Instituto Universitario de
Ciencia de Materiales Nicolás Cabrera

INC Young Researchers Meeting 2024

BOOK of ABSTRACTS

Universidad Autónoma
de Madrid

INC YOUNG RESEARCHERS MEETING

(La Cristalera, Miraflores de la Sierra, December 13th, 2024)

Program

9:30 – 9:45 Welcoming session

9:45 – 10:15 Session I (**Chair: Celia Polop**)

9:45-10:15 **Invited speaker**: **María Varela** " Atomic resolution studies of nanomaterials in the electron microscope"

10:15 – 11:10 "Chema Gómez-Rodríguez" awards to the best paper

10:20-10:45 **Angel Ibabe Avilés**, "Heat Dissipation Mechanisms in Hybrid Superconductor–Semiconductor Devices Revealed by Joule Spectroscopy"

10:45-11:10 **Carlos Sebastián Vicente,** "Photovoltaic charge lithography on passive dielectric substrates using active Fe:$LiNbO_3$ stamps"

11:10 – 11:20 Physics Students Awards

11:20 – 12:20 Coffee break + Poster Session I

12:20 – 13:30 Session II (**Chair: Mercedes Hernando**)

12:20 **Nicol Caetano Zeballos,** *"Unlocking the Potential of Gold Nanostars: Enhanced Heat Delivery through Geometry Optimization"*

12:40 **Alejandro Díez Martínez,** *"New insights into tobacco mosaic virus: stability, disassembly and uncoating"*

13:00 **Antonio Miguel Bosch Fernandez,** *"Adsorption-driven deformation and footprints of the RBD proteins in SARS-CoV-2 variants on biological and inanimate surface"*

13:20 **Pablo Tuero,** *"Unraveling different contributions to spin orbit coupling in superconductor/ferromagnet hybrids"*

13:40 – 15:00 Lunch

15:00 – 16:00 Session III (Chair: Rafael Sánchez)

15:00 **Pablo Vaquer de Nieves,** *"Transport of exciton-polaritons on halide perovskites"*

15:20 **Jose Antonio Moreno,** *"The feedback driven atomic scale Josephson microscope"*

15:40 **Jesús Díaz-Sánchez,** "Nanoscale nucleation and growth of sodium and lithium anodes in zero-excess solid-state batteries"

16:00 – 17:00 Coffee break + Poster Session II

17:00 – 18:00 Session IV (Chair: Carlos Antón Solanas)

17:00 **Liyan Ming,** *"Luminescence-enabled three-dimensional temperature mapping"*

17:20 **José Balduque Picazo,** *"Scattering theory of thermal and bipolar thermoelectric diodes"*

17:40 **Jorge Vega Martín,** *"Proton Transport through Peptide Nanotubes: Insights from Computer Simulations"*

18:00 Wrap up and closing

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Invited Speaker

Atomic resolution studies of nanomaterials in the electron microscope

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Harnessing relevant behaviors in multifunctional materials relies, now more than ever, on understanding and controlling the properties and responses of relevant point defects. The success of aberration correction in the electron microscope, in fact, has allowed electron probes to bear on this task with atomic resolution in real space and with single atom sensitivity both in imaging and spectroscopy. Recent years have also witnessed the development of specimen holders that allow modifying samples in-situ. The effects of external stimuli, such as temperature or bias, can be now explored at the flick of a switch. This talk will review examples of in-situ atomic resolution characterization of functional materials of interest for fields as diverse as spintronics or energy in the scanning transmission electron microscope (STEM). An example can be found in the study of single Bi dopants in Cu nanowires with very low doping levels. These are very interesting systems due to the spin Hall effect associated with the presence of Bi. However, the dopant size and the presence of defects such as grain boundaries may promote Bi segregation when the temperature is raised or electric polarization is applied, which may affect the electrical performance of future devices based on these wires. Other relevant electronic properties, such as the possibility of detecting orbital currents can be probed in the STEM. This talk will review preliminary results along this front and discuss future avenues for nanomaterial characterization in the STEM.

Acknowledgements: A. Guedeja-Marron, J. I. Beltran, M. Saura-Muzquiz, P. Perna, L. Perez.

“Chema Gómez-Rodríguez” award to the best paper

Heat Dissipation Mechanisms in Hybrid Superconductor–Semiconductor Devices Revealed by Joule Spectroscopy

A. Ibabe[1,3], M. Gomez[1,3], G. O. Steffensen[2,3], I. Casal[1,3], T. Kanne[5], J. Nygard[5], A. Levy Yeyati[2,3,4], and E. J. H. Lee[1,3,4]

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Hybrid superconductor-semiconductor systems have been widely studied in the past decade for the development of novel quantum devices, with focus on both the topological and trivial regimes. Heat transport, on the other hand, still remains relatively unexplored in such systems, and self-heating effects have been generally overlooked, which is surprising given that heating becomes increasingly more important at very low temperatures, with potential implications for device performance. To minimize detrimental effects, it is then crucial to understand the fundamental heating and cooling processes in such hybrid systems. In this work, we address these issues by studying devices based on full-shell InAs-Al nanowires. Concretely, we develop a technique dubbed “Joule spectroscopy” that detects Joule effect-driven superconductor-to-normal transitions in a device by means of signatures in electron transport [1].

We further make use of the Little-Parks effect to reveal the dominant heat dissipation mechanism for distinct superconducting regions of a hybrid device. We find that the primary cooling mechanism for grounded and floating superconductors is different, i.e., quasiparticle diffusion and electron-phonon coupling, respectively. As a result, we conclude that floating superconductors are significantly more susceptible to heating, with a cooling power approximately two orders of magnitude lower than that of grounded superconductors [2].

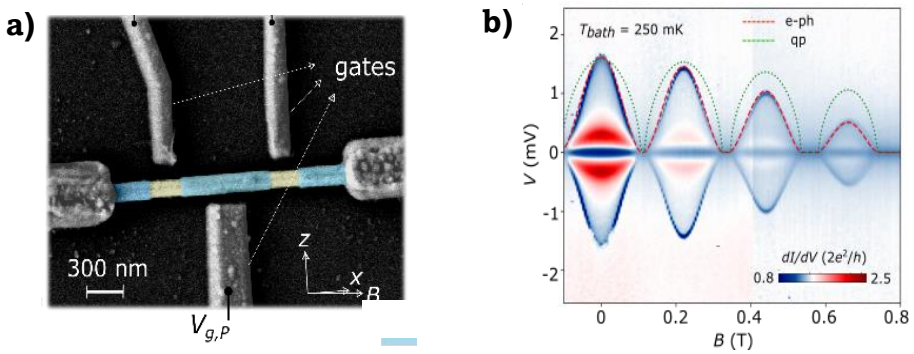

Figure 1| a) SEM micrograph of a hybrid superconductor-semiconductor nanowire device. b) Little-Parks oscillations of the Joule-driven superconductor-to-normal metal transition of a superconducting island defined in a nanowire.

[1] A. Ibabe, M. Gomez, G. O. Steffensen, T. Kanne, J. Nygard, A. Levy Yeyati, E. J. H. Lee, Nat. Commun. 14, 2873 (2023).
[2] A. Ibabe, G. O. Steffensen, I. Casal, M. Gomez, T. Kanne, J. Nygard, A. Levy Yeyati, E. J. H. Lee, Nano Lett. 24 (2024).

“Chema Gómez-Rodríguez” award to the best paper

All-optical domain inversion in $LiNbO_3$ crystals by visible continuous-wave laser irradiation

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$LiNbO_3$ is a distinguished multifunctional material where ferroelectric domain engineering is of paramount importance. This degree of freedom of the spontaneous polarization remarkably enhances the applicability of $LiNbO_3$, for instance, in photonics. Electrical poling is the standard method to create ferroelectric domain structures in $LiNbO_3$. This method consists in the application of an external electric field above the coercive threshold of $LiNbO_3$ to locally switch the spontaneous polarization [1]. In this work, we report the first method for all-optical domain inversion of $LiNbO_3$ crystals using continuous-wave visible light [2]. While we focus mainly on iron-doped $LiNbO_3$, the applicability of the method is also showcased in undoped congruent $LiNbO_3$. The technique is simple, cheap, and readily accessible. It relies on ubiquitous elements: a light source with low/moderate intensity, basic optics, and a conductive surrounding medium, e.g. water (see Figure 1a). Light-induced domain inversion is unequivocally demonstrated and characterized by combination of several experimental techniques: selective chemical etching (Figure 1b), surface topography profilometry, pyroelectric trapping of charged microparticles, scanning electron microscopy, and 3D Čerenkov microscopy. The influence of light intensity, exposure time, laser spot size, and surrounding medium is thoroughly studied. To explain all-optical domain inversion, we propose a novel physical mechanism based on an anomalous interplay between the bulk photovoltaic effect and external electrostatic screening. Finally, we also explore the possibility to fabricate arbitrary domain patterns using structured light (see Figure 1c). Overall, our all-optical method offers straightforward implementation of $LiNbO_3$ ferroelectric domain engineering, potentially sparking new research endeavors aimed at novel optoelectronic applications of photovoltaic $LiNbO_3$ platforms.

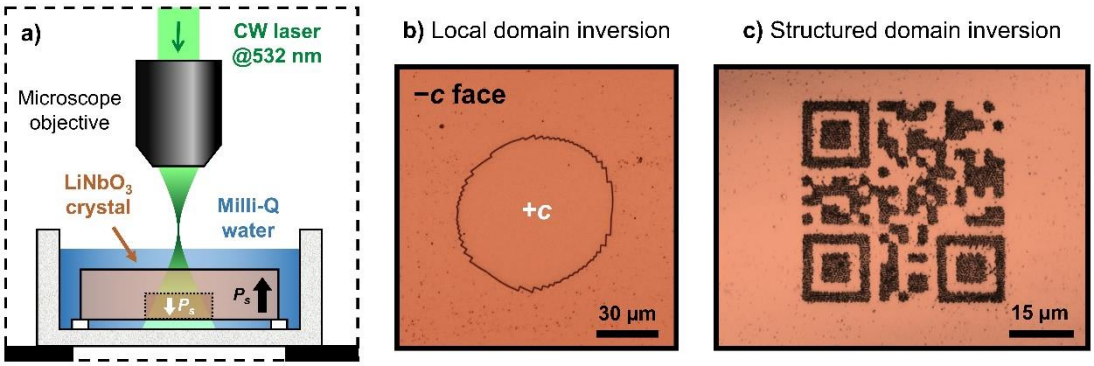

Figure 1. a) Experimental setup for all-optical domain inversion. b) Example of local domain inversion with a focused Gaussian beam in Fe:$LiNbO_3$. c) QR code of ferroelectric nanodomains obtained with structured light in Fe:$LiNbO_3$. Both images were acquired after chemical etching in HF acid.

[1] V. Shur et al., Appl. Phys. Rev., **2**, 040604 (2015)
[2] C. Sebastián-Vicente et al., ACS Photonics, **11**, 2624 (2024)

Oral Contributions

Unlocking the Potential of Gold Nanostars: Enhanced Heat Delivery through Geometry Optimization

Nicol Caetano Zeballos[1,2,3], Alejandro Casillas[4], Óscar G. Calderón[4], Sonia Melle[4], Marta Quintanilla[2,5], Antonio Benayas [1,3,5]

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Nowadays, optical biomedical applications increasingly rely on plasmonic nanoparticles due to their strong interaction with electromagnetic radiation. These nanoparticles show promise in advanced biomedical techniques such as Photothermal Therapy (PTT), Photoacoustic Imaging (PAI). [1,2] These applications are based on the large extinction cross-section of nanoparticles' plasmonic resonance, which enables either absorption or scattering of photons, depending on the application. In this sense, both PTT and PAI require nanoparticles with high light absorption to facilitate optically triggered local heat release, which can treat infections or generate pressure waves for imaging. Consequently, PAI and PTT, both relying on heat delivery probes, offer promising approaches for non-invasive and better resolved biomedicine. Through optical excitation, it is possible to activate and control the heat release of these plasmonic nanoparticles in a specific spectral range, allowing the research community to design them, so far, mainly for the first biological window (BW-I, 700-980 nm [3]). However, the second biological window (BW-II, 1000-1350 nm [3]) has advantages for biomedical imaging, as it reduces scattering in tissues, increases penetration depth, and improves control over excitation light, making it ideal for techniques such as PTT and PAI. For such heating-oriented oriented applications, and to minimize light-tissue interaction, gold nanostars constitute a particularly attractive material. That is due to the high control over the heating properties achievable by tuning the geometrical design of the nanoparticles [4] and the shifting to the longer wavelengths within the BW-II range. Upon choosing nanostars, we have developed a palette of synthesis parameters (concentration of hydrochloric acid, and the size and amount of gold seeds), rendering an effective lever to shift the extinction to larger wavelengths (BW-II). Moreover, such a synthesis toolkit allows us to maximize the absorption over the scattering, thus increasing heat delivery. Since GNSt should also exhibit high thermal stability under irradiation, we have carefully studied the changes in the structure and optical properties depending on the illumination dose. This new generation of optical actuators will become key towards upgraded PAI and PTT, able to reach deeper into biomedical systems and to act with better-resolved performance.

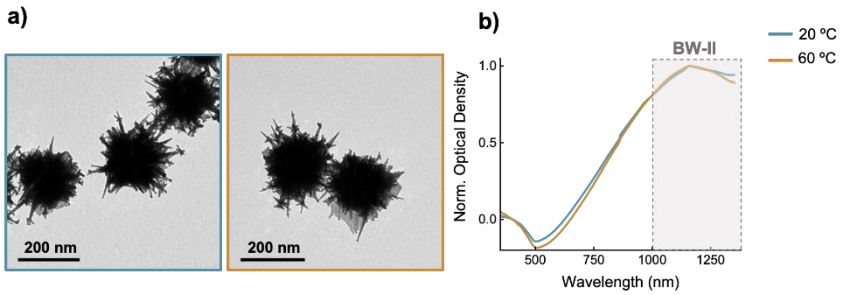

Figure 1. Thermal stability of gold nanostars synthesized in water using a gold seeds diameter of 33 nm and hydrochloric acid concentration of 13 mM A) TEM image of Gold nanostars at room temperature (left) and after heating the NPs at 60 ºC (right). Scale bar-200 nm B) Normalized extinction spectrum in water of gold nanostars at room temperature (blue line) and after heating the NPs at 60 ºC (orange line).

[1] Ge, Xiaoguang, et al. *New J. Chem.* **43**,23,8835-8851. (2019)
[2] Fang C, et.al. Biomater. Sci. 9, 367-390. (2021)
[3] Schellenberg, M. W. & Hunt, H.. *Photoacoustics* **11**, 14–27 (2018).
[4] Li, W. & Chen, X. Nanomedicine (Lond) **10**, 299 (2015)

New insights into tobacco mosaic virus: stability, disassembly and uncoating

Alejandro Díez-Martínez [a,b], Pablo Ibáñez-Freire [a,b], Diego Alonso Aldave [a,b], Salvatore Assenza [a,b], David Reguera [c], Pablo Ares [a,b], Julio Gómez-Herrero [a,b], Alexander Bittner [d] and Pedro J. de Pablo [a,b]

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Tobacco mosaic virus (TMV) serves as a key model in both virology and nanotechnology, admired for its robust structure and ease of assembly. While the mechanical resistance of TMV has attracted interest for nanostructure applications [1], the intricate details of its disassembly mechanics remain poorly understood. In this study, we integrate three key aspects of TMV behavior: its mechanical resilience, its thermal stability and the role of genome-protein interactions. By combining nanoindentation experiments with coarse-grain and finite elements simulations [2], we investigate how the viral capsid disassembles as a function of the force applied. Which reveals that the central cavity plays a critical role in the distribution of mechanical stress. We also heated TMV up to 175ºC and found almost no structural degradation. Beyond this temperature, its height follows a sigmoidal curve until its complete degradation at 250ºC. Additionally, we explore how the specific nucleotide sequence of the TMV RNA affects the weakening of specific regions during mechanical disassembly [3]. Using Atomic Force Microscopy (AFM), we correlate the formation of rifts along the capsid with the trimers in the genomic sequence, shedding light on how these interactions contribute to the mechanical stability of the virus. Together, this combined approach provides a deeper understanding of the structural integrity of TMV and the factors that govern its disassembly process.

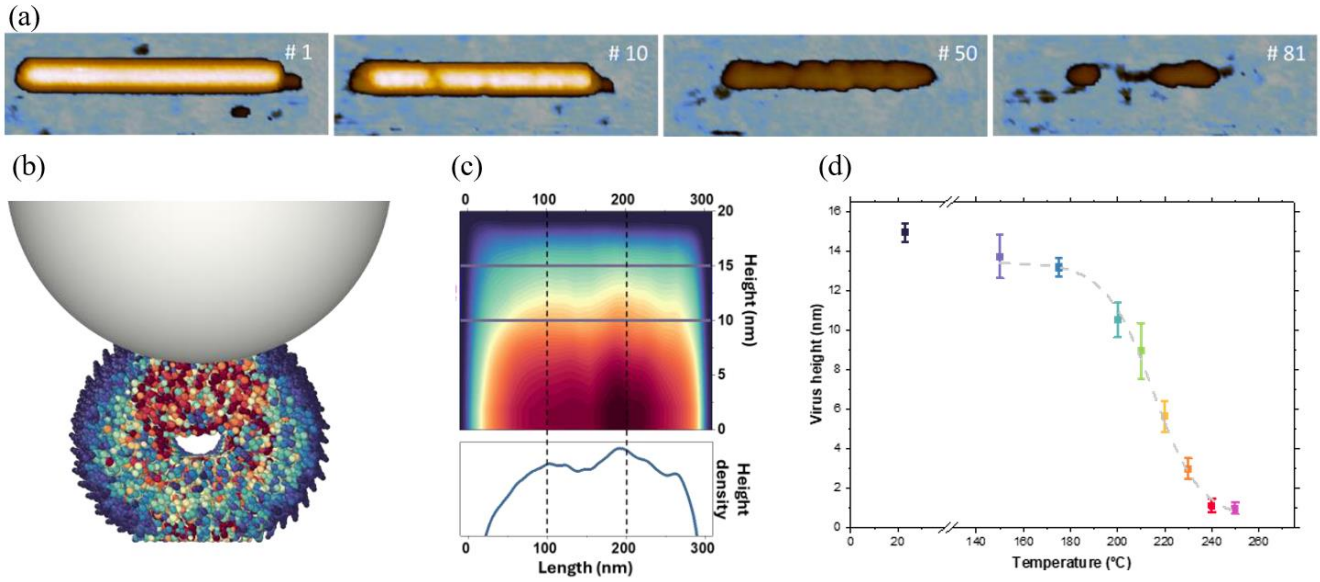

Figure 1. (a) Mechanical fatigue on TMV particle: #1 first frame, #10 beginning of disassembly, #50 disappearance of the upper half, and #81 final remains. (b) Coarse grain simulation of an indentation showing an uneven mechanical stress distribution. (c) TMV average disassembly pattern. (d) Distribution of TMV heights at different temperatures.

[1] Lee, K. Z. et al., Biotechnology Journal 16 (2021).
[2] Y. Zhao. Et al., Soft Matter Phys. 78 (2008).
[3] J. J. Steckert et al., Nature, 299, 32-36 (1982).

**The results presented here are part of three ongoing manuscripts currently in preparation.*

Adsorption-driven deformation and footprints of the RBD proteins in SARS-CoV-2 variants on biological and inanimate surface

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Computational Biophysics has provided a broad and deep understanding of molecular-scale phenomena, during the recent pandemics, the direct transmission of the SARS-CoV-2 has elucidated the mechanisms of infection for the different variants that contributed to the development of vaccines and therapies. However, respiratory viruses, carried through airborne microdroplets, frequently adhere to surfaces, including plastics and metals. Our understanding of the interactions between viruses and materials remains limited, particularly in scenarios involving polarizable surfaces. Here, we investigate the role of receptor-binding domain (RBD) mutations on the adsorption of SARS- CoV-2 to hydrophobic and hydrophilic surfaces employing molecular simulations. To contextualize our findings, we contrast the interactions on inanimate surfaces with those on native-biological interfaces, specifically the ACE2 receptor. Notably, we identify a twofold increase in structural deformations for the protein's receptor binding motif onto the inanimate surfaces, indicative of enhanced shock-absorbing mechanisms [1]. Furthermore, the distribution of amino acids (landing footprints) on the inanimate surface reveals a distinct regional asymmetry relative to the biological interface. Despite the H-bonds formed at the hydrophilic substrate, the simulations consistently show a higher number of contacts and interfacial area with the hydrophobic surface. In contrast, the adsorption of delta and omicron to hydrophilic surfaces was characterized by a distinctive hopping pattern. The novel shock-absorbing mechanisms identified in the virus adsorption on inanimate surfaces could lead to current experimental efforts in the design of virucidal surfaces and sensors.

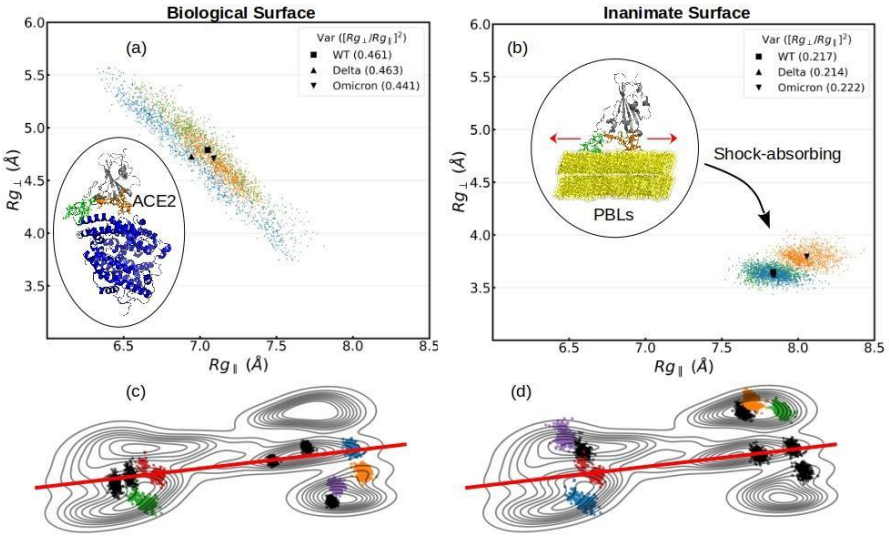

Figure 1: (a,b) Perpendicular versus parallel Radius gyration and (c,d) the landing footprints of the group 1 of the RBM(depicted in green in insets) onto the (a,c)ACE2 and PBL0 (b,d). Rg^2/Rg^2 ratio on the legend [2].

[1] A. Bosch, H. V. Guzmán, R. Pérez, (2024). Adsorption-Driven Deformation and Footprints of the RBD Proteins in SARS- CoV-2 Variants on Biological and Inanimate Surfaces. J. Chem. Inf. Model. 2024, 64, 15, 5977–5990

[2] S. Poblete et al. 2021. ACS omega, 6(48), pp.32823-32831.

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 with interfacial spin-orbit coupling. CA amplitude anisotropy in weak IP and OOP magnetic fields 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 in the same ferromagnet- superconductor junctions. When Rashba and Dresselhaus-type SOC contributions coexist, an in-plane anisotropy arises in the effective spin-orbit field. 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 polarization when under an anisotropic interfacial spin-orbit field. 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 to spin-orbit coupling. Comparison between experimental findings and theoretical modelling indicates that the Dresselhaus contribution to SOC is approximately 10% of the Rashba-type SOC. This relatively 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.

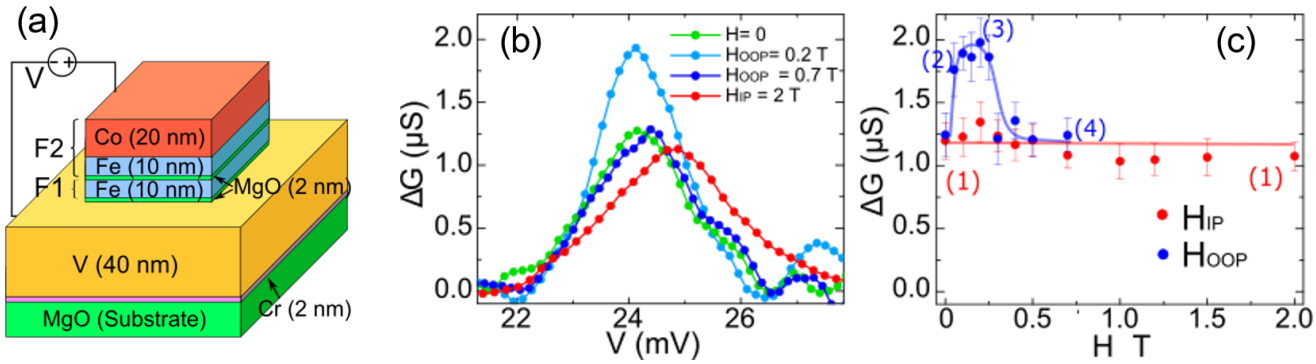

Figure 1. (a) Sketch of the F/S/F sample under study. (b) and (c) show the evolution of conductance anomaly peaks under applied IP and OOP magnetic field.

[1] P. Tuero et al., Phys. Rev. B, **110**, 094504 (2024)
[2] A. Costa and J. Fabian., Phys. Rev. B, **104**, 174504 (2021)

Transport of exciton-polaritons on halide perovskites

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This research project, currently at a very initial state, aims to develop a platform to control exciton-polariton propagation resulting from the strong coupling between cavity photons and excitons in semiconductors. The core of this investigation will be the construction and utilization of a Fabry-Perot open cavity embedding excitons in order to study the dynamics of the resulting exciton-polariton system. The study will focus on various semiconductor materials, exploring their transport dynamics as a function of the micro-structured cavity topology.

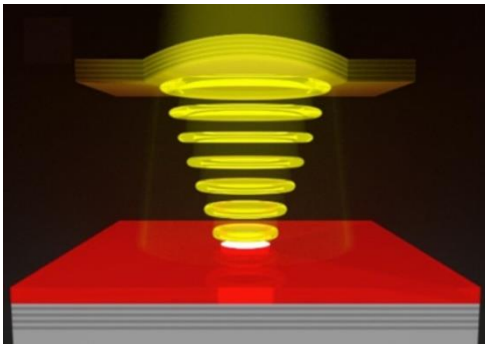

Figure 1. Visualisation of an exciton-polariton in a cavity.

Understanding and controlling transport in exciton-polaritons is essential for the advancement of polariton-based electronic and optoelectronic devices, operated at room temperature. Traditional microscopy methods often fall short in providing the spatial and temporal resolution necessary to study these processes at the nanoscale. Moreover, detailed control of polaritonic states is limited in conventional monolithic cavities. This PhD research project, part of the ERC-CoG EnVision initiative, proposes to overcome these limitations by coupling Transient Microscopy equipped with scanning open cavities. While the super-resolution capabilities of transient microscopy provide the level of detail to visualize the transport of exciton-polaritons directly, the open cavity will provide full versatility to reconfigure the light-matter coupled system (active materials of choice, mirror design) and deterministically control its coupling in space and energy.

[1] Seitz, M., Magdaleno, A.J., Alcázar-Cano, N. et al. Exciton diffusion in two-dimensional metal-halide perovskites. Nat Commun 11, 2035 (2020). https://doi.org/10.1038/s41467-020-15882-w
[2] Seitz, M., Magdaleno, A. J., Alcázar-Cano, N., Meléndez, M., Lubbers, T. J., Walraven, S. W., ... & Prins, F. . Exciton diffusion in two-dimensional metal-halide perovskites. Nature communications, 11(1), 2035 (2020). DOI https://doi.org/10.1039/D0MH01723J
[3] Anton-Solanas, C., Waldherr, M., Klaas, M., Suchomel, H., Harder, T. H., Cai, H., ... & Schneider, C. Bosonic condensation of exciton–polaritons in an atomically thin crystal. Nature materials, 20(9), 1233-1239 (2021) https://doi.org/10.6084/m9.figshare.14342471.
[4] Adrados, C., Liew, T. C. H., Amo, A., Martín, M. D., Sanvitto, D., Antón, C., ... & Viña, L.. Motion of spin polariton bullets in semiconductor microcavities. Physical Review Letters, 107(14), 146402 (2011).

The feedback driven atomic scale Josephson microscope

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The ultimate spatial limit to establish a Josephson coupling between two superconducting electrodes is an atomic-scale junction. The Josephson effect in such ultrasmall junctions has been used to unveil new switching dynamics, study coupling close to superconducting bound states or unveil non-reciprocal effects. However, coupling is weak and thermal smearing reduces the Cooper pair current magnitude. Here we show that a feedback element induces a time-dependent bistable regime which consists of spontaneous periodic oscillations between two different Cooper pair tunneling states (corresponding to the DC and AC Josephson regimes respectively). The amplitude of the time-averaged current within the bistable regime is robust against thermal smearing. By tracing the periodic oscillations in the new bistable regime as a function of the position in a Scanning Tunneling Microscope (STM), we obtain atomic scale map of the critical current in 2H-NbSe2 and find spatial modulations due to a pair density wave. Our results fundamentally improve our understanding of atomic size Josephson junctions including a feedback element in the circuit and provide a promising new route to study superconducting materials through atomic scale maps of the Josephson coupling [1].

[1] S.D. Escribano *et al*., https://arxiv.org/html/2311.12783v2 (2023).

Nanoscale nucleation and growth of sodium and lithium anodes in zero-excess solid-state batteries

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Zero-Excess Solid-State Batteries (ZESSB), in which an anode is formed in situ during charging, have received much attention in recent years. ZESSBs have great potential to increase energy density and facilitate battery production, thereby reducing cost as well as material and energy consumption. Practical application of ZESSBs has so far been limited by challenges related to the non-uniform growth of alkali anodes during cycling, leading to poor performance. To address this issue, various strategies have been reported so far to control the morphology of the alkali anodes to be homogeneous and dense, but until now, the microstructure of the anodes during the nucleation and early growth stages is unknown [1, 2, 3].

Here we have developed the virtual electrode method that enables in-situ anode plating and stripping of a ZESSB, with nanoscale chemical and morphological analysis using nanospectroscopy and nanomicroscopy. Combining Atomic Force Microscopy (AFM) at UAM and Photoemission Electron Microscopy (PEEM) at the CIRCE beamline of ALBA synchrotron, we have been able to study the nucleation and growth kinetics, morphology and chemical state of the grown anodes with nanoscale resolution. This technique circumvents issues related to the physical current collector by creating surface charge with an electron beam, which drives cation migration to form clusters of Na/Li on the electrolyte surface. For stripping, a photon beam induces positive surface charge, driving Na/Li ions back into the electrolyte and allowing in-depth analysis of stripping at the nanoscale. The virtual electrode method successfully offers insights into early-stage nucleation, with various experimental parameters significantly impacting anode morphology and growth efficiency.

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Luminescence-enabled three-dimensional temperature mapping

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Luminescence nanothermometry analyzes the changes in the luminescent properties of nanoparticles to provide remote thermal readouts with high spatial resolution and in a minimally invasive way.[1] This technology has advanced our understanding of biological mechanisms and physical processes at the submicrometric scale. However, current luminescence-based techniques typically provide only two- dimensional (2D) thermal images. This is a limiting factor in biological applications, where precise localization of temperature variations is crucial. Yet, despite first attempts,[2] a credible method that allows extracting three-dimensional (3D) thermal maps via luminescence is missing.

Here, we design such a method combining Ag_2S nanothermometers and convolutional neural networks (CNN). The approach leverages the distortions in the emission spectra of luminescent nanothermometers caused by changes in temperature and tissue-induced photon extinction. The optimized, neural network- based algorithm can extract this information and provide 3D thermal maps of complex nanothermometer patterns (**Figure 1**). Although tested for luminescence thermometry, this method has far-reaching implications for luminescence-supported 3D sensing in biological systems in general. This is because it offers a means to simultaneously capture spatial distribution information of sensors and the magnitude of the parameter of interest.

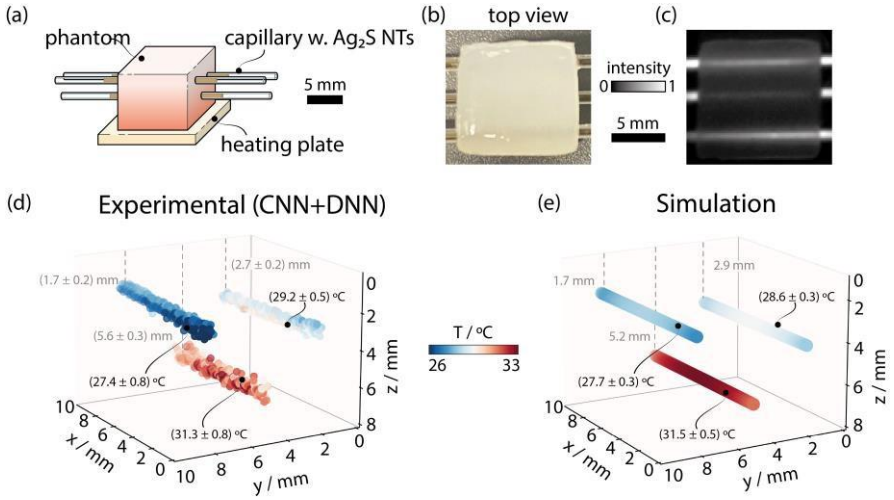

Figure 1. (a) Scheme of the phantom with inserted Ag2S NTs-filled capillaries (outer diameter = 1 mm, inner diameter = 0.5 mm). (b) Top view of the phantom and (c) corresponding hyperspectral image used to obtain the 3D thermal maps shown in (d). (e) Thermal maps obtained considering the depth measured from a photo and the temperature resulting from simulations.

[1] Adv. Mater. 35 (2023) 2302749, DOI: 10.1002/adma.202302749
[2] Adv. Mater. 36 (2024) 2309452, DOI: 10.1002/adma.202309452

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 due electron-electron interactions, 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 tunneling samples to efficiently exploit these effects, and find configurations acting as bipolar thermoelectric diodes whose current flows in the same direction irrespective of the sign of the temperature difference, a case of antireciprocity.

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Proton Transport through Peptide Nanotubes: Insights from Computer Simulations

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Peptide nanotubes consist of cyclic peptides stacked on top of each other and held together by hydrogen bonds, making them similar to carbon nanotubes in morphology. These materials are very interesting from both a fundamental point of view, as they serve as a testing ground to study proton transport in more complex biomolecular systems, and from a technological perspective, as they are promising proton conducting materials for the development of fuel cells, batteries, sensors, and other advanced technologies. However, proton transport in peptide nanotubes remains poorly understood. Recent experiments on cyclic peptides based on phenylalanine and functionalized with either lysine, arginine, or histidine [1, 2] have shown an order-of-magnitude higher proton conductivity in lysine- containing nanotubes, which also varies drastically with the system's hydration level and counter-ion doping. Motivated by these results, we carried out molecular dynamics simulations to study the structure and dynamics of these systems. We find that peptides nanotubes can form bundles with channels between them, where the water molecules and counter-ions can enter and form a rich and dynamic structure of hydrogen bonds with the lysine sidechains. This structure appears to be a viable candidate for mediating proton transport through a Grotthuss-like mechanism. We have also analyzed the influence of varying the water content and counter-ion doping on this network. Finally, preliminary QM-MM simulations have suggested that classical potentials may not accurately describe the hydrogen bonds within the peptide nanotubes, which may be an important information to consider when attempting to understand proton transport through these systems.

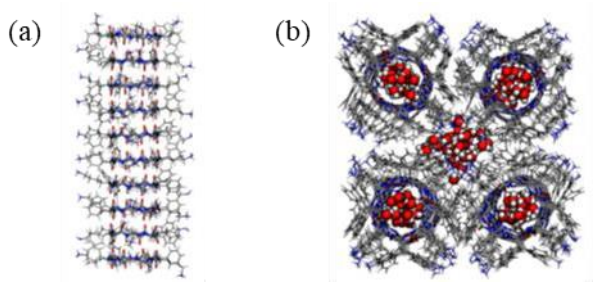

Figure 1: (a) Side view of a section of the peptide nanotube c(KF)4. Each peptide ring contains 4 lysine (K) and 4 phenylalanine (F) amino acids in an alternate fashion. (b) Top view of a bundle of 4 nanotubes. Water molecules can be hosted inside the nanotubes and in the channel between them.

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Poster Contributions

INC Awards to Undergraduate Students

Signatures of spin fractionalization in Kitaev materials

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The Kitaev model is a paradigmatic model of quantum interacting spins on a honeycomb lattice whose exact ground state is a quantum spin liquid and its spin excitations fractionalize onto Majorana fermions. The recent observation of an anomalous thermal Hall effect in the quasi-two-dimensional material, α-$RuCl_3$, suggests that it may host a Kitaev spin liquid with Majorana excitations. This has driven an intense research activity around finding materials realizing the Kitaev model such as Na_2IrO_3, α-Li_2IrO_3.

In the present project we explore the exact solution to the Kitaev spin model on a three-dimensional tri- coordinated hyperhoneycomb lattice [2] (see figure), which has been experimentally suggested to be an accurate model for describing the magnetic properties of β-Li2IrO$_3$. After revising the exact solution to the Kitaev model on a honeycomb lattice we explore the three-dimensional situation. We focus on understanding the analytical zero-flux solution to the Kitaev model on the three-dimensional tri-coordinated lattice by fractionalizing the spins into Majorana fermions. By analysing the behavior of the Majorana energy bands we conclude on the nature of the possible magnetic ground states encountered for different parameter regimes of the model. We finally discuss possible signatures of the spin fractionalization predicted from the model in experimental observations on β-Li_2IrO_3.

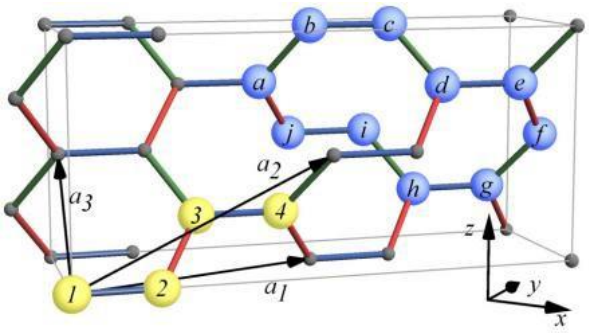

Figure 1. This figure shows the hyperhoneycomb lattice on which the Kitaev model is solved. The red, green and blue bonds correspond to the xx, yy and zz interactions on the tri-coordinated lattice. The numbering 1 to 4 denotes the sites comprising the unit cell of the lattice. [2]

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Growth and characterization hybrid systems for antiferromagnetic spintronics

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Systems composed of antiferromagnetic (AFM) and ferromagnetic (FM) layers have been investigated in recent decades because of their impact on spintronics applications, as spin-valves for commercial magnetic field sensors and magnetic random-access memories (MRAMs). Some hybrid AFM/FM systems with a strong exchange coupling at the interface [1] are able to a perfect imprint of the magnetic domain pattern of the AFM into the FM layer, so that it can be used as a read-out mechanism in antiferromagnetic spintronics. NiO is one of the most studied AFM for applications with Néel temperature above room temperature (RT) showing a very complex domain structure that depends on deposition conditions and crystalline orientation. In fact, one of the factors that can affect the exchange coupling of the NiO / FM hybrid system is related to the presence of the uncompensated spin at the NiO / FM interface that depends on the texture of the AFM layer [2].

In this work we have grown NiO / FM (FM = Fe and FeCo) bilayers with different FM thickness on single crystal MgO (100), (110), (111) and Al_2O_3 (0001) substrates by reactive ion beam sputtering. Raman spectroscopy combined with vectorial Kerr magnetometry have been used to characterize the bilayers, both as deposited and after a field cooling procedure (FC), which involves heating the bilayer above its Néel temperature in vacuum and cooling it down under the presence of an external magnetic field.

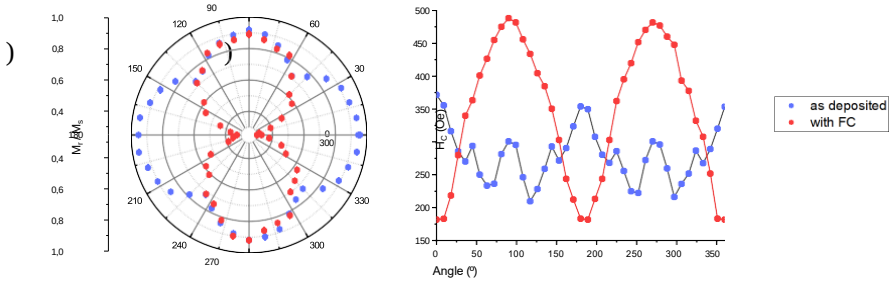

Figure 1. Both graphs are from the NiO/Fe grown on MgO (110) with measures before and after FC. a) Polar plot of remanent magnetization M_r/M_S. b) Angular dependence of the coercive field.

Figure 1 shows the results of the NiO/Fe grown on MgO (110), graph a) is a polar plot of remanent magnetization (M_r/M_s) and b) the angular dependence of the coercive field. Before FC, it exhibited biaxial magnetic anisotropy, with an easy magnetization axis (e.a) at 0º, and a slightly smaller one at 90º, and after FC, it changes to uniaxial anisotropy, with an e.a at 90º due to the direction of the external field applied, and an increase in the coercive field is observed at the e.a. Additionally, Raman spectroscopy measurements showed that, after FC, magnetite appeared, which may have been formed at the interface.

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Electron dynamics in atoms driven by intense quantum light

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High-harmonic generation (HHG) is a nonlinear process which arises when illuminating a system of atoms with an intense laser pulse in which the electric field strength approaches that of the Coulomb field binding the electrons to the nucleus. While HHG has mostly been studied under driving by classical fields, there has been a recent surge in interest in its properties using intense quantum (i.e., non-classical) light fields, which promise to enable phenomena that cannot be reproduced by classical driving. To investigate this, we study a model atom driven by an external monochromatic EM field in an arbitrary quantum state, following a recently developed theoretical approach [1]. The emission spectrum depends on the (average) intensity of the driving laser field and the quantum state of the driving light.

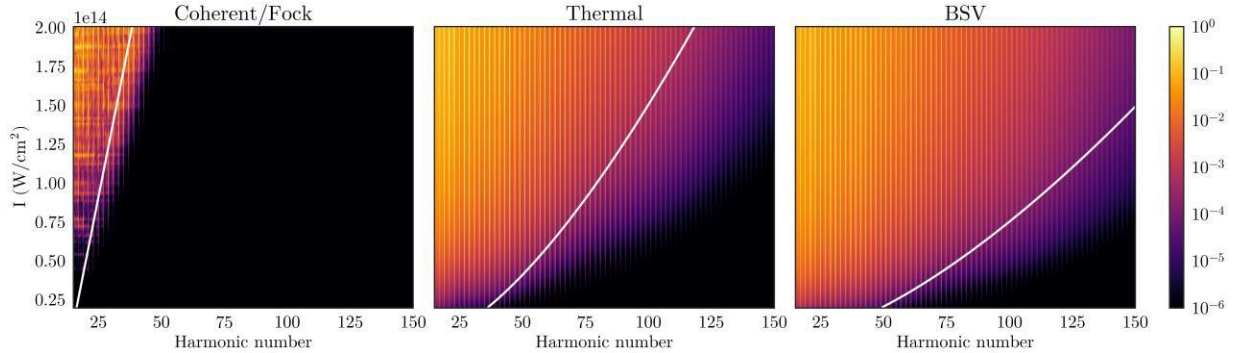

Figure 1. Spectrum of the light emitted through HHG as a function of mean intensity under driving by light in different quantum states: coherent & Fock, a thermal distribution, and bright squeezed vacuum (BSV).

We study the HHG spectrum emitted for four different states of the driving light: (i) coherent (equivalent to classical light), (ii) Fock (or number state), (iii) thermal, and (iv) bright squeezed vacuum (BSV) [2]. As shown in Figure 1, the spectra generated by these states are qualitatively different: For the same average intensity, driving by thermal light or a BSV produces significantly higher harmonics compared to coherent and Fock states, which give identical results. Our results agree qualitatively with those published in [1], but differ quantitatively – to the best of our knowledge, due to mistakes in [1]. Furthermore, it should be noted that the differences observed here are not due to quantum properties of the light, but simply because thermal and BSV states have much larger statistical uncertainty in the intensity compared to coherent or Fock states. In other words, these results can be reproduced by a statistical mixture of classical fields. We are currently working on ways to identify truly quantum effects within HHG.

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Polarisation effects in emitted light from topological lattices of exciton-polaritons

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Semiconductor microcavities, defined by a Fabry-Perot cavity embedding a quantum well, enable strong confinement of both light and electronic excitations [1]. In these heterostructures, the strong interaction between light and matter induces the emergence of hybrid light-matter bosonic quasiparticles known as exciton-polaritons. Polaritons inherit properties from their two fundamental constituents: the photonic part (providing a light polariton mass) and the excitonic component (responsible for Coulomb interactions in polaritons) [1,2,3].

The combination of the planar cavity DBRs with an additional lateral confinement results in the discretization of the optical modes in the microcavity [2], forming a micrometric lattice potential for photons. This lattice engineers polariton dispersion relations in different geometries (in this work, we focus on the Hofstadter geometry), allowing the exploration of topological polariton effects with tailored interactions [3].

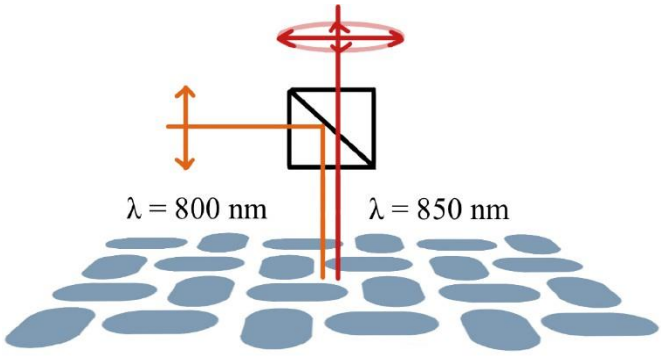

Figure 1: Scheme of the polarisation input and output

In this work, we first study the dispersion relation of polaritons in a planar microcavity at various detunings. Subsequently, we will investigate whether an asymmetry in the Hofstadter lattice design induces an intrinsic circular polarization in the emitted light under a linear, non-resonant laser pump. To address this, we developed a polarization tomography tool designed to accurately characterize the emitted polarization state [4]. Ongoing simulations of the polarisation resolved, two-dimensional Gross-Pitaevskii equation will allow us to confirm the hypothesis on the intrinsic circular polarisation effects of the emission from the lattice.

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Study of AFM tip-induced ion migration on a solid-state ion conductor

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Zero-Excess Solid-State batteries (ZESSB) refer to batteries where the anode is formed during the charge of the battery instead of being already built. This feature could lead to an increase in energy density and cost reduction for future batteries. To achieve this behavior, we need to be able to migrate ions across the solid electrolyte and grow a homogeneous layer to work as the battery anode. In this project we studied the ion migration process using the AFM tip to induce a voltage difference in the electrolyte, with the goal of mobilizing Na/Li to the surface.

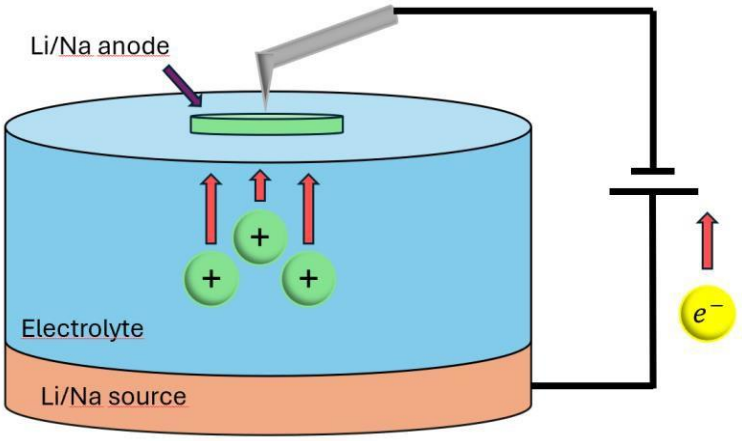

Figure 1. Diagram of the experimental setup and goal.

We studied two different types of Li/Na solid-state ion conductors: $Li_{7-x}La_3Zr_{2-x}Ta_xO$ prepared by NTNU and $Na_5GdSi_4O_{12}$ prepared at Fraunhofer IKTS. As complementary measurements we also conducted Impedance Spectroscopy to some of the samples to better understand their electrical behavior. We concluded that the sample thickness is an essential parameter to induce local ion migration with the AFM tip.

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Tunable Fabry-Pérot Microcavity for Photonic Coupling of Emission in Quantum Materials

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Light-matter interaction is responsible for many phenomena in nonlinear photonics, spectroscopy, photovoltaics, and optoelectronics. Optical microcavities constitute a fundamental platform to investigate such interactions, enabling applications in quantum photonic technologies and material science [1].

In this work we study theoretically and experimentally a Fabry-Pérot resonator, a microcavity composed by two opposed mirrors with air filling the cavity space, allowing us to freely tune their relative positions with piezoelectric nanomotors. Using Transfer Matrix Methods (TMM) simulations, we theoretically study the characteristics (reflectivity, quality factor) of such an empty open cavity. In the future, we will use this cavity for investigating light-matter coupling with various quantum materials at room temperature, such as two-dimensional perovskite excitons or single defects in hexagonal Boron Nitride. This type of reconfigurable microcavity allows its spectral tunning (changing the mirror distance) and in-plane spatial translation (displacing laterally the mirrors) [3]. Figure 1a shows the refractive index profile of the planar microcavity (designed to confine one optical mode at 650 nm) with an air gap of 1 µm, panel (b) shows the corresponding simulated reflectivity spectrum. Figure 1c shows the open cavity designed for our experiments, alongside preliminary experimental results on the dispersion relation of the microcavity reflectivity map.

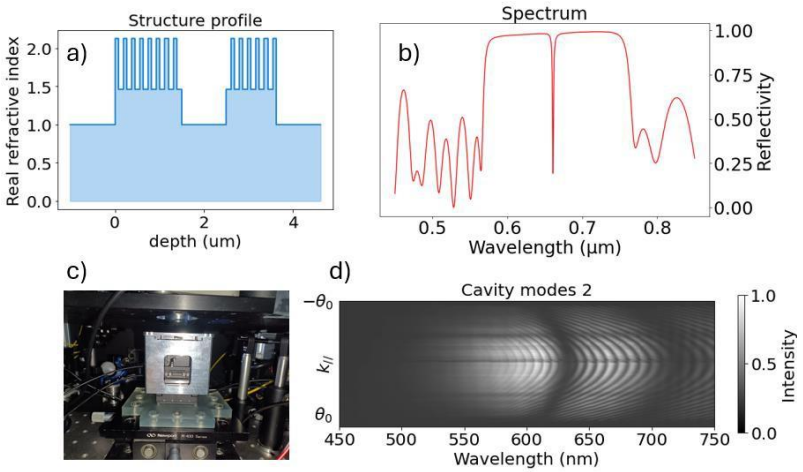

Figure 1. a) Real part of the refractive index vs depth of the cavity. b) Reflectivity vs wavelength. c) Open microcavity in the lab. d) Reflectivity map of the microcavity represented versus wavelength (horizontal axis) and in- plane momentum of the emission (vertical axis, representing the range of angles of collection).

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All-Optical Modulation of Charge Carriers in $MoSe_2/LiNbO_3$

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Charge carrier density of 2D-TMDs are typically controlled through chemical doping, electrostatic gating, or their association with ferroelectric substrates. In the latter case, periodically poled structures (i.e, antiparallel ferroelectric domains) enable the creation of reconfigurable and nonvolatile p-n homojunctions, which can also be further modulated by light [1]. In this work, we investigate the interplay between light, ferroelectricity and electronic doping in 2D materials by analyzing the photoluminescence (PL) properties of 1L-$MoSe_2$ deposited onto the polar surface of a periodically poled $LiNbO_3$ crystal. Specifically, we study the PL response as a function of the incident light intensity and/or the illumination time on domains with opposite polarity. We show that light-induced charging processes are strongly influenced by the underlying spontaneous polarization of the substrate, leading to opposite trends in the PL dynamics depending on the polarization sense. The results highlight the critical role of interfacial charge transfer in TMD-based ferroelectric heterostructures, paving the way for advanced spatial and temporal modulation of charge carriers using all- optical methods.

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Transport of colloidal particles in periodic grid of obstacles

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The objective of this project is to understand the movement of colloidal particles within fluids in the presence of a periodic grid of obstacles, which could eventually give insight on how transport occurs in certain biological systems. These colloids are solid, microscopic particles, of a few microns in size, subjected to the stochastic motion caused by the molecules in the fluid and the hydrodynamic forces created by the obstacles. The evolution of the probability density distribution for this colloidal particle is described by the Fokker-Planck equation. The density will go to equilibrium following certain relaxation frequencies, which are precisely the eigenvalues of the Fokker-Planck operator.

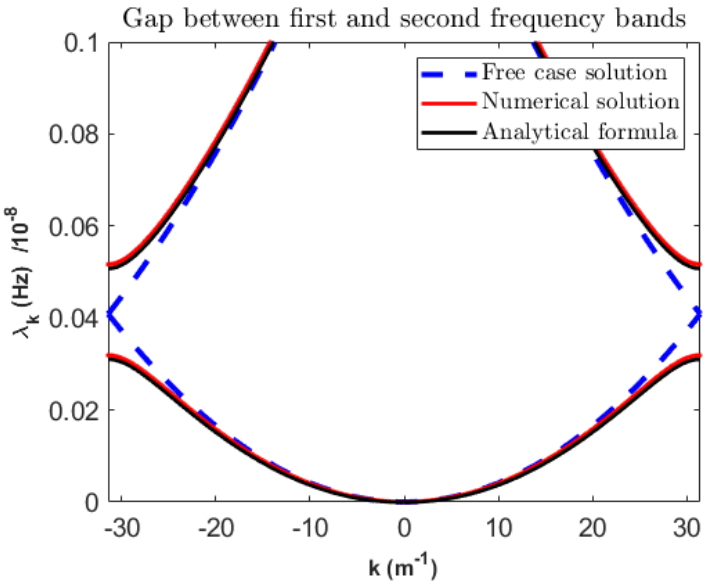

Figure 1. Eigenvalue spectrum of the Fokker-Planck operator for a certain periodic grid. A gap appears in the frequency values.

For the time being we have focused on a one-dimensional grid of obstacles. We have exploited the fact that the grid's periodicity causes the Fokker-Planck operator to commute with the translation operator, and thus Bloch's theorem can be applied to obtain the eigenvalue spectrum of frequencies, in a similar way to how the energy levels are obtained in crystalline solids. In contrast to the Hamiltonian, the Fokker-Planck operator is not Hermitian, meaning that complex eigenvalues can be obtained that lead to propagation of these colloids. Furthermore, gaps in the frequency spectrum have been shown to appear, meaning that there are certain frequencies through which the probability density cannot relax towards equilibrium. It would be of great interest to excite the system at those prohibited values to study its behavior.

Restricted Boltzmann Machines for Solving Many-Body Quantum Systems

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The goal of this project is to develop and implement a novel machine learning algorithm, inspired by principles from statistical and quantum physics, to address the computational challenges inherent in solving many-body quantum physics problems. Traditional exact methods for these problems are computationally intensive for systems with a large number of particles.

a) b)

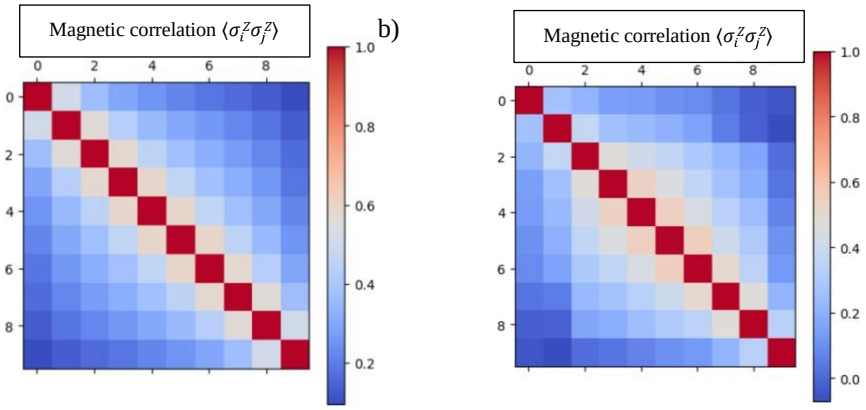

Figure 1. Magnetic spin correlation for wave function of the 1D-Ising Hamiltonian solved using exact diagonalization(a) and learnt by RBM(b).

Restricted Boltzmann Machines, recently awarded the Nobel Prize, are able to learn probability distributions from a given dataset to generate new data. As one of the first generative AI algorithms, RBMs have generally been applied to non-physics-related tasks, such as generating images or improving their resolution. In this project, RBM will be trained with quantum system measurement data to reconstruct the wave function to obtain macroscopic properties of the system and then compared to exact solutions [1].

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[2] G. Torlai et al., Neural-network quantum state tomography for many-body systems (2017)
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Optimisation of nanomaterials for their integration into lithium-ion batteries

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Magnetite nanoparticles (Fe_3O_4 NPs) are promising materials for improving the performance of lithium- ion batteries [1]; however, achieving both environmentally friendly synthesis methods and optimal particle properties is a major challenge. This study investigates two approaches to synthesize Fe_3O_4 nanoparticles using the co-precipitation method, utilizing a base to induce the reaction: one approach employs ammonium hydroxide (S1) [2], while the other uses sodium hydroxide (S2) [3].

Both methods successfully produced nanoparticles with a size of 7-9 nm. However, S2 outperformed S1 in several key areas. This resulted in more uniform deposition on the membranes, reduced aggregation, and better electrochemical performance, with oxidation and reduction peaks close to the theoretical values. Although S2 showed more aggregation compared to S1, it proved to be the more effective method overall, as cracking was evident in the S1 samples even before cycling, while S2 materials demonstrated greater resistance to such damage.

These results demonstrate that optimizing the synthesis conditions can significantly enhance the properties of nanoparticles for battery applications. Future work will focus on combining these materials with carbon nanotubes in a composite, as an electrode for ion-Li batteries, aiming to increase conductivity and establish a strong network with the nanoparticles while buffering volume expansion during cycling. This approach is likely to have a positive impact on battery efficiency, paving the way for greener and more powerful batteries. [1]

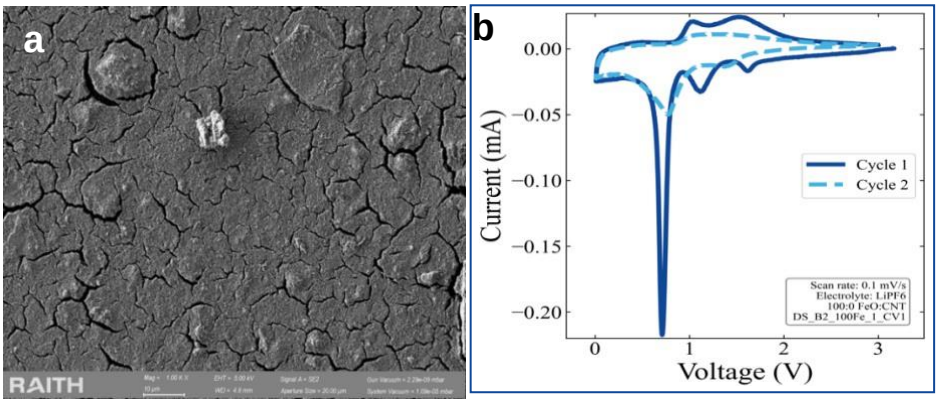

Figure 1. SEM image showing the surface morphology of the synthesized Fe_3O_4 nanoparticles (a). Cyclic voltammetry (CV) curves for Fe_3O_4-based electrodes over two cycles (b).

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[2] Braim, F. S. *et al.*, green-assisted synthesis and functionalization of superparamagnetic magnetite nanoparticles using *Sumac* extract and assessment of their cellular toxicity, uptake, and anti-metastasis property. *Ceramics International* **49**, 7359–7369 (2023).
[3] Asimakidou, T. *et al.* Continuous production of magnetic iron oxide nanocrystals by oxidative precipitation. *Chemical Engineering Journal* **393**, 124593 (2020).

Visualizing magnetic topological material NdSb

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Materials with topological band structures are one of the most active fields in condensed matter physics. Rare-earth monopnictides are known to have complex magnetic phase diagrams and some of them have been proposed to have topological properties [1]. In this project, STM studies are being carried out to determine if the topological properties of NdSb are linked to its antiferromagnetic structure below the Néel critical temperature (T_N = 15 K). We have analyzed topographical images of the samples with atomic resolution to study its crystal structure, the presence of defects and steps at low temperatures. We have also studied the density of states and identified edge states around the steps at temperatures below T_N. We will present these results and discuss preliminary measurements of the temperature dependence across T_N.

[1] B. Schrunk et al., Nature **603**, 610-615 (2022)

PhD Students

Tunneling spectroscopy through the magnetic phases of $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$

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The magnetic entropy in a compound containing magnetic ions and itinerant electrons can be reduced to reach the ground state through two competing interactions. Either Kondo screening creates a spin- singlet nonmagnetic coherent state, or Ruderman-Kittel-Kasuya-Yoshida interactions produce magnetic order. $CeRu_2Si_2$ is an archetypical heavy fermion compound with a large electronic specific heat at low temperatures and no magnetic order. On the contrary, $CeRh_2Si_2$ presents AFM order below about 36 K. $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$ shows a combined behavior, with an antiferromagnetic phase (AFM) below 4.2K, which vanishes above 2.5 T, and a metamagnetic transition at 5.5 T. The electronic properties of $Ce(Ru_{0.92}Rh_{0.08})_2Si_2$ are highly susceptible to a magnetic field. Here we present atomically resolved tunneling spectroscopy studies in a millikelvin Scanning Tunneling Microscope across the magneticphase diagram. We visualize directly atomic site dependent Kondo hybridization and its evolution across the different phases with applied magnetic field.

Oxidized is better: modifying the photoluminescence of γ-In_2S_3 nanoplatelets

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Two-dimensional (2D) semiconductor materials are being explored for applications including photocatalysis and optoelectronic devices. This class of materials showcases high surface-to-volume ratio, which imparts unique physical properties but also heightens the interaction with the environment. Large-scale application of these materials requires a deep understanding of degradation processes towards the design of strategies to increase their stability.[1] Indium sulfide (In_2S_3) is a promising material for photovoltaic and (opto)electronic applications because of its wide band gap energy, and photoconductive properties. It presents three different polymorphs: cubic (α), tetragonal (β) and trigonal (γ), in which the most stable one is the β-phase. However, the defective crystal structure presented by the β-phase makes the material more prone to oxidation. On the other hand, γ-In_2S_3 is a polymorph, that has been stabilized at room temperature as colloidal nanoplatelet dispersion.[4] In this work, the photoluminescence properties of γ-In_2S_3 were studied at cryogenic temperatures, observing that the emission of this material comes from the different intra-band gap defect levels. To study the effect of oxidation, the material was exposed to air for a prolonged time, observing the appearance of oxygen-containing chemical species in the surface of γ-In_2S_3. This oxidation is translated into a change in the photoluminescence spectra, where oxygen-related intra-band gap defects states were identified though their characteristic spectral fingerprints. By leveraging this knowledge, we were able to modify the photoluminescence properties of γ-In_2S_3 by treating it with an oxygen-containing molecule. This study offers new insight into the properties of less studied material, providing key information for its application in several fields including luminescence thermometry and oxygen sensing.

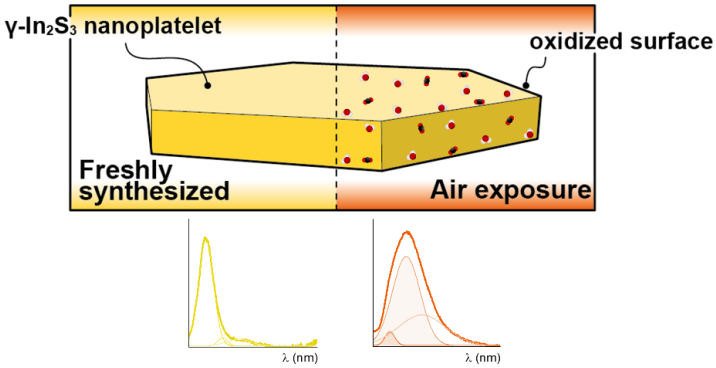

Figure 1. Change in the photoluminescence properties between a recently synthesized nanoplatelet (yellow) and a sample exposed to air formonths (orange).

[1] Dai, M. *et al.*, *Adv. Mater. Technol.* **7**, 2200321 (2022).
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Near-Infrared Luminescent Cr^{3+}-doped FluorideNanoparticles

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Transition metal (TM) and lanthanoid (Ln) ion-doped nanoparticles (NPs) are photoluminescent nanomaterials with applications across diverse fields, such as bioimaging and theranostics, sensing, light conversion and energy applications, data storage, quantum computing, and anti-counterfeiting. Fluoride NPs stand out among nanomaterials in this context owing to their unique physical properties, such as low- energy phonons, size and architecture tunability, as well as colloidal stability and low cytotoxicity. Despite the many advances in the development of fluoride NPs in recent years, most of them are primarily designed to incorporate only Ln ions. TM ions cannot be easily accommodated into the crystal lattice of fluoride NPs due to their distinct electronic configurations, ionic radii (lower sizes) and coordination preferences (lower coordination number).

Here, we present a wet-chemistry synthesis approach for the preparation of an In-based fluoride NPs that can be doped with Cr^{3+}, used as model luminescent TM ion.

The synthetic protocol of In-based fluoride NPs was optimized to identify the NPs growth mechanism,which involves a phase transition from cubic to monoclinic crystalline structure, similar to the cubic-to-hexagonal phase conversion in $NaYF_4$ NPs. The optimization revealed that reaction time and temperature (above 250 ºC) had minimal effects on NP size and morphology. Importantly, the size of these NPs can be tuned by adjusting the amounts of fluoride source and oleylamine in the reaction mixture. Additionally, these NPs can be easily made hydrophilic, enhancing their potential for biological applications, showingtheir low in vitro cytotoxicity. The efficient incorporation of Cr^{3+} ions and the crystal field experienced by them in this crystalline host matrix has been explored by photoluminescence (PL) studies at room temperature (RT) and at cryogenic temperatures (15 - 298 K). Time-resolved PL measurements of Na_3InF_6: Cr^{3+} NPs showed thermal dependence in the range of 20-50 ºC, thus paving the way for the use of luminescent TM-doped fluoride NPs in including in sensing in biological environments.

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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 Bi100-xSbx 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].

[1] J. S. Shier and D. M. Ginsberg, Physical Review 147 (1966) 84.
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[5] A. Andrino-Gómez et al., Low Temperature Physics 50 (2024) 427-433.

Thermoelectric power study of 2D dichalcogenides through Scanning Thermopower microscopy adapted in a Scanning Tunnel microscope.

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Nanotechnology requires the use of specialized experimental techniques to investigate the physical properties of materials at the nanoscale. One such powerful technique is Scanning Tunneling Microscopy (STM), which allows the study of material surfaces at the atomic level. In STM, a sharp metal tip is positioned extremely close to the sample surface, typically of the order of angstroms. At thisproximity, electrons can tunnel between the tip and the sample, generating a tunneling current [1]. Thiscurrent is measured and used to produce images of the surface topography with atomic resolution, as well as to probe the local density of states through tunnel conductance.

STM can be modified to incorporate additional measurement modes, enabling the exploration of physical phenomena beyond those addressed by the conventional technique [2]. In this poster, we present a novel approach involving the development of a high-resolution Scanning Tunneling Microscope adapted as a Thermopower Microscope (STM/SThEM), which operates in a high vacuum environment and at room temperature. This innovative setup allows for the measurement of the Seebeck coefficient (S), a critical parameter in thermoelectric studies, and offers valuable insights into material propertiesWe demonstrate the application of this technique using our custom-built STM/SThEM microscope to study the effect of chemical doping on the thermoelectric power of the transition metal dichalcogenide WSe_2, a novel material with additional properties such as ferroelectricity and ferromagnetism [3].

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Vortex lattice pinning at 20 K in the stoichiometric pnictide superconductor $CaKFe_4As_4$

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Vortices in a superconductor usually arrange themselves in an ordered lattice, but when a currentis applied vortices move under the Lorentz force, leading to dissipation and loss of the superconducting coherence [1]. Vortices can be pinned by impurities and imperfections counteracting this motion. However, thermal excitation might provide sufficient energy to releasevortices from their pinning centers. Superconducting applications require immobile vortices in the largest possible temperature range. This is particularly important in high Tc superconductors. Herewe make vortex imaging experiments in the superconductor $CaKFe_4As_4$ (T_c=35 K, H_{c2}=90 T) from 10 K up to Tc and up to magnetic fields of 14 T. This compound has been used for manufacturing superconducting wires [2]. We construct the phase diagram for the vortex lattice, delineating the optimal pinning range and directly observing the transition to the vortex liquid phase.

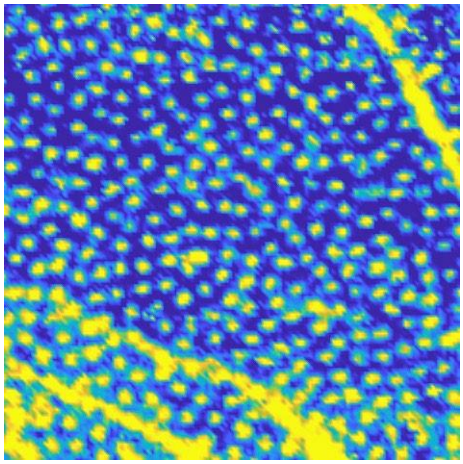

Figure 1. The vortex lattice of CaKFe4As4 taken at 10 K and under a magnetic field of 10 T.

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[2] S. Pyon et al., *Applied Physics Express*, *11*(12), 123101. (2018)

Phase transition induced carrier density modulation in monolayer MoS_2/SBN heterostructures

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This work explores the tunable optoelectronic response of monolayer MoS_2 deposited on a ferroelectric substrate (SBN) that undergoes a transition from the ferroelectric to the paraelectricphase. Transition Metal Dichalcogenides (TMDs) like MoS_2 are known for their distinctive electronic and optical properties, which can be influenced by underlying substrates through electrostatic interactions.

In this study, SBN—a relaxor ferroelectric crystal with a low Curie temperature—is used to induce electrostatic doping effects on MoS_2 in response to temperature changes. Confocalphotoluminescence (PL) measurements performed across a temperature range of 30–90°C show significant enhancement of the exciton/trion rate within the MoS_2 layer as the substrate evolves from the ferroelectric to paraelectric state. This effect is attributed to the vanishing spontaneous polarization in the paraelectric phase, which alters the polarization and screening charge balanceat the MoS_2/SBN interface and therefore the electronic doping. The findings highlight a promising method for optoelectronic modulation in TMDs and suggest potential applications fortemperature-responsive photonic devices that operate without external electric fields.

Sensing Cellular Temperature In Multicellular Spheroids Using CaF_2:Nd, Y Nanoparticles

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In biomedical research, light is an invaluable, non-invasive tool for engaging with biological samples, allowing advancements in super-resolution and live cell imaging. Although these methods are developed with in vivo applications in mind, results often vary from conventional monolayer assays conducted *in vitro*. In this context, 3D cell cultures—particularly multicellular spheroids—offer a more accurate tissue-like model, bridging the gap between *in vitro* and *in vivo*. Spheroids are spherical aggregates of single or multiple cell lines that can be easily prepared *in vitro*, providing reproducibility through size and enablingcontrolled experiments.[1] Initially, we identified safe illumination ranges according to multiple wavelengths and established a rapid visual method for monitoring the health of the spheroid.[2] The interaction of light with spheroids can raise local temperatures, which may affect cell proliferation due to their strict thermal tolerances. This study aims to assess local temperature variations within spheroids to comprehend cell-light interactions and cellular thermal responses to external stimuli.

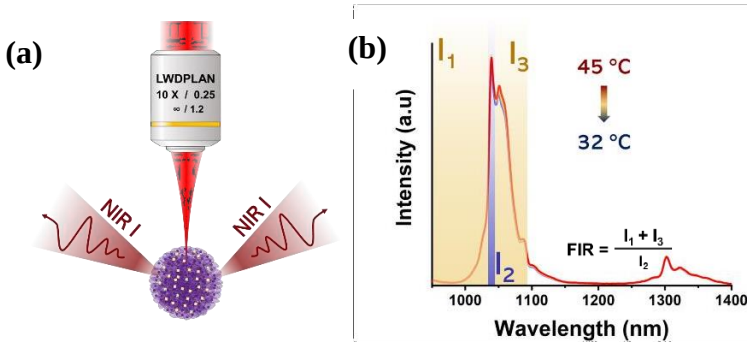

Figure 1. (a) Schema of the irradiation of the nanoparticles inside the spheroid an its emission (b) Emission spectra of the CaF_2:Nd,Y nanoparticles inside the spheroid.

Spheroids were developed by forced-floating method using U-87 MG cells from human brain cancer (glioblastoma astrocytoma), resulting in an approximately diameter of 200 μm. Given the microscale of thisbiological model, high spatial resolution for remote measurement is needed. To meet this requirement, CaF_2:Nd, Y nanoparticles were synthesized by hydrothermal method. The electronic population of the levels involved in the emission of Ln^{3+}- doped materials follows a Boltzmann distribution, making the emission temperature-dependent. After the optimization of several optical parameters (excitation wavelength, region where the Fluorescence Intensity Ratio determines the best sensitivity, …) they turn outto be nanothermometers with enough sensibility and precision. Following the internalization of the nanothermometers into the cells comprising the spheroid, emission temperature calibration was conducted.Since this, the temperature increases inside the spheroid due to 1450 nm illumination have been measured.

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Magnetic state dependent thermoelectricity insuperconducting spin valves

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Spin-splitted superconductor-ferromagnet tunnel junctions demonstrate giant thermoelectric effects (TEs), which are being exploited to engineer ultra-sensitive terahertz radiation detectors. Here, we experimentally observe the recently predicted complete magnetic control over thermoelectric effects in superconducting epitaxial spin valve junction (V/MgO/Fe/MgO/Fe/Co),including the dependence of its sign on the magnetic state of the film [1,2]. The description of theexperimental results is improved by the introduction of an interfacial domain wall in the spin filterlayer interfacing the superconductor. The application of high in-plane magnetic fields induces a double sign inversion of the thermoelectric effect, which exhibits large values even at applied fields of twice the superconducting critical field, leading up to a "giant thermoelectric effect".

We also investigated experimentally and numerically [3] thermoelectric effects in fullyepitaxial Fe/MgO/V/MgO/Fe/Co junctions as well as their dependence on the magnetic configuration of the FM electrodes. We observe sizeable Seebeck coefficients for the parallel alignment of the ferromagnetic electrodes, reaching values on about of 100 μV/K. Importantly, we find a decrease of the thermoelectric signal of more than an order of magnitude when switchingfrom a parallel to the antiparallel configuration, constituting a large thermoelectric spin-valve effect. Theoretical modeling based on a self-consistent non-equilibrium Keldysh-Usadel Green function theory, combined with micromagnetic simulations, qualitatively reproduce these experimental findings.

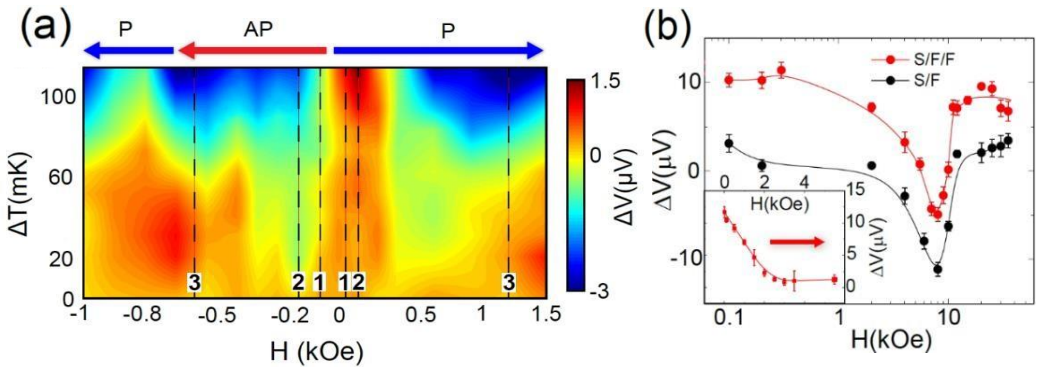

Figure 1. (a) Colormap of the thermoelectric voltage ΔV as a function of the temperature difference ΔT and the applied in-plane field for a S/F/F junction, indicating the P and AP states.The sign inversion of the TE voltage becomes apparent with different magnetic alignment of thelayers of the spin valve. (b) TE voltage of an S/F/F and S/F junctions at ΔT≈113 mK vs. appliedin-plane field at T=0.3 K. The high-field sign inversion is achieved in both samples. The inset displays the measured TE voltage in the S/F/F junction under out-of-plane field. At thesuperconductong critical field, superconductivity and its associated TE voltage vanish.

[1] C. González-Ruano et al., Phys. Rev. Lett., **130**, 11111 (2023)
[2] J. A. Ouassou et al., Phys. Rev. B, **106**, 094514 (2022)
[3] P. Tuero, et al., under preparation.

Upconversion Nanoparticles as Potential Nanothermometers: Temperature-Dependent Emission Analysis of SrF_2: Tm^{3+}, Yb^{3+}.

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The importance of the use of upconversion particles (UCNPs) in biomedical applications has been evidenced over the years, primarily due to their ability to be excited in the near infrared (NIR) and emit inthe visible or ultraviolet (UV). This property allows greater penetration into biological tissues and facilitatesobtaining cleaner images. In addition, the strong dependence between UCNPs emission and temperature iswell known [1,2]. Therefore, different samples of SrF_2: Tm^{3+}, Yb^{3+}, co-doped with bismuth and dispersed in heavy water,were excited using a 980 nm laser to obtain strong UV emission at different temperatures, ranging from 10ºC to 60 ºC. These samples have been studied in order to explore the correlation between emission and temperature, aiming to determine whether these particles are sensitive enough to function as nanothermometers [3].

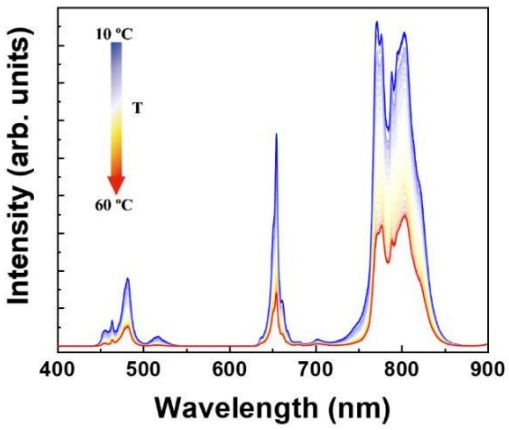

Figure 1. Upconversion luminescence spectra of SrF2: 22% Yb, 0.5% Tm, 1.5% Bi UCNPs at thetemperature range of 10 - 60 ˚C recorded with steps of 2 ˚C under 980 laser excitation.

Through a serie of experiments, we synthesized different UCNPs samples to identify which offers the highest sensitivity, and consequently, the best suitability as nanothermometer for biological systems.

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[2] Brites, Carlos DS, Sangeetha Balabhadra, and Luís D. Carlos. "Lanthanide-based thermometers: at the cutting-edge of luminescence thermometry." *Advanced Optical Materials* 7.5 (2019): 1801239.

[3] Quintanilla, M., et al. "Intense ultraviolet upconversion in water dispersible SrF 2: Tm 3+, Yb 3+ nanoparticles: the effect of the environment on light emissions." *Journal of Materials Chemistry C* 3.13(2015): 3108-3113.

Synthesis of Magnetic Iron Oxide Nanoparticles via Rapid Microwave Plasma Hydrogenation for Biomedical Applications

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Advancements in nanotechnology have led to the development of nanostructures with precise morphologies and customized surface properties for specific applications. Efforts focuson optimizing nanoparticle characteristics such as composition, shape, size, and magnetic properties [1]. Magnetic nanostructures are particularly promising for enhancing therapeutic procedures, clinical diagnostics, and biomedicine. However, synthesizing monodisperse magnetic nanoparticles larger than 30 nm remains very challenging, often requiring very long multi-step that can take over five hours.

In this study, hematite nanoparticles (NPs) were hydrothermally synthesized. NPs weresubsequently reduced using a 10-minute microwave plasma hydrogenation process. The resulting nanoparticles exhibited excellent monodispersity and saturation magnetization above40 emu/g. We examined the effects of plasma pressure and hydrogen concentration on magneticproperties, finding that higher hydrogen concentrations and lower plasma pressures increased saturation magnetization. These magnetic NPs have been tested for cellular magnetic stimulation and hold potential for other biomedical and environmental applications, such as magnetic hyperthermia, drug delivery, and water purification. [2].

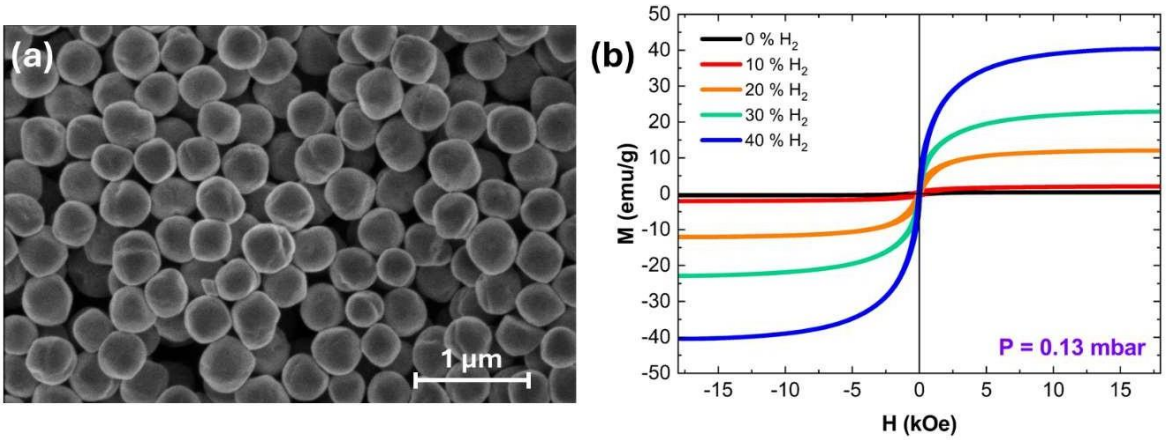

Figure 1: (a) SEM images of the magnetic NPs. (b) Hysteresis loop of the magnetic NPs as afunction of the concentration of hydrogen used in the reduction process.

[1] A. Lu, E.L. Salabas and F. Schüth, Angew Chem Int Ed 46 (2007) 1222–1244.
[2] L. Peixoto, *et al.*, Applied Physics Reviews 7 (2020) 011310.

Pyroelectric control of the electronic doping in MoS_2 monolayers deposited on ferroelectric substrates

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Monolayer transition metal dichalcogenides (TMDs), such as MoS_2, are promising two-dimensional materials for nanoscale optoelectronic applications. Making use of their strong sensitivity to the surrounding environment, we investigate the modulation of electronic doping in a monolayer of MoS_2 deposited on a ferroelectric substrate ($LiNbO_3$) as the temperature varies from 300 K to 10 K. Temperature-dependent photoluminescence measurements were performedto determine the variation of the relative concentrations of excitons and trions, which correlate with the free carrier concentration.

Our results reveal a distinct variation in electronic doping levels that correlates with changes in the electric polarization of the $LiNbO_3$ substrate across the 300 K to 10 K temperature range. These findings underscore the role of pyroelectricity in modulating the electronic environment ofMoS_2 and demonstrate that ferroelectric substrates offer an effective strategy for precise control of electronic doping in TMDs. This work opens new avenues for engineering doping profiles in 2D materials, enhancing their potential in optoelectronic applications.

Charge density wave in UTe_2 measured by STM

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UTe_2 is one of the most promising materials to show topological superconductivity. The intimate connection between bulk and boundary places the surface at the center of the debate on the topological properties. However, previous surface measurements by Scanning Tunneling Microscopy (STM) show in UTe_2 a puzzling charge density wave (CDW) [1-4], apparently unrelated to the bulk [5-7]. In this work, weshow results from STM measurements at the (011) surface of UTe_2 under high magnetic fields up to 20 T.We present new insights into the CDW, possibly solving some of the issues concerning it.

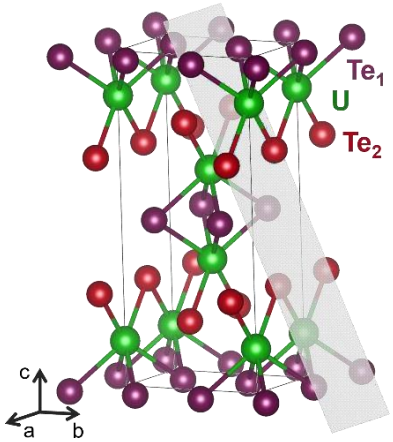

Figure 1. Orthorhombic unit cell of the UTe_2 atomic lattice. Violet, red and green spheres are Te(1),Te(2) and U atoms, respectively. The (011) cleaving plane is given in grey.

[1] L. Jiao et al., Nature **579**, 523(2020)
[2] Q. Gu et al., Nature **618**, 921 (2023)
[3] A. Aishwarya et al., Nat. Phys. **20**, 964 (2024)
[4] A. LaFleur et al., Nat. Comm. **15**, 4456 (2024)
[5] C. Kengle et al., Phys. Rev. B, **110**, 145101 (2024)
[6] F. Theuss et al., Phys. Rev. B, **110**, 144507 (2024)
[7] C. Kengle et al., arXiv:2406.14690

Experimental and theoretical investigation of the optoelectronic behavior of Lead Iodide governed by two-dimensional electron confinement

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In this study, experimental and theoretical methods are used to explore lead iodide's (PbI_2) structure and optoelectronic properties. By combining X-ray diffraction and photoelectron spectroscopy with density functional theory (DFT) simulations, the research reveals PbI_2's two- dimensional layered structure and its strong transient photocurrent effect under visible light, attributed to a surface photovoltage effect. The prolonged lifetime and long relaxation times of this photocurrent are due to slow carrier mobility, which results from 2D electron confinement in the layered material. These insights help model the behavior of more complex 2D hybrid perovskites.

Na and Li anode growth at the nanoscale by synchrotron-based PEEM and AFM

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Zero-Excess Solid-State Batteries (ZESSBs), where the anode is formed during the charge cycle, are a promising alternative to today Li-ion batteries, as they offer a higher energy density, improve safety and cut on anode production. Further advances are done in substituting Li-based electrolytes to Na-based, as itis not a critical material. Deeper knowledge is needed in the early stages of anode nucleation [1,2] tobring this technology into daily use.
We have studied the anode plating and stripping process in both Li and Na-based electrolytes, usingthe virtual electrode approach. Combining Atomic Force Microscopy (AFM) at UAM and Photoemission Electron Microscopy (PEEM) at the CIRCE beamline of ALBA synchrotron, we have been able to study the growth kinetics, morphology and chemical state of the grown anodes with nanoscale resolution. Multiple anode platings were done, varying the electron dose, current and energy, as to find the optimal growth parameters for the virtual electrode approach. With this work, we aim to unveil the mechanisms behind anode growth in ZESSBs.

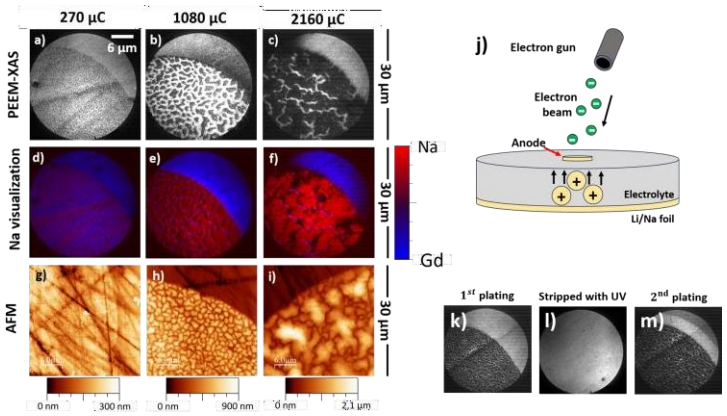

Figure 1. a) to i) study of dose effect on anode plating. a) to c) PEEM-XAS measures for chemicalcomposition information. d) to f) visualization of surface chemical composition. g) to i) anodes topographies. j) virtual electrode approach plating setup scheme. k) to l) anode cycling done by the virtualelectrode approach

[1] Li, Q., Yi, T., et al, "*In-situ* visualization of lithium plating in all-solid-state lithium-metal battery." Nano Energy 63 (2019). DOI: 10.1016/j.nanoen.2019.103895
[2] Fuchs, T., Ortmann, T., Becker, J. et al. "Imaging the microstructure of lithium and sodium metal inanode-free solid-state batteries using electron backscatter diffraction." Nat. Mater. (2024). DOI: 10.1038/s41563-024-02006-8

Langmuir-Blodgett films of plasmonic Janus Nanoparticlesfor biomedical applications

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In the past few decades, an increasingly important trend in controlling physical and chemical properties at lower scales to develop new materials has been aimed. Among a variety of approaches to address this, the Langmuir-Blodgett (LB) technique is an efficient method for making ultrathin organic and inorganic colloidal self-assembled films, which has a wide range of optoelectronic and biomedical applications [1,2]. If a metallic and biocompatible semi-shell of gold is additionally deposited on top, either to increase the scattering cross-section of the particles, or the absorption cross-section after a properthermal treatment of the gold films, the resulting structure can also induce controlled temperature increments and contribute to thermal therapies with positive effects against ongoing diseases, such as cancer [3]. Additionally, the nanoscale combination of materials with magnetic and plasmonic properties has demonstrated a synergistic potential resulting from the association of both materials [4]. In this work, we present a variety of SiO2 particles of sizes ranging from 200 to 500 nm transferred onto a substrate using a Langmuir-Blodgett trough (Figure 1a). Later, 5-20 nm layers of Fe iron are first deposited on the surface of the particles via magnetron sputtering and then oxidized in a muffle furnace toform hematite. As an intermediate step of the fabrication, the synergetic hematite-gold capabilities of the particles are sought-after by depositing an additional quasi-continuous Au layer on top of the particles that is further annealed to form individual Au nanoparticles that increase the absorption cross-section, andtherefore their heating efficiency. Their corresponding heating curves close from the plasmon resonance of the Au nanoparticles show an enhancement of the heating capabilities compared to the particles only covered with hematite (Figure 1b).

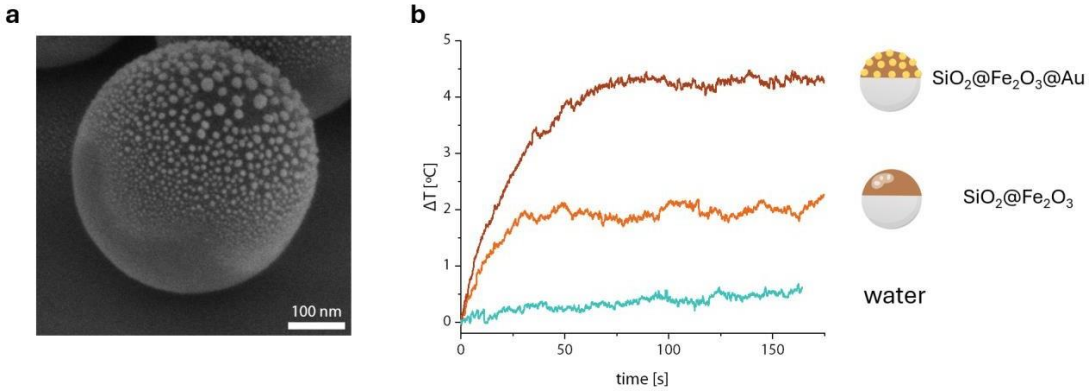

Figure 1. a) Scanning Electron Microscopy (SEM) image of commercial 200 nm SiO_2 particles transferred by LB assembly, after Fe and Au deposition via magnetron sputtering to ultimately form individual Au nanoparticles on the surface by thermal annealing. b) Heating curves recorded under 690 nm laser irradiation measurements of the $SiO_2@Fe_2O_3$ with and without Au nanoparticles on top, showing a synergistic heating with the addition of Au nanoparticles.

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[2] Z. Matharu et al., Langmuir, **23**, 13188-13192 (2007)
[3] S. C. Freitas et al., Adv. Mater. Interfaces, **10**, 2202214 (2023)
[4] T. A. Larson et al., Nanotechnology, **18**, 325101 (2007)

Targeting Inflammation: Unveiling Gold Beyond OCTDetection Using PIXE and RBS

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Optical coherence tomography (OCT) is a high-resolution optical imaging technology that is substituting other conventional cardiovascular diagnostic procedures (ultrasound, angiography). Today, OCT is used as a minimally invasive technique to detect and assess atherosclerotic plaques in vivo and to guide intervention procedures such as atherosclerotic surgery and stent placement [1]. Despite its high resolution, the lack of molecular-scale information available in OCT images makes the use of contrast agents a step-forward in the implementation of this technique. For this purpose, innovative strategies like functionalized nanoparticles are being used to achieve molecular level contrast by targeting specific biomarkers. Proteins overexpressed by cells that are undergoing inflammatory processes, like intracellular adhesion molecule 1(ICAM-1) are particularly interesting, as they are characteristic of the early stages of the atherosclerotic plaque development.

Gold nanoshells (GNSs) functionalized with inflammation-targeting molecules have already been usedas OCT contrast agents, and their specific adhesion to inflamed endothelial human cells has been demonstrated in vitro [2]. However, the translation of these experiments to tissues is challenging, since thepresence of gold on the tissue can go undetected if the OCT signal provided by the GNSs is similar to the one provided by tissues, making the optimization of the experimental conditions challenging. In this workwe have addressed this problem by determining the gold presence on inflamed rat-aorta tissue after incubation with functionalized-GNSs using Rutherford Back Scattering (RBS) and Particle Induced X-rayEmission (PIXE) with a 2 MeV proton beam. The technique has demonstrated the presence of gold undetected by OCT, and thus can be used as a guide towards a better understanding of the OCT detection of GNSs. The present study represents an important step forward for the use of contrast agents to target inflammation in the first stages of atherosclerosis by OCT.

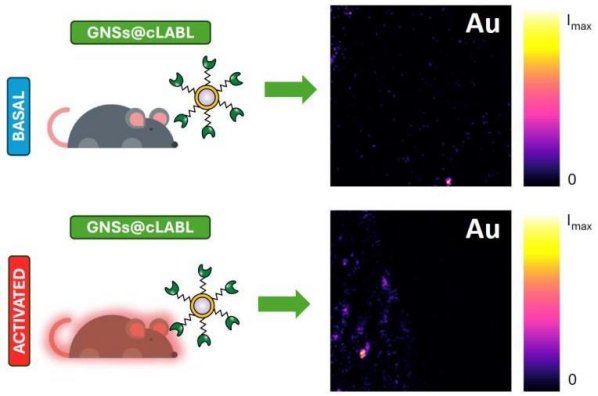

Figure 1. RBS gold signal in a basal state (top) vs. inflammed (bottom) mice aorta.

[1] Tearney, G. J., et al., (2012). Consensus standards for acquisition, measurement, and reporting of intravascular optical coherence tomography studies: a report from the International Working Group for Intravascular Optical Coherence Tomography Standardization and Validation. Journal of the American College of Cardiology, 59(12), 1058-1072.

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

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The influence of a magnetic field on single atom point contacts of nonmagnetic metals as Au and Ag isconsidered to be weak and generally negligible in the field range of a few tens of Tesla. The eventual modifications of the band structure by, say, a Zeeman shift, are nearly negligible in metals with a large bandwidth. However, it is also known that there are circumstances in which these metals respond to these values of magnetic field, particularly in nanoscale systems and surfaces. Here we measure Au and Ag atomic size contacts in magnetic fields from zero field to 20 T. We demonstrate a magnetic field induced torque which leads to atomic binding at shorter distances than those at zero field. Furthermore, the conductance drops below the quantum of conductance, $G_0 = 2e/h$, at high magnetic fields by about 15% due to (spin polarized) scattering from residual O_2 molecules which are attracted to the contact region.

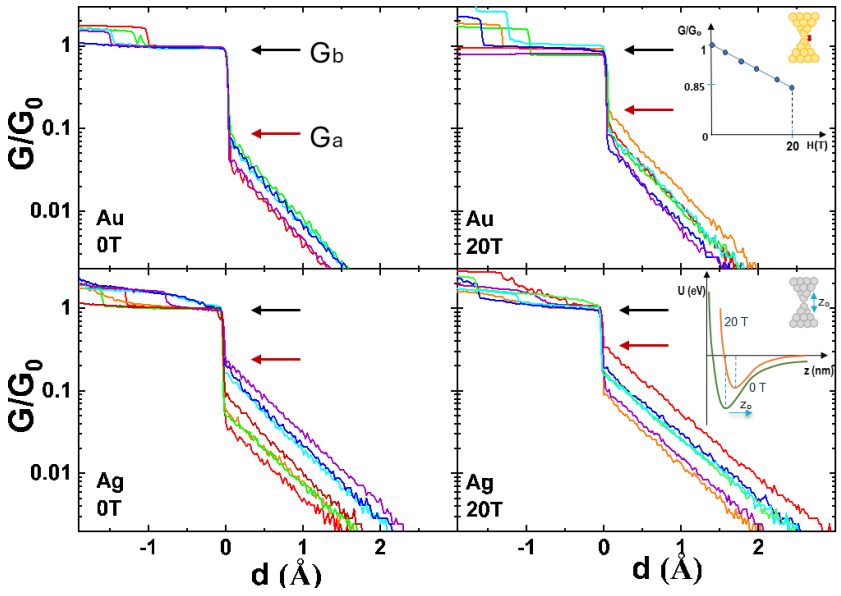

Figure 1. Dependence of the quantum tunnelling conductance regime in single atom point contacts ofAu and Ag samples under the effect of an external applied magnetic field. The tunnelling conductance isnormalized to the value of the quantum of conductance, G_0. The insets schematically show the evolution of the conductance value of the single atom point contact and the jump to contact distance whenincreasing the external magnetic field.

[1] B. Wu, et al, *Magnetic field dependence of the atomic and electronic structure of monovalent metallicnanocontacts unveiled in transport experiments*. In preparation (2024).
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[3] C. Sabater, et al, *Understanding the structure of the first atomic contact in gold.* Nanoscale Res. Lett.**8**, 257 (2013).
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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.

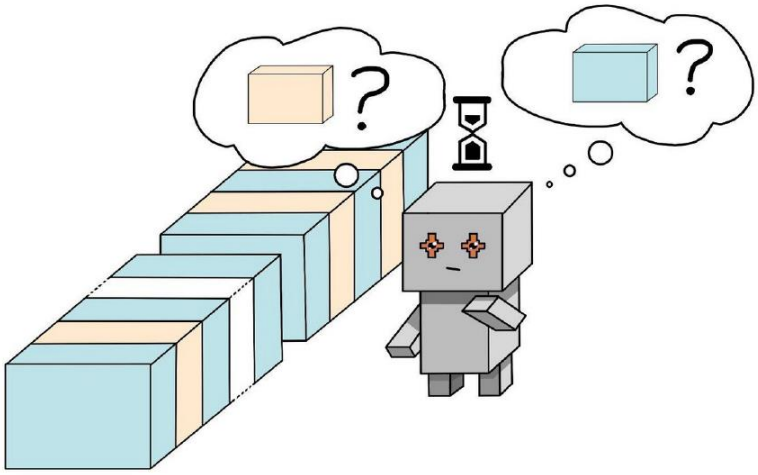

Figure 1. Reinforcement Learning schema for the enhancement of near-field radiative heat transfer through the design of a multilayer system.

[1] E. Ortiz-Mansilla, J.J. García-Esteban, J. Bravo-Abad, J.C. Cuevas, Deep Reinforcement Learning for Radiative Heat Transfer Optimization Problems, arXiv: 2408.15727, to appear in Phys. Rev. Applied.

En Route to Reliable Multiparametric Luminescence Sensing

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Luminescence sensing offers remote and minimally invasive inference of physicochemical conditions that modulate the readout of a luminescent probe. For example, biologically relevant parameters such as temperature, pressure, and dissolved oxygen may all induce a change in the steady state and temporal domain readout features (e.g., emission band peak position and shape, and luminescence lifetime, respectively).[1-3] Calibration of a specific readout feature against one or more such parameters *under controlled conditions* thus offers luminescence sensing of said parameter(s), assuming that only one unknown parameter is targeted. A simple case is one in which only one parameter induces a large change in a specific readout feature – such a sensor is deemed highly selective and sensitive. However, it is almost always the case that multiple parameters modulate the same readout feature – a popular term for this phenomenon is "cross-sensitivity", and a sensor prone to cross-sensitivity is deemed "biased". Lack of consideration of the relevant parameters during calibration of a biased sensor thus hinders accurate inference of the parameter of interest under complex physicochemical conditions in which multiple parameters are changing simultaneously. Furthermore, even if diligent parameter control was established during multiparametric sensor calibration, cross-sensitivity makes it impossible to accurately infer the magnitude of two parameters of interest from a single readout if both are unknown. Motivated by the pursuit of reliable multiparametric sensing, we implement silver sulfide (Ag_2S) nanoparticles as a platform to critically evaluate the possibility of reliable luminescence thermometry under conditions of simultaneously changing pressure and dissolved oxygen concentration (i.e., conditions of high relevance to in-vivo luminescence thermometry). In the scope of this work, we also propose new metrics for quantifying cross-sensitivity and identify machine learning strategies to decouple cross-sensitive readouts when targeting two unknown parameters simultaneously.

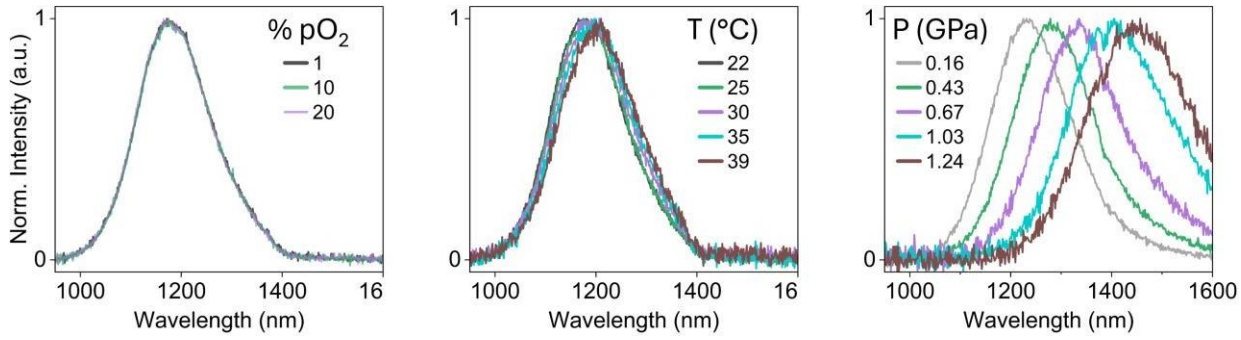

Figure 1. Differential sensitivity of Ag_2S emission toward O_2, temperature, and pressure.

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Intracellular spectroscopy of infrared emitting goldnanoclusters

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Gold nanoclusters (AuNCs) typically consist of a core made up of a few metal atoms, protected by an organic shell, with both elements influencing their photoluminescent characteristics. Although there has been progress in utilizing AuNCs emitting in the second biological window (NIR-II) as probes in biological systems,[1,2] there remains limited understanding of their spectroscopic behavior within such environments. In this investigation, we explored the spectroscopic properties of NIR-II-emitting AuNCs[3] in vitro, focusing on the alterations in their luminescence when incorporated into live cells. The infrared luminescent characteristics of AuNCs were systematically assessed as a function of pH, viscosity, ionic strength, proteins, aggregation state and the redox environment, providing deeper insights into the mechanisms underlying the modifications induced by the intracellular medium. Finally, we conducted in vivo studies to demonstrate that living organisms can modulate the response of AuNCs-based sensors, highlighting the critical need for comprehensive characterization of their properties to prevent erroneous redouts.

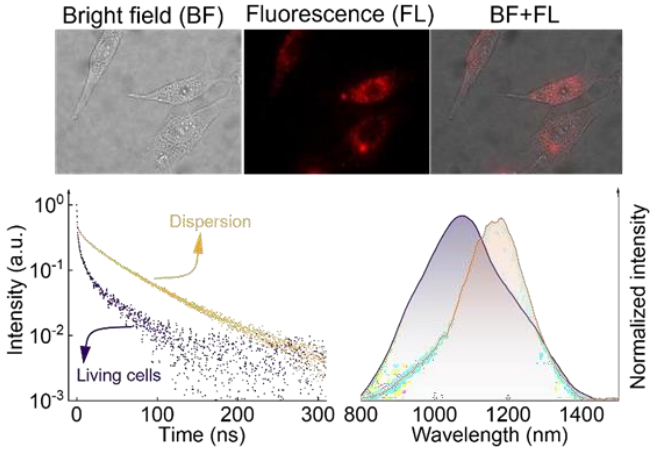

Figure 1. Bright field and fluorescence images of NIR II AuNCs in U87 cell line. Lifetime andphotoluminescence emission of AuNCs in dispersion and within living cells.

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Current-driven orbital angular momentum flow fromCu/oxide interfaces

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The angular momentum of the electrons underpins the field of spintronics, which focuses on designing materials with complementary magnetic and electrical properties for memory and logic applications [1]. Most spintronic phenomena, however, involve spin-orbit coupling (SOC) which is limited to a few number of materials, thus restricting the development of such technologies. Orbital angular momentum (OAM) has appeared as an interesting alternative to the use of spin and SOC in devices, yet holding betterefficiencies [2]. Deploying OAM currents in experiments might be challenging, particularly in magnetic devices where conversion of orbital into spin currents is necessary for angular momentum transfer to the spin-lattice. This conversion is achievable by interfacing the OAM generator with an SOC metal [3], highlighting a critical step in the experimental validation and utilization of OAM in device applications.In our study, we explore the generation and propagation of OAM at copper (Cu)/oxide interfaces [4]. By employing cobalt (Co)/ platinum (Pt) thin films interfaced with our OAM generator we can assess the impact of OAM through spin-orbit torque (SOT) measurements. We conduct such study at room temperature via harmonic magneto-transport measurements in patterned hall-bar devices [5]. We find thatorbital currents significantly enhance SOT in Co, as evidenced by an enhanced damping-like (DL) torque detected in the second harmonic response in in-plane angular dependent measurements. By interfacing copper (Cu) with AlO_x and CuOx, we demonstrated a threefold enhancement of the DL torque in Co compared to the reference Co/Pt bilayer. Therefore, the use of orbital angular momentum currents result in a massive enhancement of the angular momentum transfer to the magnetic lattice. These results highlight the potential of *orbitronics* to extend the range of materials to be employed in the nextgeneration of electronic devices.

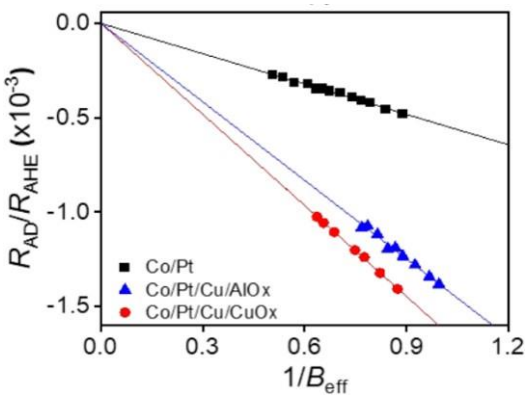

Figure 1. SOT analysis. The efficiency of the anti-damping torque is determined by the slope of the linear fit. A ~3-fold increase of the spin torque is observed in the Cu/oxide samples due to orbital angular momentum currents.

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Exploring the charge state of cancer cell spheroids viaphotovoltaic tweezers

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Photovoltaic optoelectronic tweezers (PVOT) are versatile tools widely used for manipulating and trapping micro- and nano-objects. PVOT take advantage of the electric fields generated by the bulk photovoltaic effect (PVE), present in certain ferroelectric crystals, such as LiNbO3:Fe (LN:Fe) [1]. Recently, a method for manipulating micro-droplets by PVOT has been developed, allowing for the manipulation of aqueous suspensions with biomaterials, such as DNA and sperm, homogenously dispersedwithin the droplets [2].

In this work, we report the manipulation and characterization of non-homogenous droplets containing individual multicellular spheroids — 3D models of cells whose metabolism is close to tissue metabolism [3]. Two cancerous human cell lines, U-87 MG and MCF-7, have been studied.

The cell culture medium droplets containing a distinguishable spheroid, referred to as hybrid droplets, are suspended at the air-paraffin interface (see Figure 1). Upon illumination of the ferroelectric crystal, thedroplet starts migrating due to interactions with the photo-generated electric field.

Results show differences in the migration behavior of hybrid droplets compared to only cell culture medium droplets, depending on which face of the ferroelectric crystal is illuminated. The analysis of the migration of droplets of varying aqueous suspensions (water, cell culture medium, and hybrid droplets) demonstrates that the spheroids exhibit negative charge. Additionally, a model was developed to estimate the charge density of the spheroids.

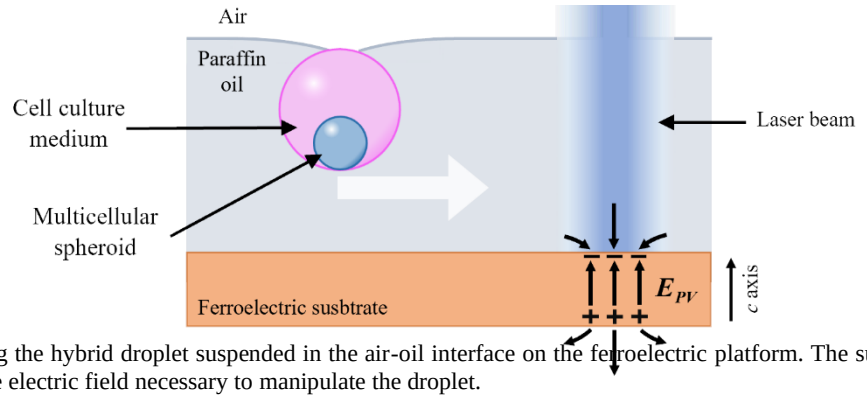

Figure 1. Schematics showing the hybrid droplet suspended in the air-oil interface on the ferroelectric platform. The substrate is illuminated by the laser beam, generating the electric field necessary to manipulate the droplet.

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Antiaromatic non-alternant heterocyclic compounds asmolecular wires

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We have theoretically studied the electron-transport properties of a family of molecular junctions containing the antiaromatic pentalene moiety stabilised with various 5-membered heterocycles [1]. By electron-transport calculations based on density functional theory, we show that the position of the heteroatom affects the shape of the transmission curves significantly. We also observed that, despite causinga reduction of the HOMO-LUMO gap, a higher degree of antiaromaticity does not necessarily lead to an increase in conductance. This is due to the appearance of destructive quantum interference. This behaviouris well-modelled by tight-binding calculations and the graphical prediction scheme [2,3] but not by curly arrow rules.
We developed an algorithm to efficiently determine analytically, using the graphical prediction method, whether destructive quantum interference will appear. This allows for a very fast and precise estimation ofthe conductive properties of different molecular.

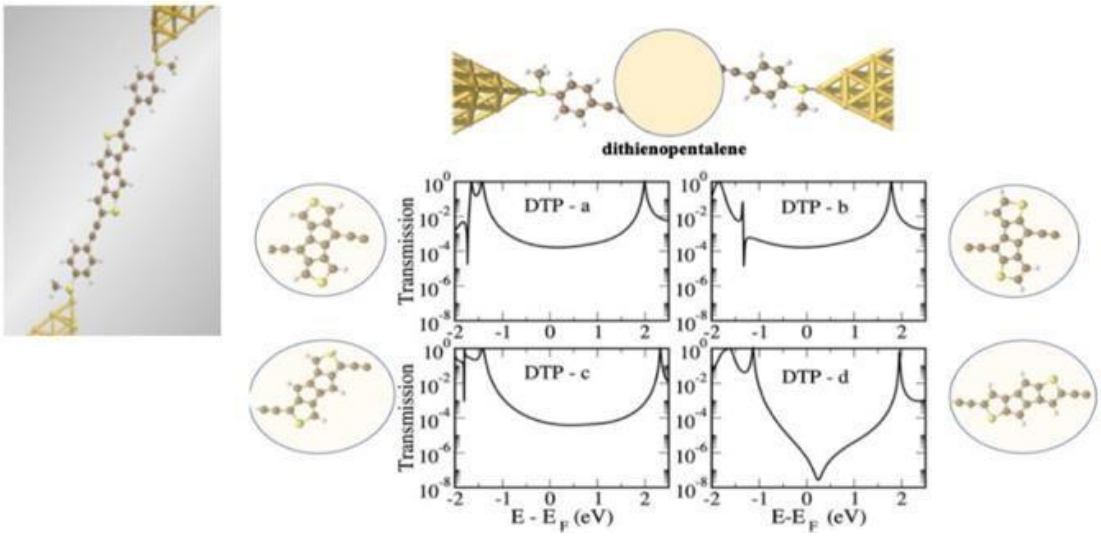

Figure 1. DFT transmission computations of different dithieno derivatives.

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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 observationof vortex lattices in superconductors or of Landau quantization. For the latter, it is of particular importanceto decrease as far as possible the size of the STM. Although efforts made during past years have led to someimprovements, 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 obtainmeasurements at different angles between the sample and the magnetic field. Both the head and the base ofthe main body of the STM have been manufactured through 3D printing in grade 3 Titanium, which couldturn 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 measurementsusing a gold tip on a gold film at 4.2 K and applying magnetic fields up to 6 T. Namely, we have obtainedtopography images and observed the conductance quantization phenomenon with the STM at different tiltedangles.

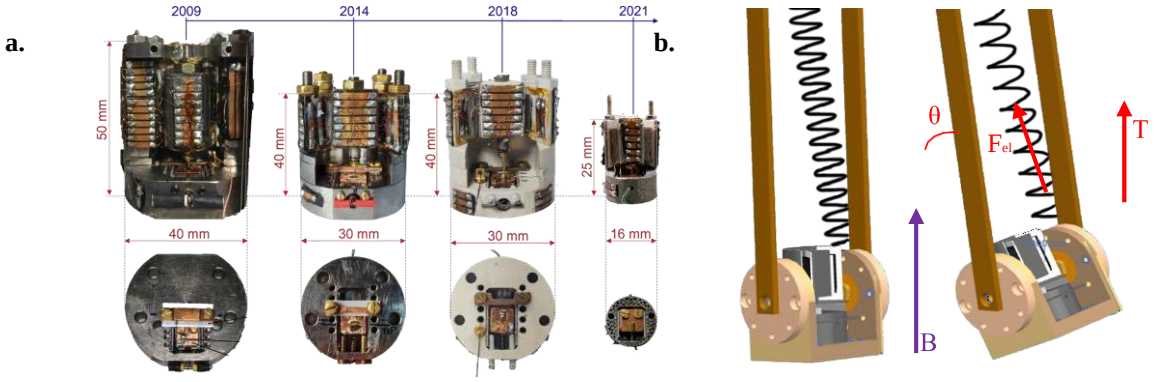

Figure 1. a) Size comparison between some other STMs developed in the laboratory and the one presented in thiswork. **b)** Scheme showing the rotatory system operation and the STM.

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General theory of cavity-mediated interactions between low-energy matter excitations

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The manipulation of low-energy matter properties such as superconductivity, ferromagnetism and ferroelectricity via cavity quantum electrodynamics engineering has been suggested as a way to enhance these many-body collective phenomena [1]. In this work [2], we investigate the effective interactions between low-energy matter excitations induced by the off-resonant coupling with cavity electromagnetic modes. We extend previous work [3] by going beyond the dipole approximation accounting for the full polarization and magnetization densities of matter. We further include the often-neglected diamagnetic interaction, and, for the cavity, we consider general linear absorbing media with possibly non-local and non-reciprocal response. We demonstrate that, even in this general scenario, the effective cavity-induced interactions between the matter degrees of freedom are of electrostatic and magnetostatic nature. This confirms the necessity of a multimode description for cavity engineering of matter systems where the low-energy assumption holds. Our findings provide a theoretical framework for studying the influence of general optical environments on extended low-energy matter excitations.

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Single photon emission from hBN defects

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Hexagonal boron nitride is a 2D material which has recently emerged as a promising platform for quantum applications. Defects in the crystalline structure hBN have been associated with single photon emission at room temperature, which makes this material ideal for the design of integrated photonic devicesfor quantum information [1]. First, we describe the experimental setup to detect and characterize single- photon emitters, which involves the study of their brightness and spectral properties, demonstration of photon antibunching via a Handbury Brown and Twiss experiment, and measurement of the lifetime of theexcited state [2]. Furthermore, the emission can be enhanced via Purcell effect by coupling the single- photon source to a Fabry-Pérot cavity in the weak coupling regime [3]. This source can be used to implement quantum key distribution protocols such as BB84, where encoding is performed by using different polarization states of the single photons [4].

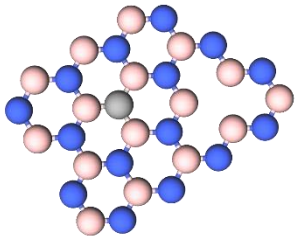

Figure 1. hBN with crystallographic defects

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Optically driven revolution and spin of Janus nanoparticlesin a Laguerre-Gaussian vortex beam

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The development of artificial nanomoter/nanomachine has attracted considerable attention due to their potential in various biomedical applications. Light, as an external stimulus, can drive the motion of nano- objects. For instance, optical tweezers create an optical potential well to confine nanoparticles within a small spatial range and transfer momentum and energy to the particles, enabling remote manipulation.

To enable diverse motions in optically trapped micro-objects, optical tweezer systems generally adopt one of two main approaches. The first one involves modulating laser beams with techniques such as optical vortex beams, Bessel beams, Laguerre–Gaussian beams, and other specialized beam types. The second approach uses specially designed particles, incorporating asymmetric micro-objects like micro- turbines, gammadion-shaped micro-rotors, birefringent particles, or Janus particles. These asymmetrical particles exhibit distinctive mechanical behaviors when placed within Gaussian or other uniquely shaped optical traps. Among these, a promising approach relies on the so-called Janus particles composed of metal and a dielectric material, which has paved a way toward optical nanomachines.

In this work, we combine the two approaches into one. A circularly polarized Laguerre–Gaussian beam, carrying both spin and orbital angular momentum (SAM, OAM), was applied to manipulate a Janus nanoparticle composed of gold and silica. The simultaneous spin and orbital rotation of the 200 nm Janus particles was experimentally observed (**Figure 1**). The rotational frequencies in both cases show a strong dependence on laser power, and a supra-linear dependence at high power (>40 mW), which can serve as an indicator of local temperature within the optical tweezers. Our work contributes to the development of optically driven nanomachines and promotes their applications in thermodynamics, microfluidics, biomechanics.

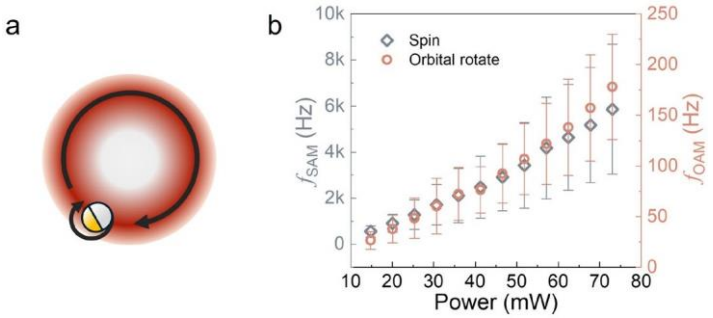

Figure 1. **(a)** Schematic diagram of the orbital revolution and spin rotation of an optically trapped Janus nanoparticle in circularly polarized Laguerre–Gaussian beam. **(b)** Spin and orbital frequencies of a 200 nm Janus nanoparticle as functions of laser power.

Acknowledgements

This work was financed by Grant TED2021-129937B-I00, CNS2022-135495, and PID2023-151078OB-I00 funded by MCIN/AEI/10.13039/501100011033 and by the "European Union NextGenerationEU/PRTR. F. Zhang acknowledges the scholarship from the China Scholarship Council (NO. 202108440235).

Universality of Nanoconfined Water within Lipid Mesophases

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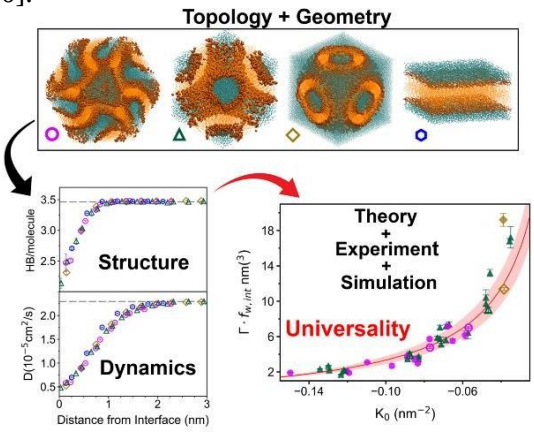
Water under confinement has a major impact in life and nanotechnology[1,2]. The exotic behavior of nanoconfined water[4,5] emerges from a complex interplay between the topological and geometrical properties of the confining space, as well as its chemical nature. The multitude and specificity of confiningsystems and geometries mask any of its potentially universal traits. In our work, we advance in this quest by resorting to lipidic mesophases as an ideal nanoconfinement system[1,3], allowing inspecting the behavior of water under systematic changes in the topological and geometrical properties of the confining medium, without altering the chemical nature of the interfaces. To detect and characterize the properties ofinterfacial water we combine Terahertz absorption spectroscopy, Small Angle x-Rays diffraction experiments and molecular dynamics simulations. The emergence of master curves from the simulations allows us to derive a parameter-free law quantitatively capturing into a single master curve both experimental and numerical data, unveiling the universal laws governing the physics of nanoconfined water,recapitulating the data collected under varying levels of hydration, nanoconfinement topologies and geometries. Overall, we believe that this study sets an important steppingstone towards a comprehensive physical understanding of water under soft nanoconfinement, allowing the optimization of applications having an impact in biology[6], medicine[7], pharmaceutical processes[8], food[9] and material science fields[10].



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