predicts in-gap photogalvanic currents of almost ~10 nA in sufficiently clean samples, which is typically one order of magnitude higher than the value predicted by independent-particle theory near the band edge.

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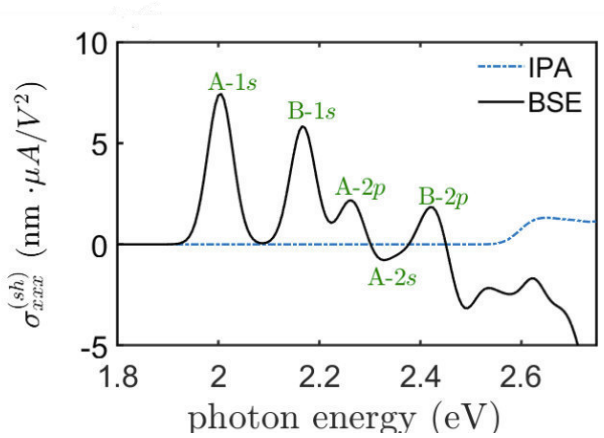

Figure 1: Frequency-dependent shift conductivity of monolayer MoS2 calculated in the independent particle approximation (DFT) approximation and including exciton effects.

Exploring the Geometry of Three-Atom-Thick Structures in Stretched Gold Contacts Through Electronic Transport Studie

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Abstract

The atomic-level geometry of electrodes is crucial in molecular electronics, but few techniques can identify electrode geometry at this scale [1]. Previous theoretical studies and experiments at cryogenic temperatures using mechanically controllable break junctions (MCBJ) and scanning tunneling microscope in break junction's configuration (STM-BJ) revealed that gold can form one- and two-atom-thick structures [2-5].

In this study, we combine electronic transport experiments through BJ with Molecular Dynamics (MD) simulations and Density Functional Theory (DFT) to investigate the geometry of gold atomic contacts. We compare STM-BJ results at 4 K with MCBJ results at 300 K, finding that the 2D conductance histograms are remarkably similar at both temperatures, including conductance values around 2.5 G_0, value that up to now didn't have a defined structure attributed. Using MD and DFT, we have correlated this conductance with specific atomic configurations, and we have observed how three-atom-thick structures evolve into one- and two-atom-thick when is stretched [5] (see Figure 1d).

Additionally, by calibrating our system *in situ* at room temperature, we introduced a novel statistical analysis to understand the sharpening of the electrode stretching. Moreover, we have extended this analysis to Sn atomic-sized contacts.

In summary, we have identified three-atom-thick gold structures and their conductance, developed a new calibration method, and introduced a technique to analyze electrode sharpness even at room temperature.

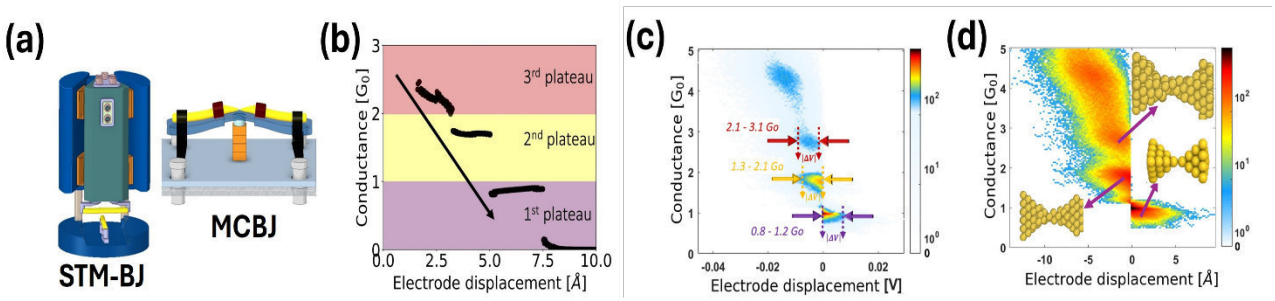

Figure 1: (a) shows an illustration of the STM and MCBJ experimental setups. (b) displays a rupture trace featuring three distinct plateaus. (c) presents a two-dimensional plot used for calibration. (d) shows a calibrated density plot of gold rupture traces, highlighting each structure.

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Hydrodynamic electron flow in antidot graphene superlattices

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In most solids, electron transport is typically determined by sample geometry, electron-phonon interaction, and electron-impurity interaction, characterized by the inelastic mean free path (l_e). In such solids, electron-electron interactions, characterized by the elastic mean free path (l_{ee}), play a secondary role ($l_{ee} >> l_e$). However, recent progress in high-quality materials have facilitated the exploration of electrical transport in the hydrodynamic regime, where increasing *le* makes elastic interactions more significant. In this regime, Coulomb interactions drive electron motion from independent particles to collective motion of a viscous "electron fluid" [1, 2].

Above a certain temperature, hBN-encapsulated graphene can exhibit large *le*, greater than *lee*, making it an ideal candidate for the study of the hydrodynamic regime. Viscous electron flow in graphene exhibits exotic signatures such as superballistic conduction [3, 4]. To enhance these hydrodynamic effects, it is crucial to modify the geometry of the device. In this work, a novel antidot superlattice geometry was designed and fabricated in encapsulated graphene heterostructures. Three graphene superlattices with different hole diameters were tested (Fig. 1.a)) to create an inhomogeneous current flow and promote viscous electron transport. The measurements revealed an enhanced superballistic effect (Fig. 1.b)), demonstrating the effectiveness of the device geometry in altering the electron flow path. Additionally, for the first time, superballistic conduction was observed to show non-monotonic behavior as a function of the magnetic field, enabling in situ modulation of the collective behavior of electrons using both temperature and magnetic field. This research could open new avenues in electronics and nanotechnology by achieving more energy-efficient devices, reducing resistance by leveraging collective effects.

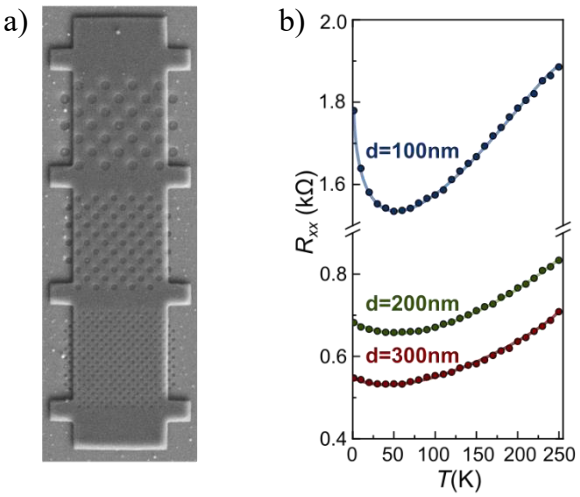

Figure 1. a) SEM images of the hole pattern.
b) Enhanced superballistic conduction

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Single defects in hBN coupled to Fabry-Pérot open cavities

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Most relevant quantum photonic applications require reliable single photon sources. They are crucial to deliver photonic qubits to be used in quantum information processing and computing, and they play an essential role in photon-based metrology and quantum communications, such as in the implementation of quantum key distribution protocols or the design of quantum repeaters for communication networks.

In this context, solid-state single photon sources are attracting interest, since their emission is remarkably more efficient than probabilistic sources (such as spontaneous parametric down conversion), [1] and can be integrated in compact devices and optical circuits. Furthermore, optical resonators can be coupled to these emitters generating ultrabright single photon emission. Fabry-Pérot cavities stand out as the leading structure to do so in different materials such as self-assembled quantum dots, [2] transition metal dichalcogenides monolayers [3] and defects in hexagonal Boron Nitride (hBN). [4]

In this work, we study the two main components of an ultrabright single photon source operated at room temperature: (1) single defects in hBN nanocrystals and (2) their reconfigurable coupling to an open Fabry-Pérot cavity. We characterize the spectral, polarization, and temporal properties of the single photon emission from these defects, and we also study the single photon character of the emission via second order correlation measurements. In Fig. 1 we show the typical spectrum of a single hBN defect under 450 and 532 nm off-resonant excitation and the saturation curve of the corresponding emitter (under 450 nm excitation). We also measure the open cavity quality factor (via resonant reflectivity) and provide preliminary results on defect coupling to the Fabry-Pérot resonator, showing Purcell enhancement of the emission.

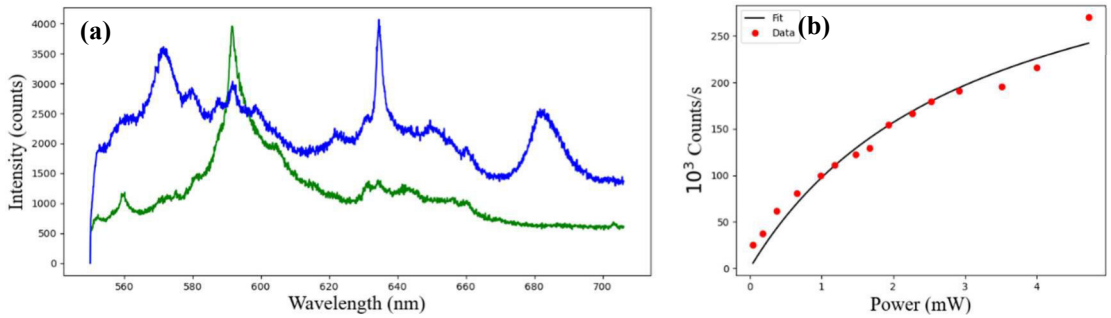

Figure 1: (a) Spectrum of emission of an hBN defect under 450 nm (blue) and 532nm (green) laser excitation and **(b)** saturation curve of the defect with ZPL at 635 nm under 450 nm excitation.

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Cavity optomechanics in MoS_2 micro-drum resonators

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The field of cavity optomechanics explores the interaction between electromagnetic radiation and nanomechanical motion. Optomechanical devices are commonly used for the optical detection of displacements in the nanometric range, small masses or forces [1], and also could serve as coherent light-matter interfaces, for applications in quantum information processing [2].

In this work we study the optomechanical properties of MoS2 micro-drum resonators. Radiation pressure and thermal effects of incoming laser light, can result in the coupling of optical cavity modes and mechanical drum modes, forcing the membrane to oscillate. The readout of the membrane response is performed via tracking the changes in the system's reflectivity. With the information gathered from this coupling, we can establish the position of the membrane which is comparable to a Fabry-Perot cavity.

By applying RF electric fields between the drumhead and the substrate in the range of 1 MHz up to 100 MHz, we can force electromechanical oscillations in the suspended region. In order to study the mechanical properties such as the pre-tension, the phase velocity in the material, and the resonant modes of the membrane we carry out several frequency sweeps of the system. This is done using a XYZ scanner to gather spatial information.

When the electrical driving and the optomechanical mode frequencies are close enough we observe and anticrossing behaviour characteristic of strongly coupled systems.

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a) b)

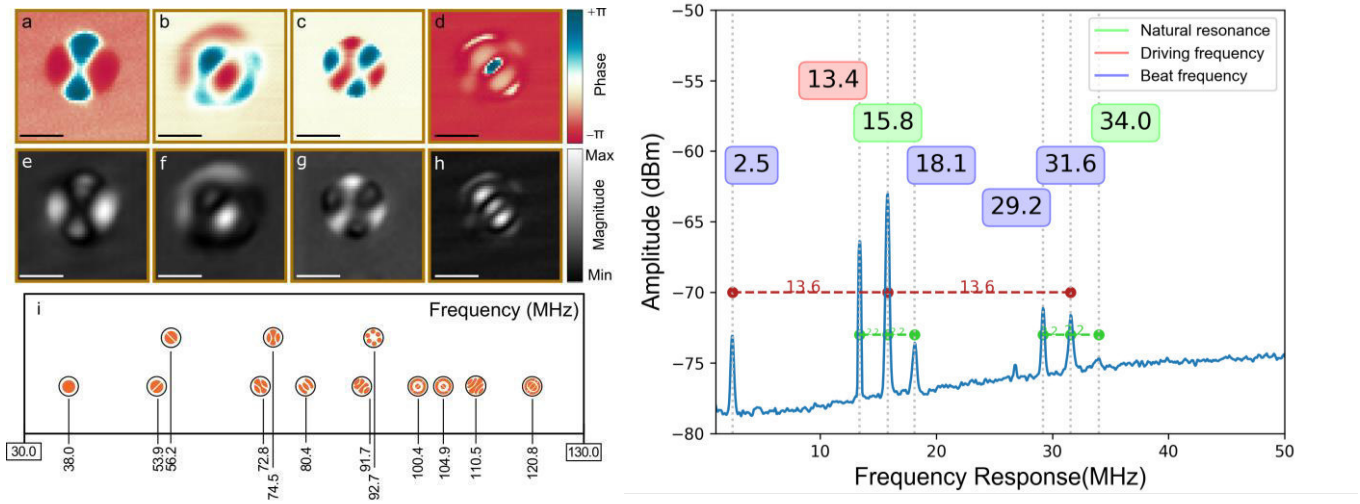

Figure 1: a) High resolution imaging of vibrational modes at 5 K. b) Spectrum analyzer response of an electrically forced resonator (driving frequency) and the lower and upper sidebands.

Revealing interfaces and buried inhomogeneities in van der Waals heterostructures by micro-reflectance mapping

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Van der Waals (vdW) heterostructures —freely stacked vdW single thin layers— allow for tailored varied physical phenomena [1, 2] that can be leveraged for electronic and optoelectronic devices, in which interfacial homogeneity is critical for optimum performance. In this study, we present an optical technique based on micro-reflectance measurements [3, 4] to assess the quality of interfaces in vdW heterostructures. We show micro-reflectance maps to be a useful tool to quickly and non-destructively study the topography of single thin layers and vdW heterostructures on large surfaces with lateral resolution of less than 1 micron. Furthermore, this method allows for optically observing the presence of trapped air between vdW flakes, whose thickness can be quantified by relating the experimental reflectance to that given by the isotropic transfer matrix (TM) model. To this end, the refractive index of widely used vdW materials h-BN and α-MoO_3 has been extracted also from micro-reflectance measurements [5]. Finally, a software application which will be soon openly available has been developed for in-situ determination of flake thicknesses as well as data post-treatment for air gap quantification.

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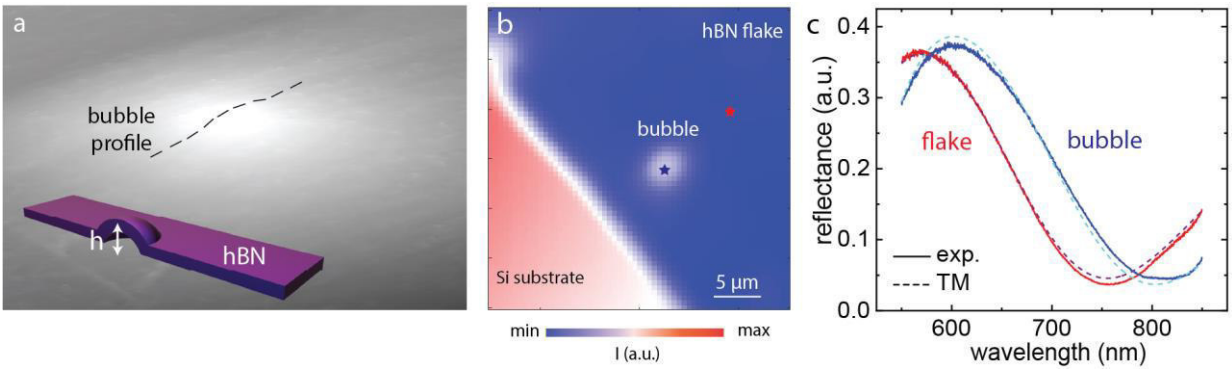

Figure 1: (a) Atomic force microscopy (AFM) map of a thin slab of hexagonal boron nitride (h-BN) in which a bubble is present. (b) Micro-reflectance map of the region, in which the bubble can be also clearly observed. (c) The fitting of the reflectance measured on both the thin slab and the bubble to the transfer matrix model (TMM) allows for extraction of the thickness of the thin slab and the height of the bubble.

Enhanced Magnetization by Oxygen Vacancies in $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ [001] Heterostructures

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O vacancies strongly influence the properties of complex oxides and give rise to novel and unexpected phenomena[1]. Here we combine *first-principles* density-functional theory (DFT) with high spatial resolution electron energy-loss spectroscopy and energy-loss magnetic chiral dichroism (EMCD) to show that O vacancies (O_{VAC}) control interface magnetism in $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ (LSMO/STO) heterostructures grown by high-pressure O_2 sputtering. EMCD measurements obtained at low temperature (<100K) are sensitive to the local magnetization with atomic resolution, revealing near the interface the formation of Ti magnetic moments and the increase of Mn magnetic moments. Comparison to the calculated electronic properties unambiguously demonstrates the O vacancy origin of the enhanced interface magnetism. The ideal interface - cleavage of bulk components -shows no charge transfer to the STO, while O vacancies induce finite occupancy of the Ti 3d ($3z^2$-r^2) orbitals and hole depletion at the Mn interface planes, enhancing interface magnetism. Our results indicate that the control of O vacancies is a promising approach to improve the magnetic properties [2] of LSMO/STO interfaces.

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Figures

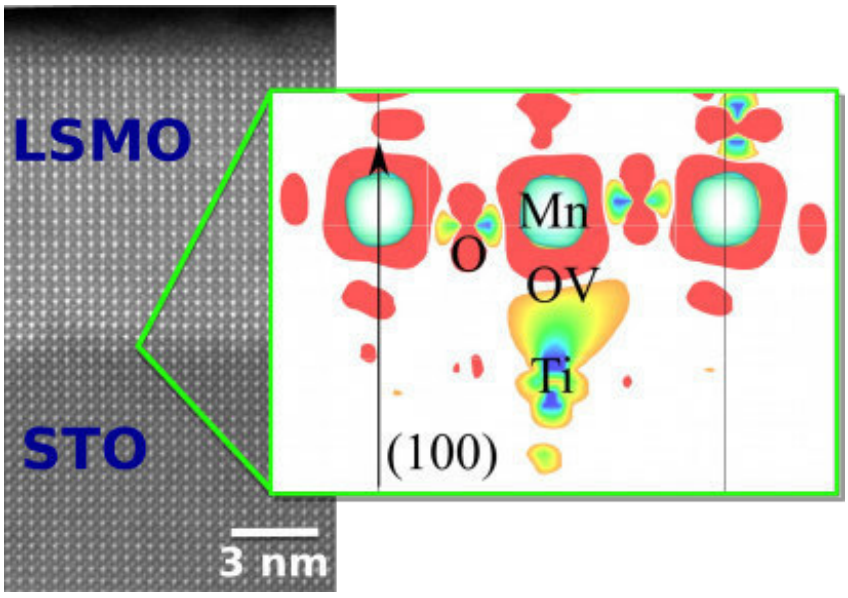

Figure 1: Scanning transmission electron microscopy image of a LSMO/STO interface including Ovac and the electronic cloud redistribution giving rise to an enhancement of the local magnetic moments.

Geometry-Enforced Topology in Amorphous Chiral Metals

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Beyond symmetry and topology, geometry has recently emerged as an additional knob for tuning the quantum properties of materials. One of the simplest manifestations of geometry is structural chirality, the notion that two 3D objects with the same symmetry can still be distinguished by their handedness. In structurally chiral crystals, there exists a profound link between lattice and wavefunction (topological) chirality, which gives rise to abundant chiral (Weyl) quasiparticles, extended Fermi-arc surface states [1], and enhanced photogalvanic effects. Despite numerous efforts, many aspects of strongly disordered Weyl semimetals remain puzzling, including whether they still carry quantized wavefunction topology that is bound by lattice fermion-doubling theorems [2], and hence exhibit topological surface Fermi arcs. In amorphous insulators with strong structural disorder, the average system symmetry [3] has been established as a tool for characterizing the bulk topology. In this work, we find that this approach overlooks a crucial additional ingredient: the average structural chirality. We find that in nonmagnetic amorphous metals, there exist generalizations of Kramers-Weyl, charge-two Weyl fermions, and spin-1 multifold, fermions that inherit their topological chirality from the system-averaged chirality of the position-space local lattice structure. We introduce an amorphous Wilson-loop numerical method to, for the first time, demonstrate the existence of Weyl fermions with quantized Berry curvature fluxes in fully disordered 3D metals. We further demonstrate the existence of vestigial surface Fermi arcs, which along with the chirality and spin textures of the bulk Weyl fermions, can be controlled via the average system chirality. Our work opens pathways to engineer geometry-enforced topological phenomena in non-crystalline materials and metamaterials.

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Tribological Properties of Mono and Few Layers of $MoTe_2$ by Frictional Force and Transverse Shear Microscopy

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Molybdenum ditelluride ($MoTe_2$), a transition metal dichalcogenide (TMD), exhibits both a metallic 1T' phase and a semiconducting 2H phase with a bandgap of 1.1 eV, making it a promising material for a variety of tribological, electronic, optoelectronic, and energy applications [1,2]. TMDs, including $MoTe_2$, have attracted significant interest in tribology due to their outstanding tribological properties. The weak interlayer interactions combined with strong intralayer bonding in TMDs promote interlayer sliding, which has driven substantial research on understanding and controlling interlayer friction [3,4]. Studies have shown that the friction force of $MoTe_2$ is lower than that of MoS_2 and $MoSe_2$ under identical testing conditions [5]. In this work, we obtained mono- and few-layer samples of $MoTe_2$ through mechanical exfoliation and transferred them onto a Si substrate with a 290 nm oxide layer. Optical microscopy was employed to locate the targeted layers for transfer, while Raman spectroscopy confirmed successful exfoliation by detecting characteristic peak shifts. Specifically, the reduced intensity of the B^1_{2g} mode relative to the E^1_{2g} mode verified the presence of 2-4 layers. Subsequently, nanoscale frictional behaviour was investigated for both bulk and few-layer $MoTe_2$ using atomic force microscopy (AFM) in Frictional Force and Transverse Shear modes. This comparative analysis aims to elucidate the effects of layer thickness and relative crystalline orientation on the tribological properties of $MoTe_2$.

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Disordered-induced topological phase transitions in Bismuth

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Crystalline bismuth is a higher-order topological insulator (HOTI) with a very low superconducting critical temperature (~0.1 mK). In contrast, amorphous bismuth is not believed to be topological, but it superconducts at 6K. These differences motivate us to explore how topological properties in bismuth evolve under strong disorder. Our analysis reveals that disorder does not necessarily trivialize bismuth. We present the phase diagram of three-dimensional bismuth as a function of disorder as given by the spectral localizer—a real-space topological marker capable of signaling the trivial to topological phase transition, even when the bulk band gap is small.

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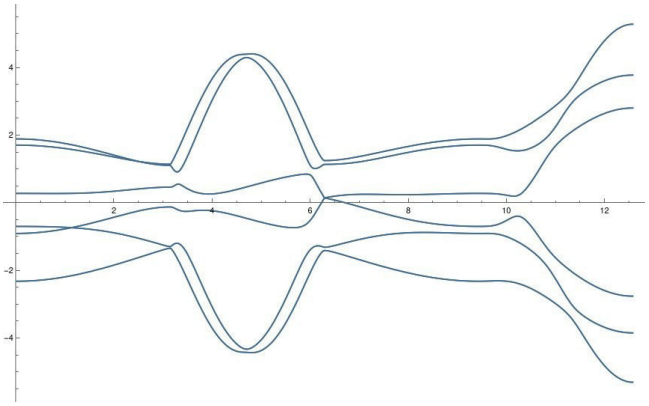
Figures



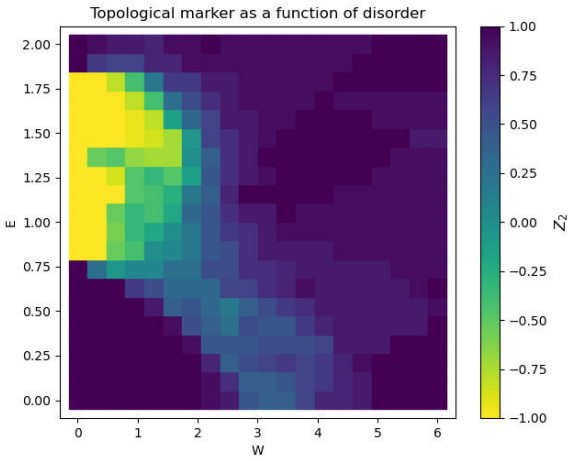


Figure 1: Bulk bands in crystalline bismuth.

Figure 2: Spectral localizer marker as a function of disorder and energy.

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-Abstract for a **poster** contribution-

Spin and charge control of topological end states in exchange biased chiral graphene nanoribbons

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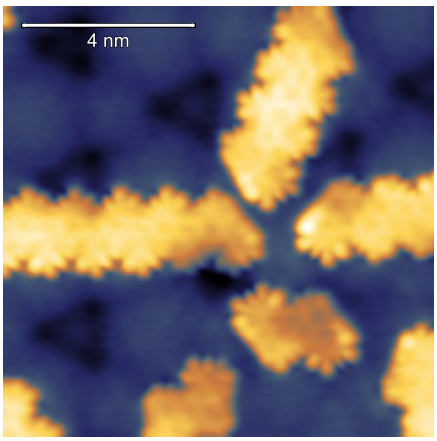

Figure 1: Scanning tunneling microscope scan of chiral graphene nanoribbons on $GdAu_2$.

Nanographene can exhibit radical states due to sublattice imbalance or nontrivial topological phases. On-surface synthesis (OSS) enables growth of such structures with atomic precision, whose electronic structure and magnetism can then be probed by scanning tunnelling spectroscopy. The magnetism of the topological end states in chiral graphene nanoribbons (chGNRs) however remains unobserved, as electron transfer of two electrons to or from the substrate readily occurs for small mismatches in electron affinity, quenching magnetism [1].
When alloyed with rare-earth metals [2], gadolinium-gold still catalyzes OSS, while exhibiting a much lower work function [3]. We show here that pristine chGNRs can be synthesized on this intermetallic surface without undergoing charge transfer. We furthermore observe that the occupancy of the two topological end states, as well as their total spin multiplicity, can be switched reversibly from a doublet to a singlet, and then to a triplet configuration by lateral manipulation.
Due to the low-temperature ferromagnetism in $GdAu_2$, prominent spin-flip excitations are observed and interpreted as a Kondo-screened π-radical state acted upon by the substrate's magnetization [4]. We introduce a many-body model that unifies the effects of local electrostatic gating, electron-electron-correlation, and exchange bias on the chGNR charge and spin state.

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Deep Learning and Twistoptics: Designing light propagation at the nanoscale

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Van der Waals (vdW) materials [1,2] stacked with a relative twist angle have garnered significant attention for their ability to control electrical -Twistronics- and optical -Twistoptics- properties. In particular, twistoptics promise precise control over the propagation of light at the nanoscale in the form of low-loss polaritons—hybrid light-matter quasiparticles—exhibiting topological transitions and exotic phenomena such as canalization or ray-like propagation. However, despite the growing interest for nanophotonics, achieving desired polariton propagations using Twistoptics remains elusive due to the large number of parameters to be controlled. In fact, the complexity of the analytical equations, the number of tunable parameters and trial-and-error approaches often employed in twistoptics make the application of artificial intelligence (AI) in this field ideal [3]. Here, we introduce, for the first time, a neural network (NN) model that in combination with Twistoptics enables the design of desired polariton propagations at the nanoscale by accurately predicting optimal multilayers [4]. In particular, we apply our model to achieve canalization and bi-canalization of phonon polaritons (PhPs) in twisted bilayer and trilayer homostructures of α-MoO$_3$. As a highly efficient predictive tool for twistoptics, our NN model enables the design of optimal twisted multilayers, offering significant potential for advancing nanophotonic applications in areas such as sensing, thermal management, or quantum computing.

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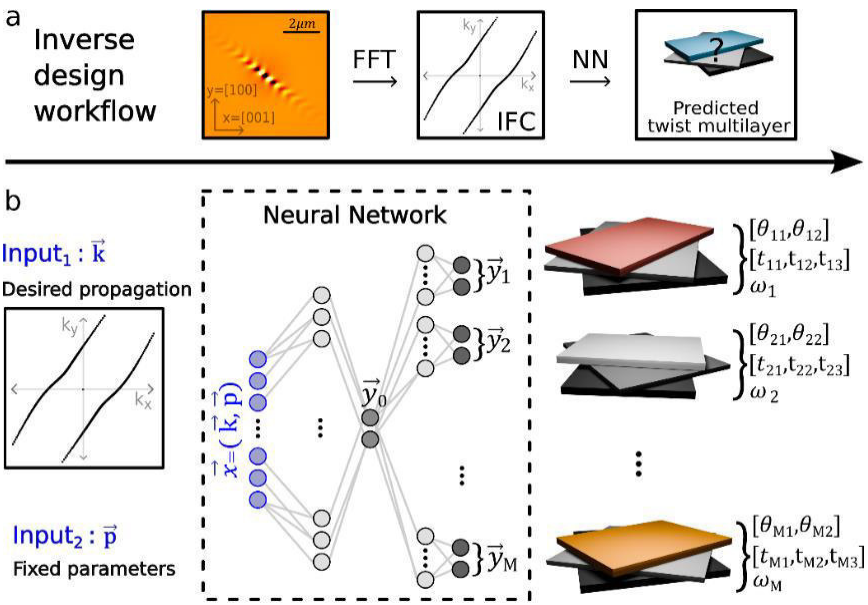

Figure 1: Designing light propagation at the nanoscale applying NNs in Twistoptics. a) Schematic representation of the inverse design workflow using a NN in Twistoptics. b) The NN operates as a unified model that can be conceptually divided into two parts: a first part that generates a vector $\vec{y}_0$ with the length of the parametric space, and a second part consisting of a set of M branches that allow finding symmetries and multivalued solutions [3].

Speeding up quantum Monte Carlo computations using set transformers

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In the study of many-body physics, the exponential growth of the cardinal of the Hilbert space with system size can represent an insurmountable complexity barrier. With analytical results rarely available, this problem forces researchers to turn to numerical practices. Quantum Monte Carlo (QMC) techniques are one of the main tools used for these studies, thanks to their ability to provide accurate solutions to complex quantum systems by efficiently sampling high-dimensional integrals. However, the computation of some physical quantities becomes very computationally expensive even with the QMC toolbox. Here, we propose the use of a modern, universal and permutation invariant neural network architecture —the set-transformer— to learn to predict observables from raw MC samples. By employing supervised learning in system configurations with known analytical solutions, we can make accurate predictions across the full parameter range. We build classifiers to identify the different phases of the system, as well as regressors to predict fluctuations and the fourth moment of magnetization, a computationally expensive quantity, as well as the second Rènyi entropy. Our results show that this architecture generalizes across the entire range of interaction, accurately predicting the different phases and observables, as exemplified in the long-range Ising model in a transverse field. Additionally, the model delivers a very significant speed-up in computation time compared to conventional QMC calculations.

Molecular Identification via Molecular Fingerprint extraction from Atomic Force Microscopy images

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Non-Contact Atomic Force Microscopy with CO--functionalized metal tips provides access to the internal structure of individual molecules adsorbed on a surface with totally unprecedented resolution [1]. However, the chemical identification of individual molecules remains a challenge. Previous works [2-4] have already shown that deep learning (DL) models can retrieve the chemical and structural information encoded in a 3D stack of constant-height HR--AFM images, leading to molecular identification. In this work, we overcome their limitations by using a well-established description of the molecular structure in terms of topological fingerprints, the 1024--bit Extended Connectivity Chemical Fingerprints of radius 2 (ECFP4) [5], that were developed for substructure and similarity searching. ECFPs provide local structural information of the molecule, each bit correlating with a particular substructure within the molecule.

In this work [6], we train a DL model to extract this optimized structural descriptor from the 3D HR--AFM stacks and use it, through virtual screening, to identify molecules from their predicted ECFP4 with a retrieval accuracy on theoretical images of 95.4%. This approach, unlike previous DL models, assigns a confidence score, the Tanimoto similarity, to each of the candidate molecules, thus providing information on the reliability of the identification. Finally, we perform a limited test with experimental images, obtaining promising results towards the application of this pipeline under real conditions.

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Study of the effect of collisional cascades on an edge dislocation dipole in FeCr.

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In this work we study the influence of 20 keV collisional cascades on an 1⁄2⟨111⟩{110} edge dislocation dipole in FeCr using the molecular dynamics code LAMMPS [1]. The interaction among the atoms is modeled by CD-EAM (Concentration-Dependent Embedded-Atom Method) [2], smoothly connected to a Ziegler-Biersack-Littmark (ZBL) potential [3] at small interatomic distances. We analyze the mobility of the dislocations, the generation and clustering of defects as well as the influence of the percentage of Cr atoms in the alloy.

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Analysis of the effects of He bubbles near a FeCr surface. A molecular dynamics study

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This work analyses the dynamics of He bubbles near the surface of a FeCr alloy. For this purpose, we have used the molecular dynamics software LAMMPS [1] together with the concentration dependent interatomic potential developed in [2] for high Cr-ferritic alloys. The He-Fe and He-Cr interaction was modeled by the potential described in [3]. We study the dependence on the size of the bubble, its He-vacancy ratio and the closeness to the surface. We also consider the effect of the Cr concentration in the alloy.

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Non-linear conductivity and wireless radiofrequency rectification in chiral Te

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Electrical transport in non-centrosymmetric materials departs from the well-established phenomenological Ohm's law. Non-linear transport effects, characterized by a quadratic relationship between voltage and current, can arise in these systems, either with or without external magnetic fields [1]. These effects are fundamentally tied to the absence of spatial inversion symmetry. However, the experimental impact of an inversion symmetry operation on non-linear electronic transport remained to be explored. In this study, we report the observation of a large zero-field non-linear conductivity in chiral Te flakes [2]. The dependence of this non-linear effect on the relative orientation between the crystallographic axes of Te and the current direction is fully explained by symmetry considerations, as it arises from the non-linear conductivity tensor of Te point group. Importantly, by measuring samples with opposite handedness [3], we demonstrate that the non-linear transport is odd under spatial inversion (Fig. 1a). We further investigate the resistivity dependence of non-linear conductivity, varying sample temperature and applying an electrostatic gate, revealing that side-jump scattering from dynamic sources is the dominant microscopic mechanism [4]. Through electrostatic gating, we achieve a tuning of the non-linear output voltage by a factor of 300, reaching the highest reported value outside of engineered heterostructures. Finally, we report wireless radiofrequency rectification that persists at room temperature (Fig. 1b) [5]. Analysis of the crystal symmetry, temperature, and gating dependence of the rectification demonstrates its origin in the non-linear conductivity. These results open the path to developing tunable microscale wireless rectifiers for energy harvesting applications.

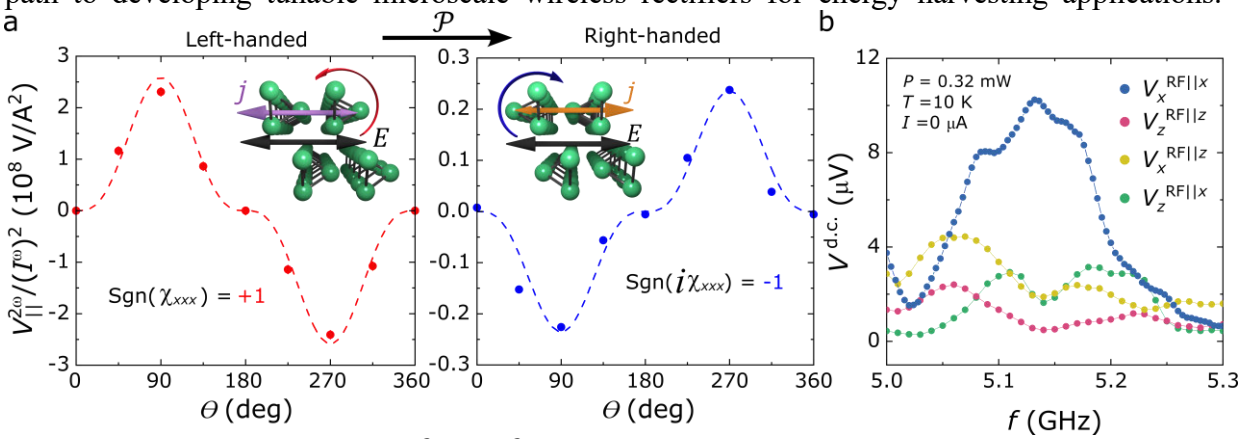

Figure 1. a, Non-linear conductivity ($V_{\parallel}^{2\omega}/(I^{\omega})^2$) as a function of the θ-angle between the applied current (I^{ω}) and the crystallographic z-axis, for left- and right-handed Te crystals. The sign of the non-linear conductivity changes sign after an inversion symmetry operation ($\mathcal{P}$). **b**, Rectified d.c. voltage along the x-axis ($V_x^{d.c.}$) and z-axis ($V_z^{d.c.}$) as a function of the frequency (f) while aligning the polarization of the incident electromagnetic wave with the x-axis ($RF \parallel x$) and z-axis ($RF \parallel z$). The maximum signal corresponds to the maximum emitting f of the antenna.

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Enhancing Light Emission of Single-Layer WSe_2 in Perylene-Doped Polymer Films through Efficient Energy Transfer

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The optical and mechanical properties of 2D semiconductors make them suitable as active components in flexible optoelectronic devices. This work investigates the incorporation of single-layer WSe_2 (1L-WSe_2) into a polystyrene (PS) film with dispersed perylene orange (PDI-O) molecules. The results show an increase in the light emission of 1L-WSe_2, observed only upon PDI-O excitation and increasing with the concentration of molecules in the PS film. Additionally, the enhancement in 1L-WSe_2 photoluminescence coincides with a reduction in PDI-O light emission intensity and a decrease in its lifetime. These observations indicate efficient long-range interactions, such as Förster energy transfer, between PDI-O (acting as the donor) and 1L-WSe_2 (acting as the acceptor), as the mechanism for the enhanced light emission in 1L-WSe_2. These findings are relevant for the development of flexible optoelectronic devices that incorporate active 2D materials; the polymeric matrix functions as both physical support and a host for organic dopants that can optimize the light emission properties of the 2D material.

Figures

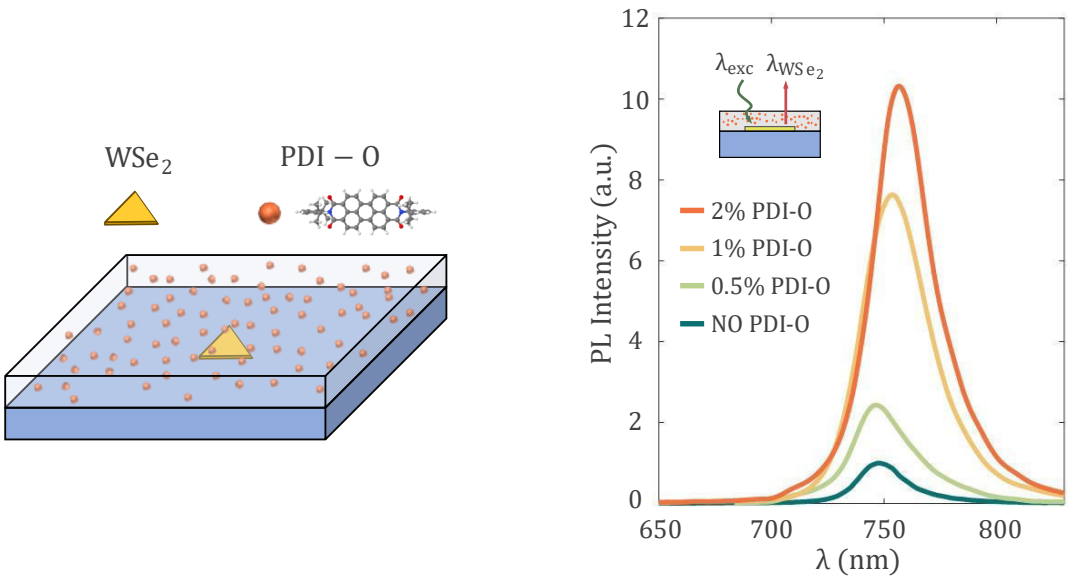

Figure 1. Left: Sketch illustrating a 1L-WSe_2 flake deposited onto a SiO_2/Si substrate, beneath a PS film with dispersed PDI-O molecules. Right: Micro-Photoluminescence spectroscopy for 1L-WSe_2 flakes (λ_{exc} = 532 nm) covered with a 100 nm thick PS film containing different concentrations of PDI-O molecules (0, 0.5, 1, and 2 wt %) as indicated in the legend. Inset: Sketch for 1L-WSe_2 on a SiO_2/Si substrate, beneath a 100 nm thick PS/PDI-O film.

Unveiling the shape of α-MoO_3 microcrystals in oxygen deficiency environment

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Nowadays, 2D transition metal oxides have a great interest in many applications in optoelectronic devices. In particular, orthorhombic molybdenum trioxide (α-MoO_3) possesses a well-known layered crystal structure that allows the fabrication of 2D morphologies with anisotropic optical behavior [1]. MoO_3 requires a high concentration of oxygen to crystallize in the orthorhombic stoichiometric phase [2]. The formation of microcrystals α-MoO_3 with tabular morphology has been shown in various reports [3]. In fact, recently we have reported the fabrication of high-quality tenths of nanometer-thick α-MoO_3 microcrystals by annealing in air of amorphous MoO_{3-x} thin films prepared by pulsed laser deposition in vacuum (10^{-6} Torr). Amorphous as-grown films become crystalline after a low temperature annealing in air (250ºC), [4]. The samples crystallized in orthorhombic phase, proved by Raman spectroscopy.

In this work, we study and unveil the morphology and internal crystal structure of individual α-MoO_3 microcrystals. We can observe a change in the growth mechanism from growth by 2D nucleation with the "bowtie" morphology to a growth mechanism by helical dislocations that give rise to tabular microcrystals with different atomic distances along (100) (short side of the crystal) and (001) (long side of the crystal) crystalline directions as shown by TEM. Whereas the inter-atomic distance along the (100) direction is in good agreement with the lattice parameters of relaxed MoO_3, the crystal, it is compressed in the [100] direction and elongated in the [001] direction. Finally, to validate the optical quality of the produced crystals, we perform scattering-type scanning near-field optical microscopy (SNOM), where an anisotropic near-field distribution is observed. Interestingly, bright regions aligned along [100] and [001] directions are revealed depending on the illumination wavelength, which clearly indicates an anisotropic and wavelength-dependent optical response, which is discussed and correlated with the structural characterization.

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Figures

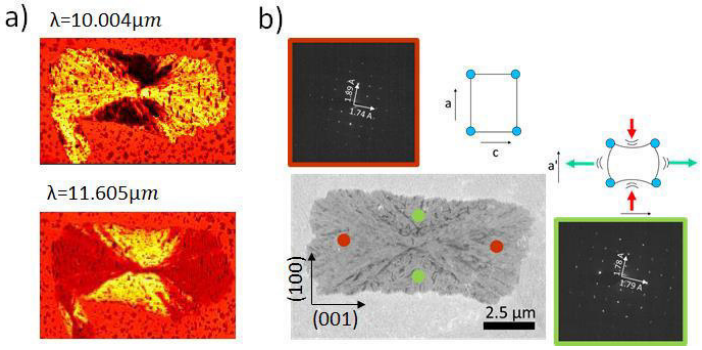

Figure 1: SNOM measurements of MoO_3 single crystals in different wavelength (a) and TEM image of a MoO_3 single crystal in the central image; the diffractograms are shown with the measured inter-atomic distances. A scheme showing the lattice shape and the deformation for the long side bowtie (b).

Magnetic behaviour of Fe-oxide nanoparticles embedded in a carbon matrix

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Fe-based nanostructured systems have been extensively investigated due to their scientific interest related to nanoscale magnetism and their promising applications in our modern society, such as biomedical, energy storage or environmental sustainability [1].

In order to optimize the final properties for these applications, the nanoparticles (NPs) can be inserted into insulating matrices. In particular, carbon provides a good protection to the NPs against corrosion, chemical stability and biocompatibility [2,3] and can decrease the magnetic interactions between the NPs [4].

In this work, carbon encapsulated γ-Fe_2O_3 NPs with emerging proximity effects were synthesized by a simple and easily scalable chemical method based on a pyrolysis at high temperature. The morphology and size distribution of the nano-entities were investigated using high-resolution transmission and scanning electron microscopies that showed γ-Fe_2O_3 NPs with an average diameter of 9 nm embedded in the porous amorphous carbon matrix. Apart from these γ-Fe_2O_3, small amount of Fe_3C and metallic-Fe phases were also detected from X-ray absorption and Mössbauer spectroscopies. These NPs exhibit exchange bias at 4 K even with a H_{cool}=14 T, and magnetic relaxation together with memory effects below 60 K, where the core magnetic moments of γ-Fe_2O_3 seems to be coupled with disordered surface magnetic moments of the Fe atoms. Our join investigation shed light on the role of the different magnetic entities and the nature of the spin-glass like phenomena.

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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.

Current induced propagation of magnetic textures in $NdCo_5/Ni_8Fe_2$ bilayers: current threshold and memory effect

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The need to develop energy-efficient devices is increasing day by day. In the magnetism community, numerous investigations have been carried out around the magnetic racetrack paradigm. Here, we work with a $NdCo_5/ Ni_8Fe_2$ bilayer with a periodic stripe domain pattern in order to develop a reconfigurable domain wall racetrack. These linear up/down stripe domains at the $NdCo_5$ layer provide a reconfigurable magnetic potential that guides the propagation of head-to-head (H2H) or tail-to-tail (T2T) domain walls (DW) within the top permalloy (Ni_8Fe_2) layer [1]. As sketched in Fig. 1, each DW hosts either a vortex or antivortex texture with skyrmionic charge close to $\pm 1/2$.

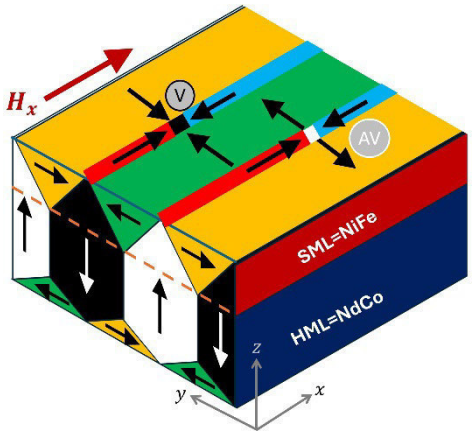

Fig. 1: Sketch of reconfigurable racetracks for H2H DWs hosting vortex/antivortex textures in the stripe domain pattern of NdCo/NiFe bilayers

Magnetic transmission X-ray microscopy experiments at MISTRAL Beamline have shown the thermally activated propagation of these DWs under the effect of pulsed currents ($\sim$20 ns) over a threshold current of 3×10^{11} A/m^2 [2]. DW propagation direction is determined by its H2H/T2T character and applied magnetic field orientation, irrespective of the sign of the applied current pulse. In the remnant state, it is found that DW propagation direction is controlled by magnetic history, i.e. by the sign of the magnetic field used to previously saturate the sample. Micromagnetic simulations reveal that this memory effect is created by an exchange-bias effect at the $NdCo_5/ Ni_8Fe_2$ interface that acts as a magnetic spring selecting a favourable sense for the movement of the V/AV textures with an equivalent bias field $\mu_0 H_{bias} \approx 9$ mT.

Planar Hall effect measurements [3] and micromagnetic simulations in NiFe/Pt and NdCo/NiFe/Pt multilayers will be presented in order to assess the magnitude of Spin Orbit Torques in our system and their possible contribution to reduce the threshold current for DW propagation in the reconfigurable racetracks.

Work supported by Spanish AEI and Asturias FICYT.

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Commensurability peaks in graphene antidot lattices

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Commensurability oscillations in magnetotransport, resulting from the interplay between cyclotron orbits and periodic patterning [1,2], are foundational in mesoscopic physics. Achieving similar control in two-dimensional materials like graphene has been challenging due to the need for ballistic transport over large scales [3]. Here, we present the observation of magnetoresistance peaks in high-quality perforated graphene (antidot lattices), where collective electron motion – a key ingredient for the emergence of hydrodynamic flow - is evident. We find that scattering between states bound to individual or grouped antidots drives these commensurability features. Our findings provide key insights for advancing experiments in nanostructured graphene.

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Figures

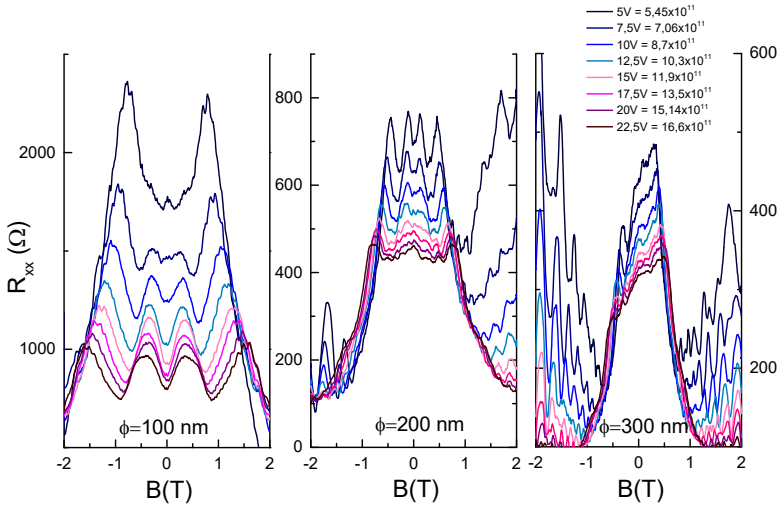

Figure 1: Commensurability oscillations in graphene antidot lattices as a function of the external magnetic field for various electronic densities. The antidot regions present different diameters ranging from 100 to 300 nm.

Rashba spin-orbit coupling in 2D semi-Dirac materials

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Two-dimensional semi-Dirac materials exhibit an anisotropic dispersion relation, being linear in one direction and quadratic in the perpendicular one. In a finite size system described by this model in the topological regime, edge states emerge along one-direction, localized on either upper or lower edge. Notably, only a single-momentum value, corresponding to a zero energy mode, is topologically protected and can be rigorously founded on the zak phase of the one-dimensional reduction of the Hamiltonian. This study explores the impact of the Rashba spin-orbit coupling (RSOC) on this picture. RSOC lifts the spin degeneracy of the quadratic bands except at k_x=0, splitting them into four bands polarized in the s_y-direction, while preserving the sublattice polarization. We also explore the spin-dependent conductance which shows signatures of spin-flip conductance. This mechanisms is sensitive to the length of the nanoribbon and the strength of the electric field, which can be tuned externally. The interplay between momentum, spin and sublattice degree of freedom highlights the potential of semi-Dirac materials as a platform for spintropic devices.

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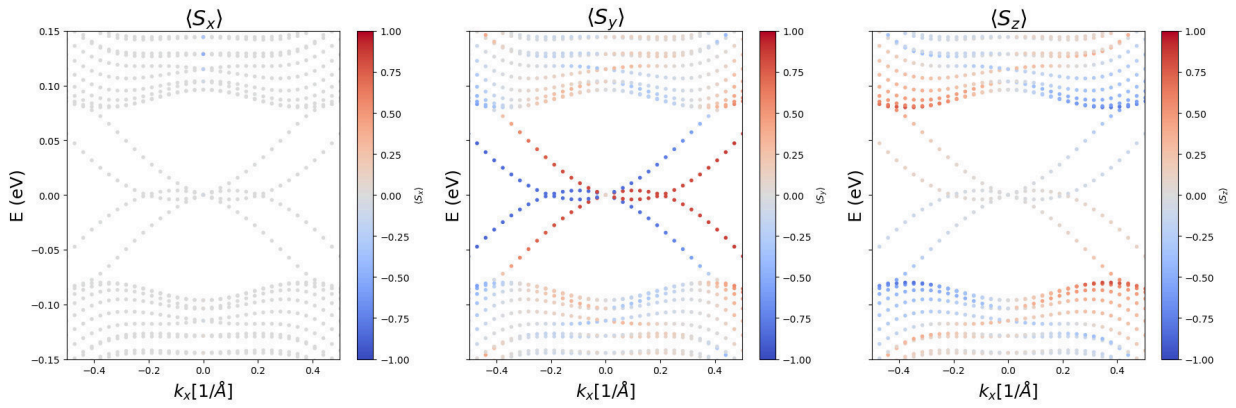

Figure 1: Components of the expected-spin value of a finite system describe by semi-Dirac model in the topological regime with Rashba spin-orbit coupling.

LOREA: the new ARPES beamline at ALBA Synchrotron

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LOREA (*flower* in basque language), the ninth beamline of the ALBA synchrotron radiation source, started its operation in 2021 and is dedicated to electronic structure investigation of quantum materials by means of Angle Resolved Photo-Emission Spectroscopy (ARPES).

The beamline covers the photon energy range of 10-1000 eV, with continuously variable polarization, resolving power of more than 10^4 in the whole range, and a spot size of about 10x10 μm^2. The beamline allows to perform high resolution VUV ARPES as well as Soft X-ray ARPES and resonant PES. The MBS A-1 hemispherical electron analyser can be used in the deflector map mode to get isoenergy maps in the energy range 10-600eV, while ARPES is available in the 10-850eV range. The analyser includes an MBS spin manipulator and a Focus-VLEED spin detector to perform Spin-Resolved ARPES in all 6 components at once.

The 6-axes cryo-manipulator can reach low temperatures better than 7.5K and is provided with 4 electrical contacts for characterizing the ARPES samples with transport measurements and to perform "operando" experiments on simple devices with dimensions of the order of about 20 micrometers. The beam positioning is facilitated by a microscope looking at the sample surface in the direction collinear with the beam and with a spatial resolution of about 10μm.

The two preparation chambers allow to sputter clean surfaces and to deposit thin films of a wide range of materials, from noble metals to alkali and rare earth elements. The presence of a plasma source gives a further possibility of cleaning surface and to grow oxides or nitrides. Atomic layer deposition (ALD) of oxides is also possible thanks to a customised ALD reactor attached to the main preparation chamber.

In this contribution we will show some results on topological insulators measured at low energy, on charge density waves materials measured with soft X-ray ARPES, on spin polarised surface and bulk states, and preliminary results of gated oxide heterostructures used in "operando" resonant PES experiments.

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Unraveling Pines' Demon in Sr_2RuO_4

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In certain multiband metals, electrons in different bands can oscillate in anti-phase under the influence of an electric field. This results in the formation of a neutral mode termed the Pines' demon, a collective mode comprising two species of charged particles collaborating to sustain the collective motion's neutrality—an acoustic plasmon mode in three-dimensional metals.

The theoretical prediction of this phenomenon dates back to 1956 by D. Pines[1], yet its experimental validation materialized only recently[2] in Sr_2RuO_4. This work explores the Pines' demon in Sr_2RuO_4, incorporating beyond-RPA effects and accounting for surface contributions to the material's susceptibility.

While conventional approaches such as RPA and beyond-RPA corrections in both bulk and surface models predict the existence of an acoustic plasmon, they predict a linear dispersion intersecting the origin different from the experimentally observed dispersion reported[2]. Our analysis reveals that the inclusion of momentum-relaxation effects results in a modification of the linear acoustic plasmon for any 3D system hosting acoustic plasmons, leading to a universal phenomenon of momentum-gapping in any 3D system with momentum relaxation. These results rule out many-body interactions or surface effects as the origin of the experimental measurements of the Pines' demon in Sr_2RuO_4. Furthermore, the predicted and observed acoustic plasmon dispersion constitutes the first detection of a momentum-gapped dispersion in a 3D electronic system.

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Magnetically Induced Modifications of Topological Surface States Mediated by Rare-Earths Surface Doping.

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Magnetic topological insulators (MTIs) are a unique class of materials where the coexistence of a topologically protected band structure with long-range ferromagnetic order can break time-reversal symmetry (TRS). This symmetry breaking introduces a bandgap in the Dirac cone-shaped topological surface state (TSS), a prerequisite for realizing the quantum anomalous Hall effect (QAHE). The QAHE, characterized by dissipationless, spin-polarized edge currents, offers promising applications in spintronic devices but remains challenging to achieve experimentally, especially at practical temperature conditions [1].

In this study, we investigate the effects of Er doping on two prototypical three-dimensional topological insulators: Bi_2Se_2Te and Bi_2Te_3. Using angle-resolved photoemission spectroscopy (ARPES) performed at the LOREA beamline at the ALBA Synchrotron, we explore how Er surface doping influences the TSS. For Bi_2Se_2Te, low concentrations of Er induce TRS breaking, evidenced by a bandgap opening at the Dirac point and a transition of the TSS Fermi surface from a hexagonal to trigonal symmetry [2]. Increasing Er coverage further allows for tunable p-type doping, bringing the Dirac point—and the associated magnetic bandgap—closer to the Fermi level. These effects are modeled with a Zeeman magnetic out-of-plane term in the TSS Hamiltonian, providing insights into magnetic interactions with the TSS. For Bi_2Te_3, which exhibits a more warped Fermi surface [2], Er doping leads to distinct modifications of the TSS, further highlighting the substrate-dependent nature of these interactions. The comparative analysis of these materials underscores the potential for tuning magnetic properties and band structure in MTIs. Our findings open a viable pathway toward achieving the QAHE and integrating MTIs into spintronic technologies.

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Implementing neuron functionality with an $La_{0.7}Sr_{0.3}MnO_3$ synaptic transistor

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Neuromorphic computing aims to create efficient information-processing hardware inspired by the brain's parallelism, sparsity, and low power consumption.[1] Developing large-scale neuromorphic systems requires densely integrating large numbers of neurons and synapses into compact networks. A significant milestone toward achieving this goal is the implementation of synaptic and neuronal functionalities using the same material and, ideally, the same device. This is challenging due to the distinct properties of neurons (volatile) and synapses (non-volatile). Interestingly, three-terminal transistors, which can exhibit both volatile and non-volatile resistive switching, offer a promising solution for integrating neuronal and synaptic functionalities within a single system.

In this work, we demonstrate neuronal functionality by leveraging the volatile regime of a three-terminal synaptic transistor based on an ultra-thin film of $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) near a metal-insulator transition.[2] The LSMO channel is connected to the gate terminal through an ionic liquid, so that a gate voltage creates a strong electric field on the LSMO surface. This field can induce electrostatic effects (electron or hole accumulation) and electrochemical effects (creation/annihilation of oxygen vacancies) in the LSMO channel, enabling volatile and non-volatile modulation of its electronic properties. These mechanisms have previously been used to implement synaptic properties related to short-term and long-term memory and plasticity.[2]

Here, we focus on the fully volatile regime, where the device exhibits relaxation dynamics analogous to those of biological neurons, to demonstrate important neuron functionalities, including leaky integration, frequency filtering and rate coding. Using the rate-coding mechanism, we experimentally implement the sigmoid activation function (Figure 1), a fundamental component of artificial neural networks. These results represent a significant step toward the development of neuromorphic networks that integrate neuron and synapse functionalities using identical devices.

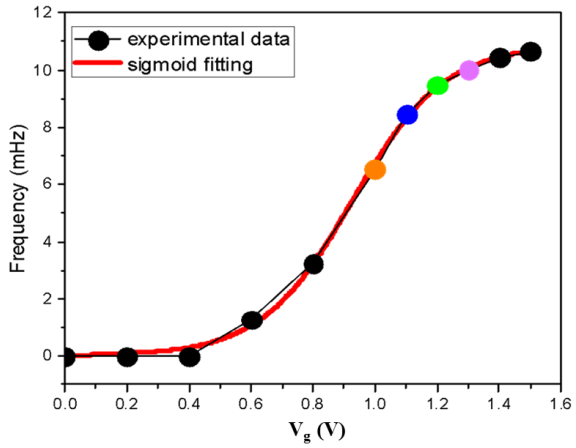

Figure 1: Experimental representation of the firing frequency for different gating voltages (dots), following a sigmoid dependence (red line).

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Localized nanoscale formation of vanadyl porphyrin 2D MOF nanosheets and their optimal coupling to lumped element superconducting resonators

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A strategy for realizing a quantum spin processor involves coupling spin qubits and qudits to resonant photons within superconducting resonators.[1,2,3,4] In this work, we take a step toward such a hybrid architecture by designing a chip featuring multiple lumped-element LC superconducting resonators, optimized for coupling to specific transitions of a vanadyl porphyrin electronuclear qudit.[5,6] The in-situ formation of nanosheets derived from a 2D framework where the vanadyl qudit serves as a node allows a precise control over the number and orientation of the qudits onto the superconducting device. Low-temperature transmission experiments reveal the coupling between photons in resonators of different frequencies and the targeted electronuclear transitions of the vanadyl qudit. The observed collective spin-photon couplings in the 0.3–1.6 MHz range enable the estimation of enhanced single-spin photon couplings, reaching optimal values of up to 4 Hz.

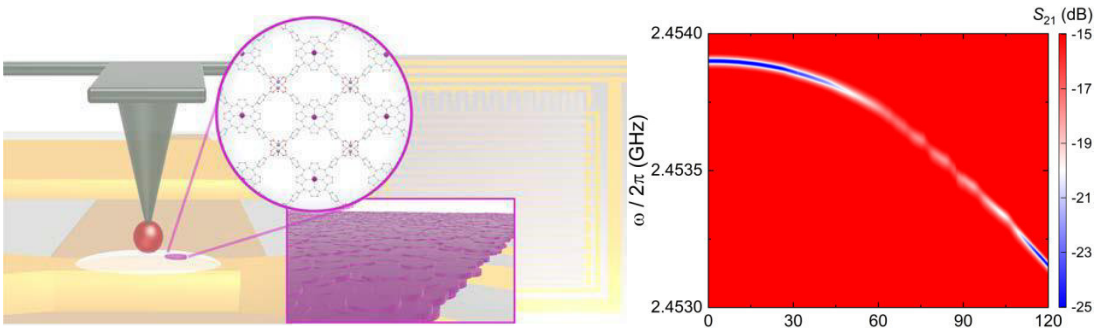

Figure 1: Scheme of in-situ formation of isolated nanodomains of the [{VOTCPP}$Zn_2(H_2O)_2$] 2D MOF on an LC resonator (left) and color plot of the microwave transmission of a resonator coupled to 10 MOF 2D planes (right).

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Nanofabrication and Anisotropic Non-linear Transport of the Kagome Metals AV_3Sb_5 (A = K, Rb, Cs)

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Kagome metals represent a new class of materials ideal for experimental research on various physical phenomena, including spin liquid states, charge density waves (CDW), and superconductivity. These materials are characterized by having a kagome crystal lattice where the atoms form the vertices of adjacent triangles, thus creating a kagome basket or Star of David-like network [1]. Recently, researchers have discovered the AV_3Sb_5 (A = K, Rb, Cs) family of kagome metals, sparking significant scientific interest. These metals possess a 2D kagome lattice composed of vanadium atoms, a superconductive ground state, and exhibit notable properties like a pronounced anomalous Hall effect (AHE) and high magnetoresistance. These effects arise from the breaking of time-reversal symmetry triggered by the CDW transition as temperature decreases [2].

Although initial observations reveal quantum oscillations in the second-order response on transport (Figure 1a), the non-linear conductivity and electrical magnetochiral anisotropy (two types of non-linear transport effects) in AV_3Sb_5 remain largely unexplored. To investigate these properties in detail, devices are fabricated using kagome metals from the AV_3Sb_5 family. For this purpose, a mechanical exfoliation technique is used, through which 2D flakes are obtained from 3D crystals of these metals. A crucial aspect of the fabrication is giving them the appropriate shape to study the electrical transport in various crystallographic directions. Therefore, a star-shaped design is used (Figure 1b) [3], which is defined by electron-beam lithography and an etching process. Once this nanofabrication step is optimized, the legs of the device are electrically contacted using electron beam lithography and metal deposition.

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Figures

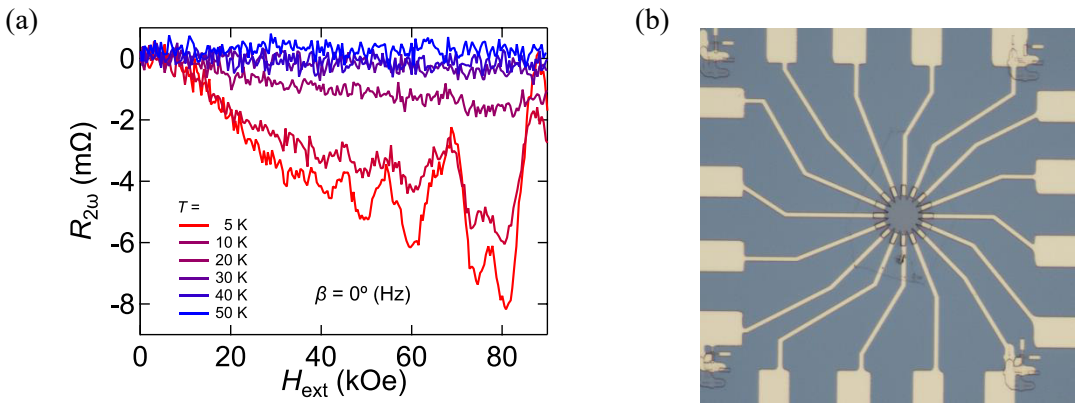

Figure 1: a Magnetic field dependence of the second harmonic resistance for different temperatures in a CsV_3Sb_5 flake. Quantum oscillations can be observed for high magnetic field applied and low temperatures. **b** Star-shaped device used for the study of the electrical transport along different crystallographic directions of the metals AV_3Sb_5 (A = K, Rb, Cs).

Spatial Modulation of Thermal Conductivity in Oxides for Thermal Memory Devices

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In this work, we introduce a novel technique for precise control of thermal conductivity in thin films of charge-transfer oxides. Using a voltage-biased AFM tip, we can induce the local accumulation of oxygen vacancies,[1,2] continuously and under ambient conditions, creating micron-size patterns with a perfectly defined value of thermal conductivity. Frequency Domain Thermoreflectance measurements reveal that the thermal conductivity within these regions depends on the applied voltage, achieving reductions of up to 55% (Figure 1).
By optimizing the oxide's chemical composition, these modified thermal states remain stable in normal atmospheric conditions, but they can be fully reset to their original state through thermal annealing, enabling repeated cycles of thermal conductivity modification. In comparing Mott-Hubbard and charge transfer oxides, we highlight the key role of redox-active lattice oxygen in enabling full reversibility of the process.[3]
This AFM-driven approach opens promising avenues for designing oxide-based microthermal elements, advancing the creation of thermally tunable circuits with potential applications in thermal management and nanoscale device engineering.

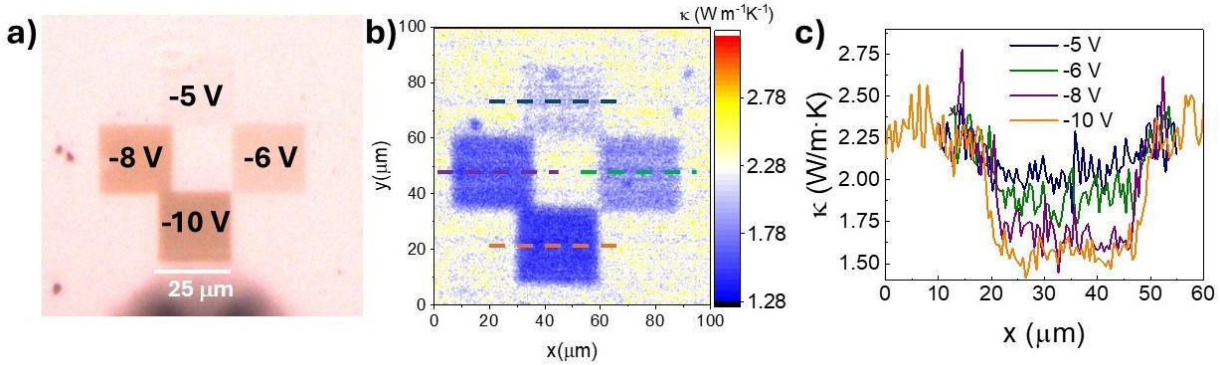

Figure 1: a) Optical microscope image of a 40 nm thick $SrFeO_{3-x}$ thin film after scanning regions of 25x25 μm^2 with an AFM tip biased at different voltages. b) Thermal conductivity map of the written pads shown in (a), observing a decrease in the thermal conductivity. c) Thermal conductivity profiles along the lines shown in (b).

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Excess energy and countercurrents after a quantum kick

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Motivated by the study of non-equilibrium quantum systems, we describe here some formal results and some of their consequences for systems undergoing a sudden onset of motion. A system of interacting quantum particles under the influence of a static external potential is here described as kicked when this potential suddenly and rigidly starts to move with a constant velocity, **v**. This is of experimental relevance for the study of electrons in an atom when its nucleus recoils after a neutron (or dark matter particle) hit, known as Migdal's sudden jolt [1], well known in particle detection. The generalization presented here has no direct experimental relevance (rigidly moving the external potential generated by nuclei in a molecule or solid is not a realistic way to describe a multi-nucleus system when hit in any physical way, see e.g. [2]), but it is a useful reference result for time-dependent simulations, and it could stimulate experiments on optical lattices where kicks as defined quantum could be realized. If the system is initially in its ground state, the excess energy at any time after the kick is given by $\mathbf{v}\cdot\langle\mathbf{P}\rangle(t)$, where **P** represents the total momentum of the system. Being *M* the mass of the system, if the system remains bound, the long-time average of the excess energy approaches $M\cdot\mathbf{v}^2$, which is twice the excess energy it would have if the onset of motion were infinitely smooth. A related expression is trivially obtained when particle emission occurs. For a macroscopic solid, an electronic current can arise that opposes the motion of the potential lasting for a longer time scale than other channels of thermalization. For non-metallic systems, there may be a threshold velocity below which transient currents remain only on very short time scales. Results are presented based on real-time time-dependent density functional theory calculations using its implementation in the SIESTA code [3], [4].

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Enhanced Water Resistance of halide $CsPbI_3$ Perovskite through Graphene Flake Encapsulation

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The stability of halide perovskites, such as $CsPbI_3$, in humid environments remains a key challenge for their integration into durable photovoltaic and optoelectronic devices.[1, 2] This work investigates the use of graphene flake encapsulation as a method to enhance the water resistance of $CsPbI_3$ perovskite films. Given graphene's impermeable and chemically stable nature, we hypothesize that applying pristine graphene flakes that are amphithatic and conductive as a protective layer over the $CsPbI_3$ perovskite will mitigate moisture-induced degradation by creating an effective barrier against water ingress.[3] Our approach combines experimental fabrication and theoretical modeling (DFT calculation) to evaluate the structural and chemical interactions between the graphene flakes and the perovskite surface. By examining these interactions, we aim to gain insight into the encapsulation's protective efficacy under various environmental conditions. Although results are forthcoming, we anticipate that graphene encapsulation will significantly improve the water resistance of $CsPbI_3$, advancing the viability of perovskite-based technologies for practical applications.

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Discovering symmetries from physical data via machine learning

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In recent years, machine learning (ML) and neural networks (NNs) have emerged as powerful tools for uncovering relevant physical insights from measured or simulated data, such as governing equations, symmetries, and conservation laws. Particularly, symmetries play a crucial role in modern physics, providing a deep understanding of physical theories and efficient ways to simplify calculations. Moreover, incorporating symmetries into ML models enhances generalization and improves accuracy in physical simulations.

When the governing dynamics of a physical system are unknown and only a dataset is available, discovering the underlying symmetry becomes a challenging task, especially in high-dimensional systems. Here, we present two ML-based approaches for identifying the symmetry group of a given dataset. These methods uncover two key manifestations of symmetry: invariance and equivariance. To demonstrate the effectiveness of the algorithms, we provide several toy examples of applications across different fields in physics.

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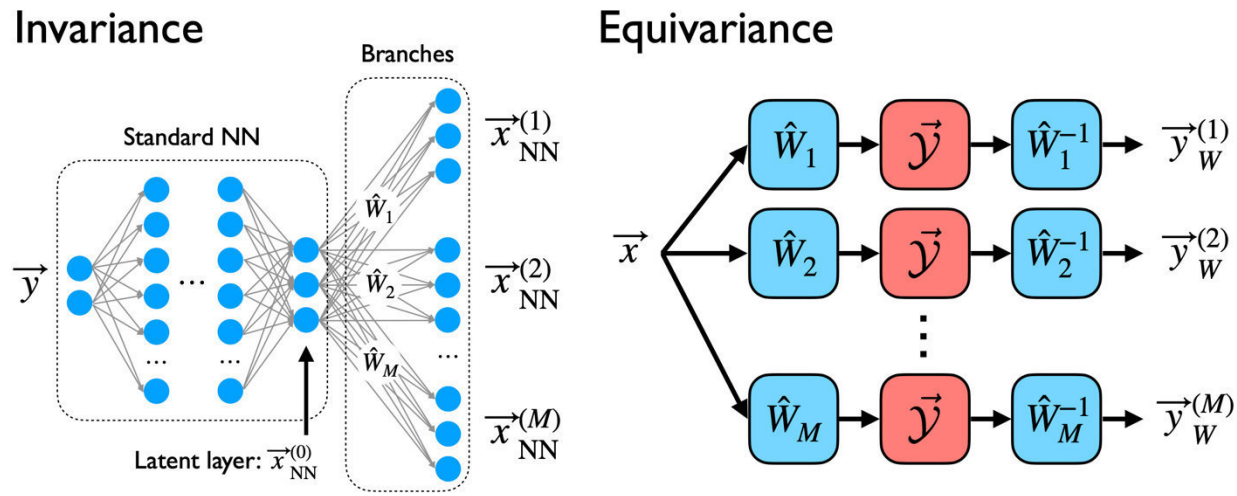

Figure 1: ML-based approaches for symmetry detection: Symmetry Seeker Neural Network (left) and Equivariance Seeker Model (right).

Phononic Casimir effect

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Fluctuation-induced interactions are a universal effect that need a fluctuating field and the induction of noise to generate a macroscopic transport of energy (heat transfer) or momentum (Casimir effect) between macroscopic objects. Here we present the phononic Casimir effect, a fluctuation-induced interaction mediated by phonons instead of the usual electromagnetic field. We will show, on one hand, how to couple the phononic modes of separated compact objects that opens a new channel for heat transfer and Casimir effect in the very close regime, and on the other, how the coupling with the electromagnetic field will modify the em Casimir effect, leading even to an unusual repulsive Casimir effect for a kind of piezoelectric materials. Those results pave the way for an understanding of the forces on a superconducting sphere immersed on a superfluid, an experiment that is being carried out by our group, where we expect that the phononic modes will be one of the relevant contributions on the forces over the sphere.

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Unraveling different contributions to spin orbit coupling in superconductor/ferromagnet hybrids

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Over the past decade, it has been proposed theoretically and confirmed experimentally that long-range spin-triplet (LRT) superconductivity can be generated in superconductor/ferromagnet hybrids either by the presence of spin textures (ST-LRT) or owing to spin-orbit coupling (SOC-LRT). Nevertheless, there has been no theoretical or experimental investigation to date suggesting that both contributions could simultaneously exist within an experimental system. First, we show that there is an interplay between SOC-LRT and ST-LRT in the samples under study, and disentangle these two contributions. In [1] we present a comprehensive study of superconducting quasiparticle interference effects taking place inside a ferromagnetic layer interfacing a superconductor, through the investigation of above-gap conductance anomalies (CAs) related to MacMillan-Rowell resonances. The magnetic field dependence of the CAs is studied under a wide range of in-plane (IP) and out-of-plane (OOP) magnetic fields in two types of epitaxial, V/MgO/Fe-based ferromagnet-superconductor junctions allows us to distinguish between the field independent SOC and the field "controlled" ST contributions to LRT generation.
Second, we aim to investigate the physical origin of interfacial SOC when Rashba and Dresselhaus-type SOC contributions coexist. Theory [2] predicts that LRT contribution to zero bias conductance (ZBC) in FSF hybrid junctions could be strongly dependent on the in-plane angle of the ferromagnets. Here we present experimental study of the dependence of ZBC on IP magnetic field orientation in Fe/MgO/V/MgO/Fe junctions, observing an anisotropy that allows to estimate the relative Rashba and Dresselhaus contributions. Comparison between experimental findings and theoretical modelling indicates that the Dresselhaus contribution to SOC is approximately 10% of the Rashba-type SOC. This small addition to interfacial SOC could be associated with extended defects caused by the ~3% lattice mismatch between the Fe(V) and MgO bcc lattices in Fe/MgO/V-based superconducting spintronic devices.

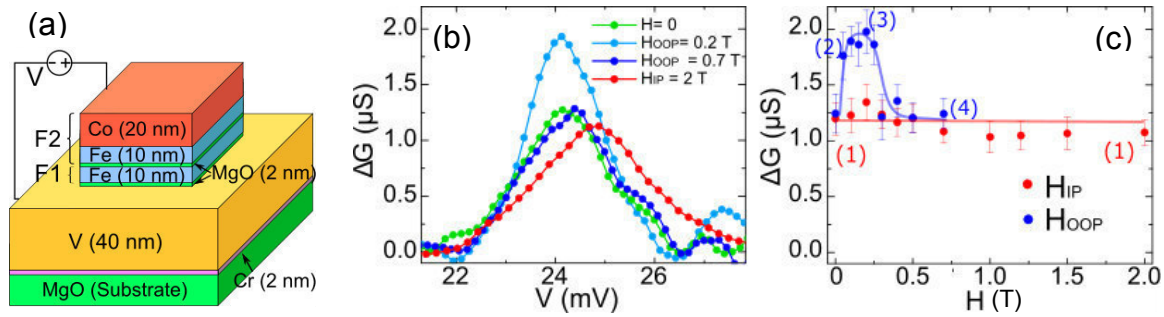

Figure 1: (a) Sketch of the F/S/F sample under study. (b) and (c) show the evolution of conductance anomaly peaks under applied IP and OOP magnetic field.

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GEFES 2025

Anisotropic spin dynamics in proximitized graphene

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While electronics exploits the charge degree of freedom of electrons, spintronics benefits from their spin to process and store information. Graphene stands out as a medium for spin transport due to its carbon-based composition, which ensures very low spin-orbit coupling (SOC), and allows spins to propagate over very long distances. However, weak SOC limits spin manipulation. Two-dimensional (2D) layered materials, integrated into vertical van der Waals heterostructures, offer unique opportunities for engineering novel physical properties through proximity-induced phenomena [1]. In this work, we investigate spin dynamics in hybrid graphene–transition metal dichalcogenide (TMDC) systems, where proximity-induced SOC is introduced into graphene by adjacent high-SOC TMDCs. Graphene/TMDC spin devices with spin-sensitive contacts were fabricated to study spin dynamics in pristine graphene (as a reference) and in graphene partially covered by a TMDC crystal.

Prior studies have reported strong spin lifetime anisotropy in graphene with the hierarchy $\tau_z >> \tau_x;\tau_y$ and isotropic in-plane spin lifetimes $\tau_x = \tau_y$ for highly symmetric TMDCs such as WSe_2, WS_2, MoS_2 and $MoSe_2$ [2]. We demonstrate that low-symmetry TMDCs, such as pentagonal $PdSe_2$ [3], further modify this hierarchy, yielding in-plane spin lifetime anisotropy ($\tau_{x'} \neq \tau_y$ where *x'* and *y'* are orthogonal directions in the graphene plane, with *x'* defined as the direction of maximum spin lifetime). Our experiments also reveal a directional dependence of the spin lifetimes across all spatial directions, underscoring the richness and versatility of proximity-induced phenomena in these hybrid systems.

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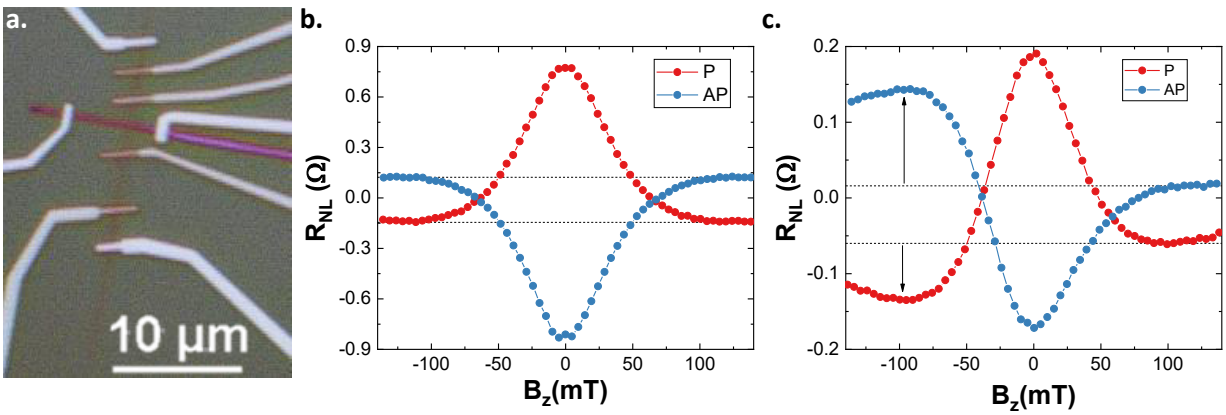

Figure 1: a. Graphene/TMDC spin valve. b. Parallel and antiparallel spin Hanle precession curves in bare graphene. c. Parallel and antiparallel Hanle spin precession curves in graphene showing in-plane anisotropy.

Solvents in Molecular Electronics: Their Role in the Conductance of Molecular Junctions

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Conductance measurements in metal/molecule/metal junctions are essential for understanding electron transport at the nanoscale. While previous studies have primarily focused on the intrinsic conductive properties of the molecules within the junction, the role of the solvent environment in which the molecule is deposited has been less explored. The choice of solvent can affect not only the mechanical stability of the molecular junctions but also the interaction between the molecule and the electrodes, thereby influencing the conductance results.
Our studies using STM and STM-BJ reveal that commonly used solvents in molecular electronics, such as benzene, cyclohexane, and toluene, remain adhered to the gold surface, significantly impacting the electronic transport properties of the system. This highlights the importance of understanding the solvent's role in these measurements.
In this study, we evaluate the influence of chloroform and dichloromethane as solvents in conductance measurements of molecular junctions, using mechanically controlled break junction (MCBJ) and scanning tunneling microscopy break junction (STM-BJ) methods, to determine their impact on system stability and conductance.

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Magnetic Field dependence of the atomic and electronic structure of monovalent metallic nanocontacts unveiled in transport experiments

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We measure Au and Ag atomic-size contacts in magnetic fields, from zero field to 20 T. We find a magnetic field induced torque which leads to atomic binding at shorter distances than at zero field. Furthermore, the conductance drops below G_0 at high magnetic fields by about 15% in Au. We calculate the conduction through nanosized Au contacts containing residual O_2 molecules attached to the contact region and find a spin polarized current when O_2 is located at the atomic contact. We discuss the role of spin-orbit coupling in the magnetic properties of O_2 attached to Au.

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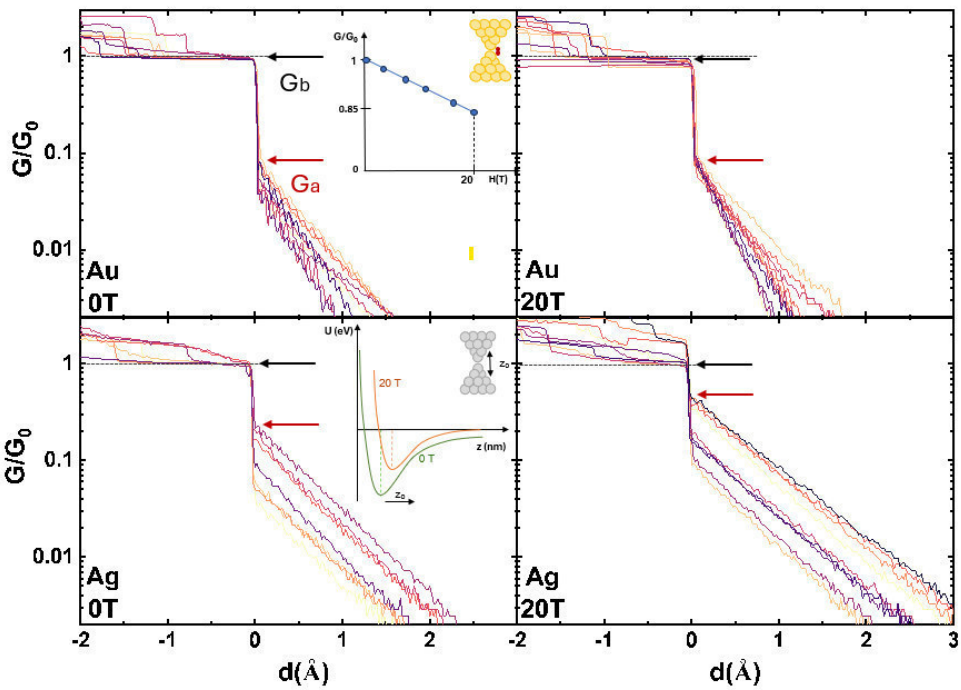

Figure 1: Dependence of the quantum tunnelling conductance regime in single atom point contacts of Au and Ag samples under the effect of an external magnetic field. Insets in the top right corner schematically show the decrease of the conductance value in the contact regime for Au and the decrease in the jump to contact distance for Ag with the increase of the applied magnetic field.

On the Superconductivity in Graphene Multilayers

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During the last six years, we have been investigating the emergence of unconventional superconductivity (SC) in graphene multilayers mediated by a screened long-range Coulomb interaction. We have been using a diagrammatic approach based on a Kohn-Luttinger-like Random Phase Approximation (KL-RPA) analysis[1–3], which includes direct electronic interactions as well as phonon-mediated electronic interactions. In this context, a successful theory of SC in graphene multilayers should reproduce as many experimental observations as possible in all stacks, within a unified framework with the least number of parameters with not well-known magnitude. Interestingly, our SC-from-repulsion, KL-RPA mechanism fulfills these criteria, as shown in Figure 1, it yields critical temperatures in twisted and non-twisted graphene multilayers in agreement with experiments, and, more importantly, it reproduces reasonably well the global trend observed in graphene stacks within two orders of magnitude. Our approach has being used to describe emergence of SC in transition metal dicalcogenides[4]. We also predict SC in helical TTG[5] and Terbium doped single layer graphene (SLG)[6].

In this talk, I will give an overview and an unified theoretical methodology to describe unconventional SC in twisted graphene systems as bilayers[1], trilayers[5,7], doble bilayers[5] as well as in non-twisted systems of graphene like doped monolayers[6], Bernal bilayer[8,9], rhombohedral trilayer[8,10] and tetralayers[8].

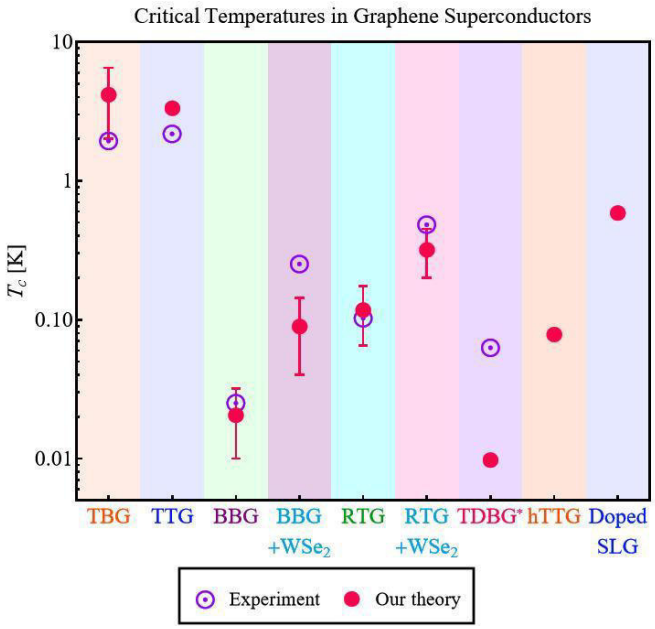

Figure 1.- Superconducting critical temperature obtained with our KL-RPA approach (red dots) and experimental values (purple circle-dot). Error bars indicate the variation with different model parameters. Our predictions for hTTG and Doped SLG are waiting for experimental confirmation. Figure adapted from Herrera S. *et.al.* arXiv:2408.05271 (2024)

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Fragile and orbital-obstructed topology in threefold-symmetric two-dimensional materials

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The signatures of fragile and higher-order orbital-obstructed topological phases are systematically studied in a number of nonmagnetic two-dimensional materials belonging to space group P-3m1, most of them transition metal dichalcogenides. Using group theory analysis in the framework of topological quantum chemistry, as well as a minimal tight-binding models and first-principles calculations, fragile topological bands near the Fermi level are reported for all the materials studied [1]. In these two-dimensional topological systems, corner states hosting fractional corner charges can arise [2]; we report the presence of anomalously filled corner states, that can be foreseen from the bulk configuration. Several material examples are presented to illustrate the ubiquity of these nontrivial features, and each particular ground state configuration is discussed [3].

Additionally, we present a list of threefold-symmetric two-dimensional material candidates that host fragile and obstructed topology, and their potential signatures. The presence of these topological phases, specially orbital-obstructed topology, is particularly interesting since their corresponding material realizations are scarce. Our work aims to broaden the scope of experimentally accessible materials with these topological features.

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Ferroelectric hysteresis in Moire single layer Graphene/hBN heterostructure

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Abstract

Ferroelectric materials have the unique ability to maintain and reverse electric polarization with an external applied electric field, making them valuable for applications such as non-volatile random-access memory, transducers, actuators and electro-optic modulators.[1] Traditionally, this property was thought to be exclusive to insulating materials, as insulators are crucial for sustaining polarization and enabling field-induced switching. However, recent research on two-dimensional (2D) material has shown that ferroelectric properties can also exist in semiconductors and metals.[2] Recently, emergent unconventional ferroelectricity has been demonstrated in the moiré superlattices of bilayer graphene and hexagonal boron nitride (hBN), hosting non-centrosymmetric stacking order [3,4]. Whether such phenomenon can persist in non-centrosymmetric single layer graphene (SLG)-hBN moiré superlattices has still remained elusive. Here we demonstrate a ferroelectric response in SLG-hBN moiré superlattice. Through Hall measurements, we pinpoint the origin of the hysteretic behavior to abnormal charge screening due to the moiré superlattice band and estimate the spontaneous polarization magnitude moiré in the superlattice structure. Temperature dependence measurement confirming hysteretic behavior persists from 2K to room temperature, offering further opportunities for high-mobility, ultrathin non-volatile devices.

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Figures

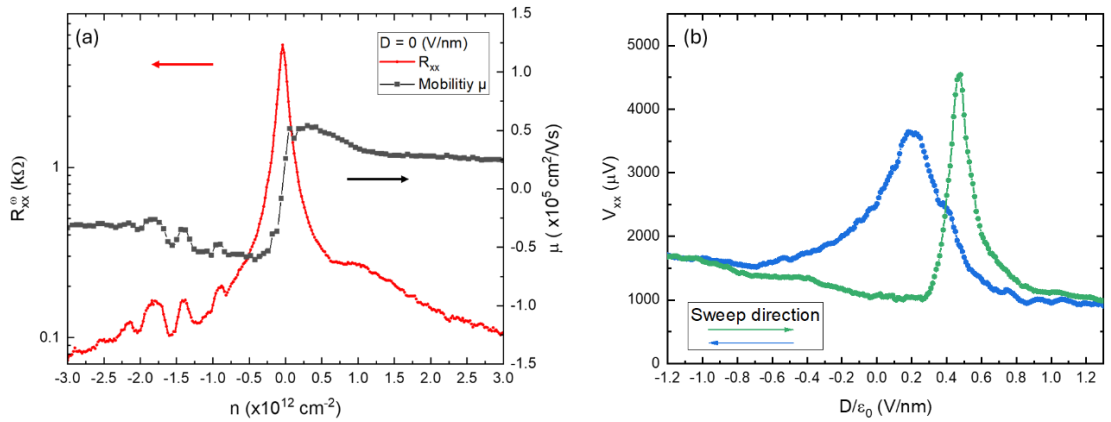

Figure 1: (a) Transport properties of moiré graphene/hBN heterostructure. (b) Hysteretic behavior while sweeping displacement field D at fixed carrier concentration.

Dimensionality control of magnetotransport properties in La0.7Sr0.3MnO3 [111] epitaxial ultra-thin films.

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Transition metal oxides interfaces offer a unique platform to explore many novel phenomena and functionalities that cannot be attained in bulk form. These epitaxial heterostructures have been predominantly grown along the perovskite [001] direction. However, the crystallographic [111] direction has emerged as a new frontier in material science due to the possibility of creating unique interfacial engineering thanks to the stronger oxygen octahedral coupling at the interface, and because it can be used for geometrical lattice engineering [1,2], which can create novel strongly correlated and topological states [2].

In this work, we have studied magnetic and transport properties of high quality $La_{0.7}Sr_{0.3}MnO3$ epitaxial ultrathin films of different thicknesses grown on [111] and [001] direction. While all [001] LSMO samples present an ordinary Hall Effect dominated by holes, reducing the thickness of the [111] samples produce a change in the sign of the Hall coefficient R_H (from positive to negative) at low temperatures. This change indicates a reduction of hole mobility, consistent with an enhancement of the electron correlations, which has been proposed in similar perovskite oxide grown in [111] direction [3]. Moreover, although samples in both orientations exhibit very similar magnetic properties (magnetic moment, anisotropy…), [111] films show an enhancement in the anomalous Hall effect (AHE) at low temperature in the thinner samples ($t < 10$ nm). Our results indicate that dimensionality plays an important role in the magnetotransport properties of $La_{0.7}Sr_{0.3}MnO3$ [111] epitaxial ultrathin films.

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Optoelectronics of magic-angle twisted bilayer graphene *pn*-junctions

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Magic-angle twisted bilayer graphene hosts flat electronic bands where exotic ground states appear, driven by electronic correlations. Here, we study the electronic and phononic structure of MATBG by probing its optoelectronic response. First, we study the thermoelectric transport in the flat bands, governed by the Seebeck coefficient. We leverage the extreme sensitivity of the Seebeck coefficient to electron-hole asymmetry to inspect the electronic spectrum of correlated states in MATBG. Our devices are optically excited pn junctions on high-quality MATBG samples. Our findings reveal strong asymmetry of the low energy bands at the correlated states which can be naturally attributed to the co-existence of incoherent and coherent excitations in the electronic spectrum of MATBG[1]. Second, we investigated the dynamics of the hot carriers in MATBG through time-resolved optical measurements of the electronic temperature. Combining two complementary techniques (CW photomixing and time-resolved photovoltage) we resolved ultrafast cooling time for hot carriers in MATBG, even at cryogenic temperatures where the cooling time of non-twisted graphene slows down due to reduced phonon density. We propose a novel scattering mechanism between hot carriers and moire phonons to account for our observations[2].

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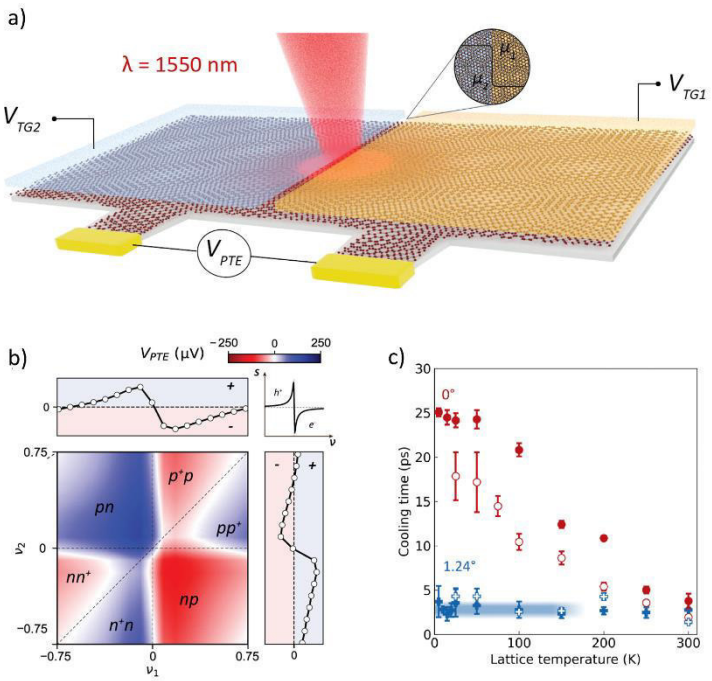

Figure 1: a) Schematic representation of the experiment, where a gate-defined *pn*-junction is excited by a near-infrared continuous-wave laser, inducing a hot carrier distribution in the system. b) Photo-thermoelectric response of magic-angle twisted bilayer graphene around its Dirac point. c) Carrier cooling time as a function of lattice temperature for Bernal-stacked bilayer graphene and magic-angle twisted bilayer graphene, where the latter strikingly exhibits ultrafast cooling down to cryogenic temperatures.

Electromechanical modulation of light using MoS_2 MEMS

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In this work we report frequency and amplitude modulation of visible laser beams using micro electromechanical systems based on two-dimensional drum resonators. These devices have been extensively studied in the last years due to their high quality factors and potential applications in sensing and signal transduction [1, 2]. Using few-layer MoS_2 flakes suspended over microcavities of different shapes carved in SiO_2/Si we manage to couple the mechanical modes of the resonator to the optical cavity. This allows us to increase the optical contrast and modulate the amplitude of the incident laser in the range of tens of MHz by electrical actuation of the resonator. Furthermore, the optomechanical coupling gives rise to the excitation of the mechanical modes by a CW laser beam without the need of electrical actuation. The excited mode order depends on the excitation point and its frequency can be tuned by the power of the incoming light. These developments highlight the potential of two-dimensional drum resonators as compact electromechanical systems for integrated photonics.

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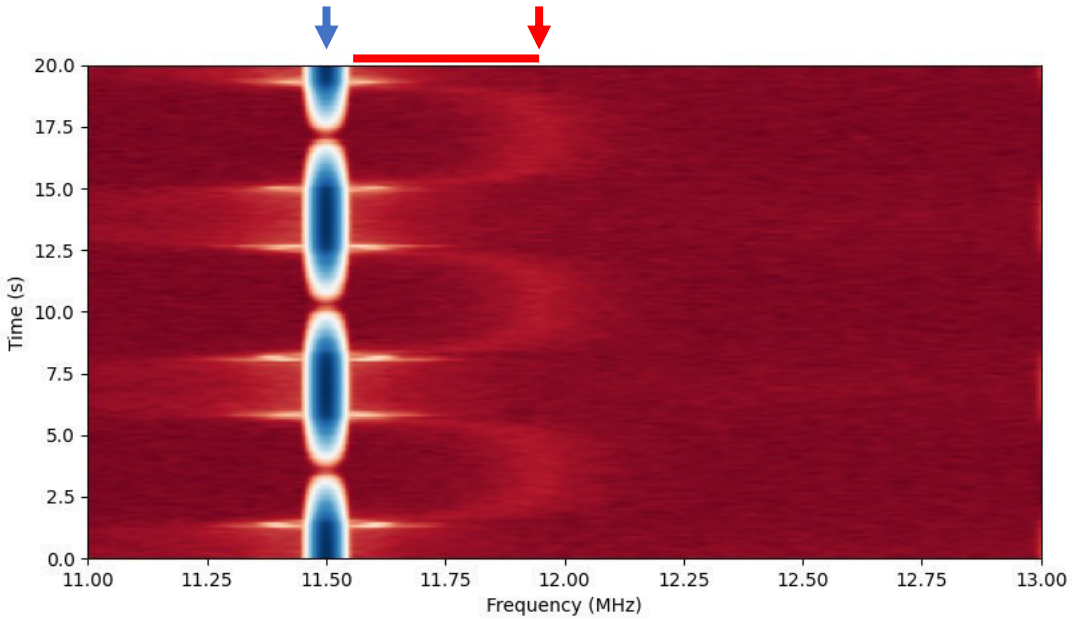

Figure 1: RF spectrum of reflected signal from a MoS_2 drum resonator illuminated with a 532 nm CW laser (2 mW) and driven by an amplitude-modulated 11.5 MHz RF signal. The electromechanical response is transduced as an amplitude modulation of the reflected signal at the actuation frequency (blue arrow). The optical response from the coupled optomechanical resonator (red arrow) is shifted towards the driving frequency as the amplitude increases.

Alternative materials to coarse grained W for plasma facing applications in nuclear fusion reactors

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Nuclear fusion is a promising option for future large-scale green energy supply fitting squarely into the 2030 agenda within the sustainable objective goals. There are two main approaches to fusion energy: magnetic confinement fusion (MCF) and inertial confinement fusion (ICF). Both of them achieved important milestones during 2022 (long plasma confinement times and ignition with gain, respectively), supporting that the scientific community is on the right path to make fusion energy a reality. These breakthroughs have motivated a notable increase in public and private funding for the development of projects aimed at the conceptualization of commercial power plants.

Despite the achievements, there are still a number of several challenges that need to be addressed prior to up-scaling to a commercial facility. One of them is the development of plasma facing materials (PFMs) able to withstand the combined effects of large thermal loads and radiation environments taking place in these reactors.

In this contribution, we will show the different radiation environments that PFMs have to withstand in MCF and ICF reactors [1]. We briefly introduce the limitations of coarse-grained W acting as PFM in both fusion approaches [2]. Finally, based on a combination of experimental and multiscale computer simulation data, we will discuss the capabilities and limitations of alternative W-based materials to act as PFM: nanostructured W, with a large density of grain boundaries [3–6], and W nanocolumns, with a large surface area [7–10].

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Biological interaction *in-vitro* cancer cells-magnetic nanodisks

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Magnetic particles are increasingly valuable in biomedicine for cell manipulation, targeted drug delivery, advanced diagnostics, and therapeutic innovations. Among these, disk-shaped magnetic nanodisks (MNDs) show exceptional potential due to their high magnetic moments and shape anisotropy, which make them ideal for applications involving mechanical stimulation [1]. These properties may affect biological processes like neuron signaling [2] or even targeted cell destruction [3].

MNDs in a spin-vortex state were fabricated using top-down lithography techniques, combining interference lithography and electron beam evaporation to create Permalloy ($Ni_{80}Fe_{20}$) disks with diameters of 300 and 700 nm and a thickness of 50 nm. Gold protective layers were added to prevent oxidation and enhance biocompatibility. The MNDs were characterized with scanning electron microscopy (SEM) for morphological analysis and SQUID magnetometry to confirm the spin-vortex configuration and quantify nanodisk concentrations.

MND-cell interaction has been investigated in vitro using SQUID magnetometry, SEM, cryo soft X-ray tomography and immunofluorescence assays. We have quantified MND internalization and externalization on skin cancer cells for both dimensions to understand cellular uptake dynamics.

Findings show that both cell-disk interaction and cellular dynamics depend on both MND morphology and cell metabolism, providing insights into optimizing MND size, surface functionalization, and internalization timing for magnetic field treatments for cancer disease.

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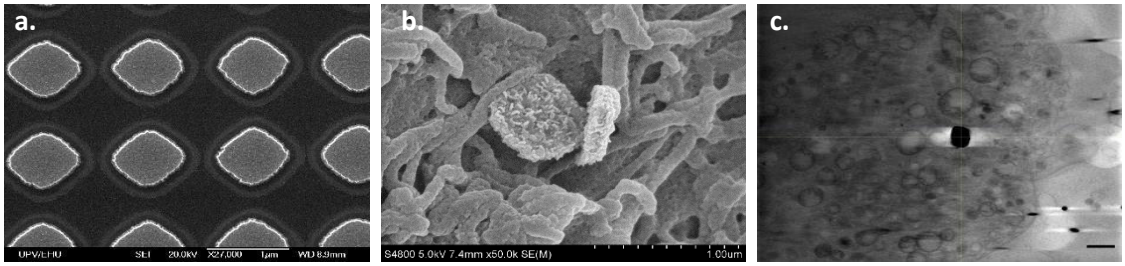

Figure 1: SEM images of MNDs with a diameter of 700 nm and a thickness of 50 nm, shown (a) in an array on the silicon wafer, and (b) interacting with the microvilli of a tumor cell membrane. (c) Cryo Transmission X-ray image of MNDs inside the cellular cytoplasm. Scale bar 1µm.

4D-STEM for the observation of emergent phenomena in complex oxide heterostructures

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Complex oxide heterostructures present platforms with a wealth of exotic interactions to explore, owing to the interplay between degrees of freedom associated with the physical and electronic structures of their constituent materials. Such interactions can lead to emergent phenomena that are not observed in their individual bulk counterparts, such as two-dimensional electron gases, or interfacial superconductivity [1]. Particularly, in heterostructures with ferroelectric materials, the organization of domains arises from the combination between strain imposed by the non-matching crystal structures at either side of the interfaces and the polarisation of interfacing domains. Reducing the thickness of the ferroelectric layer to a few unit cells further modifies the system's interaction between the layers and may trigger the appearance of exotic phenomena. [2]. Here, the interplay between the electrostatic and mechanical boundary conditions can be responsible for stabilising complex polar structures like charged domain walls [3] or topological polar structures such as vortices [4].

In this work we show the potential of scanning transmission electron microscopy to harness the physical properties of such systems. The STEM offers detailed structural and chemical analysis of samples down to atomic resolution, moreover, recent advances in detector technology expanded the capabilities of this technique. The recent ability to acquire full probe diffraction patterns (4D-STEM) has enabled high-resolution phase, orientation and strain mapping, as well as phase-retrieval methods which allow for resolution improvements or the imaging of electromagnetic features [5]. These methods can be used to conduct an extensive characterisation of the structure and the electrostatic configuration of interfaces in complex oxide heterostructures, increasing our understanding of the mechanisms behind the emergent phenomena in these systems. However, analysis of such measurements often requires large computational efforts due to large dataset sizes, complex interference effects observed in diffraction space, and experimental artifacts, such as instrumental noise and electron lens aberrations. For these reasons, machine learning algorithms are now being developed to improve and automate the analysis of 4D-STEM datasets, increasing the depth of information that can be obtained from experimental observations.

In this work, a 4D-STEM investigation of emergent phenomena in complex oxide heterostructures is presented, based on a detailed treatment of experimental and simulated datasets to detect and analyse relevant features.

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GEFES 2025

Optical Studies in Van der Waals Heterostructures using Micro-Photoluminescence

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Transition Metal Dichalcogenides (TMDs) are a family of semiconductors characterized by a layered structure, which enables mechanical exfoliation down to the monolayer limit. In this single layer conditions, TMDs exhibit a direct band gap within the visible spectrum and support the formation of excitonic quasiparticles at room temperature, namely the exciton (X^0), charged excitons or trions ($X^{\pm}$) and biexcitons (XX) among others. These properties lead to significant light absorption and complex light-matter interactions. TMDs are held together by van der Waals forces, which allow for the stacking of monolayers to obtain heterostructures using the dry transfer method. Thanks to the stacking, interactions between layers allow for interlayer excitons (IX) to form [1]. Additionally, it facilitates the creation of moiré superlattices and moiré excitons (MX), enhancing the optical tunability and properties of these heterostructures [2].

In this work, we exploit the above properties of 2D materials, stacking them to create heterostructures with tailored optical properties. We fabricated type II heterostructures composed of hexagonal boron nitride (hBN), tungsten disulfide (WS_2), and tungsten diselenide (WSe_2). Photoluminescence (PL) spectroscopy is employed to study the formation of excitons in these heterostructures and the effect of twist angle between the monolayers and annealing on the excitonic formation and emission. Low-temperature PL measurements were performed to understand the excitonic complexes originating in these heterostructures. Mainly, incident power dependence and incident light polarization angle dependence measurements were carried out to map the excitonic emissions of the heterostructure to the different excitonic complexes present in these heterostructures [3].

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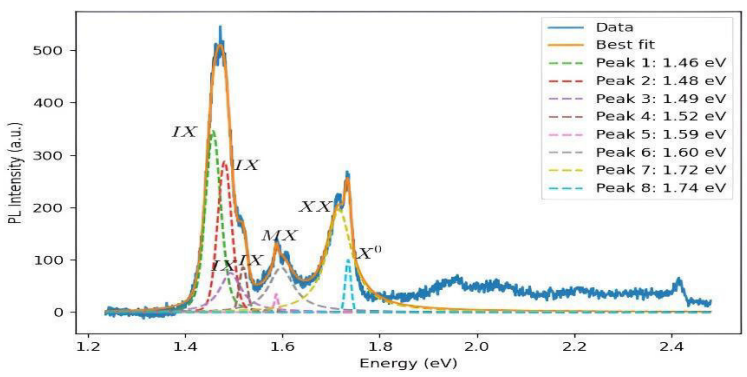

Figure 1: Preliminary results of a $hBN/WS_2/WSe_2/hBN$ heterostructure measured at 4K using photoluminescence spectroscopy with a 532nm laser with an incident power of $400\mu W$

High responsivity THz graphene detector embedded in a Fabry Perot cavity

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Terahertz (THz) technologies have recently gained attention due to their wide range of promising applications, for example for non-destructive imaging of polymers, sensing and for next generation (6G) wireless communication. However, developing efficient THz photodetectors represents a challenging task, with conventional devices typically suffering from operation at cryogenic temperatures, difficult integration with CMOS platforms, a relatively low responsivity or a slow response. Recently, graphene-based photodetectors have emerged as a promising platform to implement compact THz detectors with low energy consumption, CMOS-compatible, while offering a high responsivity and a fast response [1,2].

In our recent work [3], we developed an hBN-encapsulated graphene photodetector integrated inside a sub-THz Fabry-Perot cavity, designed to strongly enhance the absorption of incoming sub-THz light and thereby the detector responsivity. The absorption enhancement occurs in combination with a dipolar antenna that gates two sides of the graphene channel to create a pn-junction while focusing the incoming sub-THz light on the photo-active area in the junction. The absorbed THz radiation heats up electrons [4] and leads to the generation of a photo-thermoelectric current in the device due to the varying Seebeck coefficient across the pn-junction. The resonant cavity, whose thickness matches one quarter of the sub-THz wavelength, is formed mostly by the silicon substrate with the dipolar antenna on one end and a metallic back mirror on the other end. This cavity plays an important role in increasing the absorption in the photoactive region at the graphene. We obtain an enhanced responsivity at the cavity resonance, as compared to the reference case that does not include the sub-THz cavity. These results pave the way for high-responsivity passive sub-THz detectors for a plethora of applications.

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Micromagnetic simulations of domain walls dynamics and Spin Waves propagation in FeB stripes.

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Micromagnetic simulations have been conducted using MuMax3 code [1] in order to investigate the characteristics of the magnetization structures stabilized in high aspect ratio magnetic stripes due to the local induction of a transverse-to-the-stripe-long dimension magnetization easy axis. These structures have been shown to be responsible of phase-shifting for longitudinally propagating spin waves [2,3]. To this end, a systematic study of the structure, symmetry and dimensions of the afore mentioned structures was performed as a function of the width and thickness of a stripe with a length of 100 µm, employing the magnetic parameters of FeB. The results are summarized in Figure 1, which identifies the regions at which specific energy minimizing structures occur.

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Figures

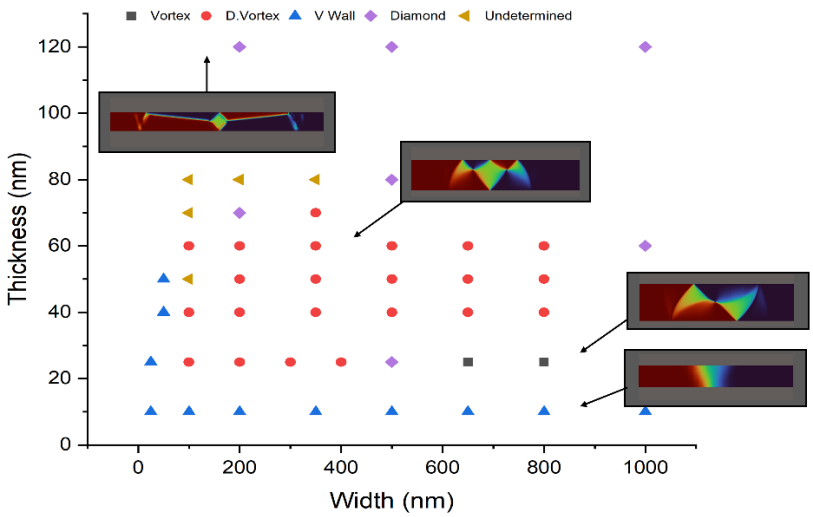

Figure 1: Energy minimizing structures identification as a function of the stripe thickness and width.

Thermal and electrical transport at the nanoscale

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The limited sensitivity and resolution of current thermal sensors pose a fundamental obstacle to conduct thermal measurements at the nanoscale. Addressing this challenge requires the development of advanced instruments capable of detecting minute temperature variations across nanometer-scale junctions [1]. Progress in nanoscale thermal measurement techniques hinges on overcoming the inherent limitations of existing sensor technologies through innovative methodologies and approaches that enable accurate thermal, electrical, and thermoelectric measurements [2,3].

In this talk, I will detail how commercial Pt and $PtRh_{10}$ Wollaston wires can be used to develop thermoelectric-resistive sensors using micromanipulation and welding techniques, along with a patented novel in-situ calibration method [4] using the Peltier effect generated at the welded junction of the two wires.

Integrating these thermoelectric-resistive probes to an AC-STM under High Vacuum (~2×10^{-6} mbar) conditions enables the direct simultaneous measurement of the thermal and electrical conductances in various transport regimes, from tunneling to contact [5]. With a resolution of 0.1 nW/K, the thermoelectric-resistive sensors enable the detection of the thermal conductance of metallic gold atomic junctions, as well as the contributions of adsorbates to thermal transport several nanometers before electrical contact is established. Complementary, molecular dynamics simulations suggest that water is the dominant adsorbate, yielding thermal conductance values consistent with experimental observations.

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Improved real-time propagators for a moving basis in SIESTA

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When dealing with the time-dependent Schrödinger equation (or the Kohn-Sham equation in the density-functional context) for the study of the dynamics of any system using a non-orthogonal basis set that evolves with time, it is essential to account for that basis set evolution. In the SIESTA code [1] the Crank-Nicholson algorithm has been used quite successfully to solve these equations [2]. It includes two different approaches for dealing with moving basis set: the Löwdin orthonormalization [3] and the affine connection [4] methods. The first one was proposed by Sankey and collaborators. It orthonormalizes the basis before displacing the nuclei with a Löwdin transformation (using the $S^{-1/2}$ matrix, S being the overlap), then moves the atoms (and the basis orbitals) keeping the coefficients, and then it undoes the transformation for the displaced basis. It has shown good performance and fidelity for low-velocity dynamics.

The affine connection method extends the time-dependent Schrödinger equation to include the evolving basis effects through the D-matrix, where $D_{\mu\nu} = < e_\mu \mid \delta_t \mid e_\nu >$. This modifies the Hamiltonian as $H - iD$, where D can be seen as introducing a gauge potential that modifies the dynamics [5]. While the affine connection method offers superior accuracy for high-velocity dynamics, it does not strictly conserve unitarity for arbitrarily long-time steps [4] (Sankey's method does).

There have been several techniques proposed and tried for improving the efficiency of the integration for static basis sets, using modifications of the algorithm keeping the accuracy for longer time steps. They were trivially extended to the moving basis problem for the Löwdin method. We have extended and tested those techniques to the affine connection method. In particular, results for tests for the extrapolation and two-step schemes [3] will be presented.

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Fabrication and study of freestanding $SrRuO_3$ thin films

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The emergence of novel collective states in twisted freestanding bilayers has attracted significant interest for their unique physical properties. Recent studies have shown that in twisted oxide ferroelectrics polar topologies appear with the modulation of the underlying Moiré pattern [1, 2]. In this communication we investigate remote Moiré interaction in twisted perovskite oxide ferromagnets. Our focus is on the transition metal oxide $SrRuO_3$ (SRO), known for its itinerant ferromagnetism, perpendicular magnetic anisotropy, and strong spin–orbit coupling. The SRO samples are grown epitaxially via pulsed laser deposition (PLD), with $La_{0.7}Sr_{0.3}MnO_3$ serving as a sacrificial layer to enable the detachment of freestanding flakes.

It is well established that many properties of SRO—such as the Curie temperature, magnetic easy axis, and anomalous Hall conductivity—can be modulated by epitaxial strain, due to the strong coupling between lattice distortions and the electronic structure [3] enabled by the spin orbit interaction. In this work, we study how strain release affects the physical properties of freestanding SRO through electronic and magnetic measurements. Notably, some properties of the freestanding SRO appear to be modified compared to the strained material. To understand this behavior, we explore potential underlying mechanisms. Some studies suggest that strain from the sacrificial layer may persist in the flake after separation [4], although establishing a clear correlation remains challenging. Additional factors, such as device fabrication or processing could further alter the lattice parameter and, consequently, the fundamental properties of SRO.

Furthermore, we explore the potential for generating polar topologies in non-ferroelectric materials. Recent work by Wei Peng et al. [5] demonstrated the induction of flexoelectric polarization in $SrRuO_3$ (SRO) heterostructures, paving the way for investigating polar structures in freestanding SRO. To this end, we prepared bilayers of SRO with varying twist angles. Scanning Transmission Electron Microscopy (STEM) is used to resolve the atomic positions within each layer, and special attention is paid to the off-centering of Ru atoms within individual unit cells, as this displacement could indicate induced polarity arising from interlayer interactions in the bilayer system.

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Atomic-scale mapping of superconductivity in the incoherent CDW mosaic phase of a transition metal dichalcogenide

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The emergence of superconductivity in the octahedrally coordinated (1T) phase of TaS_2 is preceded by the intriguing loss of long-range order in the charge density wave (CDW). Such decoherence, attainable by different methods, results in the formation of nm-sized coherent CDW domains bound by a two-dimensional network of domain walls (DW)-mosaic phase-, which has been proposed as the spatial origin of the superconductivity. Here, we report the atomic-scale characterization of the superconducting state of 1T-TaSSe, a model 1T compound exhibiting the CDW mosaic phase. We use high-resolution scanning tunneling spectroscopy and Andreev spectroscopy to probe the microscopic nature of the super conducting state in unambiguous connection with the electronic structure of the mosaic phase. Spatially resolved conductance maps at the Fermi level at the onset of superconductivity reveal that the density of states is mostly localized on the CDW domains compared to the domain walls, which suggests their dominant role in the formation of superconductivity. This scenario is confirmed within the superconducting dome at 340mK, where superconductivity is fully developed, and the subtle spatial inhomogeneity of the superconducting gap remains unlinked to the domain wall network. Our results provide key new insights into the fundamental interplay between superconductivity and CDW in these relevant strongly correlated systems.

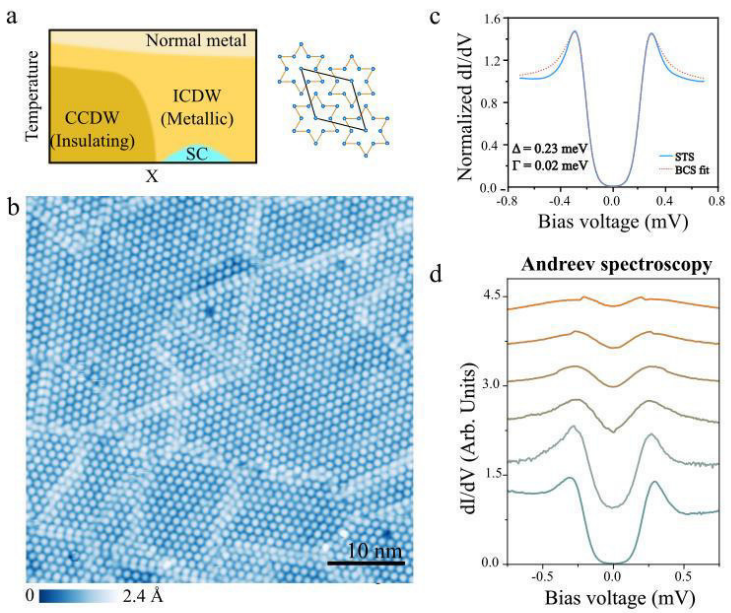

Figure 1: Mosaic CDW and superconductivity in 1T-TaSSe.

Intrinsic Stripe Charge Density Wave in 4Ha-$NbSe_2$

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Polytypism in transition metal dichalcogenides (TMDs) refers to distinct structural variations that emerge due to different stacking sequences of their atomic layers. These structural variations play a crucial role in determining the electronic properties of TMDs. For instance, $NbSe_2$ has two stable polytypes that share common ground in exhibiting charge density waves (CDW) and superconductivity, the $2H_a$ polytype (normally referred to as 2H) of space group $P6_3/mmc$ and the $4H_a$ polytype (space group P-6m2 with no central inversion symmetry). However, the additional complexity of $4H_a$'s stacking sequence may lead to significant differences in the CDW and superconducting properties between the two polytypes.

Using high-resolution scanning tunneling microscopy and spectroscopy (STM/STS) at 340 mK, we carried out the characterization of the CDW and superconductivity phases of $4H_a$-$NbSe_2$ in comparison with the well-known 2H-$NbSe_2$ polytype. In the $4H_a$ polytype, we uncover a striking striped, CDW pattern of wavelength of $\lambda \approx 3.5a$ (a the lattice parameter), corresponding to a k-vector of $q = \frac{2}{7}\bar{Q}_0$ with $\bar{Q}_0$ the Bragg vector. Surprisingly, the striped phase is observed uniformly over the entire surface and, while it coexists with the 3×3 phase, it clearly dominates over the latter configuration. This result is in stark contrast to the CDW in the 2H polytype, where the ground state is the 3×3 CDW and the striped pattern only appears under external strain [1]. This result highlights the crucial role of stacking order and structural anisotropy in stabilizing distinct CDW configurations, with the $4H_a$ structure naturally favoring the striped pattern without external perturbation. Regarding the superconducting phase, our STS data reveal that the $4H_a$ polytype is also a two-band superconductor but with gap sizes $\Delta_1 = 0.35$ meV and $\Delta_2 = 0.98$ meV, which are smaller than those of the 2H polytype and that result from a more complex Fermi surface [2].

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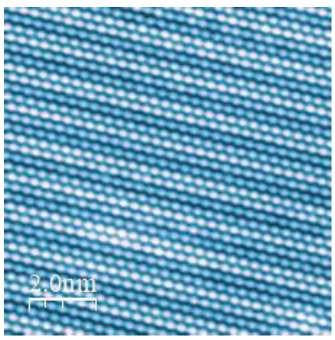

Figure 1: Intrinsic stripe order in $4H_a$-$NbSe_2$

GEFES 2025

Graphene Quantum Dots as Quantum Materials for Optoelectronics, Spintronics, and Sensing

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Graphene Quantum Dots (GQDs) stand out as quantum materials with unique properties arising from quantum confinement and edge-state effects [1, 2]. As nanoscale graphene fragments, GQDs offer tunable electronic and spin characteristics, making them prime candidates for applications in optoelectronics, spintronics, and sensing [3]. Here, we demonstrate synthesis routes to obtain high-quality GQDs, including those prepared from CVD-derived graphene and controlled chemical assembly, yielding crystalline structures with controlled sizes and diverse edge configurations. We performed various high-resolution characterizations—using HRTEM, Raman spectroscopy, XPS, and EELS—to provide detailed insights into their atomic structure and electronic composition [4, 5]. Also, we present theoretical models that predict critical size thresholds and edge configurations for the emergence of robust edge states in GQDs. We demonstrate real-world applications of GQDs in the environmental and energy sectors, including efficient photodegradation of industrial contaminants for wastewater treatment, selective fluorescence detection of Hg^{2+} and Fe^{3+}, and enhanced solar energy harvesting using GQDs as co-sensitizers, highlighting not only their potential for spintronic and quantum devices but also their versatility in monitoring and renewable technologies [6-8].

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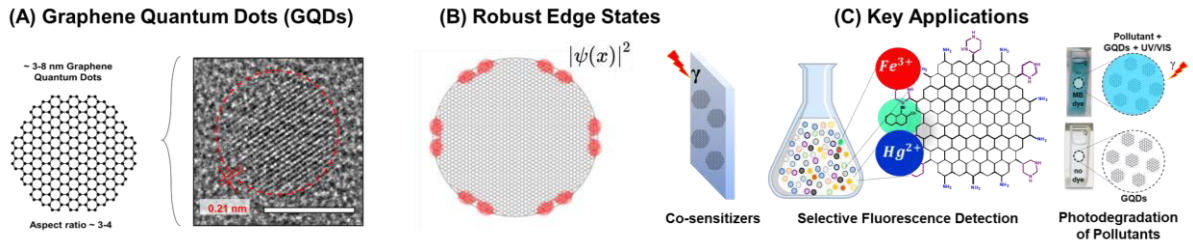

Figure 1. (A) High-resolution TEM image of GQDs showing crystalline structure; scale bar 5 nm. (B) Schematic of quantum confinement and edge states in GQDs. (C) Key applications of GQDs.

Magnetic Structure Investigation of the Ternary Rare-Earth Based Compound TbFeSi

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In recent decades, magnetocaloric materials have proven to be more efficient and environmentally friendly than traditional gas compression technology. RFeSi intermetallic compounds (where R represents a rare earth element) have an application range between 10 and 150 K, which makes them suitable for hydrogen liquefaction. These compounds exhibit a second-order magnetic transition that varies with the radius of the rare earth element [1]. They crystallize in a tetragonal cristal structure with the *P4/nmm* space group, where R and Si occupy the 2*a* Wyckoff position and Fe occupies the 2*c* Wyckoff position [2]. However, the thermal treatments required to obtain a single phase are expensive and time-consuming (taking 35 days at 1373 K) [1]. In this context, the melt spinning method emerges as a fast and easy technique for obtaining single and nanostructured phases.

In this work, we investigate the magnetic structure of TbFeSi ribbons produced by this melt spinning method, using magnetic measurements, neutron powder diffraction and Density Functional Theory (DFT) calculations. Through ZFC-FC measurements, the magnetic ordering temperature was determined being 130 K, 20 K higher than in polycrystalline bulk state. Furthermore, we obtained the magnetization of saturation to calculate the magnetic moment from isothermal magnetic measurements. We have also studied the evolution of the volume with temperature, revealing anomalous behaviour around the Curie temperature (T_C), related to magnetovolume effects. These effects were evaluated through the spontaneous volume magnetostriction, which showed negative values in this range. In contrast to previous neutron analyses, the Fe atoms exhibit a non-zero magnetic moment with antiparallel coupling with Tb ions. This finding aligns with the value obtained from the approach to saturation law and band structure calculations.

Acknowledgements

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Neural-network wave functions for quantum many-body models

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While the race for breakthroughs in quantum computing continues, classical techniques are simultaneously expanding their capabilities to tackle more difficult challenges. The rapid development of machine learning has led to neural networks establishing themselves as efficient ground state ansätze for quantum many-body systems [1]. In this talk, we will explore how the use of such neural quantum states, particularly those generated with the game-changing transformer architectures [2], in conjunction with variational quantum Monte Carlo techniques, allow us to reproduce the phase diagrams of Ising-type models with long-range interactions [3,4], to elucidate the nature of the phase transition (first or second order), or to tackle frustrated models such as the elusive spin liquids [5] – a challenge even for established techniques like matrix product states (MPS), dynamical mean field theory (DMFT), or tensor networks. The inherent flexibility in constructing different types of neural networks enables us to circumvent issues like the sign problem characteristic of frustrated systems—an Achilles' heel of other quantum Monte Carlo methods—or to reproduce correlation lengths that exceed those achievable with DMFT. Those techniques can also be useful in connection with experiment, assisting for instance in the characterization of real materials believed to exhibit physics consistent with spin liquids, like 2D heterometallic oxalate complexes [6].

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ZX Christmas Trees: a graphical diagnose of topological order

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The topological entanglement entropy γ [1,2] of a system's bipartition (A,B) as in Fig.1a, is a key diagnostic of the type of topological order, as it measures long-range entanglement. However, γ is not universal [3,4], and can be computationally expensive to obtain. In this work, we introduce a new characterization of topological order, which helps to circumvent practical and non-universal issues in computing γ. The boundary-reduced density matrix $\rho_{\partial A}$ is a reduced density matrix that keeps the relevant degrees of freedom at the boundary of the bipartition. When simplified as a ZX diagram, as we show in Fig.1b, it resembles a Christmas Tree, and has a number of non-local nodes which are related to γ.

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Figures

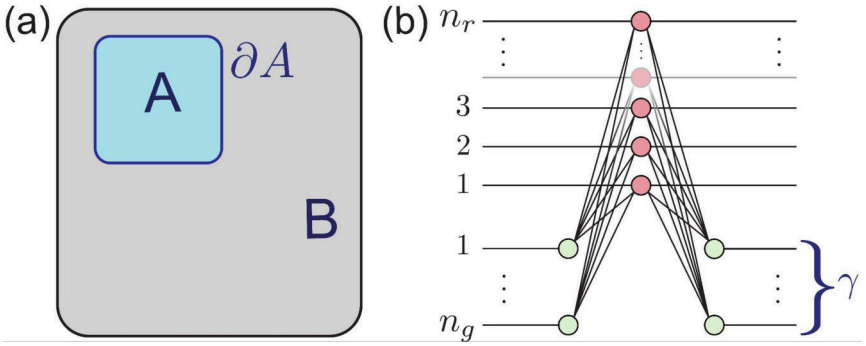

Figure 1: Schematic of how a ZX-diagram characterizes topological order. (a) Bipartition of a system into two regions A and B with a boundary ∂A. (b) The boundary-reduced density matrix $\rho_{\partial A}$ is equal to a ZX-diagram that resembles a Christmas tree. The bottom green node pairs connect non-locally to the red nodes, a signature of long-range entanglement. The total number of red nodes grows linearly with the number of relevant degrees of freedom at the boundary ∂A, while the total number of green node pairs n_g, is a topological invariant that characterizes the type of topological order. $n_g = 1$ for the square and hexagonal Toric codes, and $n_g = 2$ for the color codes, which match with the γ of the models.

Novel Approach for Normal Incidence Excitation of Out-of-Plane Lattice Resonances

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Two-dimensional periodic arrays of nanoparticles give rise to collective modes known as lattice resonances, which result from the mutual, coherent interactions between the individual nanostructures composing the array [1]. Specifically, out-of-plane lattice resonances correspond to those modes for which the nanoparticles in the system are polarized perpendicular to the plane of the array. Out-of-plane lattice resonances exhibit exceptional optical properties, including minimal losses, substantial field enhancements, and very high Q-factors, positioning them as ideal candidates for applications in nanotechnology and biosensing [2].

Due to their potential, it is of utmost interest to achieve an efficient excitation of out-of-plane lattice resonances. Earlier research efforts have employed oblique incidence excitation [3], although this approach comes with important disadvantages. Not only does it introduce experimental complexity, but it also compromises the properties and quality of the resonance. In turn, the use of normal incidence excitation would address these shortcomings; however, this strategy has been traditionally neglected based on the transversality condition of the electromagnetic field.

In this work, we introduce a novel methodology for the efficient excitation of out-of-plane lattice resonances in bipartite arrays of metallic nanoparticles at normal incidence [4]. Thanks to the electric-magnetic interaction between the nanostructures composing the array, we show that it is possible to achieve sharp resonances with outstanding quality factors (Fig. 1). Furthermore, we explore a potential application of our results by analyzing a periodic array of nanodisks, mounted on a substrate and embedded in a dielectric coating.

The conclusions of our study are broad and extendible to different lattice geometries and particle shapes, introducing a novel approach towards the efficient excitation of out-of-plane lattice resonances at normal incidence. This breakthrough opens up opportunities to harness their valuable properties in a wide range of applications.

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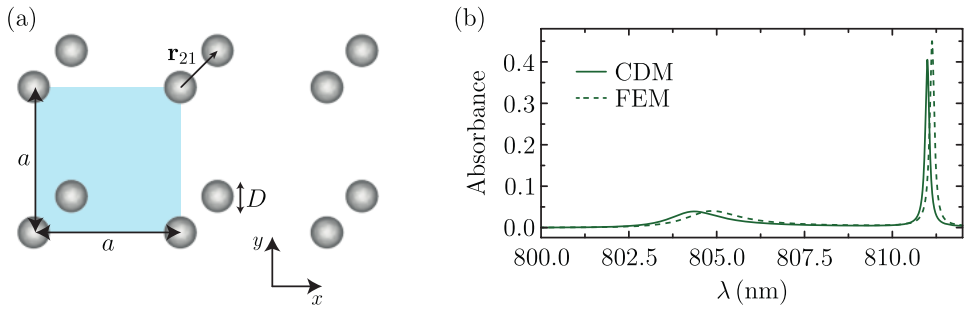

Figure 1: (a) Two-dimensional periodic, square array composed of silver nanoparticles, located in the XY plane. (b) Absorbance of the system for a = 800 nm, D = 160 nm, and $\mathbf{r}_{21}$ = (1,1,0)a/4. A very sharp and narrow out-of-plane lattice resonance appears at around 811 nm.

Inversion of the radiative heat transfer between rotating nanostructures

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The fluctuations of the electromagnetic field are responsible for the radiative heat transfer between material structures [1, 2]. Another phenomenon induced by the fluctuations of the electromagnetic fields is the Casimir forces and torques between neutral nanostructures, which can serve as a platform to transfer linear and angular momentum in the nanoscale [3, 4]. Despite their shared physical origin, radiative heat transfer and Casimir interactions are typically studied independently. In the former, nanostructures are usually considered steady, while in the latter, thermalized conditions are assumed. However, as we demonstrate in our study, Casimir interactions can exert a notable influence on radiative heat transfer.

In this work, we analyze the simultaneous transfer of energy and angular momentum in a pair of nanostructures with different temperatures, rotating around a common axis [5]. We find that, as a consequence of the rotation of the nanostructures, radiative heat transfer between them can be increased, decreased, or even reversed compared to the transfer in the absence of rotation, only determined by the temperatures of the nanostructures (See Figure 1). These results indicate the possibility of modulating radiative heat transfer between nanostructures through their motion.

Our study is grounded on the fluctuational electrodynamics framework, which we employ to derive analytical expressions for the force, torque, and power transferred between the nanostructures. This work unravels nontrivial phenomena stemming from the interplay between Casimir interactions and radiative heat transfer, paving the way for utilizing moving nanostructures to gain control over radiative heat transfer.

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Figures

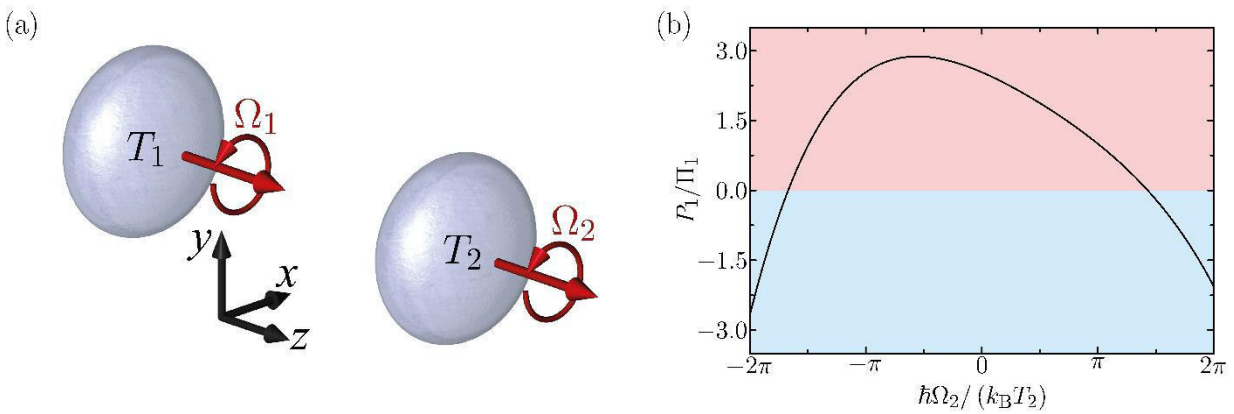

Figure 1: (a) Schematics of the system under consideration. (b) Power transferred between the nanostructures P_1, normalized to the power transferred in the absence of rotation Π_1, as a function of Ω_2 for $T_1 = 1.5T_2$, $\Omega_1 = \pi k B T_2/\hbar$. The red (blue) background indicates positive (negative) values of the normalized power transferred.

On the coupled magnetoelastic transition in $Fe_{49}Rh_{51}$ alloy using high-magnetic field- neutron thermo-diffraction experiments

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Fe-Rh alloys with near-equiatomic composition undergo a thermally and/or magnetically driven magnetoelastic phase transformation, around RT, from a low-temperature antiferromagnetic (AFM) state to a high-temperature ferromagnetic (FM) state [1, 2]. This first-order phase transition (FOPT) exhibits a hysteretic behavior on heating/cooling procedures. The unit cell volume increases by approximately 1.0%, while the crystalline structure (CsCl, B2-type) remains unchanged [1, 2]. Accompanying the FOPT, remarkable giant magnetocaloric and magnetostrictive effects emerge [2].

The aim of this work is to analyze the dynamics and spin-lattice coupling within the phase transition. Neutron thermo-diffraction (ND) experiments under a magnetic applied field up to 10 T have been carried out to investigate the FOPT in a bulk $Fe_{49}Rh_{51}$ metallic alloy. The evolution in zero-magnetic-field of both the lattice parameter and the AFM phase fraction with temperature reveals a kinetic arrest of the AFM phase, which coexists with the FM phase even 70 K above the FOPT. It is inferred that the structural and magnetic transformations occur simultaneously, evolving hand-in-hand across the FOPT. Further analysis of isothermal and iso(magnetic)field ND patterns evidence that the observed features mentioned above are intrinsic to the sample and remain unchanged under the influence of the applied magnetic field. We have used a new method based on the temperature first order reverse curve (T-FORC) applied to neutron thermo-diffraction measurements, to investigate in detail the evolution of the cell parameter and the AFM phase fraction in zero-magnetic-field (see Fig. 1) and under 8 T. Finally, the critical magnetic field required to induce the FOPT was determined from the isothermal evolution of the lattice parameter.

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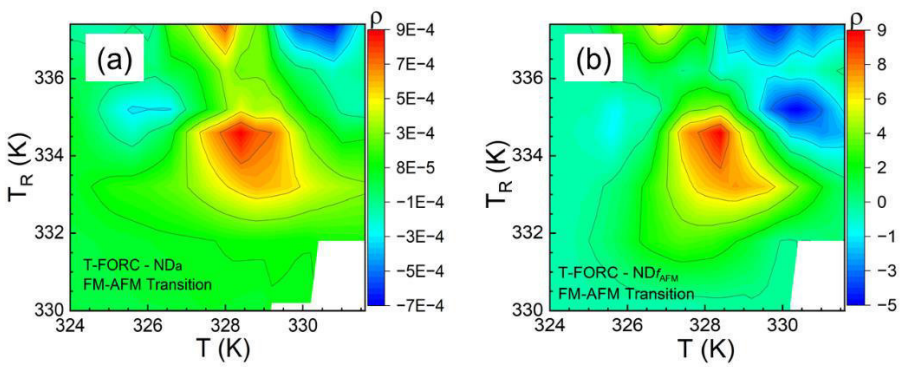

Figure 1: T-FORC distributions linked to the FM-AFM transition in terms of the temperature evolution of (a) the cell parameter *a*, and (b) the AFM phase fraction f_{AFM}.

Nano-scale Microscopy of GaN Nanowires for Optoelectronic Applications

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The development of high-quality GaN-based semiconductors has laid the foundation for advances in optoelectronics and high-frequency devices. Despite challenges in GaN growth due to defect-prone substrates, nanostructures, particularly nanowires (NWs), have emerged as a promising solution, enabling low-defect growth, enhanced strain relaxation, and improved light efficiency. GaN nanowires, which are valuable for applications in LEDs, lasers, and sensors, have been grown using Metalorganic Vapor-Phase Epitaxy (MOVPE) [1] and characterized through Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). Here we present the results of SEM and AFM measurements which reveal the hexagonal structure and orderly arrangement of the nanowires (Fig. 1a, b), with AFM providing detailed resolution of the nanowire edges. AFM measurements report a nanowire height of approximately 3.6 µm, differing from SEM estimates due to (i) the presence of a stabilizing medium used to support nanowire growth in fixed positions and (ii) the ~5 µm depth resolution limit of our AFM instrument. By imaging a scratched region of the sample with AFM, we obtained enhanced resolution of the hexagonal base of the nanowires. We estimated an average transverse (x-axis) diameter of ~735.7 nm and a vertical (y-axis) diameter of ~686 nm. Additionally, scratched nanowires imaged on a silicon substrate (Fig. 1c) displayed only three sides of the hexagon, as the AFM tip could not reach the area where the nanowire is leaning. These imaging techniques, along with Scanning Tunnel Microscopy, Raman spectroscopy, and, Kelvin probe force microscopy which are currently work in progress provide deeper insights into the nanowire growth process, defect structures and functional response for next generation devices.

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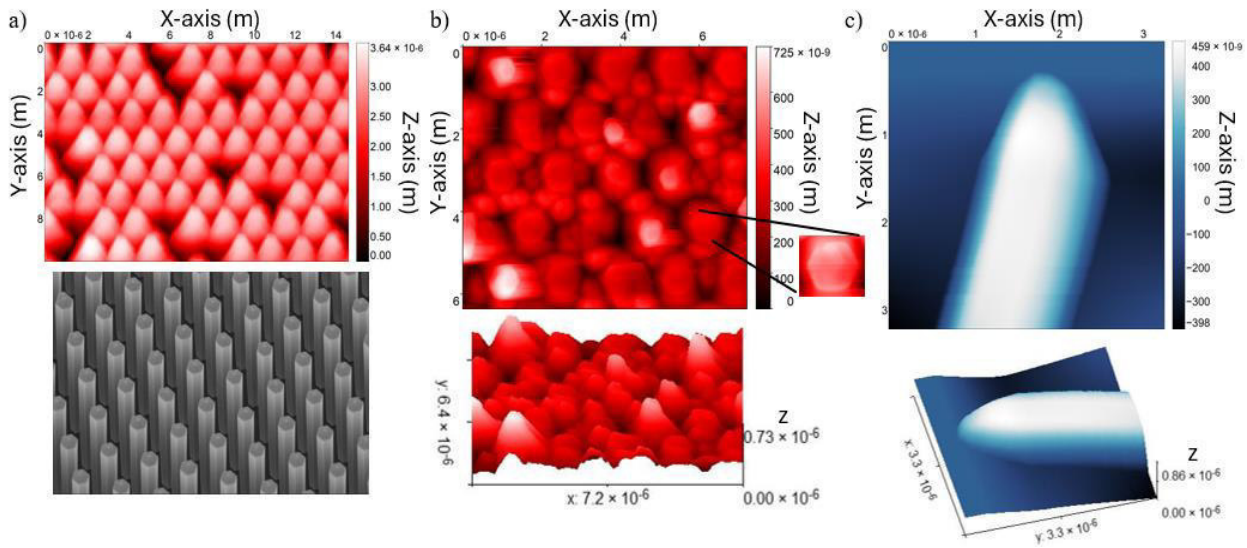

Figure 1: a) Comparison of AFM and SEM images for two regions of the sample. b) 2D and 3D images of the nanowire regions after scratching. The inset shows a typical nanowire base with a hexagonal shape. c) 2D and 3D images of one end of a nanowire after scratching, showing only three sides of the hexagon because the tip cannot reach the region where the nanowire is leaning.

Localized vibrational states in Silicon Grain Boundaries: phonon-lifetimes

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The study of heat transport in nanocrystalline silicon (nc-Si) is critical in materials science, particularly for understanding the profound influence of grain boundaries (GBs) on thermal conductivity. While mesoscopic models based on bulk phonon properties struggle to capture vibrational dynamics in nanostructured systems, microscopic approaches such as Non-Equilibrium Green's Function (NEGF), perturbation theory or *ab initio* molecular dynamics (MD) are limited by the large number of atoms required to describe GBs. Recently, machine learning interatomic potentials (MLPs) have emerged as a promising solution, offering ab initio accuracy with computational efficiency. However, the structural complexity of nc-Si introduces spatially localised vibrational modes (LVMs), which trap energy, impede heat flow and affect interfacial Kapitza resistivity. These modes can decay to bulk modes with weak coupling and extended lifetimes, significantly affecting thermal conductivity.

To study these dynamics, a supercell approach is used, which allows controlled excitation of specific vibrational modes and direct observation of their relaxation. This method mitigates thermal fluctuations, avoids artefacts from non-thermostatic techniques and allows detailed analysis of the LVM-bulk mode coupling. This coupling, although weak, can significantly affect thermal properties.

Here, we integrate state-of-the-art machine learning interatomic potentials [3] with the supercell approach to study LVMs on silicon GBs. We aim to elucidate their coupling with bulk modes and their broader impact on the electronic, optical and thermal properties of nc-Si.

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Advanced multi-purpose SPM lab at ALBA: enabling correlative experiments in controlled gas and liquid environments

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As part of the pioneering InCAEM initiative, a new Scanning Probe Microscopy (SPM) platform will be installed at the ALBA synchrotron facility. This platform, in combination with synchrotron radiation and electron microscopy techniques, will facilitate correlative experiments on advanced materials within controlled measurement environments at ALBA. The two multi-purpose SPMs with multi-technique capabilities (KPFM, MFM, EFM, LFM, PFM, SCM, Phase Contrast, C-AFM, ECM), and one of them will operate inside a glovebox, will offer unique opportunities for ALBA users to investigate advanced funtional materials under controllable gas and liquid conditions. In this presentation, the design, technical capabilities, and scientific examples of the multi-purpose SPMs will be explained, in line with InCAEM's objectives.

Acknowledgments: We acknowledge the State Investigation Agency through the Severo Ochoa Programme for Centres of Excellence in R&D (CEX2023-001263-S). Our research is funded by the Spanish MICIN under project PID2022-136802NB-I00 (AEI/FEDER, UE) and the InCAEM project, supported by MCIN through NextGenerationEU funds (PRTR-C17.I1) and the Generalitat de Catalunya, within the Advanced Materials Complementary Plan.

Impact of bound states in the continuum on magnetotransport in InSb nanowire networks

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Bound states in the continuum (BICs) are exotic, localized states even though their energy lies in the continuum spectra. Since its discovery in 1929, the quest to unveil these exotic states in charge transport experiments remains an active pursuit in condensed matter physics. Here, we study charge transport in InSb nanowire networks in the ballistic regime and subject to a perpendicular magnetic field [1] as ideal candidates to observe and control the appearance of BICs. We use the Kwant toolkit [2]. We find that BICs reveal themselves as distinctive resonances or antiresonances in the conductance by varying the applied magnetic field and the Fermi energy. Finally, the investigation focuses on the effect of the Rashba spin-orbit interaction of InSb on the occurrence of BICs in nanowire networks. We believe that this work could pave the way for the unambiguous observation of BICs in charge transport experiments and for the development of advanced spintronic devices.

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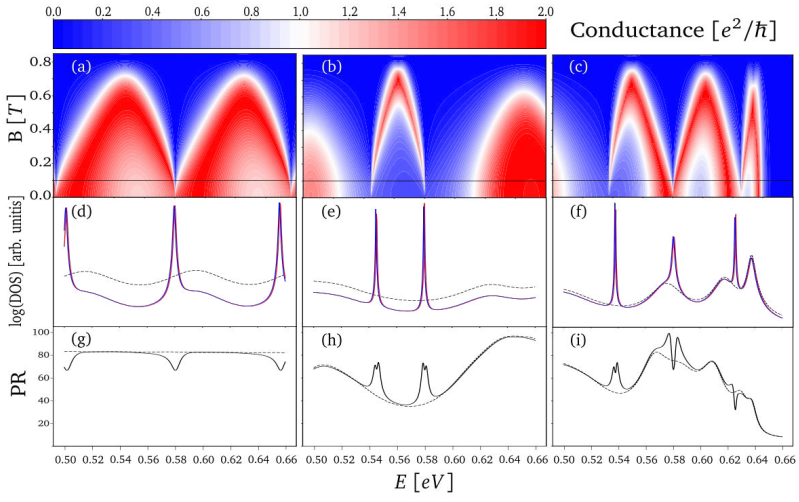

Figure 1: (a), (b), (c) Map of conductance against magnetic field and Fermi energy. (d), (e), (f) Density of states with and without magnetic field for different spin orientations. (g), (h), (I) Participation ratio with and without magnetic field. Different columns represent different nanowire configurations.

Enhancing the thermoelectric figure of merit of BiN via polymorphism, pressure, and nanostructuring

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The discovery of new materials and their properties is crucial for technological advances. The emergence of high-throughput experimental methods combined with artificial intelligence has sped-up the pace in which new compounds are discovered and synthesized. Occasionally, there are compounds that remain unused for many years until their functionality and commercial potential are eventually recognized. Bulk BiN is a good example.
Two-dimensional BiN has been attracting attention for its potential use in transistor technology. Nonetheless, its bulk structure and properties have remained a mystery for a century after the first reported synthesis in 1905. Glazyrin et al. recently synthesized and characterized two bulk BiN polymorphs at different pressures [1]. Pbcn BiN represents the stable polymorph at pressures higher than 12.5 GPa, whereas $Pca2_1$ is the prevailing phase under ambient conditions. The structural characterization of these compounds has revealed various features that make them candidates for thermoelectric materials. For example, Pbcn BiN shares the same structural prototype as SnSe, which is one of the most efficient thermoelectric materials reported. Bismuth is also commonly used in thermoelectric materials due to its electron lone pair and the anharmonicity of its bonds with other elements [2]. Moreover, the difference in mass between Bi and N should increase the anharmonicity of the material and reduce its thermal conductivity.
Despite these interesting features, experimentally characterizing the thermoelectric properties of BiN is difficult due to its reactivity in the presence of O_2 or H_2O. Therefore, theoretical modeling becomes essential to study its performance as a thermoelectric material. In this work, DFT calculations are combined with Machine Learning to explore the transport properties of bulk BiN material to determine its potential application as thermoelectric material, its deficiencies, and venues for improvement. Our approach underscores the necessity of a tight collaboration between experimental and theoretical communities to enhance progress in modern material science and chemistry, thus contributing to the advancement and inspiring future experiments development tailored to specific material properties.

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Optimization of soft X-ray Fresnel Zone Plate fabrication through joint Electron Beam Lithography and cryo-etching techniques

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The ability to manufacture complex 3D structures with nanometer-scale resolution such as Fresnel Zone Plates (FZPs) is crucial to achieve state-of-the-art control in X-ray sources to be used in a diverse range of cutting-edge applications. The synergic employment of Electron Beam Litography and cryoetching techniques is applied to the production of silicon-based FZP prototypes as a test bench useful to assess the strong points and limitations of this fabrication method. The work shows promising results in the fine shaping control of the critical parts of the FZP device. This, would in turn reflect into an enhanced optical resolution and improved efficiency of the FZP

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Figures

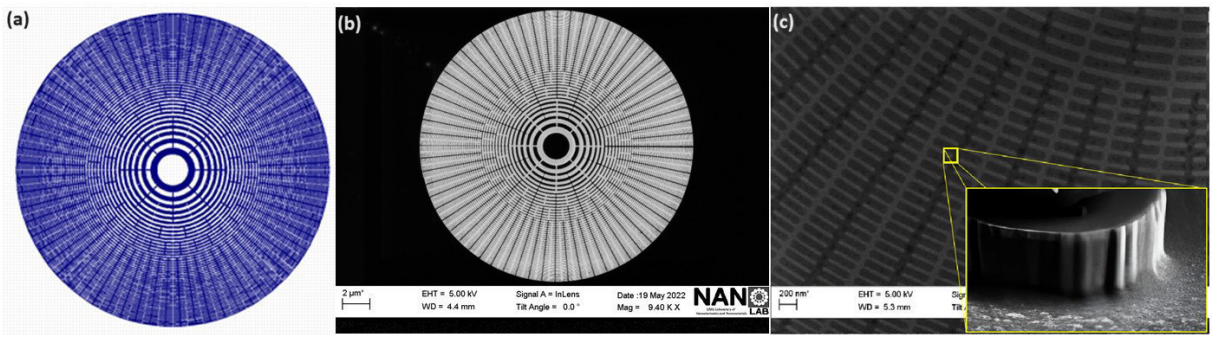

Figure 1: (a) CAD design of Fresnel zone lens, (b) Scanning electron microscope (SEM) image of FZP that has a diameter of 20 µm and an outermost zone width of 50 nm, (c) SEM overview of FZP after 02mn of Silicone cryogenic -etching.

Annealing effect on self-supported high entropy oxy-hydroxides for the acidic oxygen evolution reaction

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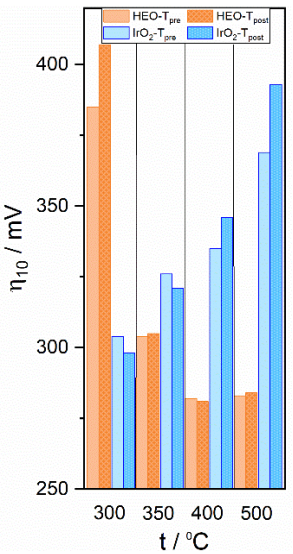
Keywords: High entropy oxides, iridium oxide, electrocatalysis, oxygen evolution reaction.

Background and motivation. To produce green hydrogen from water electrolysis and renewable electricity is one of today's major challenges. Proton exchange membrane water electrolysers (PEM-WE) have several advantages over alkaline electrolysers.[1] However, the use of iridium oxide (IrO_2) as electrocatalysts at the anode limits the widespread implementation of PEM-WE. Ir is a critical raw material because of its scarce abundance,[2] thus, for PEM to become viable the EU has the aim to reduce Ir from current loadings (1-2 mg cm^{-2}) to 0.4 mg cm^{-2} by 2035.[3] Recently, high entropy oxides (HEOs) are gaining interest in electrochemical reactions due to their inherent properties: high structural and chemical stability, and synergistic effects.[4] Nevertheless, research on HEO that are active and stable towards acidic OER is still infrequent.[5] In this work, MnFeCoNiIr HEOs were synthesised through thermal treatment and assessed towards the acidic OER.

Materials and methods. Materials synthesis: MnFeCoNiIr HEO and IrO_x self-supported on carbon fibres were synthesised through the thermal decomposition (300-500 °C, 1h, air) of metal chlorides. Catalysts were characterised by means of XRD, XPS, Raman spectroscopy, HRTEM, and assessed towards the OER in 0.1 M $HClO_4$.

Results and discussion. The effect of annealing on HEOs was compared against IrO_2 samples prepared on a comparable way. Upon annealing, both HEOs and IrO_2 started to crystallise at 350 °C. Catalytic activity and stability were assessed by linear sweep voltammetry (LSV) and chronopotentiometry (CP, 10 mA cm-2). As seen on the adjacent figure, IrO_2 (blue bars) deactivates and becomes less stable with increasing annealing temperature, whilst HEOs followed the opposite trend. The higher the temperature the better the catalytic activity towards OER. In addition, no deactivation was observed after 70 h operation at 10 mA cm^{-2} for the HEO sample annealed at 500 °C, nor structural changes were detected by XRD.



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