



Instituto Universitario de  
Ciencia de Materiales Nicolás Cabrera

**INC Young Researchers Meeting 2023**  
**BOOK of ABSTRACTS**

# Talk 1

## Elastic response of deformed nucleic acids

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The genetic material is densely compacted inside the nucleus of the cell. Knowledge of the sequence-dependent elastic response of DNA is crucial to understand chromatin conformation, whose alterations may cause important diseases [1]. Experiments reveal that when mechanical stress is exerted on DNA, e. g. by helicases, its elastic response changes [2]. In a recent work [3], we introduced a fluctuations-based approach to characterize the stress-dependent elastic response of nucleic acids, thus overcoming the limitations of the widely-used Linear Theory of the Elastic Rod.

By inspecting the force-dependent elasticity of short sequences of double-stranded DNA and RNA in all-atom simulations [3], we unveiled a number of striking physical effects whose origin can be traced down to microscopic deformations of the chains. In particular, we found that DNA becomes stiffer when pulled, while RNA softens. This unexpected discrepancy among both double-stranded nucleic acids emerges from the alignment or misalignment of the base pairs as the stretching force increases, ultimately resulting in a different variation of the stacking interactions. The same effect was later found in atomistic MD simulations with different forcefields [4]. It can be very relevant in a number of biological phenomena and for the design of DNA-based nanomaterials.

In this contribution, I will present our results concerning the variation of the elastic response of pulled nucleic acids with short sequences (all-atom simulations) and with longer sequences (coarse-grained simulations). Additionally, I will sketch our efforts to couple polymer models to fluctuations-based approaches to establish a connection with experiments.

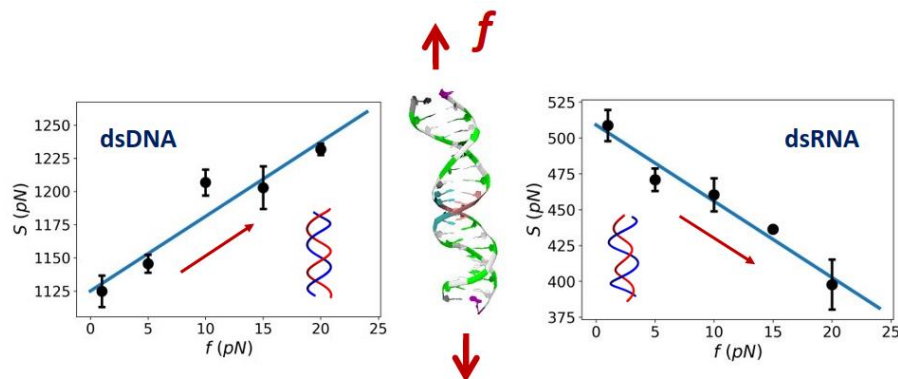


Figure 1. DNA stiffens and RNA softens upon stretching.

[1] Á. Dos Santos, and C. P. Toseland, *J. Mol. Sci.*, **22.6** (2021) 3178.

[2] . Gore, Z. Bryant, M. Nöllmann, M. U. Le, N. R. Cozzarelli, and C. Bustamante, *Nature*, **442**.7104 (2006) 836-839.

[3] J. Luengo-Márquez, J. Zalvide-Pombo, R. Pérez, and S. Assenza, *Nanoscale*, **15.14** (2023) 6738-6744.

[4] C. Roldán-Piñero, J. Luengo-Márquez, S. Assenza and R. Pérez, *bioRxiv*, 2023-09 (2023).

## Talk 2

# MoS<sub>2</sub> photo-electrodes for hydrogen production: tuning the S-vacancies content in highly homogeneous ultrathin nanoflakes

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The rational design of advanced electrocatalysts for green hydrogen production by supplying electricity from renewable sources is a key issue to be addressed in order to reduce CO<sub>2</sub> emissions. Two-dimensional transition metal dichalcogenides, such as MoS<sub>2</sub>, have been widely investigated as cathodes for electrolytic water splitting. The electrocatalytic activity of these layers is substantially enhanced by creating defects such as grain boundaries or sulfur vacancies [1].

To our knowledge, this work [2] is the first to report the growth of highly homogeneous MoS<sub>2</sub> ultrathin nanoflakes (having 1-2 layers in thickness and lateral dimensions of 2-3 nm) over large area substrates (of about 1 cm<sup>2</sup>). We have also shown that the introduction of an H<sub>2</sub> flux during the synthesis method creates sulfur vacancies in the sample. Furthermore, we demonstrated a relationship between the S/Mo ratio obtained by XPS and the position of the Raman bands (A<sub>1g</sub> and E<sub>2g</sub>) characteristic of 2H-MoS<sub>2</sub>.

Next, we tested our MoS<sub>2</sub> samples as cathodes for the water splitting reaction, which show outstanding properties, with a Faradaic efficiency of 100% and being stable for more than 80h in acidic aqueous media. In addition, we show that there is an optimal vacancy concentration of around 14% for improving the electrocatalytic performance, which is in agreement with previous results [3].

All in all, this work can open new possibilities to tune the properties of MoS<sub>2</sub> through nanostructuring and defect engineering, playing with the growth conditions and the chance of growing homogeneous thin films, which brings applications closer.

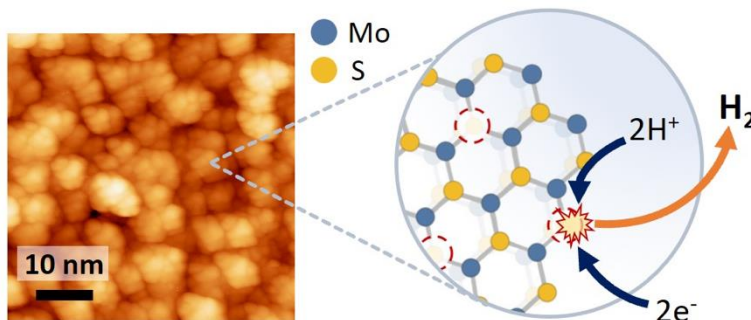


Figure 1. From left to right: STM image, which evidences the nanoflake structure of our layers. Schematic of hydrogen production on the MoS<sub>2</sub>.

[1] J. Zhu, et al. Nature Communications, **10**, 1-7, (2019).

[2] N. Jiménez-Arévalo, et al. ACS Appl. Mat & Int., **15**, 33514–33524, (2023).

[2] H. Li, et al. Nature Materials, **1**, 48-53, (2016).

## Talk 3

### Bringing Together Lanthanide and Chromium Ions for Brighter Emission

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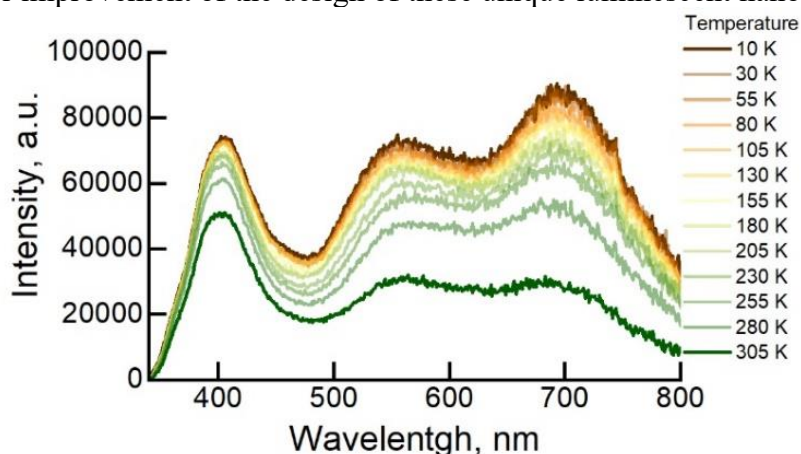
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Semiconductor nanocrystals (SNCs) are tiny crystalline particles characterized by high molar absorption coefficient ( $10^4$ - $10^6$  M<sup>-1</sup> cm<sup>-1</sup>) and strong emission. From an optical standpoint, doping these structures with different luminescent ions impart optical properties that SNCs alone do not display, such as tuning of the emission over a wide spectral range. For this purpose, lanthanide (Ln<sup>3+</sup>) and transition metal ions (TM<sup>n+</sup>, such as Cr<sup>3+</sup>) are suitable dopants. The combination of SNCs and luminescent Ln<sup>3+</sup> and TM<sup>n+</sup> is convenient also to solve an intrinsic drawback of these ions. Indeed, their optical features stem from Laporte-forbidden (i.e., parity-forbidden) electronic transitions, and hence they feature low molar absorption coefficients (0.1-10 M<sup>-1</sup> cm<sup>-1</sup>).<sup>1,2</sup> Doping of Ln<sup>3+</sup> and TM<sup>n+</sup> ions in SNCs can address this problem. The semiconductor host material can effectively absorb the incident photons, transfer the energy to the dopants, which in turn re-emit it at the desired wavelengths dictated by which specific dopant ion was chosen: a process known as *sensitized luminescence*.<sup>3</sup>

$\beta$ -Indium sulfide ( $\beta$ -In<sub>2</sub>S<sub>3</sub>) is an ideal host material for this purpose:<sup>4</sup> In<sup>3+</sup> has similar ionic radius compared with Ln<sup>3+</sup> and slightly bigger than Cr<sup>3+</sup>, same oxidation state, and it occupies an octahedral crystallographic site. These conditions allow an easier incorporation of the ions into the host material. In this work, we synthesized  $\beta$ -In<sub>2</sub>S<sub>3</sub> nanoplatelets and doped them with Cr<sup>3+</sup> and Ln<sup>3+</sup> ions with the aim of obtaining energy transfer from the host material to the dopant ions. Elucidation of the energy transfer mechanisms involved in the sensitization of the dopants' emission is currently ongoing, by means of low temperature photoluminescence measurements, thus also opening the door to their use as possible cryogenic luminescent thermometers. This study sets the stage for further improvement of the design of these unique luminescent nanomaterials.



**Figure 1.** Temperature-dependent photoluminescence spectra of In<sub>2</sub>S<sub>3</sub>:Cr (5%) sample.

1. Liu, Y. et al., *J. Lumin.*, **217**, 116775 (2020)
2. Pavlov, R. S. et al., *J. Mater. Chem.* **12**, 9, 2825-2832 (2002)
3. Li, Z. et al., *Phys. Chem. Chem. Phys.* **19**, 25, 16758-16764 (2017)
4. Park, K. H. et al., *Angew. Chem. Int. Ed.* **45**, 28, 4608-4612 (2006)

## Talk 4

# Emergence of Spinon Fermi Arcs in the Weyl-Mott Metal-Insulator Transition

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The Weyl-Mott insulator (WMI) has been postulated as a novel type of correlated insulator with non-trivial topological properties. We introduce a minimal microscopic model that captures generic features of the WMI transition in Weyl semimetals. The model hosts a bulk Mott insulator with spinon Fermi arcs on its surfaces which we identify as a WMI. At finite temperatures, we find an intermediate Weyl semimetallic phase with no quasiparticles which is consistent with the bad semimetallic behavior observed in pyrochlore iridates,  $A_2\text{Ir}_2\text{O}_7$ , close to the Mott transition. Spinon Fermi arcs lead to a suppression of the bulk Mott gap at the surface of the WMI, in contrast to the gap enhancement found in conventional Mott insulators, which can be detected through angular resolved photoemission spectroscopy (ARPES).

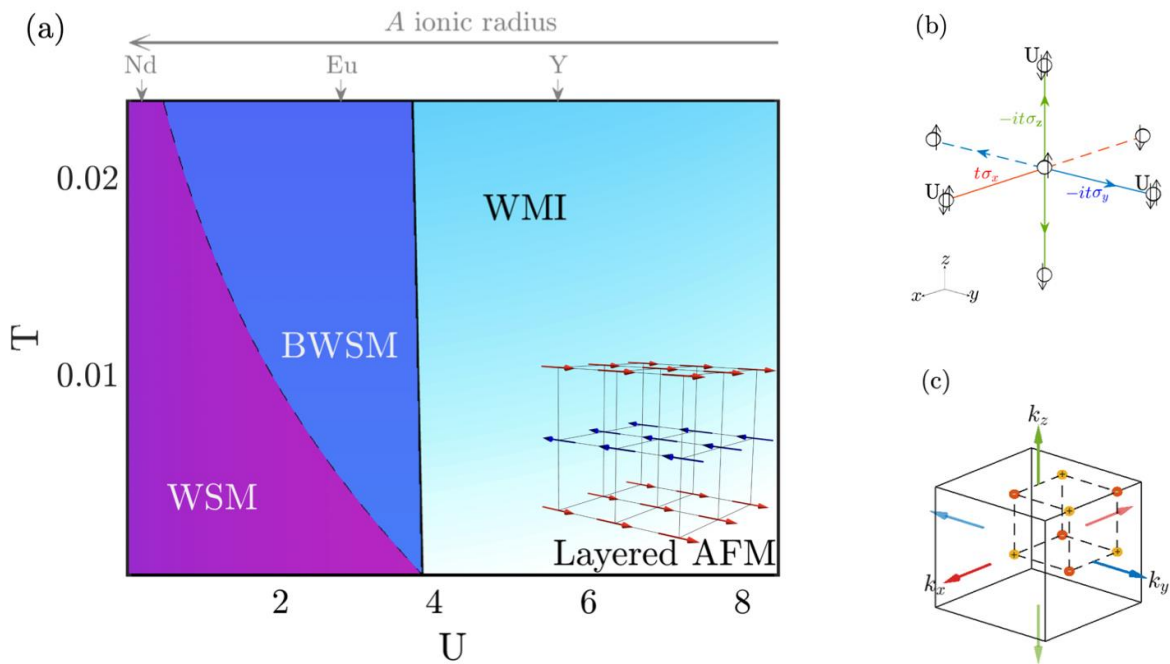


Figure 1. (a) Temperature vs. Hubbard strength phase diagram of the Weyl-Mott metal insulator transition. The WMI featured by a finite charge gap and spinon Fermi arcs occurs at large  $U$ . Layered antiferromagnetic (AFM) order arises at low  $T$  in the WMI. (b) Real space illustration of our Weyl-Hubbard model. (c) Location of the spinon Weyl nodes in the first Brillouin zone of the cubic lattice.

[1] M. F. López, I. García-Elcano, J. Bravo-Abad, and J. Merino, arXiv:2307.10102 [cond-mat.str-el] (2023).

## Talk 5

### Wide band gap $\text{Cu}_2\text{ZnGe}(\text{S},\text{Se})_4$ thin-film semi-transparent solar cells

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Kesterite-type material  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  has gained interest to be used as absorber for thin-film solar cells in the last years because of consisting of elements of low toxicity and high abundance in the earth's crust, having a high absorption coefficient and stability. Currently, efficiencies in the range of 14 % have been achieved for  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  photovoltaic (PV) devices [1]. The substitution of Sn with Ge leads to a higher band gap energy. In addition, the substitution of Se with S enables a higher band gap for  $\text{Cu}_2\text{ZnGe}(\text{S},\text{Se})_4$ -based (CZGSSe) solar cells, from 1.4 eV (CZGSe) to 2.2 eV (CZGS). The broad window of band gap energy values guarantees the multiple applications of the solar cells using this absorber layer through PV integration.

Semi-transparent solar cells are the next step for PV in our daily life. A key parameter to control the transparency of the solar cells is to increase the  $E_g$  of the active layer, as well as the thickness of the absorber film. In this work, CZGSSe thin films have been grown by sulfurization of co-evaporated CZGSe with thicknesses of 400 and 800 nm. The absorber layers were deposited on two different semi-transparent back contact configurations: Mo (30 nm)/FTO and Mo (15 nm)/ $\text{V}_2\text{O}_5$  (15 nm)/FTO. The structural, compositional, morphological, vibrational and optical properties of the CZGSSe thin films are investigated by GIXRD, GD-OES, SEM, Raman spectroscopy and transmittance measurements. The kesterite phase is detected by GIXRD and Raman spectroscopy, but also secondary phases as ZnS are present. In addition, a  $\text{Mo}(\text{S},\text{Se})_2$  layer is formed at the back interface. All the absorber layers are characterized by a columnar structure with large grain size, free of pinholes. A non-uniform distribution of S through the thickness of CZGSSe layer is observed in all the cases, with a much higher S content near the surface. Solar cells with efficiencies of 0.8 %,  $E_g = 2.1$  eV and transmittance in the range of 40 % in the near infrared region are achieved. Despite the low device performance, probably limited by the presence of secondary phases and the back recombination between other factors, these are the best semi-transparent kesterite solar cells with such a high band gap value up to now.

[1] Y. Gong, Q. Zhu, B. Li, S. Wang, B. Duan, L. Lou, C. Xiang, E. Jedlicka, R. Giridharagopal, Y. Zhou, Q. Dai, W. Yan, S. Chen, Q. Meng, H. Xin, Nat. Energy 7 (2022) 966–977. <https://doi.org/10.1038/s41560-022-01132-4>.



## Talk 6

# Joule heating effects in superconducting InAs nanowire islands

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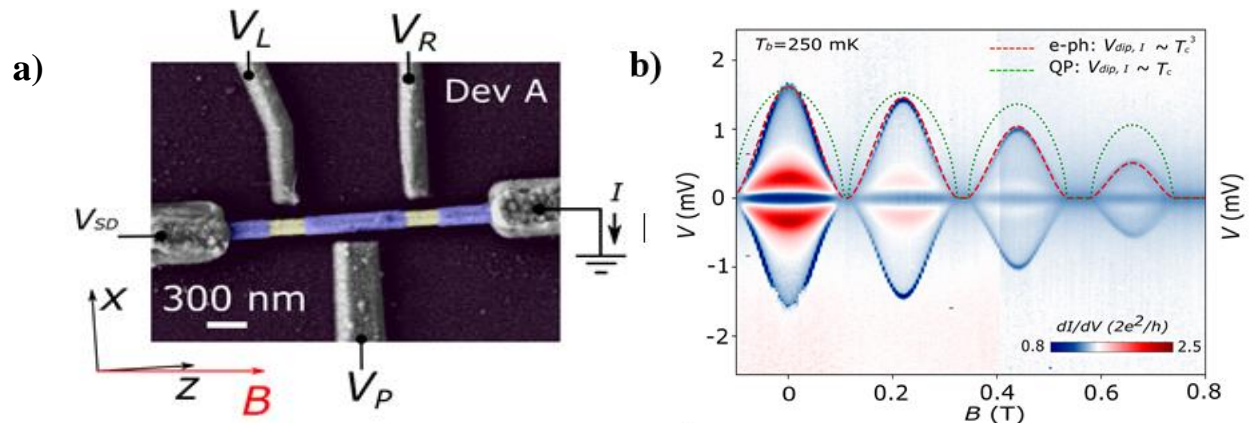
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Mesoscopic superconducting islands in hybrid superconductor-semiconductor nanowires have been intensively studied in the context of topological superconductivity, motivated by their potential for the realization of a topological qubit [1]. Interesting experimental results have been reported in the past years, including a  $2e$ -to- $1e$  transition in the periodicity of Coulomb oscillations and a related dependence with the island length, which has been interpreted in favor of topology and of exponential protection of Majorana zero modes [2-4]. Heating effects, however, have not been considered in the interpretation of the above experiments, nor has its impact been evaluated in the context of proposals for quantum devices. In this work, we study Joule and microwave heating effects in devices based on hybrid mesoscopic Al/InAs islands, which can be used to gain information on the heat relaxation mechanisms in each part of the device independently (**Fig.1a**). Interestingly, we show that the island undergo a transition to the normal state at relatively low powers  $\sim 100 - 300$  pW, which could have a strong impact on the device performance under standard operational conditions (**Fig.1b**).



**Figure 1| a) SEM image of a typical device and set up for the transport measurements. b) Little-Parks oscillations of the differential  $dI/dV$  dips associated with the superconducting-Normal phase transition of the island, showing the electron-phonon dominant heat mechanism in red dotted lines.**

- [1] D. Aasen et al., Phys. Rev. X., **6**, 031016 (2016).
- [2] A.M. Whiticar et al., Nat Commun, **11**, 3212 (2020).
- [3] A. Vekris., NanoLetters., **14**, 5765-5772 (2022).
- [4] S. M. Albrecht et al., Nature., **531**, 206-209 (2016)

## Talk 7

# Mechanical disassembly of human picobirnavirus like particles indicates that cargo retention is tuned by the RNA–coat protein interaction

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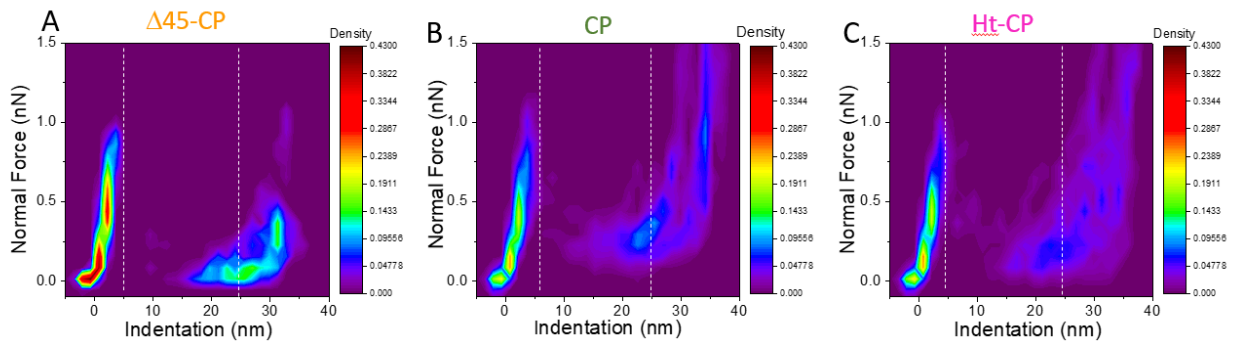
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We investigate the cargo retention of individual human picobirnavirus (hPBV) virus-like particles (VLPs) which differ in the N-terminal of their capsid protein (CP): (i) hPBV CP contains the full-length CP sequence; (ii) hPBV  $\Delta$ 45-CP lacks the first 45 N-terminal residues; and (iii) hPBV Ht-CP is the full-length CP with a N-terminal 36-residue tag that includes a 6-His segment. Consequently, each VLP variant holds a different interaction with the ssRNA cargo. We used atomic force microscopy (AFM) to induce and monitor the mechanical disassembly of individual hPBV particles. First, while  $\Delta$ 45-CP particles that lack ssRNA allowed a fast tip indentation after breakage, CP and Ht-CP particles that pack heterologous ssRNA showed a slower tip penetration after being fractured (Fig. 1). Second, mechanical fatigue experiments revealed that the increased length in 8% of the N-terminal (Ht-CP) makes the virus particles to crumble  $\sim$ 10 times slower than the wild type N-terminal CP, indicating enhanced RNA cargo retention. Our results show that the three differentiated N-terminal topologies of the capsid result in distinct cargo release dynamics during mechanical disassembly experiments because of the different interaction with RNA.

Figure 1. Mechanical unpacking data of the single indentation assay. Density maps of force



indentation curves obtained for  $\Delta$ 45-CP (A), CP (B) and Ht-CP (C) VLPs.

[1] Rodríguez-Espinosa et al. *Nanoscale Horizons* (2023).

[2] Ortega-Esteban et al. *Journal of Virology*, 94(24), e01542-20 (2020).



## Talk 8

# Strain effects and quasi-particle conversion in monolayer MoS<sub>2</sub> deposited on chains of metallic nanoparticles

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Monolayer (1L) transition metal dichalcogenides (TMDs) are promising candidates for the development of the next-generation optoelectronic devices due to their direct optical gap and atomic thickness. TMD electronic properties can be readily tuned by mechanical strain, which enables gap width control as well as quasi-particle conversion.

Here, we study the combined effects of strain and electron transfer on the optical properties of a MoS<sub>2</sub> monolayer when it is placed on top of a plasmonic chain of silver NPs (see Figures 1a and 1b) on a LiNbO<sub>3</sub> substrate. For that purpose, spatially resolved photoluminescence (PL) microscopy at cryogenic temperatures is employed. In the proximity of the chain, the strain gradient produced by the metallic chain results in a pronounced redshift (24 meV) and broadening (30 meV) of the spectral line associated with the A exciton of MoS<sub>2</sub>, which sharply contrast with the smoother spectral changes observed at room temperature (see Figures 1c and 1d). This behavior is related to the strong thermal expansion coefficient mismatch between the LiNbO<sub>3</sub> substrate and the 1L MoS<sub>2</sub>, which leads to a notable strain increment at 10 K. In addition, opposite to the exciton-to-trion transformation usually observed under inhomogeneous strain in TMDs [1,2], a trion-to-exciton conversion is detected in the vicinities of the metallic chain. This effect is attributed to the presence of the metallic chain, which allows electron transfer from the MoS<sub>2</sub> monolayer to the Ag NPs localized in the strained region.

The results show the potential of the integrated hybrid plasmonic-2D semiconductor platforms for exploring strain and electronic driven quasiparticle manipulation, and opens a pathway for controlling quantum emitters in 2D strained systems.

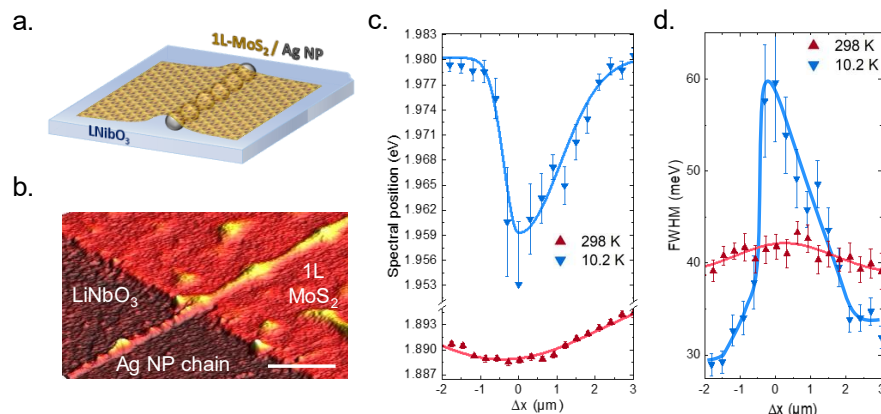


Figure 1. a) Scheme and b) AFM image of the studied sample. c) Spectral position and d) linewidth of exciton A in the proximity of the plasmonic chain at room temperature (red) and 10 K (blue).

[1] M. G. Harats *et al.*, Nat. Photonics **14**, 324-329 (2020)

[2] H. Lee *et al.*, Sci. Adv. **8**, eabm5236 (2022)

## Talk 9

# Coherent electron-vibron interactions in Surface-Enhanced Raman Scattering (SERS)

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Surface-enhanced Raman scattering (SERS) allows the fingerprinting of single molecules via their vibrational degrees of freedom. Inspired by its analogy with the field of cavity optomechanics [1], a first model was proposed considering the optomechanical dynamics between plasmonic electric fields and molecular vibrations [2]. This molecular optomechanical approach allowed both, to describe new effects in the field of SERS arising from the dynamical backaction and to offer new possibilities in cavity optomechanics due to the resulting large coupling strengths involved – orders of magnitude larger than in previous configurations. Despite recent experimental works evidencing such optomechanical nature of SERS, large spectral discrepancies have arisen with current theoretical predictions [3] that call for new mechanisms for its understanding. Inspired by the microscopic molecular Hamiltonian [4], in this work we propose an optomechanical SERS model that considers the internal mechanisms of the molecule. In this model, the electronic transitions involved in the Raman processes are treated as a set of two-level systems that mediate the interaction between plasmons and molecular vibrations via electron-vibron couplings [4]. Since such electronic levels typically lie in the ultra-violet range, we can adiabatically eliminate them and recover the original optomechanical Hamiltonian [2]. Beyond such adiabatic approximation, we further consider a near-resonant transition coexisting with the off-resonant ones, showing interesting cooperative behaviours such as enhancements of anti-Stokes lines and modifications of spectral widths. For ultrastrong interaction scenarios with electron-vibron couplings close to the mechanical frequency, we consider the resulting phonon-dressed states in the master equation that show incoherent contributions to the anti-Stokes peaks, decisive for understanding the spectrum. Our model shows the importance of treating the molecular degrees of freedom with equal footing in SERS and offers new perspectives of the mechanisms involved in molecular optomechanics.

[1] M. Aspelmeyer et al., *Rev. Mod. Phys.* 86 (2014) 1391

[2] P. Roelli et al., *Nature Nanotech.* 11 (2016) 164-169

[3] F. Benz et al., *Science* 354 (2016) 6313 726-729

[4] M. Reitz et al., *Phys. Rev. Research* 2 (2020) 033270

## Talk 10

# A ratiometric thermo-induced fluorochromatic probe for temperature sensing in living cells

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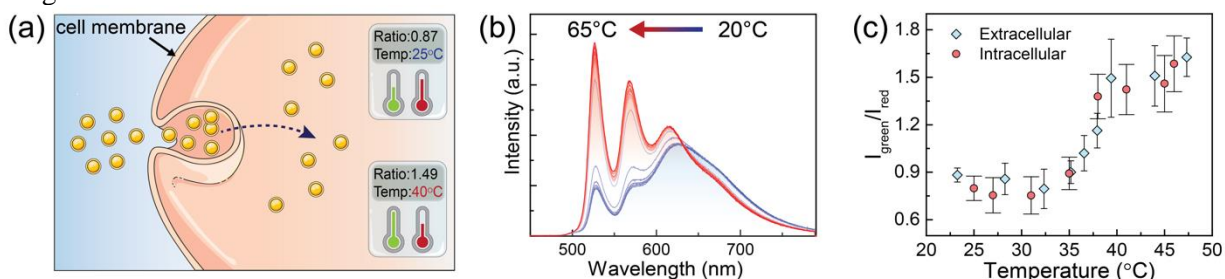
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Intracellular temperature sensing plays an important role in understanding the biological reactions and physiological conditions inside living cells. A considerable amount of works about intracellular thermometer has been published.<sup>[1]</sup> Among them, fluorescence thermometers have been widely used due to their non-contact and non-invasive characteristics. However, the reliability of their intracellular thermal readouts is still a question of debate. The change in the compositional properties of intracellular medium can induce changes in the fluorescence signal that can be erroneously interpreted as thermal variations.<sup>[2]</sup> To overcome this drawback, we proposed an inert thermal probe where the fluorescent nanoparticles are with a silica shell to isolate them from the environment.

We used the thermo-induced fluorochromatic nanoparticles as a ratiometric nanothermometer for measuring the intracellular temperature (**Figure 1a**). The fluorescent dye in nanoparticle achieves the fluorescence modulation through the solid-liquid transition of phase change materials. The dominant fluorescent color changes from green to red when the temperature is over the phase change temperature. Therefore, the temperature readout can be obtained by measuring the change of fluorescence ratio. **Figure 1b** is the emission spectra of the suspension of nanoparticles under 20°C to 65°C. The ratio changes at 38°C. This phase transition point is useful because cells will lose the viability above 40°C. We experimentally demonstrated that its green-red fluorescent ratio and phase change temperature is not sensitive to pH, viscosity, and the physical change of the cells. This can be attributed to the silica shell of the nanoparticles. We successfully internalized these nanoparticles in living cells (Uppsala 87 Malignant Glioma cells). The high viability of cells (90%) after 24h incubation indicates good biocompatibility of the nanoparticles. The intracellular temperature calibration is consistent with the extracellular results (**Figure 1c**). There is a sharp change of ratio after the phase transition point, which can be used for alarm of cellular overheating. The proposed ratiometric thermo-induced fluorochromatic probe is a reliable thermometer for living cells.



**Figure 1.** (a) Schematic diagram of the intercellular ratiometric thermometer. Yellow circles represent the nanoparticles. (b) Evolution of emission spectra with temperature from 20°C to 65°C. (c) Temperature dependence of the extracellular and intercellular fluorescence intensity ratio.

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### Acknowledgements

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## Talk 11

# Spontaneous symmetry breaking in diffraction

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The connection between symmetries and conservation laws is a cornerstone of physics. It underlies Bloch's theorem, which explains wave phenomena in all linear periodic systems. Here we demonstrate that, in a nonlinear grating with memory, diffracted waves can spontaneously acquire momentum parallel to the lattice vector in quantities unconstrained by the grating period. In this breakdown of Bloch's theorem, which we also evidence in solutions to nonlinear Maxwell's equations, wave amplitudes no longer respect the discrete translation symmetry of the grating. Our findings reveal a rich phenomenology for waves in nonlinear periodic systems and point to numerous opportunities for nonlinear lattices with broken symmetry in the context of imaging, sensing, and information processing in general.

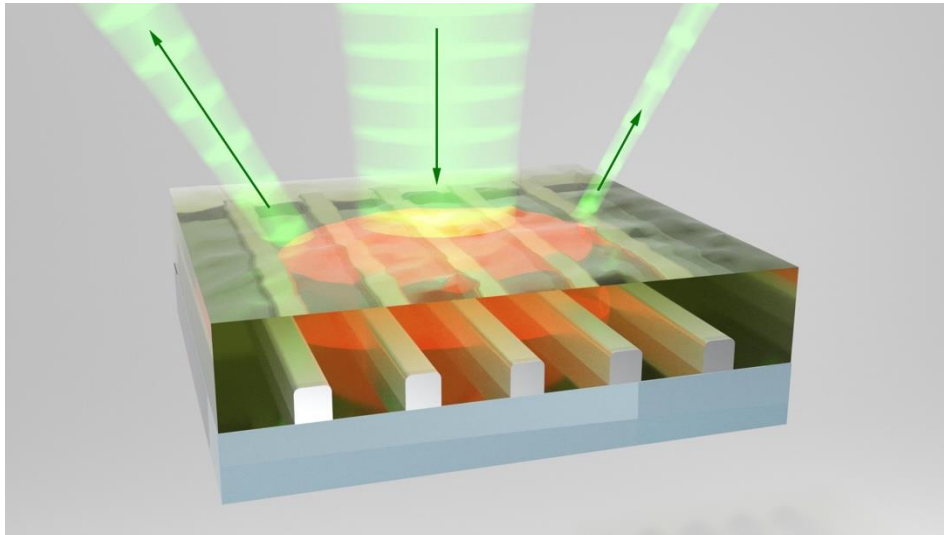


Figure 1. An unblazed metallic grating coated with oil is illuminated by a laser at normal incidence. Due to the thermo-optical nonlinearity of the oil, the symmetry of the diffraction pattern can spontaneously break implying a breakdown of Bloch's theorem.

## Talk 12

# Mechanical tomography of an archaeal lemon-shaped virus reveals membrane-like fluidity of the capsid and liquid nucleoprotein cargo

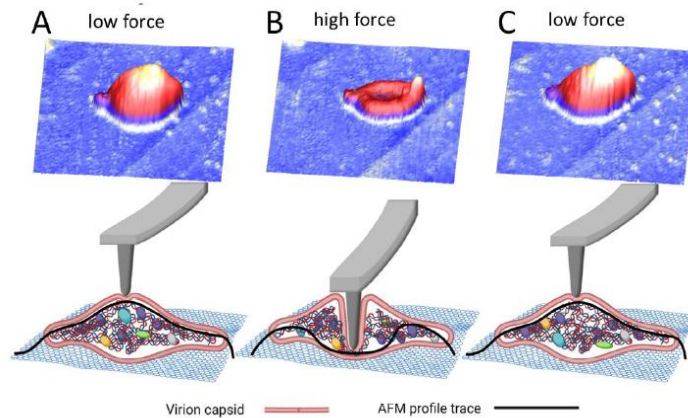
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Archaeal lemon-shaped viruses have unique helical capsids composed of highly hydrophobic protein strands which can slide past each other resulting in remarkable morphological reorganization. Here, using atomic force microscopy, we explore the biomechanical properties of the lemon-shaped virions of *Sulfolobus monocaudavirus 1* (SMV1), a double-stranded DNA virus which infects hyperthermophilic (80°C) and acidophilic (pH2) archaea. Our results reveal that SMV1 virions are extremely soft and withstand repeated extensive deformations, reaching unprecedented strains of 80% during multiple cycles of consecutive mechanical assaults, yet showing scarce traces of disruption. SMV1 virions can reversibly collapse wall-to-wall, reducing their volume by 90%. Beyond revealing remarkable malleability of the SMV1 protein shell, our data also suggest a fluid-like nucleoprotein cargo which can flow inside the capsid, resisting and accommodating mechanical deformations without further alteration. Our experiments suggest a packing fraction of the virus core to be as low as 11%, with the amount of the accessory proteins almost 4 times exceeding that of the viral genome. Our findings indicate that SMV1 protein capsid displays biomechanical properties of lipid membranes, which is unprecedented among protein capsids of other viruses. The remarkable malleability and fluidity of the SMV1 virions are likely necessary for the structural transformations during the infection and adaptation to extreme environmental conditions.



**Recreation of the SMV1 particle mechanical reaction.** A. SMV1 virus particle imaged at low force without presenting deformation (top B. The same virus at high force (top) shows a depressed apparent plateau (bottom, black line) that forms only at the pixel where the tip is touching the virus (bottom, capsid line). C. The same virus imaged again at low force (like in panel A) shows no apparent damage.

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## Study of the oxidation processes of $Zn_3N_2$ layers sensitive to the temperature and humidity conditions

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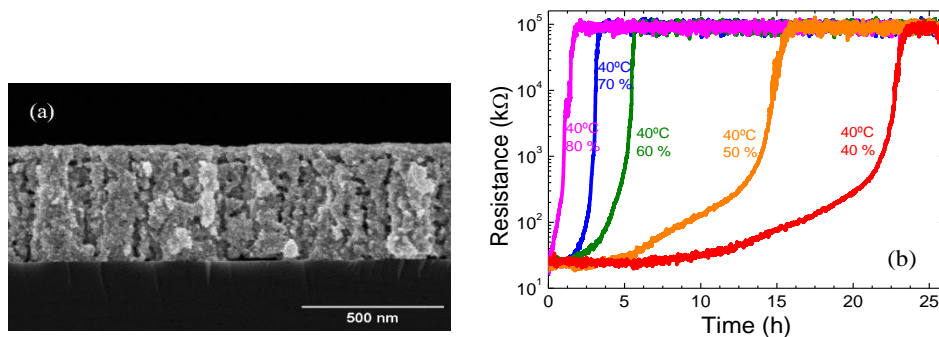
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Metastable materials have long interested researchers because of their remarkable ability to undergo significant transformations in response to external factors, including not only thermodynamics but also environmental causes [1]. Zinc nitride ( $Zn_3N_2$ ) is one of this cases, where a particularly interesting transformation occurs when exposed to humidity, resulting in its conversion into zinc oxide (ZnO). This transition has found significant innovative applications for sensing moisture [2] and body dehydration [3].

This study investigates the interplay between temperature and humidity during the oxidation process of  $Zn_3N_2$ , ultimately leading to the formation of ZnO. The synthesis of  $Zn_3N_2$  samples is conducted by RF magnetron sputtering [2]. The samples are then exposed to controlled environmental conditions inside a climate chamber, with temperature variations ranging from 40°C to 80°C, and relative humidity (RH) levels between 40% and 80%.

The structural and morphological properties of the layers are analyzed (Fig. 1a) by scanning electron microscopy (SEM), atomic force microscopy, and spectroscopic ellipsometry; while the electrical response is measured in real-time (Fig. 1b) by means of a state-of-the-art Arduino module and a voltage divider circuit [3]. We have analyzed the evolution of the roughness, porosity, and thickness during the oxidation process in a set of samples with different temperatures and RH.

Our results confirm the swelling effect of the oxidation [3], but also indicate differences in the porosity and roughness of the samples. These changes can be responsible of the fast dynamics observed for high RH and high temperatures. A proper calibration of these effects will help to produce more reliable humidity sensors.



**Figure 1.** (a) SEM cross-sectional image of a sample revealing its internal microstructural details. (b) temporal evolution of resistance during oxidation for representative samples of this study.

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# P2

## RNA-Protein capsid interaction: The influence of specific nucleotide sequences on mechanical virus disassembly

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Genome-protein interactions are known for their crucial role in the assembly and stability of viral capsids. However, the impact of nucleotide sequence on the mechanical resistance of viral capsids remains largely unexplored. Here, we focused on the Tobacco Mosaic Virus (TMV), a widely recognized model in plant virology known for its robustness and simple structure. TMV packs a helically distributed genome along the capsid from the 5' end to the 3' end, making it an ideal model system to examine whether the nucleotide sequence affects the stability of the virus capsid. To probe this hypothesis, we used Atomic Force Microscopy (AFM) to perform mechanical fatigue on single TMV particles, inducing gradual degradation that informs us about the weakest regions of the virus particle. These weak regions are denoted by the creation of rifts along the capsid, which can be compared with specific known sequences of nucleotides that play a key role during the assembly.

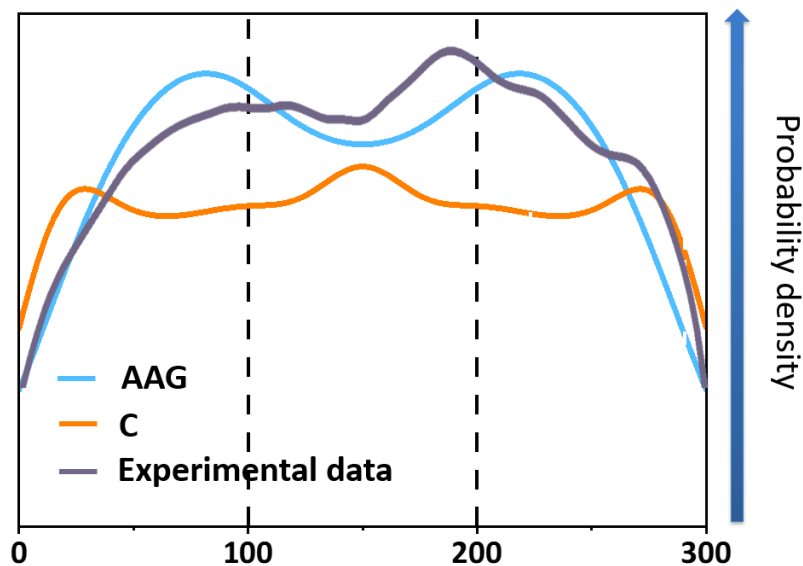


Figure 1. Disassembly pattern along the whole structure of the TMV rod. Comparison between the experimental data, the occurrence of the strongest binding trimer AAG and the destabilizer nucleotide C.

### References

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- [4] J. J. Steckert et al., Nature, 299, 32-36 (1982)

## Quantitative study of TGF- $\beta$ pathway activation dynamics

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TGF- $\beta$  pathway is an important cell-communication mechanism involved in development, neurogenesis, proliferation and apoptosis, among other processes [1]. It is known to be related to diseases such as fibrosis or cancer [1], so a better understanding of how it works will provide valuable information to develop new treatments. We focus on studying this pathway dynamics using R-Smads colocalization inside the cell through fluorescence microscopy [2]. We provide an explanation for the observed differential translocation based on R-Smads complexes formation using a simple mathematical model that can fit experimental data from cell cultures under control and Activin-treated conditions. Using FLIM-FRET [3], we obtained preliminary results confirming our hypothesis that Activin enhances complex formation, but further investigation is required.

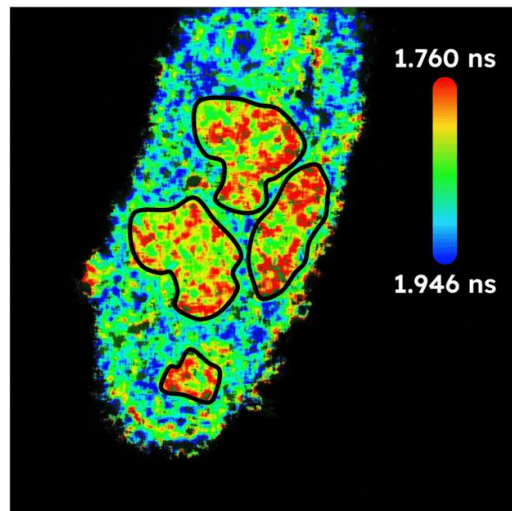


Figure 1. Experimental donor (CFP) lifetime data from U2OS S2C-S3Y cell samples. It shows a representative cell from the sample under Activin conditions. Donor lifetime shifts towards shorter lifetimes in the nuclei (black contours).

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## Harnessing virus-like particles as individual nanoreactors for controlled cargo loading

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Viruses have long fascinated researchers due to their intricate structures and biological significance. Beyond their role as pathogens, viruses possess remarkable self-assembly capabilities, often forming complex nanostructures that can serve as versatile platforms for various applications in nanotechnology and biomedicine, like targeted drug delivery, vaccine development, and synthetic metabolons for enhanced biocatalysis.

Virus-like particles (VLPs) are bio-inspired nanocages that mimic the architecture and self-assembly characteristics of viral capsids while lacking genetic material, rendering them non-infectious. These nanocontainers can be tailored to encapsulate a wide range of synthetic and gene product cargos, such as enzymes, proteins, nanoparticles, polymers or drugs. The former has recently garnered significant attention for the production of nanoreactors since enzyme internalization can enhance its stability and catalytic activity. The VLP capsid has shown to act as shield against protease digestion, thermal degradation, organic solvents, and chaotropic agents.

Here, we present not only the first real time monitorization of individual nanoreactors, but also the modulation of their catalytic activity at will. We use VLPs derived from bacteriophage P22 that encapsulate Sortase A, an enzyme catalyzing protein cleavage and ligation. In presence of calcium ions, this peptidase recognizes the sequence motif LPXTG (where X is any amino acid) and cleaves after the threonine. Enzymatic activity of our nanoreactors can be tracked by fluorescence labeling a peptide containing this motif (here: LPETGGHG in between a FRET-pair), that is cleaved by the sortase and further attached to the polyglycine chains anchored to the coat proteins in the capsid lumen. Thus, fluorescence intensity of the VLPs starts increasing as the capsids are getting filled with peptide cargo. Varying independently the concentrations of calcium and peptide in dilution permits fine-tuning the nanoreactor's performance, accelerating or slowing down and even stopping the reaction. This research opens the door to a controlled, sortase-mediated encapsulation method that allows to enclose any amount of desired cargo molecules in protein nanocages by N-terminal fusion to the LPXTG peptide.

## Proton Transport through Peptide Nanotubes

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Peptide nanotubes consist of cyclic peptides piled on top of each other and held together by hydrogen bonds, making them similar to carbon nanotubes in morphology and aspect ratio. These materials are interesting from both a fundamental and a technological perspective. They are promising proton conducting materials for the development of fuel cells, batteries, sensors, and other advanced technologies. However, proton transport in peptide nanotubes is far from being well understood. Recent experiments on cyclic octapeptides 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 with the system's hydration level. Inspired by these results, we carried out molecular dynamics simulations on these systems to gain insight into how water molecules can mediate proton flow. To do this, we considered bundles of nanotubes, which are known to be formed in the experiments. We found that water molecules can enter the space between the nanotubes and form a rich and stable structure of hydrogen bonds with themselves and the nanotubes' sidechain residues. This structure appears to be a viable candidate for mediating proton transport through a Grotthuss-like mechanism. We have studied the influence of varying water content on the network structure through simulations of a periodic system that allows precise control over the number of water molecules present. Finally, preliminary QM-MM simulations have suggested that classical potentials may not accurately describe the hydrogen bonds within the peptide nanotubes, which might play a pivotal role in proton transport through these systems.

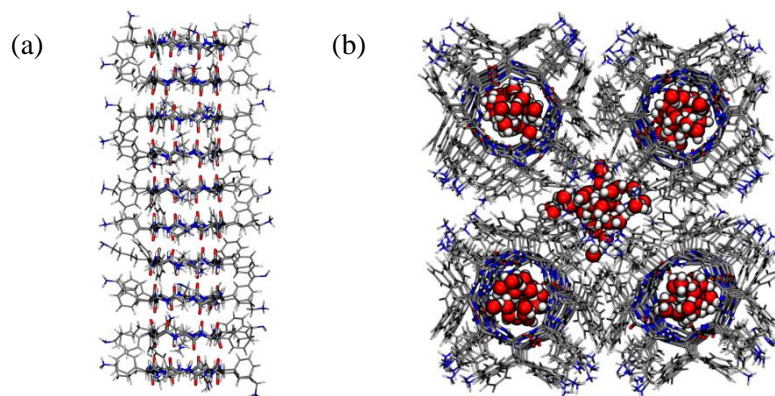


Figure 1. (a) Side view of a section of the peptide nanotube  $c(KF)_4$ . Each peptide ring contains 4 lysine (K) and 4 phenylalanine (F) amino acids in an alternate fashion. (b) Top view of a bundle of 4 nanotubes. Water molecules can be hosted inside the nanotubes and in the region between them.

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# Playing with the Geometry of Gold Nanostars: Shifting to the Second Biological Window for Biomedical Applications

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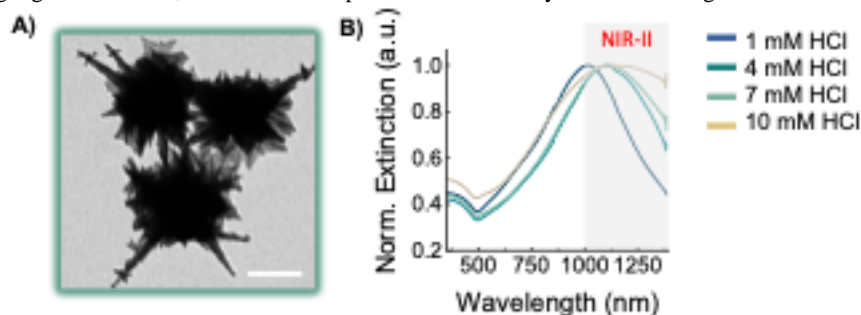
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In recent years optical biomedicine has been developing intensively, expectably becoming a fundamental part of healthcare in the coming decades, both at imaging and therapy fronts. A particular area within such field is based on the optically triggered local release of heat [1]. That heat delivery, very frequently mediated by nanoparticles, can be used for either photoacoustic imaging (PAI [2]) or photothermal therapy (PTT [2]). The former is based on the ultrasound signal generation under optical excitation, and the latter allows the removal of physiological malignances -e.g., tumors- by way of local heating, in areas that are difficult to access. In this sense, PAI and PTT, both relying on heat delivery probes, represent promising pathways for a better and harmless biomedicine, whether to achieve deeper and better resolved sensing or to non-invasively and locally eradicate diseases [2].

Clinical studies have reported promising results, but the search for more efficient and biocompatible heat release agents is ongoing.[3] Plasmonic nanoparticles (NPs), strongly interacting with excitation light, shown high heat conversion efficiency (HCE) because they feature intense absorbance and reduced scattering of the incoming photons. This means that through optical excitation we can activate and control the heating release of these NPs in the desired spectral range.[4] Specifically, the so-called “second transparency window” (NIR-II, 1000–1400 nm [4]) is particularly advantageous due to less energy dissipation and higher penetration depth into tissues compared to the nowadays widely used first near-infrared window (NIR-I, 700-980 nm [4]). From this optical viewpoint, gold is particularly attractive material due to the high control over the heating properties achievable by tuning the geometrical design of the nanoparticles [5]. 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 (NIR-II). Moreover, such synthesis toolkit will also become the key, -manifesting in nanostars’ overall size, plus number and shape of spikes- to maximize the absorption over the scattering, thus increasing heat delivery. Our carefully optimized synthesis thus paves the way to a new generation of optical probes or actuators, for PAI and PTT respectively, featuring high HCE values, able to reach deeper into biomedical systems and acting with better resolved performance.



**Figure 1.** A) TEM image of Gold nanostars in water using a seeds diameter of 29 nm and hydrochloric acid concentration of 4mM. Scale bar-100 nm B) Normalized extinction spectrum in water of gold nanostars using a seeds diameter of 29 nm. Different concentrations of hydrochloric acid used in the gold nanostars synthesis are shown (1 mM, 4mM, 7mM, 10 mM HCl).

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# Dark exciton-current conversion in quasi-1D topological insulators

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Electron-hole separation after excitation with light is at the heart of photovoltaic phenomena in semiconductors. Here we present a mechanism unique to two-dimensional topological insulators by which the exciton splits into a separate electron and hole on opposite edges where helical edge states collect the quasi-particles. This mechanism coexists with the non-radiative same-edge recombination, but it can favorably compete with it when the width of the ribbon is of the size of the exciton, giving rise to edge charge accumulation in open-circuit conditions. More importantly, since the absorption spectral weight is dominated by the excitons in two-dimensional materials, thermal excitons are less likely to shadow this phenomenon under a broad spectral light illumination. For excitons with finite center-of-mass momentum, which cannot be recombined radiatively, this dissociation results in a net current forming at the edges. This is all shown within a tight-binding model for the electronic structure of Bi(111) monolayer along with an efficient implementation of the Bethe-Salpeter equation for point-like orbitals [1, 2].

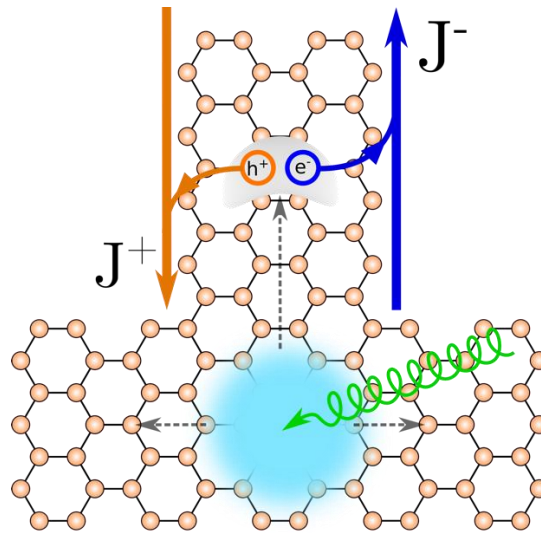


Figure 1. Schematic representation of the dissociation mechanism proposed for the exciton, where each of its components has a preferred dissociation direction resulting in an accumulation of charge at the edges of the material. If the exciton has momentum, then the charges also form a current made of helical states, intrinsic to the edges of the sample.

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# Synthesis and Characterization of Silver Nanoparticles as contrast agents in Optical Coherence Tomography

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In recent years, the use of Optical Coherence Tomography (OCT) is widely being implemented for clinical imaging in lots of medical specialties [1]. Nowadays it plays an important role in dentistry, ophthalmology, and cardiology among others. In particular, its use in this last-mentioned discipline is rising rapidly, stablishing as the general go-to imaging technique substituting the conventional Intravascular Ultrasound (IVUS) technique. The use of different contrast agents to enhance the recorded signal has been tested where noble metal nanoparticles (Au, Ag) have stood out over the rest [2]. Thanks to its plasmonic properties, well-known synthesis methods and chemical resistance they are great candidates to be used for OCT imaging.

In this work we explore viability of silver nanoparticles (Ag NPs) for OCT imaging as they present an extinction cross-section ten times higher than gold ones. For that purpose a series of Ag NPs of different sizes have been synthesized via seeded-growth strategy [3]. Initially, silver ions are reduced by citrate ions and tannic acid (TA), this results in the formation of relatively monodisperse nanoparticles stabilized by citrate that can be grown further by reducing more silver onto them. The plasmonic properties, size, morphology and stability have been studied by different techniques. In addition, citrate stabilized NPs can easily undergo ligand exchange, allowing further functionalization via bifunctional thiolated molecules.

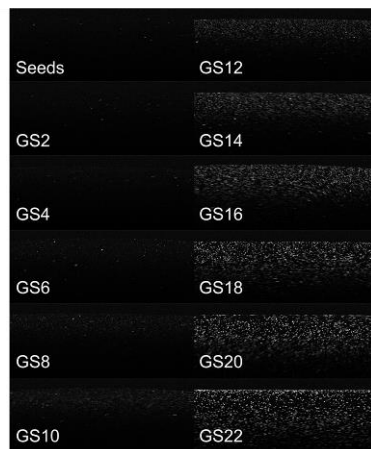


Figure 1. OCT images of different sizes of Ag NPs suspended in a water droplet.

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# Vortex lattice pinning at 20 K in the stoichiometric pnictide superconductor $\text{CaKFe}_4\text{As}_4$

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Superconductors bring macroscopic quantum coherence into concrete applications, such as levitating trains, superconducting quantum interferometric devices, quantum computers or magnetic resonance imaging. The advent of large-scale liquid hydrogen temperatures (20 K) faces superconductivity with a new frontier. 20 K is a temperature low enough to use robust and malleable metallic superconductors as  $\text{CaKFe}_4\text{As}_4$  ( $T_c=35$  K) [1]. The upper critical field of this superconductor is close to 100 T, for which it is very promising for applications. It is however important to understand the behavior of the vortex lattice in this temperature range. The vortices are arranged in an ordered vortex lattice, but when a current is applied to the superconductor, the vortices begin to move due to the effect of the Lorentz force and the property of dissipation-free current is lost [2]. Vortices are pinned by impurities and imperfections. The collective pinning of vortices depends on the elasticity of the vortex lattice. Macroscopic measurements suggest that the lattice is soft at 20 K, which allows to establish improved pinning properties. Here, we critically analyze this by imaging the vortex lattice as a function of temperature and magnetic field. We establish the phase diagram, including the optimal pinning range and observe directly the transition to the vortex liquid.

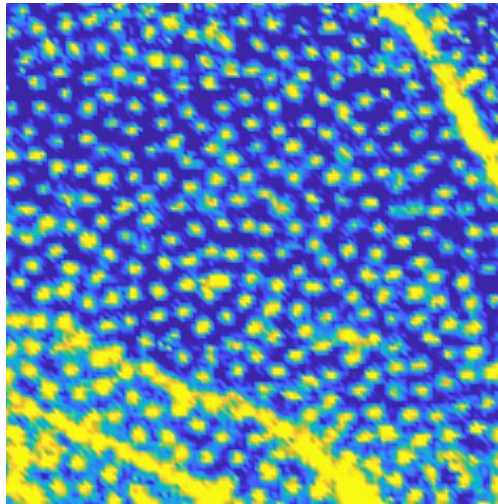


Figure 1. The vortex lattice of  $\text{CaKFe}_4\text{As}_4$  taken at 10 K and under a magnetic field of 10 T.

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

[2] G. Blatter et al., *Reviews of modern physics*, 66(4), 1125 (1994)

## Langmuir-Blodgett films of plasmonic Janus Nanoparticles for biomedical applications

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In the past few decades, an increasingly important trend in controlling physical and chemical properties at smaller scales to develop new materials has emerged. Among of the various approaches to address this trend, 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 nanoparticles (NPs), or the absorption cross-section after a proper thermal treatment of the gold films. This resulting structure can also induce controlled temperature increments, contributing to thermal therapies with positive effects against ongoing diseases, such as cancer [3].

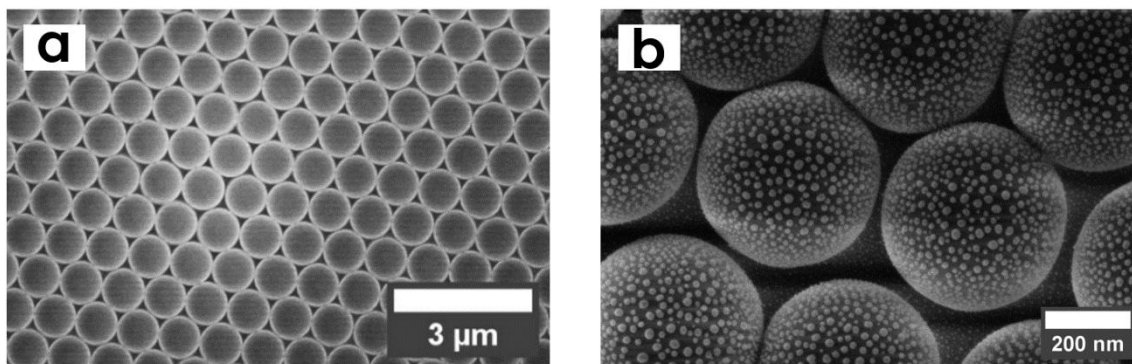


Figure 1. **a** Scanning Electron Microscopy (SEM) image of commercial 1  $\mu\text{m}$  polystyrene nanoparticles transferred onto a silicon substrate by LB assembly. **b** SEM image of 400 nm silica nanoparticles with gold nanospheres on top after thermal annealing of a gold film of 10 nm.

In this work, we present a variety of polystyrene and silica NPs with sizes ranging from 200 to 1000 nm, which are coated with gold semi-shells of different thicknesses (10-20 nm) to optimize their plasmonic properties. A spheroidizing annealing process of the gold on top of the silica NPs has also been carried out to reduce the continuous gold film on top of the silica NPs into spheres, thereby enhancing their heat conversion efficiency. Furthermore, the influence of particle size and gold semi-shell thickness in the absorption spectra will be presented, as well as COMSOL simulations of their extinction cross-section and their behavior in Optical Coherence Tomography (OCT) imaging. The results of this study present the possibility of using this type of nanoparticles for photothermal therapy purposes.

[1] P. Pellacani et al., *Materials*, **13**(5), 1244 (2020)

[2] Z. Matharu et al., *Langmuir*, **23**, 13188-13192 (2007)

[3] S. C. Freitas et al., *Adv. Mater. Interfaces*, **10**, 2202214 (2023)

# Accumulation of micro- and nano-plastics by optoelectronic platforms for sensitive detection

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The numerous advantages of plastics (inexpensive, light weight and biodurability) [1] over other materials lead to an undue daily use of them. This excessive consumption increases the appearance of secondary micro- and nano- plastics, causing an environmental pollution in terrestrial and aquatic ecosystems (soil, sediments, air, freshwater and foodstuff).[2] However, the detection and identification of low concentrated samples can be difficult, because of the weak signal of single micro- and nano-plastics. In this work, we propose and demonstrate a technique based in an optoelectronic platform whose objective is the accumulation of micro- and nano-plastics to facilitate sensitive detection.

The optoelectronic platform is based in the high light-induced electric fields generated by the bulk photovoltaic effect in  $\text{LiNbO}_3:\text{Fe}$ , a reference ferroelectric material. The method is illustrated in Fig. 1: First, a water reservoir drop is deposited on a slide located  $\sim 0.5$  mm under the crystal. A laser beam focused on the crystal is used to photo-generate the high electric field. In turn, this electric field induces the ejection of a high number of droplets from the reservoir drop (see Fig. 1.(a)). The ejected droplets reach the bottom part of the crystal and, when evaporating, they leave the micro- and nano- plastics on the crystal surface. Fig. 1(b) and 1(c) show the successful accumulation of micro- and nano-plastics on the optoelectronic platform, both giving rise to a gaussian-like distribution (see Fig. 1(d)). The influence of the initial concentration of micro- and nano-plastics in the reservoir drop on the structure of the gaussian- patterns has been also investigated. Finally, the role of the ejection time as well as the ejection from multiple reservoir drops have been explored to still enhance the accumulation capabilities.

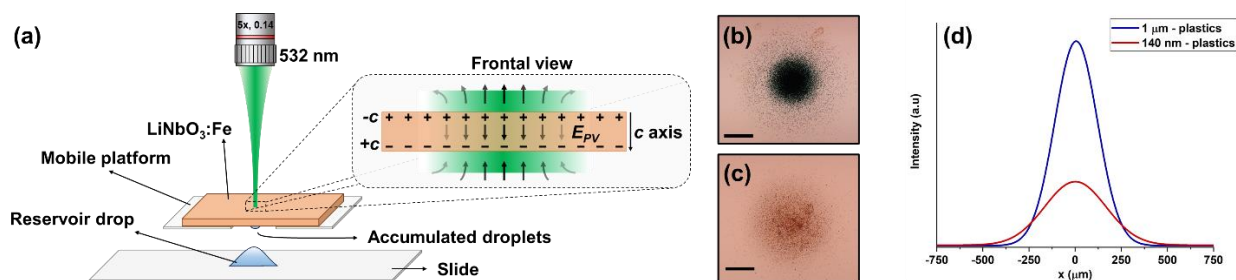


Figure 1. (a) Experimental set up: the 532 nm laser beam is focused in the  $\text{LiNbO}_3:\text{Fe}$ . Under the mobile platform, the reservoir drop is located. On the right, a frontal view of the crystal shows the electric field distribution generated by the photovoltaic effect. (b) and (c) Micro-photographs of the distributions of the accumulated micro- and nano-plastics, respectively. Scale bar: 200 $\mu\text{m}$ . (d) Gaussian profile of the micro- (blue) and nano- (red) plastics.

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[2] Mariano, S., et al., Micro and Nanoplastics Identification: Classic Methods and Innovative Detection Techniques. **3**, (2021).

## Preparation and study of potential amorphous topological superconductors of Bi-Sb

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Exotic properties of topological superconductivity are expected to pave the way towards quantum computing [1,2]. However, a stable topological superconductor has not yet been found experimentally. Good candidates have been proposed to be bismuth and its alloys (particularly, bismuth-antimony, Bi-Sb), which are among the most studied topological insulators [3,4] and which, in amorphous state, become superconductors below a critical temperature close to 6 K [5].

The aim of this work is to grow  $\text{Bi}_{100-x}\text{Sb}_x$  alloys and induce, by ion beam irradiation, enough damage to their internal structure as to amorphize the material. Although amorphous Bi-Sb tends to recrystallize unless at low temperatures [5,6], our idea to overcome such difficulty is trying to amorphize only a region of the material a few  $\mu\text{m}$  deep from the surface. To do so, we use ions in the MeV range, exploiting the capabilities of CMAM's 5 MV ion-beam accelerator [7]. By characterizing the morphological, structural and electrical properties of the resulting material, we analyze its potential as an amorphous topological superconductor.

We present here preliminary experiments, including our current work focused on testing different strategies in order to optimize all the steps in our research: alternative sample substrates, growing techniques, irradiation parameters and measurement setups.

[1] C. Beenakker and L. Kouwenhoven, *Nature Physics* **12**, 618-621 (2016)

[2] R. Aguado and L. Kouwenhoven, *Physics Today* **73**, 44-50 (2020)

[3] D. Hsieh et al., *Nature* **452**, 970–974 (2008).

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## High-throughput three-dimensional characterization of morphogenetic signals during the formation of the vertebrate retina.

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The precise differentiation of neural progenitors during development ensures the correct cognitive, sensory and motor functions of higher organisms. This balance between self-renewal and terminal differentiation is highly regulated by a complex interplay of signaling pathways, that set the spatial and temporal cues that ultimately form and organize neurogenic tissues. The developing vertebrate retina is ideal to study how these key signaling cascades modulate the mode and rate of division of neural progenitors, despite its complex three-dimensional architecture of the retina, the asymmetric differentiation dynamics, and the multiple feedbacks and cross-talks between these signaling cascades. Here, we present a multi-step framework that combines in toto experiments with three dimensional image analysis and theoretical tools [1] to obtain a quantitative characterization of the dynamics of growth and differentiation of the developing vertebrate retina. Next, we use small molecule inhibitors to study the specific roles of Hh, Wnt, Notch and FGF signaling in the regulation of the cell cycle length and/or the mode of division. Our results represent a detailed quantitative characterization of the development of the vertebrate retina and its regulation with unprecedented accuracy. We propose that the same framework can be directly used to characterize other in vitro and in vivo tissues.

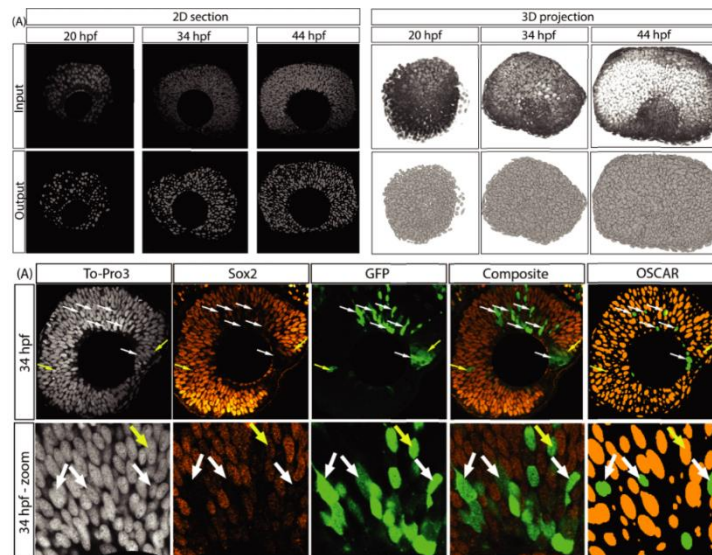


Figure 1. Original confocal images against digital reconstruction in 2D and 3D

[1] Míguez DG. A Branching Process to Characterize the Dynamics of Stem Cell Differentiation. Sci Rep. 2015 Aug 19;5:13265. doi: 10.1038/srep13265.



## Scanning Tunneling Microscopy on Van der Waals ferromagnet $\text{Fe}_3\text{GeTe}_2$

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$\text{Fe}_3\text{GeTe}_2$  is a van der Waals compound with bulk ferromagnetic ordering at  $T_c=220\text{K}$ . This material also shows a large effective mass renormalization, with a Sommerfeld coefficient reaching  $135 \text{ mJ}/(\text{K}^2\text{mol})$ , classifying it as a heavy fermion. However, contrary to usual heavy fermions, there heavy band formation is without f-electrons. Scanning Tunneling Microscopy (STM) measurements at zero magnetic fields present a Fano anomaly due to coherent co-tunneling into heavy and light electrons [1]. Here we study this compound with STM under a magnetic field. We observe the Fano anomaly and discuss its dependence as a function of the position and magnetic field.

[1] Zhang et al., Sci. Adv., **4**, eaao6791 (2018)

# Role of salinity in the accumulation of micro-plastics on photovoltaic substrates by electrohydrodynamic droplet dispensing

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Due to its versatile properties and its low price, plastics are a worldwide used materials whose utilization have augmented considerably in the last century [1]. As a result, about 1.15 – 2.41 million tones of plastic wastes are released into the ocean annually [2]. These plastics degrade into micro- and nano-plastics which have been detected in aquatic ecosystems, thus, posing a risk for the environment and human health [1]. Therefore, detection and identification of plastics in marine and freshwater is essential.

Recently, it has been reported the use of  $\text{LiNbO}_3:\text{Fe}$  (LN:Fe) platforms to accumulate micro- and nanomaterials by liquid ejection. In particular, the bulk photovoltaic effect (PVE), present in these ferroelectric crystals, has been used for the accumulation of micro-particles [3]. This method takes advantage of the light-induced electric field  $\mathbf{E}$  generated by the PVE. When a reservoir micro-droplet is near the crystal, and if  $\mathbf{E}$  is strong enough, the droplet is deformed by the electric field causing the release of nano-liter droplets towards the surface of the crystal. This way, the material contained within the nano droplets is concentrated onto the ferroelectric crystal's surface showing a gaussian-like distribution.

Lately, in our group we have proposed and demonstrated the possibility of accumulating plastics in pure water with this technique (see P. Camarero's work). With the detection of micro- and nano- plastics in marine water in mind, studies with saltwater solutions were done but initial attempts were not successful. Thus, in this work we have investigated the role of salinity (saltwater, PBS, marine water) on the accumulation of polystyrene micro-spheres by light-induced droplet ejection. The results show that the method can be also applied to saline plastic solutions, but the full width at half maximum (FWHM) of the gaussian distribution is reduced as NaCl concentration increases (see figure 1). A further study on the mechanisms is under development.

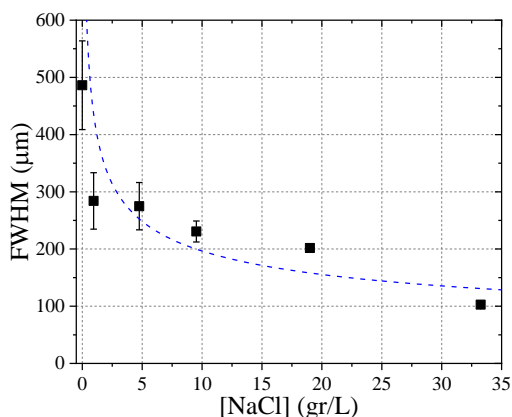


Figure 1. FWHM of the gaussian distribution of polystyrene micro-spheres accumulated onto the substrate versus the NaCl concentration. The blue line is added to guide the eye.

[1] M.R.M Zaki et al., *Science of the Total Environment*, **831**, 154757 (2022)

[2] M. Le Breton et al., *Nat. Commun.*, **8**(1), 15611 (2017)

[3] A. Puerto et al., *Adv. Mat. Int.*, **8**(22), 2101164 (2021)

## Dissipation in a superconductor viewed by impedance measurements

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A resistance can be measured by applying an AC current and recording the real part of the AC voltage drop. When measuring the resistance as a function of temperature, a sufficiently large AC current might produce a self-heating effect that leads to a delay in the voltage response. The delay depends on the thermal conductivity between the sample and the heat reservoir and the specific heat of the sample. The delay can be measured by recording the imaginary part of the AC voltage. This effect is, for nearly all purposes, negligible in a usual metal, where the resistance changes by a very small amount per Kelvin. However, in a superconductor the resistance drops abruptly to zero in a temperature range of just a few mK. This abrupt temperature dependence produces a strong imaginary component [1]. Here we show that the imaginary component persists below the superconducting transition, even when the real part is nearly zero. We associate the newly observed imaginary component to the heat dissipated from vortex motion in a current carrying wire. We discuss vortex motion in presence of a current and the associated generation of voltage and heat.

[1] D. Perconte et al, Phys. Rev. Appl., 13(5), 054040 (2020)

## Optical trapping of single nanoparticles

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Since Arthur Ashkin experimentally demonstrated that light could manipulate microparticles in the 1970s<sup>1</sup> (Figure 1), optical tweezers have been used to manipulate a wide range of areas, such as Physics and Chemistry. Optical tweezers are a technique that makes use of the optical forces exerted by a laser beam on the nanostructure, these forces are based on conservation momentum where the linear momentum of light is transferred to the nanostructure and has become fundamental to improving single nanoparticle analysis. Some advantages of using optical tweezers lies in their high precision to study the properties of nanoparticles in great detail and their non-invasive nature that does not require physical contact with the object, which eliminates the risk of damage and is important for studying delicate nanoparticles. Due to these versatile properties, the optical tweezers can be used to develop ultrasensitive sensors like electrochemical detectors for study reactions in nanoscale<sup>2</sup> and platforms for screening of drugs and environmental monitoring<sup>3</sup>. Another promising application is the possibility of using plasmonic nanostructures to enhance optical trapping because of the great interaction of it with light and the generation of localized electric fields that trap them with much higher precision<sup>4</sup>. Therefore, the importance of optical trapping in the manipulation and investigation of single nanoparticles and its ability to trap, manipulate, and characterize individual nanoparticles has the potential to unlock new frontiers in nanoscience and nanotechnology.

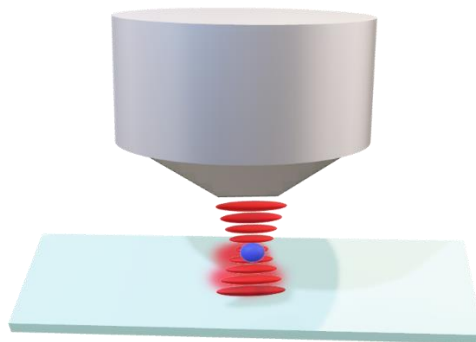


Figure 1. Representation of single-particle optical trapping.

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4. Ren, Y. *et al.* Plasmonic Optical Tweezers for Particle M

# Interplay of magnetic textures and spin-orbit coupling in the generation of equal spin triplet superconductivity

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Over the last decade, it has been proposed theoretically and confirmed experimentally that long-range spin triplet (LRT) superconductivity in superconductor-ferromagnet (S/F) hybrids may be generated either by the presence of magnetic textures in the ferromagnet (MT-LRT) [1,2] or thanks to interfacial spin-orbit coupling (SOC-LRT) [3]. However, it was never suggested nor probed experimentally that in a real experimental system both contributions could coexist. In order to disentangle these two contributions, we present a comprehensive study of electron interference effects under in-plane (IP) and out of plane (OOP) magnetic fields in epitaxial S/F junctions with spin-orbit coupling. By studying the bias-dependent conductance in S/F/F and F/S/F tunnel junctions based on V/MgO/Fe, we observe conductance anomalies (CAs) below the superconducting critical temperature, resulting from quasiparticle interference in the Fe electrode. Previously, above gap CAs in these samples were investigated only for remanent magnetization orientations of the Fe layer [3]. Interestingly, these CAs were more pronounced for an OOP orientation of the magnetization, i.e. when the IP and perpendicular magnetic anisotropies competed and induced magnetic textures at the MgO/Fe interface. In this context, a comparative investigation of CAs in a wide range of applied magnetic fields, both IP and OOP, provides a unique tool to distinguish two main physical contributions to LRT formation: magnetic textures and interfacial spin-orbit coupling. This is because SOC-LRTs could be more robust to the applied field than MT-LRTs, as the magnetic textures would be destroyed by a large applied field.

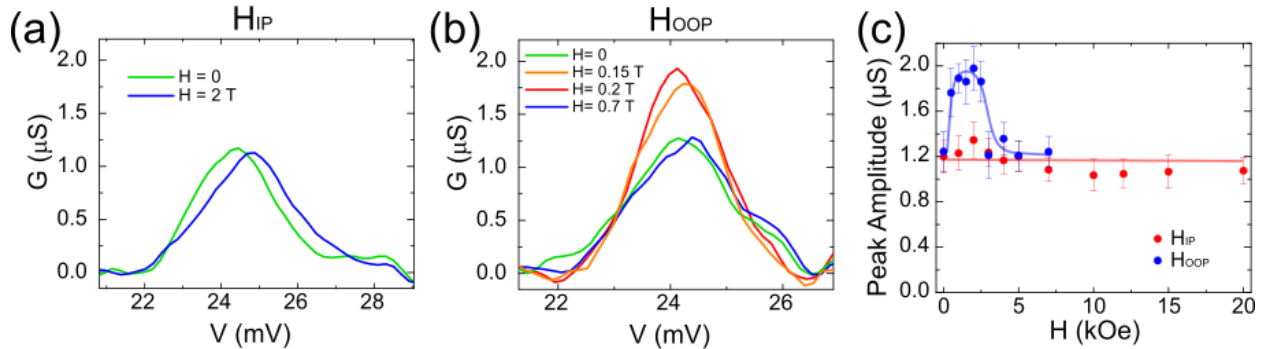


Figure 1: Example of the behavior of a CA in a S/F/F sample under different applied fields. (a, b) differential conductance around the CA peak (after a baseline conductance subtraction) for different applied magnetic fields, both IP (a) and OOP (b). (c) CA peak amplitude versus applied IP and OOP magnetic field: an increase in the CA amplitude is observed for low OOP fields due to MT-LRT generation, while the IP field saturates the magnetization yielding an approximately constant amplitude granted by SOC-LRT formation.

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[3] I. Martínez, Physical Review Applied **13**, 014030 (2020).

## Superconducting gap in PtPb<sub>4</sub>

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PtPb<sub>4</sub> has attracted attention recently due to its similar structure with the Dirac nodal arc semimetal PtSn<sub>4</sub>, which makes it a potential platform for coexisting superconductivity and topology. There have already been reports of a large Rashba splitting and possible topological properties [1-3]. This work presents the first measurements and characterization as a function of temperature of the superconducting gap in the density of states of PtPb<sub>4</sub>. Reaching temperatures as low as 100 mK, we provide through STM the critical temperature T<sub>c</sub> of this material, where superconductivity vanishes. This value corresponds to roughly 5 K, quite above the previously reported T<sub>c</sub> of 2.8 [2,5]. This considerable change of the critical temperature can occur only close to the surface, suggesting that there are changes impinging on the electron-phonon coupling. Recent measurements in AuSn<sub>4</sub> [6] show that polytypism and stacking faults lead in that material to a considerably increased T<sub>c</sub> close to the surface. We discuss here similarities and differences with PtPb<sub>4</sub>, which could be related to the observed features.

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## Manipulation of superconducting Pb islands on graphene.

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When a superconductor (SC) is at close spatial proximity and in good electrical contact with a metal, the Cooper pairs diffuse from the former to the latter. This results in the metal exhibiting superconducting characteristics on a mesoscopic range near the interface between both materials [1]. Such a phenomenon is called superconducting proximity effect. On this work, we take advantage of the proximity effect to induce superconducting properties on graphene, an extremely promising material which lacks superconducting properties. Sublimating Pb on top of a graphene sample, grown epitaxially on SiC(000-1), we are able to grow two-dimensional Pb islands directly on top of it. Here we show that the Pb islands induce a SC gap in graphene by proximity. Furthermore, we show the unprecedented manipulation of Pb islands with nanometric precision, which enables us to selectively induce SC in specific regions of our graphene samples. In addition, we also investigate how graphene SC is induced locally, showing, for example, that moiré patterns affect the SC properties, modulating the gap periodically with the distance.

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## Non-linear magnetoresistance due to magnon creation-annihilation in Pt/Y<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub> thin films

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Magnons are magnetic excitations in magnetic ordered materials that carry quanta of spin angular momentum. Recent works have shown that non-equilibrium magnons can be electrically excited and detected in magnetic insulators interfaced with heavy metal layers by exploiting charge-to-spin conversion phenomena in the metal and spin-flip scattering processes at the metal/magnetic insulator interfaces [1]. Up to now, all experiments performed in this topic have focused on investigating magnon injection/detection, transport and modulation efficiencies by measuring the build-up voltage at the detector stripe in non-local device structures, but the effect of magnon creation and annihilation processes on the local magnetoresistance at the injector stripe has remained overlooked. In this work we investigate a novel magnetoresistance phenomenon occurring in Y<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub>(YIG)/Pt bilayers originated from current-induced magnon creation and annihilation processes in YIG. The creation and annihilation of magnons results in a change of the magnetization in YIG thereby resulting in a non-linear longitudinal and transversal resistive response in the Pt layer for those magnetoresistances that depend on the magnetization. This novel non-linear magnetoresistance phenomena appears in the second harmonic voltage response upon the application of an ac current to the Pt current line. Fig 1a shows an optical image of a representative Pt Hall bar device patterned on top of YIG along with the electrical connections used in our experiments. Fig. 1b shows a representative second Harmonic Hall voltage response measured in YIG(100nm)/Pt(4nm) where the variation of the magnetization in YIG is negligible (0.1-0.01 %), therefore only exhibiting field-like torque and spin Seebeck effect contributions to the second harmonic Hall voltage response  $R_{2\omega}^H$ . In contrast, for thin YIG layers, the variation of the magnetization due to magnon creation/annihilation is large (>>1%) resulting in a sizable non-linear magnetoresistance associated to the non-linear response of the planar Hall effect (NLPHE). In our work we demonstrate that the non-linear magnetoresistance originated from the creation and annihilation of magnons is strongly dependent on the thickness and Gilbert damping of the magnetic layer. In addition, we show that the variation of the magnetization decay as a power law with the magnetic field as  $B^{-\rho}$  with a strong dependence of  $\rho$  on the thickness of the YIG layer and current density. We rationalize our results by considering the modulation of the effective Gilbert damping in our films with current.

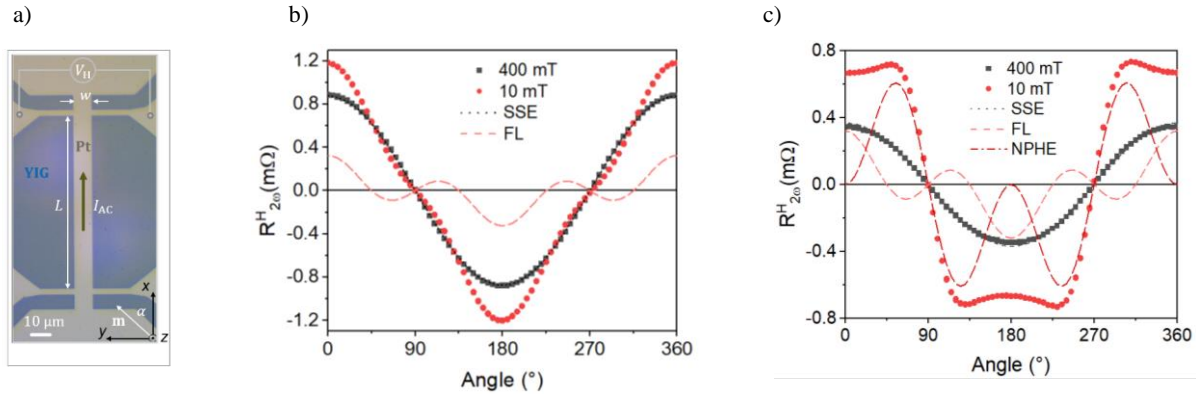


Figure.1.a) Local device schematics and coordinate system are shown. b) Second harmonic transverse signal of YIG(100nm)/Pt bilayer. c) Second harmonic signal transverse signal of YIG(10nm)/Pt bilayer

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# Optical Forces at the Microscale: Size and Electrostatic Effects

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Optical tweezers (OT) are a widely used tool in fields such as biology and physics as they facilitate the manipulation of nanometer and micrometer elements. Most of the particles used in optical tweezers (OT) with a biological interest usually have a micrometer radius, as well as being manipulated with lasers in the infrared range. Such particles lie in between the Mie Regime and the Rayleigh Regime, but neither is an accurate model for particles in the 1 to 10 micrometer range [2]. Furthermore, the optical forces acting on dielectric microparticles have only been related to parameters such as volume, and size has traditionally been identified as a key parameter, but it has now been found that electrostatic properties could be an important factor to consider [1].

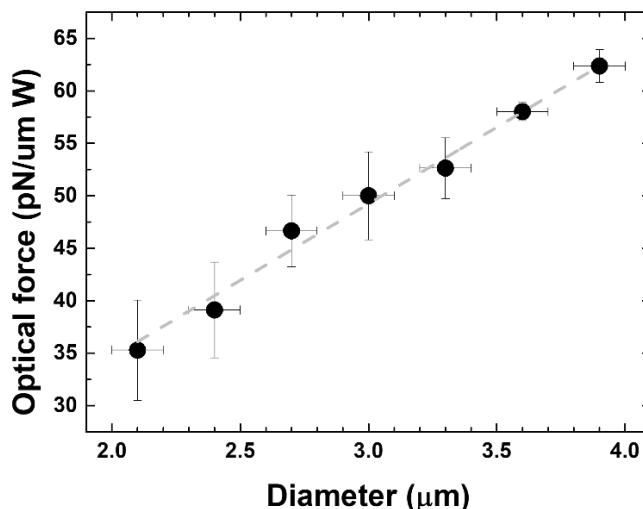


Figure 1. Optical force as a function of the diameter of particles.

For this reason, in this work we have designed a set of experiments that aim to test which parameters and properties are relevant when trapping a dielectric microparticle. Within the experiments, we will measure the trapping constant of particles of different materials, sizes, and also, we will produce changes in the zeta potential of the samples using HCl.

This work was financially supported by the Spanish Ministerio de Ciencia e Innovación, through projects (CNS2022-135495 and TED2021-129937B-I00).

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## Ion-induced bias in luminescent nanothermometers embedded in physiological media

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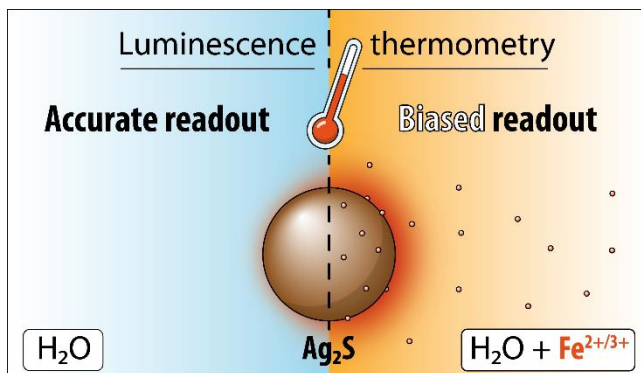
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Luminescence nanothermometry is one of the most innovative techniques for remote sensing of temperature at the subcellular range. However, this technology has been questioned in the recent years due to the presence of bias sources that reduce the reliability of the thermal sensing. Bias emerges when the environmental conditions not related to temperature, for example physiological media, modifies the luminescence of the nanothermometers. In this work, we unveil an unexpected source of bias induced by metal ions. We show that Ag<sub>2</sub>S luminescent nanothermometers are biased during the monitoring of photothermal heating produced by iron oxide nanoparticles. The observed bias arises due to the release of iron ions when iron oxide nanoparticles are heated. The interaction between the surface of the Ag<sub>2</sub>S nanoparticles and the iron ions enhances the emission of the nanothermometers. The results reported are intended to raise a warning to the community that works with nanoparticle luminescence sensing. Since different sources of bias can emerge in complex biological environments, which have a great variety of molecules and ions, the study of this interactions can be important for the development of new synthesis routes.



## Superconducting Density of States and Vortex Lattice in $\text{LaRu}_2\text{P}_2$

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Pnictide superconductors are single crystalline metallic materials with a pnictogen in the chemical composition. By far, most pnictide superconductors have non-stoichiometric compositions.  $\text{LaRu}_2\text{P}_2$  ( $T_c=4\text{K}$ ) is one of the few exceptions. Electronic band structure and other macroscopic measurements suggest that, unlike most pnictides superconductors,  $\text{LaRu}_2\text{P}_2$  presents no strong electronic correlations. That is, the effective mass has a value like the one obtained from density functional band structure calculations [1]. Here, we make first measurements of the superconducting gap and vortex lattice of  $\text{LaRu}_2\text{P}_2$  single crystals. We describe the growth and characterization of single crystals of  $\text{LaRu}_2\text{P}_2$  and how we performed STM measurements. We find features suggesting that this material is a conventional phonon mediated superconductor. This provides an indication of the maximum  $T_c$ s achievable with phonon interactions in pnictide superconductors.

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# Structural defects on graphene generated by deposition of CoO: Effect of electronic coupling at the graphene/substrate interface

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The understanding of the interactions that takes place in hybrid systems based on graphene and functional oxides is crucial to the applicability of graphene in real devices. Here, we present a study of the structural defects occurring on graphene during the early stages of the growth of CoO tailored by the electronic coupling between graphene and the substrate in which is deposited. For that we compare two substrates: graphene deposited on polycrystalline copper, cleaned in UHV to remove oxygen contamination, and graphene transferred to SiO<sub>2</sub> substrate. The CoO growth has been carried out by thermal evaporation of metallic Co under an oxygen atmosphere at room temperature and the interaction, since the early stages of CoO growth, with both graphene-based substrates have been studied “in situ” by X-ray photoelectronic spectroscopy and “ex situ” by Raman spectroscopy and atomic force microscopy. The decoupled G/SiO<sub>2</sub> substrates show low initial crystalline quality and during the growth of CoO on it is identified a wetting layer of CoO, absent on the G/Cu substrate. For low CoO coverages, the oxidation of graphene is really low in both substrates however structural defects, that are developed on both substrates during the growth of CoO, are significantly higher on decoupled G/SiO<sub>2</sub>. For low coverages small islands of CoO are formed, that group together to form CoO nanowires with diameters ranging between 70 to 150 nm for the highest coverages [1-3].

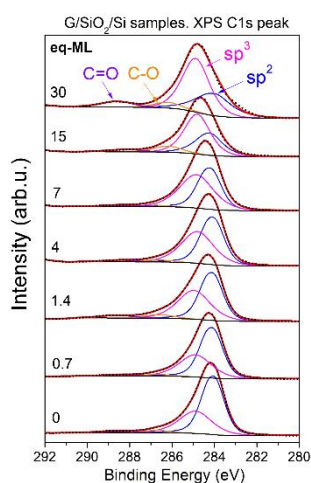


Figure 1. C1s XPS spectra of CoO/G/SiO<sub>2</sub> samples.

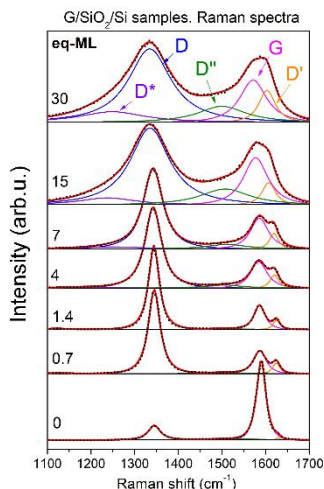


Figure 2. Carbon Raman bands of CoO/G/SiO<sub>2</sub> samples

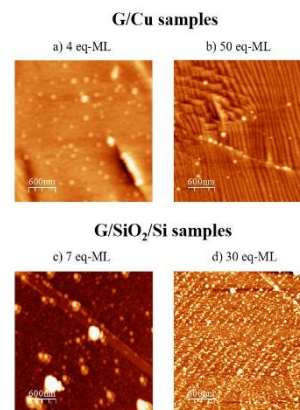


Figure 3. AFM topographic images (size: 3×3 μm) of Co grown on G/Cu and G/SiO<sub>2</sub> substrates.

- [1] C. Morales et al; *Appl. Surf. Sci.*, **509**, 145118 (2020). [2] L.M. Malard et al; *Physics Reports*, **51**, 473 (2009). [3] Z. Luo et al; *J. Phys. Chem. C*, **115**, 1422 (2011).



## Checking the suitability of $\text{Li}_3\text{InCl}_6$ as coating for Ni-rich cathodes in sulfide based all-solid-state batteries through XPS measurements

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Argyrodite-based  $\text{Li}_6\text{PS}_5\text{Cl}$  (LPSCl) has attracted much attention due to its high Li-ion conductivity and ease in processibility, which allows large-scale applications of solid-state batteries. However, when combined with high-voltage cathodes, LPSCl suffers from detrimental side reactions and structural instabilities. Due to the relatively high Li-ion conductivity and high voltage-stability  $\text{Li}_3\text{InCl}_6$  (LIC) has been recently proposed as catholyte with the potential to overcome the shortcomings of LPSCl.

Based on the evidence found through XPS measurements, among other techniques, LIC is proposed to be a good choice for coating Ni-rich cathodes when argyrodite-based  $\text{Li}_6\text{PS}_5\text{Cl}$  is used as solid electrolyte on a battery. Analyzing and fitting S 2p and P 2p peaks on the spectra from isolated electrolyte samples, cathode contacted with electrolyte samples and coated cathode contacted with electrolyte samples, it shows that the presence of the coating inhibits the apparition of some components that can be associated with the degradation of the battery as a consequence of electrolyte and cathode interaction when cycling.

SEM images of the samples, as well as XRD measurements, are coherent with this result.

## Spectral and spatial characterization of the photon statistics in the emission by a quantum dimer

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In this work, we study a dimer formed by two interacting quantum emitters, modelled as two-level systems, that are driven in two different ways: first with a coherent pump and second with that same coherent and an additional incoherent pump. The latter effectively describes the optical pump of the dimer through another, off-resonant, blueshifted, coherent driving, and it modifies drastically the results achieved with the coherent pump. We take into account the on-resonant and off-resonant interactions between the emitters, described within the Macroscopic Quantum Electrodynamics (MQED) formalism via the dyadic Green's function, and their dependence with the interatomic distance [1]. We also include the spatial information in the electric field operator, which enables us to investigate interference phenomena that modifies drastically the statistics of the scattered light according to the directions at which photons are emitted [2,3].

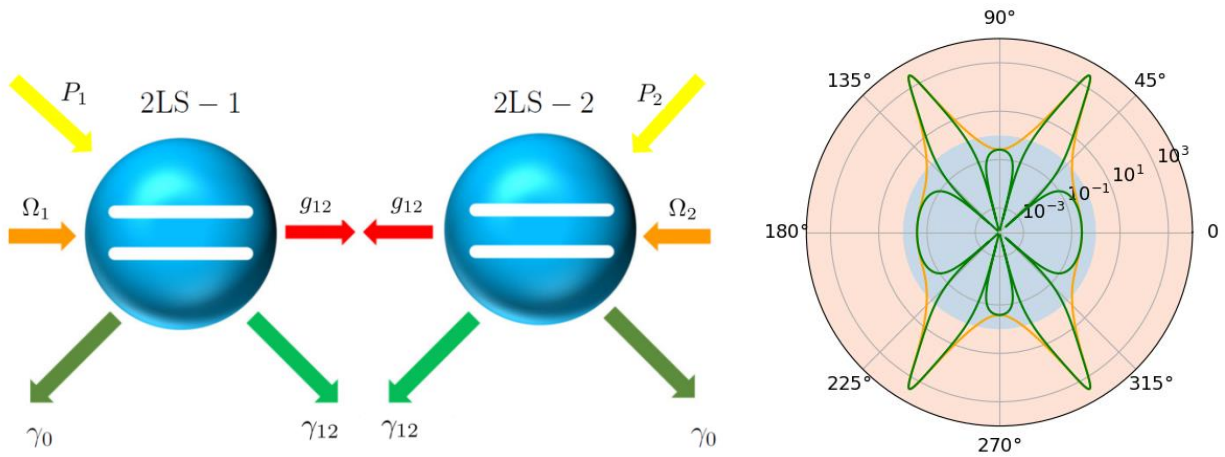


FIG 1. Left: schematics of the system formed by two interacting two-level system. Right: second order correlation function with zero delay ( $g^{(2)}(0, r, r')$ ), measured at equal directions ( $r = r'$ , orange line) and opposite directions ( $r = -r'$ , green line), as functions of the photon-emission direction.

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## Synthesis and characterization of rare earth doped luminescent nanoparticles for biological applications

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### Abstract

Our work describes a simple chemical route for preparing silver sulfide nanoparticles (Ag<sub>2</sub>S) stabilized with thioglycolic acid (TGA). The structural and the optical properties of the obtained product were characterized by using different spectroscopic techniques. The obtained Ag<sub>2</sub>S nanoparticles are highly luminescent in the NIR-I biological window. These NIR NPs present excellent cytocompatibility even at 100 ug/mL with U87 cells. These results have opened up the possibilities of using our nanoparticles for cell imaging and luminescence thermometry.

### Acknowledgements

We would like to mention our funding institution, Ministerio de Ciencia e Innovación de España (PID2019-105195RA-I00, PID2019-106211RB-I00, CNS2022-135495, and TED2021-129937B-I00). P.C. thanks the regional government of Comunidad de Madrid for the Programa Investigo (Plan de Recuperación, Transformación y Resiliencia) which was developed thanks to SEPE, Ministerio de Trabajo y Economía Social and the European Union through NextGenerationEU. The main text of the article should appear here with headings as appropriate.

# Light-induced switching of ferroelectric spontaneous polarization in iron-doped LiNbO<sub>3</sub>

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Iron-doped LiNbO<sub>3</sub> (Fe:LiNbO<sub>3</sub>) is a promising ferroelectric platform thanks to its prominent bulk photovoltaic effect. Over the past ~15 years, this material has garnered significant attention for a wide range of optoelectronic applications: assembly of micro/nano-objects [1], optofluidics [2], orientation and manipulation of liquid crystals [3] or graphene metasurfaces [4], among others. So far, only monodomain Fe:LiNbO<sub>3</sub> crystals have been explored in the literature for such applications, overlooking the additional degree of freedom provided by domain-engineered substrates. Nonetheless, the traditional electrical method for domain engineering is complex and costly, involving lithography steps [5]. Herein, we present a novel all-optical approach for local domain inversion, only using continuous-wave visible light ( $\lambda = 532$  nm). By enclosing *z*-cut Fe:LiNbO<sub>3</sub> crystals in a conductive medium during irradiation (e.g. water), we indisputably demonstrate the local reversal of the spontaneous polarization upon light excitation with low/moderate intensities. Moreover, we study the impact of light intensity, exposure time, laser focusing conditions and surrounding medium on the morphology and depth of the light-inverted domains (see some examples in Figure 1a). By tuning these parameters, ensembles of nanodomains, intricate self-assembled nanostructures or quasi-circular micro-domains may be generated. Finally, we show the feasibility to fabricate arbitrary-shaped domains by using structured light (see Figure 1b and 1c), thus proving the remarkable versatility of this all-optical ferroelectric switching technique.

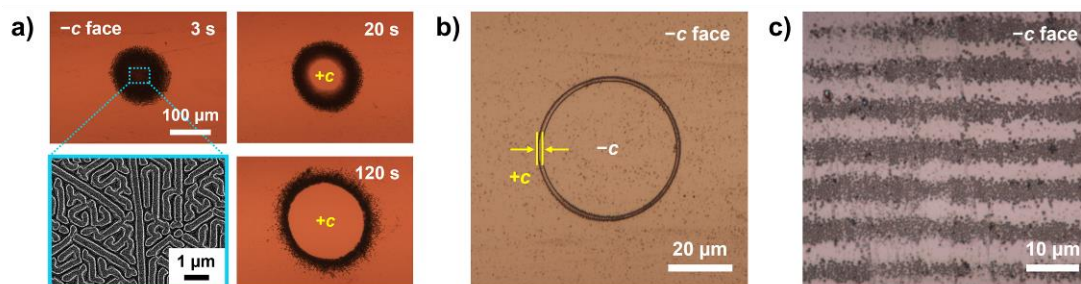


Figure 1. a) Inverted spots using a Gaussian laser beam ( $d = 150 \mu\text{m}$ ,  $I = 0.82 \text{ kW}/\text{cm}^2$ ) with different exposure times. b) Inverted ring using a spatial light modulator ( $I = 0.54 \text{ kW}/\text{cm}^2$ ,  $t_{\text{exp}} = 6 \text{ s}$ ). c) Periodic fringes of nanodomains obtained by two-beam interference ( $t_{\text{exp}} = 2 \text{ h}$ ). The intensity of the interfering beams is  $83 \text{ mW}/\text{cm}^2$  and  $76 \text{ mW}/\text{cm}^2$ . All images were taken after selective chemical etching in HF acid.

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## Ultraquantum Limit of Axionic Charge Density Waves

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### Abstract

Magnetic Catalysis (M.C.) of Chiral Symmetry Breaking is the mechanism whereby a magnetic field induces a gap in an otherwise gapless system of weakly-interacting chiral fermions [1]. It has been explored extensively in the context of the QCD phase transition in high-energy physics. However, the advent of 3D Dirac/Weyl semimetals has raised the possibility of observing the phenomenon in condensed matter systems as well in the form of Axionic Charge Density Waves [2,3].

Models of the phenomenon often rely on the fact that the energy scale provided by the magnetic field is lower than the UV cutoff of the theory, which in condensed matter systems is at most of the order of the inverse lattice spacing. We consider the opposite scenario where the magnetic field scale is of the order or larger than the UV cutoff, a scenario originally proposed in the context of the QCD [4]. Among other consequences, we find that in that case there is a wider parameter window for which M.C. can observably take place and that dimensional reduction from 3 to 1 spatial dimensions becomes stronger than in the moderate magnetic field regime, enabling a beyond mean-field description through 1D bosonization [5].

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### Acknowledgments

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## All-Dry Deterministic Transfer of Thin Gold Nanowires for Electrical Connectivity

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Metallic nanowires exhibit a number of interesting properties, such as high conductivity, flexibility and cold welding capabilities, making them ideal for nanocircuitry. They are commonly adsorbed on a substrate by simply depositing a colloid of NWs on the surface. However, they are randomly scattered on the substrate and solvent residues might contaminate and/or degrade the sample.

In this work, we present a procedure for electrical connectivity using thin gold nanowires based on all-dry deterministic transfer.[1] The process begins with the adsorption of gold nanowires via drop casting onto a viscoelastic substrate. We transfer these wires to selected locations on the substrate, precisely placing the NWs near their final destination, thus minimizing manipulation, preserving surface and sample conditions, and improving the fabrication of nanocircuits. We employ atomic force microscopy to locate the NWs and manipulate them for the final electrical connections. To illustrate the technique, we present three different examples of applicability: the electrical characterization of a four-terminal graphene device, the repair of gold nanoelectrodes, and the electrical characterization of few-layer MoS<sub>2</sub> device under different illumination conditions. We also show that the work time on the sample substrate can be minimized manipulating the gold nanowires on the viscoelastic substrate and transferring the entire nanoelectrode at once.

We anticipate our work to be a starting point to extend the potential of deterministic transfer methods successfully used in 2D materials assembly. For example, to study local electrical transport in heterogeneous samples such as van der Waals heterostructures and twisted layers of 2D materials.

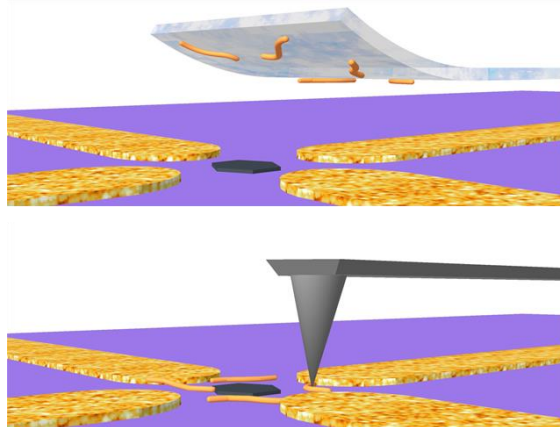


Figure 1. Schematics of the transfer (top) and nanomanipulation assembly (bottom).

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# Au – loaded Se – doped Ta<sub>2</sub>O<sub>5</sub> porous thin films for enhanced visible-light photocatalytic activity

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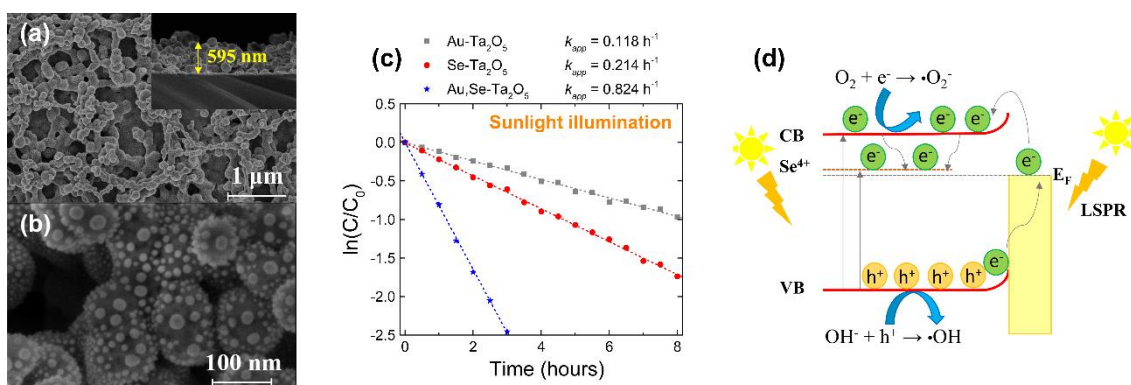
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In recent years, interest in processing materials with visible light photocatalytic activity has grown due to the need to develop new methods of energy production, pollutant degradation, or water splitting or purification, among others [1,2]. In the present work, porous, thin films of oxygen-deficient Se-doped Ta<sub>2</sub>O<sub>5</sub> have been synthesized by the sol-gel method and characterized. Their photocatalytic activity in the degradation of methyl orange has been studied both under solar and UV light and compared with that of compact thin films of Ta<sub>2</sub>O<sub>5</sub>. The UV photocatalytic efficiency of porous samples is a factor of 10 higher than that of compact samples, which is attributed to their much larger specific surface area. Also, it has been observed that photodegradation under solar illumination occurs exclusively for Se-containing samples. This is attributed to a synergistic contribution of the narrowing of the band gap caused by Se-doping and a suppressed electron-hole recombination due to Se<sup>4+</sup> associated energy levels, that act as electronic traps.

The effect of Au nanoparticle loading on the structure has also been studied. A synergistic effect has been observed between Se-doping and loading with Au nanoparticles. Our study points to a plausible reduction in radiative recombination at Se<sup>4+</sup> mid-band levels of the electrons promoted to the conduction band because of the excitation of the Au nanoparticles by the local surface plasmon resonance.



**Figure 1.** SEM images of the porous Se-doped Ta<sub>2</sub>O<sub>5</sub> films (a) before and (b) after Au nanoparticle loading. (c) Temporal evolution of the concentration of methyl orange under solar illumination. Note that  $k_{app}(\text{Au,Se-Ta}_2\text{O}_5) > k_{app}(\text{Se-Ta}_2\text{O}_5) + k_{app}(\text{Au-Ta}_2\text{O}_5)$ . (d) Proposed mechanism for enhanced visible-light photocatalytic activity.

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## Antibody/nanoparticle targeted imaging with bioorthogonal click chemistry as near-infrared contrast agents for lung cancer.

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Click chemistry is a versatile chemical approach that has found significant application in the field of biotechnology, particularly in the conjugation of antibodies and nanoparticles. This approach enables precise and efficient development of novel materials for diagnostic and treatment of cancer. When the nanoprobe binds to the biomarker with high specificity thanks to the click chemistry, it can detect and potentially treat cancer depending on the functionalities and imaging modalities of the nanoparticle. In this study, we are focusing on lung cancer, which is one of the deadliest types of cancer worldwide, causing more deaths than breast, prostate and colorectal cancers combined. We are using Ag<sub>2</sub>S semiconductor luminescent nanoparticles, which offer a dual imaging and therapeutic approach with low side effects and high emission in the second biological near-infrared window. For the click chemistry reaction, we choose one with high reaction kinetics and low toxicity, Inverse-Electron-Demand Diels-Alder Cycloaddition (IEDDA) between trans-cyclooctenes (TCO) and tetrazine (Tz), which have shown impressive results in recent years. (Rondon & Degoul, 2019). To identify lung cancer we selected four cellular surface markers (EPCAM, PD-L1, CD133 and TROP2) and functionalized antibodies against them with TCO. The Ag<sub>2</sub>S nanoparticles were functionalized with Tz, which are then delivered to react in situ and in vivo in the malignant cells, offering hope for earlier detection and improved outcomes against lung cancer.

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# Efficient Electron Hopping Transport through Azurin-Based Junctions

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Proteins have been proven to be promising candidates for molecular electronics, showing in some cases much higher conductance than one would naively expect from their size. In particular, the blue-copper azurin extracted from *Pseudomonas aeruginosa* has been the subject of many experimental studies. The exact nature of the transport mechanism, however, is still under debate [1-7].

In this work, we have conducted theoretical simulations to shed light on this issue. We found that single-site hopping can lead to either higher or lower current values compared to fully coherent transport. This depends on the structural details of the junctions as well as the alignment of the protein orbitals. Moreover, we show how the asymmetry of the IV-curves can be affected by the position of the tip in the junction and that, under specific conditions, such a hopping mechanism is consistent with a low temperature dependence of the current. Finally, we show that increasing the number of hopping sites leads to higher hopping currents [8].

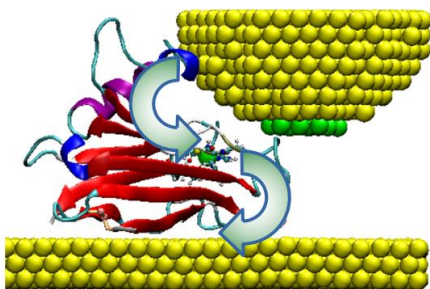


Figure 1. Geometry for the MD simulation mimicking junction formation through side-indentation. Arrows represent the one-site hopping process through copper.

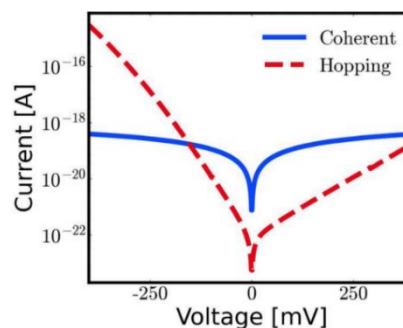


Figure 2. Representative IV curve comparing fully coherent tunneling current against one-site hopping current.

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## Towards hybrid van der Waals Josephson junctions based on NbSe<sub>2</sub>

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The emergence of van der Waals heterostructures has paved the way for a “designer” approach, in which novel devices and new physics can be obtained by combining the properties of distinct two-dimensional materials. Among the many possibilities in this context, heterostructures based on superconducting few-layer NbSe<sub>2</sub> attract great interest for studying Josephson effects and the superconducting proximity effect in 2D systems [1]. Interestingly, recent work has reported on signatures of a topological superconducting phase in heterostructures based on NbSe<sub>2</sub> and 2D ferromagnets [2]. Moreover, first demonstrations of magnetic vdW Josephson junctions have been recently reported using a similar material combination [3, 4, 5, 6]. Motivated by the above developments, we present here our first results on nanodevices based on NbSe<sub>2</sub>, including electronic transport and microwave measurements of Josephson junctions with and without antiferromagnetic tunnel barriers.

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# Multiterminal Josephson-Andreev junctions in superconducting quantum circuits

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In quantum circuits, a conventional tunnel Josephson junction is described in terms of its macroscopic degrees of freedom: the number of tunneled Cooper pairs and its conjugate variable, the phase difference. But this approximation is only valid when the fermionic excitations of the junction itself are far from the lowest circuit levels. In fact, these junctions are just a particular case of a weak link between superconductors, where their internal structure combines with the superconducting leads to form Andreev bound states, typically examined at a fixed phase difference. Here, we explore the intermediate regime, *i.e.*, a weak link where the phase fluctuations are important, which is now becoming experimentally accessible [1]. We consider a multiterminal junction embedded in different kinds of circuits and discuss, on the one hand, its application to the design of protected qubits [2] and, on the other hand, more fundamental questions that arise about its topological properties and the proper quantization rules [3].

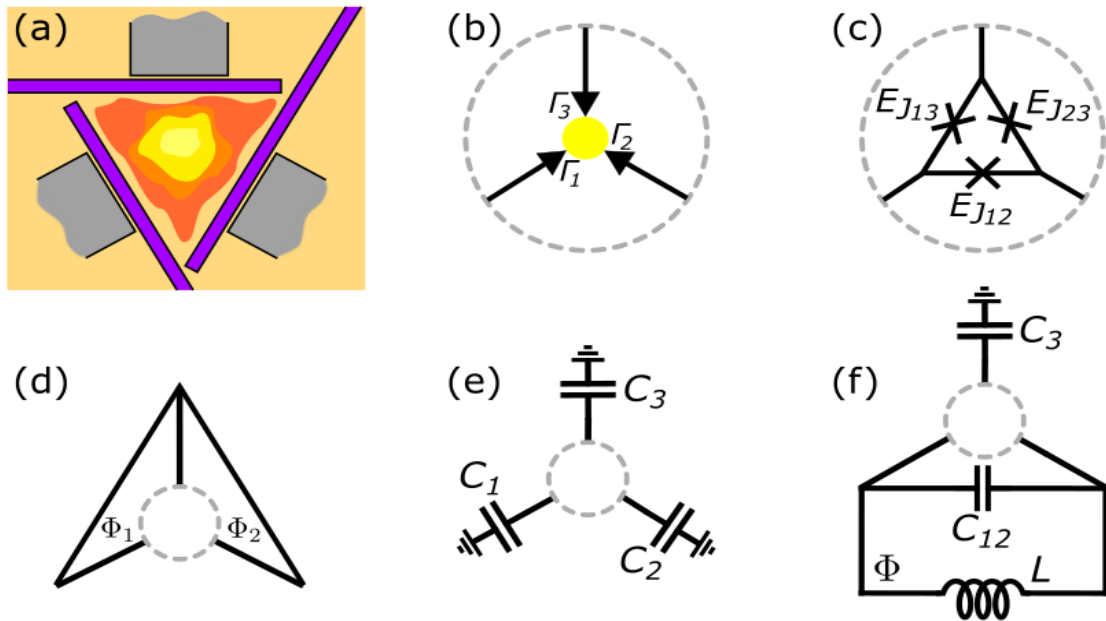


Figure 1. (a) Possible realization of the trijunction with 3 superconducting leads (grey) and a central region confined by tunable barrier gates (violet). (b) Model accounting for the effect of the central region. (c) Effective model with 3 tunnel Josephson junctions. (d-f) Three circuits we explore - the dashed grey edge is a visual guide for the placement of (b,c): in (d), the phases are fixed by external fluxes; in (e), the leads are islands with finite charging energy; in (f), two leads form a loop with finite inductance.

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# Low energy wavefunction localization in a superconductor/antiferromagnet interface

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Topological superconductors are promising building blocks for robust and reliable quantum information processing [1]. However, most platforms for engineering topological superconductivity use a combination of materials with intrinsic spin-orbit coupling and external magnetic fields, which can be challenging to manipulate [2]. In a previous work, we analyzed a conventional Josephson junction connecting two-dimensional (2D) superconductors via a narrow, magnetically textured barrier [3], demonstrating the feasibility of topological phase formation in the 1D interface. Here, we explore the impact of magnetic textures placed in proximity to finite-sized 2D superconducting surfaces. Both noncollinear magnetic components and antiferromagnetic order significantly impact the localization of low energy wavefunctions. The lattice symmetry of the textures also significantly impacts the topological phases that can appear when considering interlayer spin-orbit coupling.

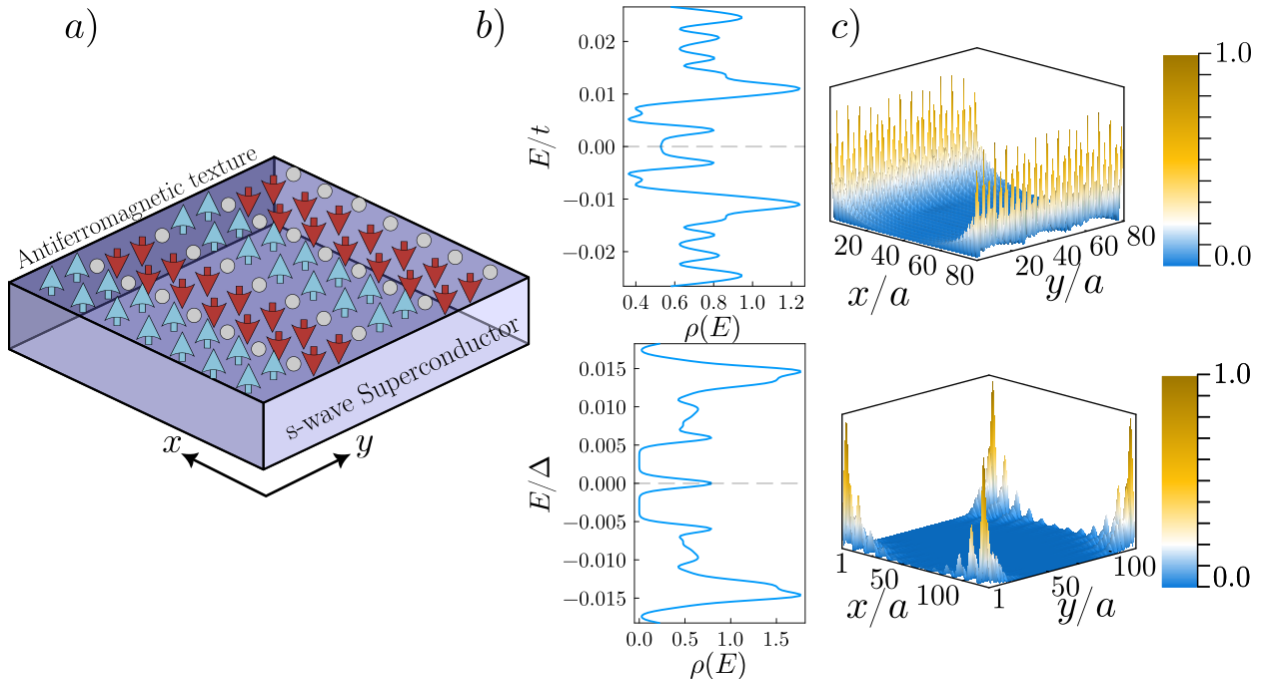


Fig.1. a) Model for the superconductor/antiferromagnet surface tight-binding Hamiltonian. b) Spectral density for two different sets of parameters, showing a dense DOS close to zero energy (above) and a zero bias peak well separated from the continuum of states (below). c) Corresponding local density of states of the corresponding lowest energy wavefunctions.

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## **Quartz Crystal Microbalance Studies of Encapsulins: Experiments and Theory**

**Noel F. Bonet, Rafael Delgado, Diego Gauto, Marisela Vélez**

Encapsulins are protein nanocompartments found in various microorganisms and play multifaceted roles in numerous biological processes. These icosahedral protein assemblies have emerged as promising candidates for diverse biotechnological applications in recent years. Despite the strong interest in these nanocompartments not all their properties and functions have been fully characterized. This study investigates and compares the physical properties of two encapsulins found in two bacteria from different ecosystems (*Thermotoga marítima* and *Mycobacterium tuberculosis*) with a Quartz Crystal Microbalance (QCM). This technique is a highly sensitive and versatile tool for studying adsorption and mechanical properties of soft materials on surfaces immersed in solution. We interpret the measurements obtained in a liquid medium within a hydrodynamic theoretical framework developed for this purpose.

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

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

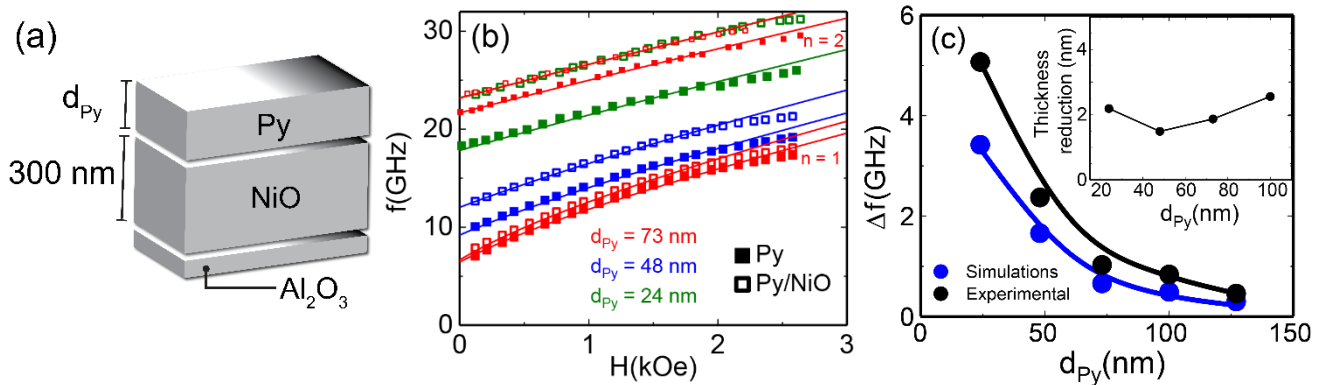


Figure 1. (a) Sketch of the Py/NiO samples. (b) PSSWs on the Py and Py/NiO for 73, 48 and 24 nm thick Py against frequency and bias field. (c) Frequency shift of the first order PSSW in our films upon the addition of the NiO layer at an applied magnetic field of 2 kOe and simulated frequency shift at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

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# Measuring magnetic coupling in graphene by Inelastic Electron Tunneling Spectroscopy

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Graphene offers unique opportunities for future technological applications in the fields of spintronics and quantum information, while also providing a playground for fundamental studies and the exploration of exotic physics [1]. Despite being non-magnetic in its pure form, the ability to induce magnetic moments in graphene was experimentally realized by the use of individual hydrogen (H) atoms [2].

In this work, we have used Inelastic Electron Tunneling Spectroscopy (IETS) to study the spin excitations of magnetized graphene states, tailored with different atomic arrangements of H (see Figure 1). In particular, we have measured the exchange energy ( $J$ ) of both ferromagnetic and antiferromagnetic configurations of H pairs on graphene. The measured values are of the order of 15-40 meV, in good agreement with previous theoretical estimations [2]. Our results show the notable spatial extension of the magnetic coupling (at least up to 6 nm) and the possibility to probe the magnetic spectra of more complex arrangements. We provide, as well, preliminary results regarding the interaction of these magnetized states with graphene superconductivity. The presence of in-gap states in superconducting graphene constitute an additional confirmation of magnetism and prepare the system for the controlled introduction of Yu-Shiba-Rusinov states, which could be used as building blocks for topological quantum computation [3,4].

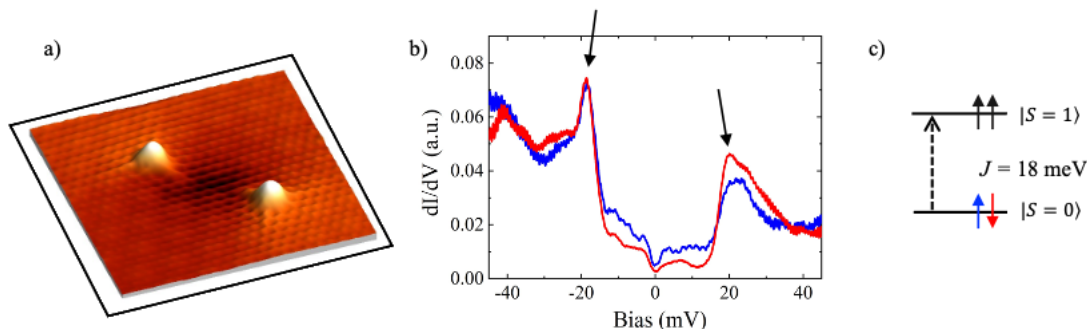


Figure 1. a) STM image of 2 H atoms adsorbed on opposite graphene sublattices ( $S=0$  ground state). b)  $dI/dV$  spectra measured on each of the H atoms. Black arrows indicate inelastic tunneling peaks associated with the energy of the spin excitation. c) Energy levels of the configuration. By IETS we are probing the singlet ( $S=0$ ) to triplet ( $S=1$ ) transition.

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# A Lindblad master equation capable of describing hybrid quantum systems in the ultra-strong coupling regime

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Light-matter interaction between confined electromagnetic fields formed in cavities and quantum emitters is of great interest because it allows to change the fundamental properties of the hybrid systems constituents. This topic has been already widely investigated for different types of systems ranging from cold atoms in optical cavities [1,2] to superconducting qubit-oscillator circuits [3]. However, despite a large theoretical effort devoted to considering light-matter interaction in different regimes, the so-called ultra-strong coupling regime [4] still presents significant challenges for theoretical treatments and prevents the use of many common approximations. In the present work, we propose a model that can describe such systems to any level of accuracy for an arbitrary electromagnetic environment. We extend an approach developed in our group for few-mode quantization of arbitrary systems [5] to the case of large light-matter coupling constants and/or ultrabroad-bandwidth resonances and show that even such systems can be treated using a Lindblad master equation where decay operators act only on the photonic degrees of freedom. We also provide a comparison with state-of-the-art master equation approaches, which show quite noticeable disagreement with our model for the considered problems.

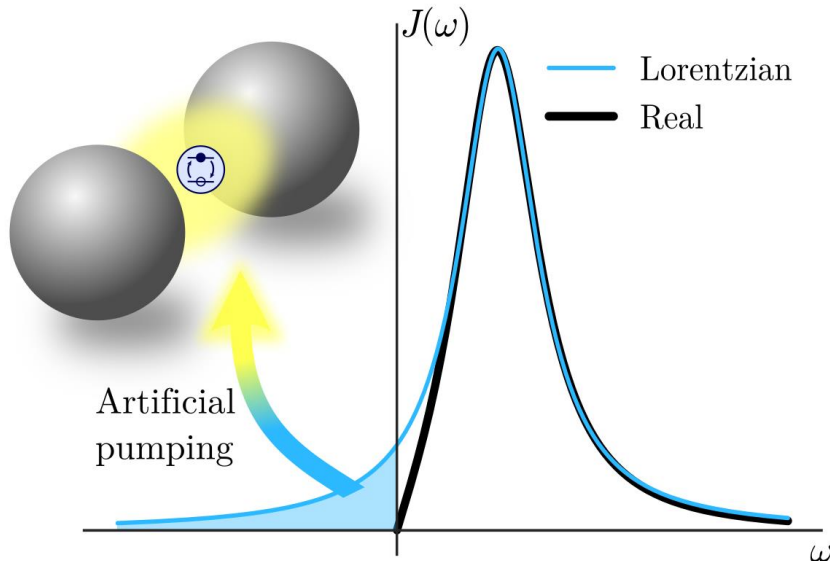


Figure 1. A realistic spectral density at zero temperature and its Lorentzian approximation, corresponding to a single-mode Lindblad master equation. The tail at negative frequencies causes artificial pumping of energy into the emitter, leading to incorrect dynamics.

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# Frequency-resolved Purcell effect for the dissipative generation of steady-state entanglement

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Generating, manipulating and preserving entanglement are essential tasks for the development of quantum technologies. However, the unavoidable interaction between the quantum system and its environment leads to the major obstacle of decoherence, i.e., the degradation of properties such as quantum coherence and entanglement. One strategy to overcome this problem is reservoir engineering [1,2], whereby interactions between the system and environment are designed to dissipatively stabilize a quantum state. Solid-state quantum emitters---like quantum dots, molecules or color centers---embedded in photonic structures stand out as particularly promising platforms for quantum technologies given their prospects of scalability and on-chip implementations.

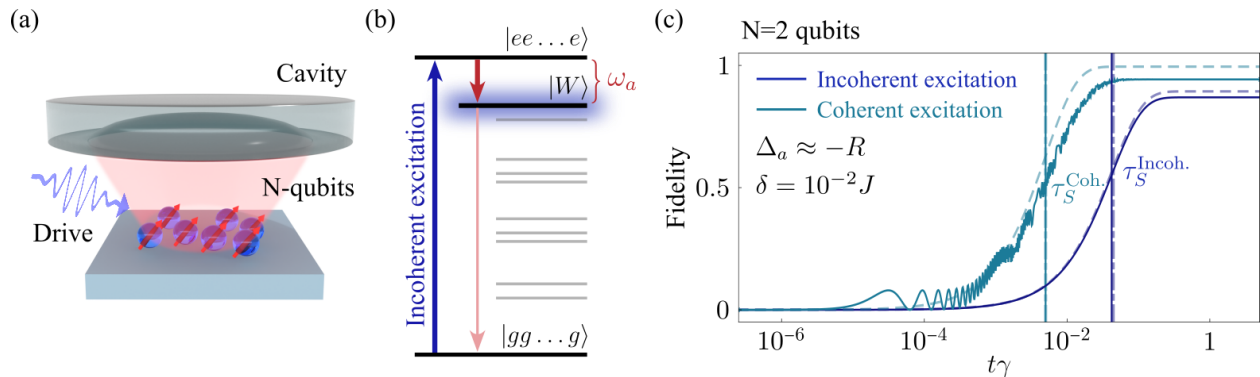


Fig 1. (a) Sketch of the system. (b) Energy diagram depicting the stabilization process of the W-state. (c) Time evolution of the fidelity to the W-state for the case of two qubits.

In this work, we present a fundamental mechanism for generating stationary states of nearly maximal entanglement among nonidentical interacting quantum emitters placed inside a cavity in a driven dissipative setting. Via a frequency-resolved Purcell effect, the cavity serves to amplify the transition from the highest excited state of the system to an entangled state, in which a single de-excitation is shared coherently among all the emitters. This phenomenon occurs when the emitters interact coherently, resulting in hybridized states, and the linewidth of the cavity is sufficiently narrow to distinguish the internal energy structure of the excitonic eigenstates. This allows us for resonant enhancement of the desired transition through frequency tuning. We show that this mechanism can be implemented using both coherent drive, specifically for the case of two emitters [3], and incoherent drive for any number of emitters---resulting in a totally scalable mechanism of entanglement generation in the presence of dissipation [4]---. We also show that the stabilization of entanglement translates into particular features in the classical and quantum optical properties of the light emitted by the system at frequencies that are perfectly resolved, allowing to isolate the optical signatures of entanglement by simple spectral filtering.

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# A mixed perturbative-nonperturbative treatment of strong light-matter interactions

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The placement of a quantum emitter in close proximity to nanophotonic structures results in promising enhanced light-matter interactions. The description of such interactions is a nontrivial problem since these nanostructures support a complex electromagnetic (EM) environment where all the light degrees of freedom must be taken into account [1]. Recently, a novel approach [2] has addressed this scenario, achieving a few-mode quantization of arbitrary EM environments. It exploits the quantity encoding the full information of the emitter-environment interaction: the spectral density. The original environment is then replaced by a model involving only a small number of lossy interacting discrete modes and providing a closed expression for its spectral density. A fitting procedure of this model spectral density to the original one then guarantees the equivalence between the two pictures. The main downside of this approach is that, depending on the complexity of the EM environment, the number of discrete modes involved can still be larger than ideally wished to ensure low computational cost.

In the present work, we tackle this issue by leveraging the underlying physics of the light-matter interaction. We divide the spectral density into two contributions in order to effectively separate the part of the EM environment strongly coupled to the emitter from that one which is weakly coupled to it. The strongly coupled part, potentially non-Markovian, is treated nonperturbatively using the technique described above [2]. The residual environment is instead treated perturbatively under the assumption of Markovianity, such that its effect is reduced to an energy shift on the emitter energy levels [3], which does not induce any additional numerical cost. We demonstrate that our model allows the description of the emitter dynamics through a Lindblad-like master equation in any coupling regime. Finally, we illustrate its validity through numerical calculations in three different setups, encompassing both the strong and the ultra-strong coupling regimes.

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## Molecular identification from hr-afm images by Predicting molecular fingerprints with deep learning

M. González Lastre

One of the fundamental challenges for the AFM is the possibility to perform chemical identification of molecules. This has only been achieved by combining HR-AFM with other techniques such as STM, KPFM or simulations [1]. Only a few works explored the possibility of finding distinctive features in images or 3D force maps that could be used as a fingerprint of the chemical species of the atoms [2]. Based on these works the hypothesis arose that a stack of HR-AFM images holds chemical information of the molecules

but that it is very subtle and depends not only on the chemical species of the atoms but also on their neighborhood, the molecular moieties. Machine Learning techniques are perfectly suited to extract this information from HR-AFM image stacks [3, 4].

In this work, we propose a method of molecular identification by extracting topological molecular fingerprints of the molecules with a convolutional neural network [5]. The network is trained with simulated HR-AFM image stacks for ~700,000 molecules, included in the QUAM data set, and provides very good accuracy.

They even produce promising results with experimental images.

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## Neural networks push the limits of luminescence lifetime nanosensing

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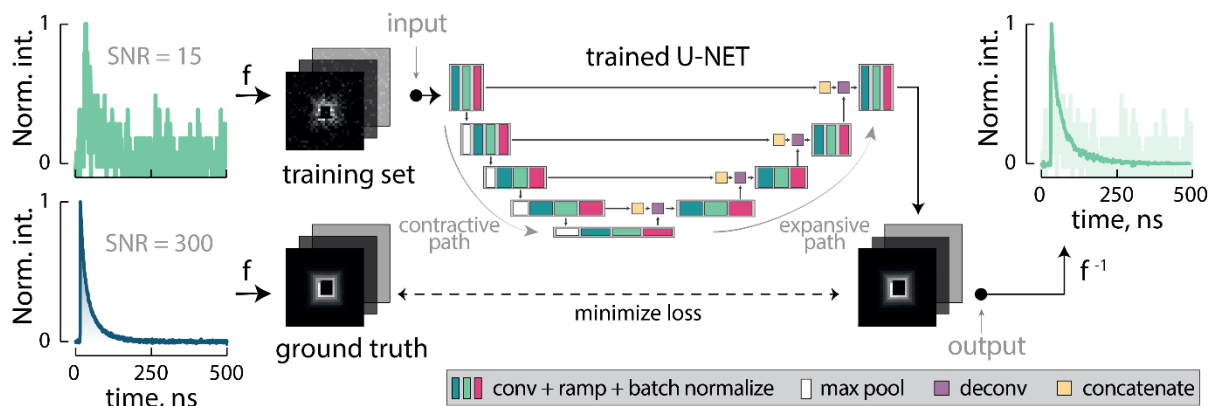
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Luminescence lifetime-based sensing relies on the analysis of changes in the decay curves of a luminescent sensor to monitor a parameter of interest. This technology is ideally suited to study biological systems due to its minimal invasiveness and remote working principle.<sup>[1]</sup> Yet, in conditions of low signal-to-noise ratio (SNR) the high uncertainty associated with the lifetime value extracted from decay curves often translates to limited precision in the readout for, e.g., short exposure times or in the presence of highly opaque media. Convolutional Neural Networks (CNNs) are emerging as a solution to several issues in luminescence sensing—thermometry above all—to ensure high spatiotemporal resolution and increased reliability.<sup>[2]</sup> U-Shaped CNNs (U-NETs) in particular, which have been proven effective in image segmentation tasks in the medical context and in image denoising,<sup>[3]</sup> show potential in overcoming the effect of noises on the performance of luminescence lifetime-based sensing.

In this work, we apply a U-NET to improve the precision of luminescence lifetime-based thermometry in conditions of extremely low SNR. To showcase this improvement, we use Ag<sub>2</sub>S nanothermometer, we first convert luminescence decay curves into images suitable to be used as input in the U-NET. The algorithm learns the relevant features from noisy images and improve luminescence lifetime estimation under conditions of extremely low SNR (**Figure 1**) compared to traditional analysis methods of decay curve fitting and integration. Specifically, we showcase the prowess of the U-NET in improving the precision of luminescence lifetime thermometry with two experiments characterized by extreme measurement conditions: thermal monitoring of free-falling droplets and monitoring of thermal transients in suspended droplets through an opaque medium. These results broaden the applicability of luminescence lifetime-based sensing in fields including in vivo experimentation and microfluidics, while, hopefully, spurring further research on the implementation of machine learning in luminescence sensing.



**Figure 1.** Flowchart representing the architecture and use of the selected U-NET.

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## Including electron-hole interactions in non-linear optical responses of semiconductors

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Optical probes are often used to extract fingerprints of materials, that later can be thought for potential device applications. In the theoretical side, first-principles DFT calculations have allowed the evaluation of macroscopic frequency-dependent responses, both in the linear and beyond-linear field regime. These response functions are found after a self-consistent calculation of the band structure, and therefore do not include many-body correlations beyond mean field. In some scenarios, as in gapped materials, including electron-hole correlations in the theory is a must to correctly match with experiments, even in a qualitative picture. While the inclusion of electron-hole interactions in linear-response calculations is being standardized nowadays, less effort has been put yet in including this theoretical ingredient in the non-linear response. Here, we show our on-going implementation of electron-hole interactions in the second-order AC response to a uniform electric field. We set a workflow to (i) set a gap-corrected band structure in the whole BZ, (ii) solve the exciton many-body states through the BSE equation and (iii) evaluate the shift-current DC response as a first calculation. Our approach is planned to work by using any Hamiltonian in a local orbital basis as the starting point; those include tight-binding models, Wannier functions-based interpolations or first-principles DFT codes using atomic orbitals basis sets.

### References:

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# P47

## Study of the localized surface plasmon resonance (LSPR) and electrical near field using classical electrodynamics calculations

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Of the wide family of plasmonic materials currently available, liquid metal nanoparticles are one of the most attractive systems due to their easy production and good control of localized surface plasmon resonance (LSPR). LSPR is the principle behind the manipulation of light as a result of interaction with the collective oscillation of electrons confined in nanoparticles. The energy of that resonance can be modified depending on the metal's permittivity, particle size, shape, and the surrounding medium.

The aim of this project is to study the LSPR of nanoparticles based on liquid metals alloys such as eutectic GaIn (EGaIn), evaporated on different substrates that allow the nanoparticles to be organized and produce uniform and adjustable sizes. The experimental results will be compared with classical electrodynamic calculations and the use of discrete dipole approximations.

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## Molecular adsorption of ClAlPc on h-BN/Rh(110)

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Exploring molecular adsorption on 2D materials holds high expectations for both the observation of novel physicochemical phenomena and the future design of nanodevices [1]. In this work, molecular adsorption of the Chloro-Aluminum-Pthalocyanine (ClAlPc) on hexagonal boron nitride (h-BN) monolayers, grown on Rh(110) surfaces, has been studied by means of scanning tunneling microscopy under ultrahigh-vacuum. After room temperature deposition, molecules are assembled into a bilayer structure with square lattice, forming islands scattered over the h-BN/Rh(110) surface. This structure coexists with regions, where molecules are not arranged into ordered assemblies. After annealing at 400 K, the molecular structure undergoes a transition to a monolayer structure, giving rise to ClAlPc clusters scattered over the h-BN/Rh(110) surface. This finding is in clear contrast with the formation of one-dimensional ClAlPc chains, previously reported on the analogue graphene/Rh(110) surface [2], which as the h-BN/Rh(110) one, is characterized by exhibiting quasi-one-dimensional moiré patterns. These differences are explained in terms of the different electronic properties of graphene and h-BN.

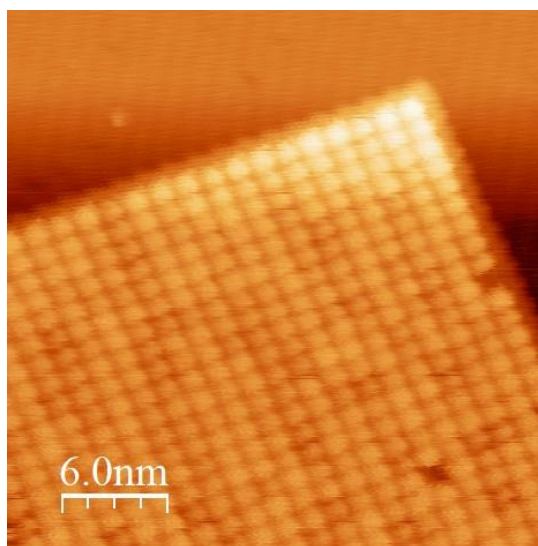


Figure 1. STM image displaying a molecular island with bilayer structure following a square lattice. Size: 30x30 nm<sup>2</sup>.

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# Growth and characterization of ferromagnetic-superconductor systems with spin-orbit coupling

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Josephson junctions (JJs) are devices where two superconductors are separated by a thin barrier exhibiting a quantum phenomenon, where supercurrent flows without dissipation. Their importance lays on their ability to create and control quantum states needed for quantum computers. Recent articles [1] show that by placing two superconducting electrodes in contact with a ferromagnetic film via spin orbit coupling (SOC) could provide a new and simpler way to generate controllable spin-polarized supercurrents. In this research, we have grown and characterized ferromagnetic/superconducting films interfaced by MgO providing spin filtering and SOC with the goal of using them to fabricate the JJs with supercurrent controlled by the direction of magnetization [2]. We have grown MgO/V/MgO/Fe ferromagnetic-superconducting hybrid systems, capped with an Al layer to prevent oxidation, by ion beam sputtering technique, on MgO (100) and Al<sub>2</sub>O<sub>3</sub> (0001) substrates. The samples have been characterized by vector magnetometry based on the Kerr effect (v-MOKE) [3] and ferromagnetic resonance (FMR) measurements (see Fig. 1). By doing this, it is seen that the samples show biaxial anisotropy when it is grown on MgO (100) substrate. In addition, the zero field FMR frequency can be increased by changing the substrate, being greater on the MgO samples. These results points on our capability to grow fully epitaxial MgO(001)/V/MgO/Fe heterostructures need to fabricate epitaxial JJs and verify predictions [1].

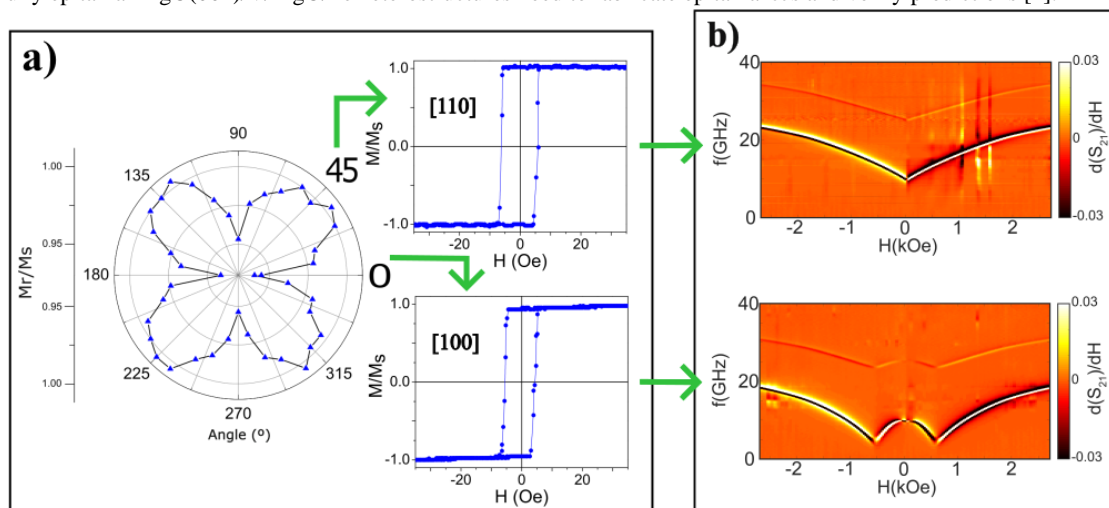


Figure 1. This figure shows the analysis of a sample MgO(13nm)/V(40nm)/Mg(2nm)/Fe(20nm)/Al(2nm) epitaxially grown on MgO. Fig.1a shows results obtained with the MOKE system: polar graphic showing the  $M_r/M_s$  and two hysteresis loops corresponding to the easy axis (diagonals of the squared sample, broader and straighter loop) and hard axis (bisectors of the sample, thinner and less straight loop) directions. Fig.b show FMR measurements, one in the easy axis and another one in the hard axis of the sample. From the FMR study (in the easy axis figure) we have obtained a low value of the damping of the sample ( $5 \cdot 10^{-3}$ ) and an anisotropy field that matches the minimum in frequency in the study for the hard axis (598 Oe).

[1] Johannes R. Eskilt et al. [PhysRevB.100.224519 \(2019\)](#).

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[3] E. Jiménez et al. [Rev. Sci. Instrum. 85, 053904 \(2014\)](#).

# Ferroelectrically driven SHG spatial modulation in monolayer MoS<sub>2</sub>-LiNbO<sub>3</sub> heterostructures

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The integration of ferroelectrics into Transition Metal Dichalcogenides (TMD) devices has recently emerged as a powerful tool to fabricate reconfigurable and nonvolatile 2D optoelectronic devices owing to the electrostatic doping provided by the remnant spontaneous polarization [1]. However, while the electric and linear optical properties of these heterostructures have been widely investigated, their nonlinear optical features remain almost unexplored, with only two works devoted to the study on how second harmonic generation (SHG) can be modulated at the heterointerface [2,3].

In this work, we study the effect of ferroelectricity on the SHG response of monolayer MoS<sub>2</sub> deposited on the polar surface of a periodically poled LiNbO<sub>3</sub> substrate. We show that the second order susceptibility values  $\chi^{(2)}$  of MoS<sub>2</sub> are affected by the underneath spontaneous polarization. Consequently, domain-engineering of the LiNbO<sub>3</sub> substrate results in a periodic spatial modulation of the SHG intensity between adjacent domains (see Figure 1).

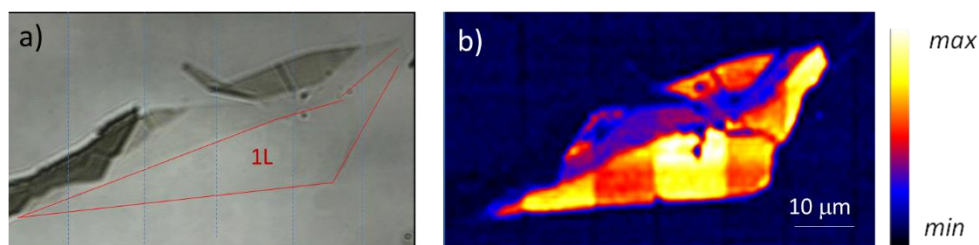


Figure 1. (a) Optical image of monolayer MoS<sub>2</sub> transferred on domain patterned LiNbO<sub>3</sub>. Dashed blue lines indicate the domain wall position. (b) Spatial distribution of the SHG intensity generated in the MoS<sub>2</sub>-LiNbO<sub>3</sub> heterostructure for a fundamental wavelength of 800 nm. The SHG spatial modulation is close to 35%.

The analysis of the SHG spatial modulation as a function of the fundamental wavelength, pump power and polarization of the incident light suggests photo-induced charge-transfer processes across the interface as the mechanism responsible for such modulation. The interfacial charge-transfer process is influenced by the domain orientation and generates an imbalanced charge distribution in the system that effectively modify the nonlinear properties of the Van der Waals heterostructure.

The results highlight the importance of interfacial charge-transfer processes in the study of the optical properties of TMDs based heterostructures and open new routes to manipulate and control their nonlinear response using patterned ferroelectric substrates.

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## **Mach-Zender interferometer for the measurement of the Hong-Ou-Mandel effect**

**Diego Marni Sobrino**

We have assembled and characterized a fiber-based Mach-Zender Interferometer, for the measurement of two-photon interference, known as Hong-Ou-Mandel effect [1]. As maximum photon transmittance is required, we have improved the free-space to fiber coupling, by applying gaussian beam analysis and mode-matching. We have developed a simple phase-locking algorithm, based on maintaining a controllable phase between the two interfered wave packets [2]. This tackles the possible phase drifting problems that may arise during the measurements by continuously readjusting one interferometer's arm-length with a piezoelectric actuator. Our plan is to use this interferometer to test the degree of photon indistinguishability emitted by semiconductor quantum dots.

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## Theory and simulation of moiré patterns in graphene-type rotated bilayers and bidimensional systems

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Since the achievement of isolation of graphene, by Geim and Novoselov, the study of two-dimensional systems has been of great interest in theoretical and experimental physics. Recently, the discovery of superconductivity and the magic angle between layers in bilayer graphene, by Pablo Jarillo-Herrero and his group [1], gave an insight of the new properties these materials can exhibit due to their geometry. These materials may seem interesting in another phenomenon called the bulk photovoltaic effect (BPVE for short). In the BPVE, non-centrosymmetric materials can generate a DC current when exposed to light [2].

In this work, we will take advantage of the moiré patterns periodicity to calculate the band structure of the material, an important electronic property, in the tight-binding approximation. We will apply this information to calculate the DC shift current and we will see how it changes depending on the angle between layers.

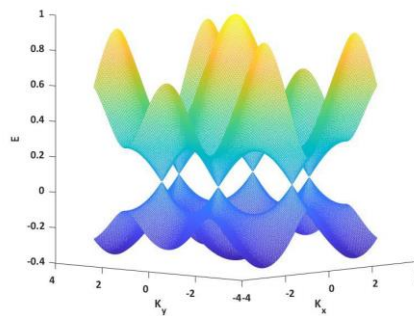


Figure 1: graphene band structure.

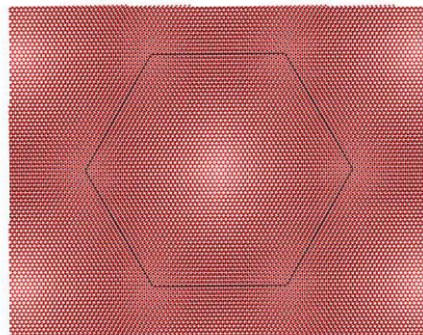


Figure 2: graphene bilayer supercell in magic angle configuration.

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## Development of an efficiently UHV modulable system, to atomically characterize and clean 2D flakes

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2D materials have recently demonstrated an extraordinary potential, not only for being revolutionary in fundamental physics [1-2], but also for their prospective applications in industry [2]. One of their most interesting features is that the existence of point defects changes drastically the macroscopic properties of the material. In our group, we aim to explore the exciting prospect of combining the strengths of both STM/AFM and transport experiments to study the rich physics of 2D devices, whereby global properties are strongly affected by the local atomic arrangement (owing to, e.g., interlayer stacking, twist angle, defects, proximity effects, etc.). To this end, we are developing the technology to employ both tools to characterize exactly the same sample under UHV conditions. Our group has recently developed a system to characterize micrometer sized flakes with an UHV-LT-STM/AFM microscope, which can also perform in-situ transport measurements. However, due to the mentioned sensibility of these materials to the presence of defects, one of the biggest challenges in this kind of study consists in preparing clean samples. Here, I present the development of a new system designed to be able to investigate both the macroscopic and the microscopic worlds in a very efficient way. It will be capable of making a fast inspection of the sample of study and also to prepare 2D samples in UHV environments. The system consists in AFM/STM microscope, working at RT in UHV environments. The AFM is accompanied by a preparation chamber equipped with heating capabilities, several interchangeable evaporation cells, a quartz microbalance and a H cracker. The whole system has been designed to be fully versatile, so, after the optimization of sample preparation in this system, the samples can be easily transferred to the LT-STM one, to do more accurate experiments. What's more, the system remains perfectly modulable to add more specific preparation chambers in the future, in order to improve our comprehension on these materials.

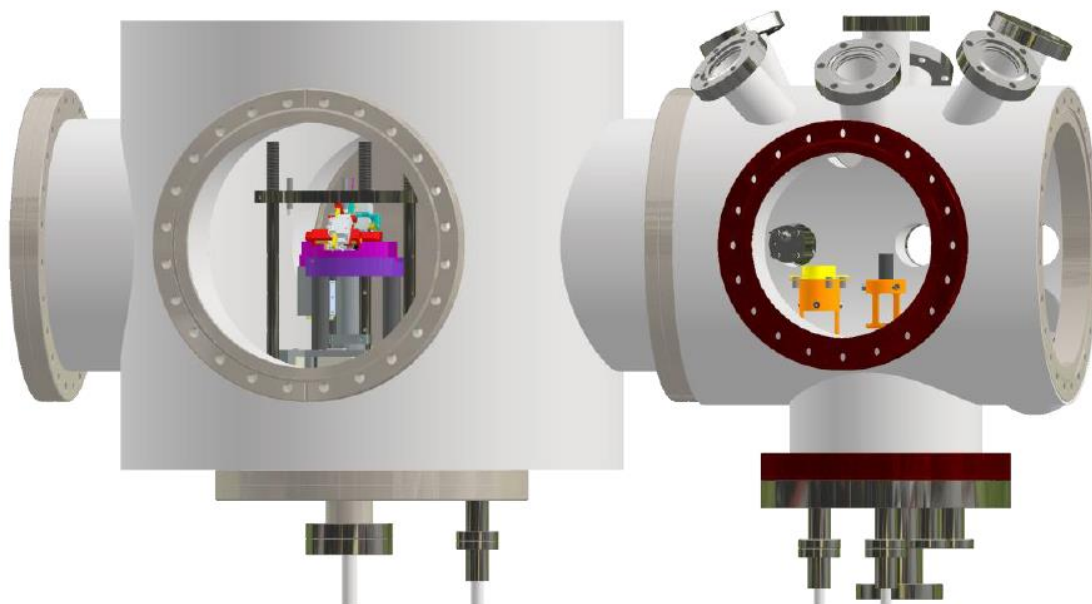


Figure 1. Design of the UHV system. To the left, the AFM chamber with the microscope to characterize and clean the samples and a parking to store samples and spare cantilevers. To the right, the preparation chamber, with a heater, an evaporator, a quartz microbalance and a cracker to deposit hydrogen.

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## Computational simulation of bioinspired materials: peptide nanotubes.

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Peptide nanotubes are bioinspired materials made up of peptide rings piled up forming nanotubes. The properties of these materials are very interesting, and in particular, the high proton conductivity<sup>[1]</sup> that some of these materials present is very interesting for its possible applications in electronics. The aim is to analyze the properties of these materials using molecular mechanics simulations at atomic scales using the AMBER<sup>[2]</sup> suite. Specifically, we wish to observe and explain the mechanism of proton transport that causes the conductivity, as well as how it varies depending on the conditions of the system. Early experimental evidence suggest that water molecules play a very important role in this phenomenon. Therefore, to study this system, we have turned our attention to the water, and have explored different water models to determine which one is best suited. For the future, we will use QM/MM mixed quantum simulations with DFT to better model the behavior of the system and allow for actual proton transport in the model.

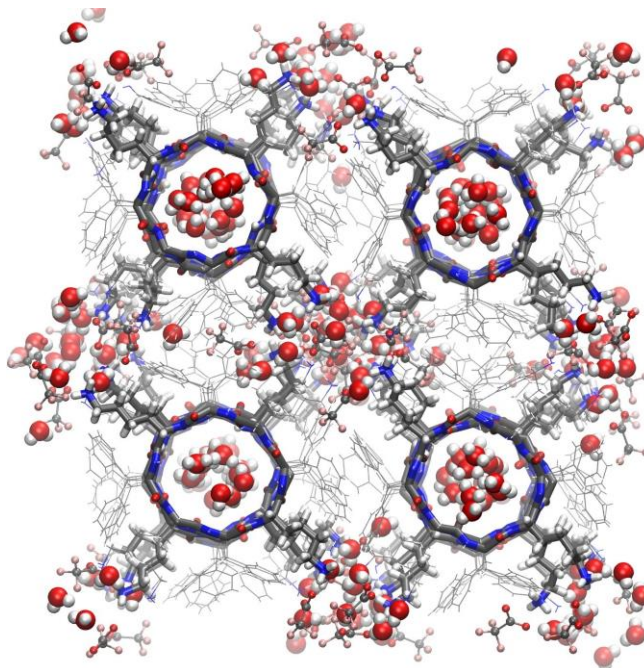


Figure 1. Top view of the unit cell of the system. There are 4 tubes consisting of 8 peptide rings piled up. The water molecules are located inside the tubes, called lumen, but also channels form between the tubes. Some of the lysines, one of the amino acids that form the peptides, are protonated, so we expect the conductivity to occur in the channels where the extra protons are available.

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# Nonlinear vibration-phonon interactions in molecular crystals

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It is well established that when polycyclic aromatic hydrocarbon (PAH) molecular crystals are doped with larger guest molecules such as dibenzoterrylene (DBT), their interaction can be studied in the frame of perturbation theory. Phonon degrees of freedom from the crystal couple to the internal vibrations of the DBT molecule (Figure 1a), resulting into energy transfer between vibrations. Due to the smaller number of vibrational modes of DBT compared to the quasi-continuum of crystal phonon modes, the crystal can be regarded as a bath that dissipates the vibrational energy and eliminates coherence in the system.

Internal vibrational frequencies lie beyond the cut-off frequency  $\omega_{max}$  of the phonon modes, so single phonon-vibron resonant processes are inhibited as there are no modes with high enough frequency to ‘store’ the vibrational excitation. However, anharmonic interaction involving two phonons and one vibron allow coherent energy transfer between the guest molecule and the surrounding crystal (Figure 1b). It has been observed that the predominant interaction involves two phonons of equal frequency  $\omega_{vib}/2$  [1]. In this work we study the coherent energy transfer between the vibrational and phonon modes, which are both coupled to a bath corresponding to the rest of the crystal. We study how selective excitation of an IR-active phonon mode with an external laser can lead to coherent population of a molecular vibrational mode due to anharmonic interactions between the phononic and vibrational modes.

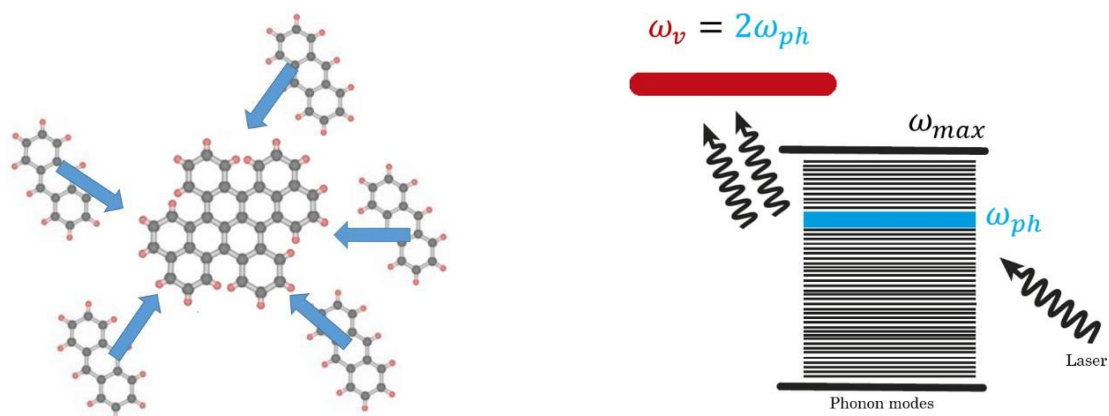


Figure 1: (a) Sketch of a DBT molecule (large) in a molecular crystal (small molecules). The blue arrows represent the forces applied on the DBT molecule by lattice phonons. (b) Representation of the coherent energy transfer process. A laser excites a phonon mode (blue) at half the frequency of the vibrational mode (red). Anharmonic coupling between the phonon and the vibration enables vibrational excitation. Both images are modified versions of those presented in reference [2].

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# Artificial neuron based on reversible control of the Bloch-Point Domain Wall in Ferromagnetic Nanowires

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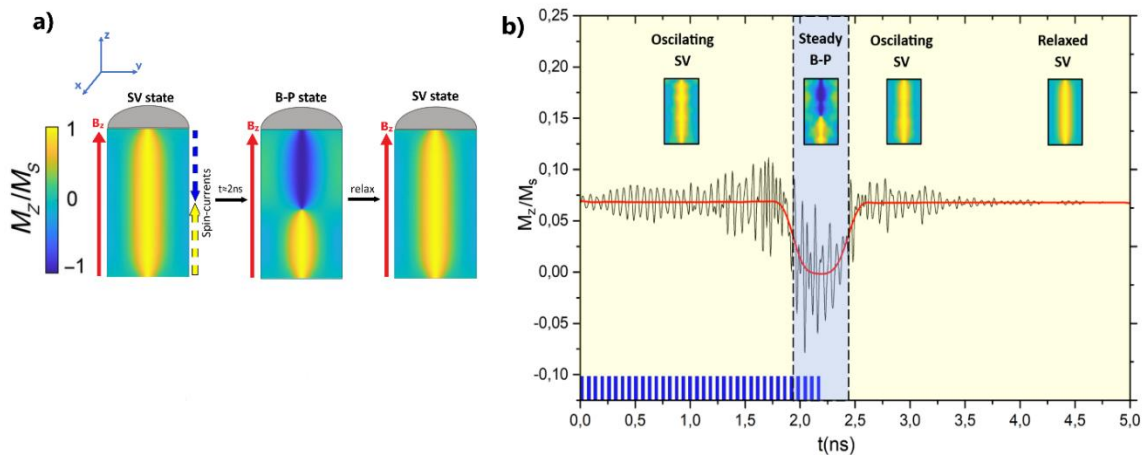
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Nanomagnetism and spintronics are fields actively researching in future magnetic memories based on switching nanomagnets. These could also be applied to neuromorphic computing by creating artificial neurons which could emulate the leak-integrate-fire-refractory characteristics that biological neurons possess [1]. In this research, we have carried numerical simulations in a ferromagnetic nanowire with a length of 250nm. The simulations have been made in Mumax<sup>3</sup>, an open software code that solves numerically the Landau-Lifshitz-Gilbert (LLG) equation. With the aim of reproducing the integration (receiving pulsed signals) we applied pulse trains of spin-currents at the opposite faces of the cylinder. These currents (previously studied in continuous form [2]) are responsible of the transition between the stable single vortex state (SV) to the metastable Bloch-Point Domain Wall state (B-P). In order to force the system to have the leak and refractory properties the nanowire was placed in a constant and homogeneous magnetic field in the axial direction on the order of mT. (see Fig.1).

This suggested set-up fulfills the requirements and characteristics of a biological neuron, which could lead to creation in future of Artificial Neural Networks (ANNs) based on the reversible changes of topology on magnetic nanowires.



**Figure 1. a)** Cross-section of the magnetization component  $M_z/M_s$  in a 250nm long NW where  $M_s$  is the saturating magnetization of the material. It is also shown the different procedures and states that the system experiences. **b)** Evolution of the average axial magnetization of the NW. Blue bars represent spin-current pulses. These pulses have an amplitude of current density  $J=5 \cdot 10^{12} \text{A/m}^2$  and a frequency of 16.26 GHz. The applied magnetic field is  $B_z=1 \text{mT}$ . There are also different identified regimes with colours. The inset images represent snapshots of the longitudinal cross section of the axial component  $M_z$  in the NW in each of the regimes.

**Acknowledgements:** This work was supported by the Instituto Nicolás Cabrera in Madrid with their INC Research Awards for Physics students 2023

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# Theory of Electron Spin Resonance in Scanning Tunneling Microscopy

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Electronic spin resonance (ESR) spectroscopy in the context of scanning tunneling microscopy (STM) is a novel technique used to probe and control the magnetic excitations in single magnetic atoms and molecules deposited on surfaces [1]. Moreover, ESR-STM is emerging as an efficient platform for quantum information processing. Despite all the recent successes of this spectroscopic technique, there are still many open questions related to its operation and the interpretation of the experimental data. In this work, we present a microscopic theory of ESR-STM that sheds new light on those open questions. Our theory is based on the use of Green's function techniques to describe the electron tunneling and quantum master equations to account for the dynamics of the magnetic system coupled to microwave radiation, which also interacts with the tunneling electrons. We show here that, with the help of this theory, we are able to reproduce quantitatively the experimental results for a spin 1/2 system (TiH molecules on a MgO substrate), see Fig. 1. Thanks to this quantitative agreement, we can also extract the decoherence and relaxation rates in this system.

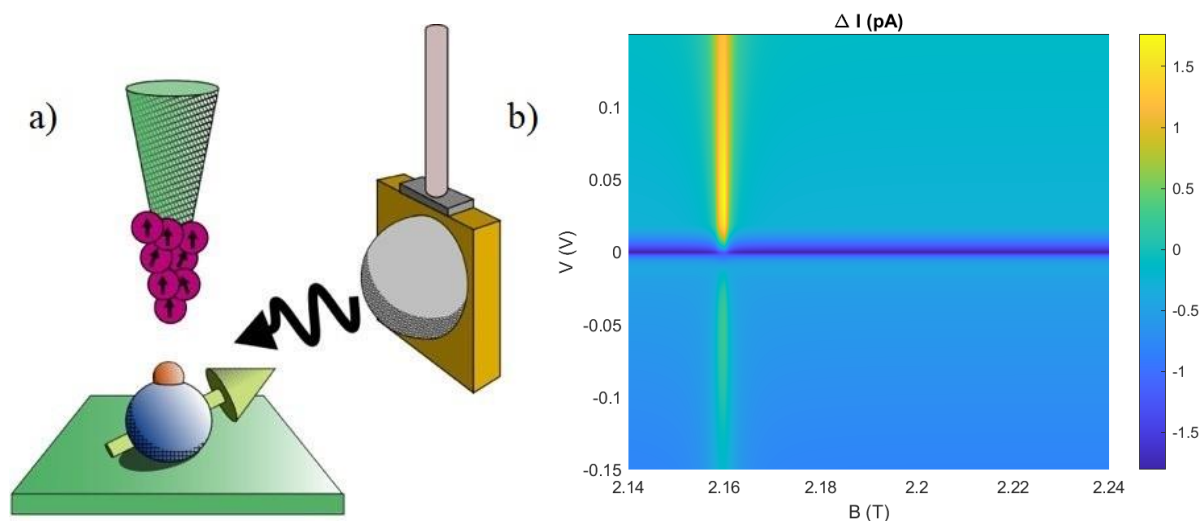


Fig. 1. (a) Schematic representation of an ESR-STM setup. (b) Calculated ESR-STM spectrum as a function of the dc voltage and static magnetic field for a spin 1/2 system.

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# Enhancement of exciton recombination in MoS<sub>2</sub> deposited on a substrate undergoing a ferro- to paraelectric transition

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MoS<sub>2</sub> monolayer (1L-MoS<sub>2</sub>) is a 2D semiconducting material with excellent optoelectronic properties holding potential for a variety of applications in spintronics, optoelectronics and integrated circuitry [1]. Due to its atomic thickness nature, this material provides the possibility of engineering its properties by means of its surrounding environment. In particular, ferroelectric-driven electrostatic doping has been previously demonstrated [2].

In this study, a relaxor-ferroelectric SBN crystal featuring a low Curie temperature ( $T_c \sim 70^\circ\text{C}$ ) is used as a substrate for a 1L-MoS<sub>2</sub>. The objective is to investigate the influence of the ferro-to-paraelectric transition on the optical properties of 1L-MoS<sub>2</sub>. By means of confocal microfluorescence, the evolution of the 1L-MoS<sub>2</sub> photoluminescence (PL) in the 30-90°C temperature range is analyzed. The results reveal a significant modification of the electrostatic doping of 1L-MoS<sub>2</sub> when the substrate undergoes the relaxor phase transition. Namely, an enhancement of the MoS<sub>2</sub> PL, which correlates with a boost of the MoS<sub>2</sub> excitonic recombination is observed. This behavior is interpreted in terms of the different polarization/screening-charge balance in the ferro- and paraelectric phases.

The work paves the way for novel devices such as temperature sensors and switches without the need of external electrical modulation.

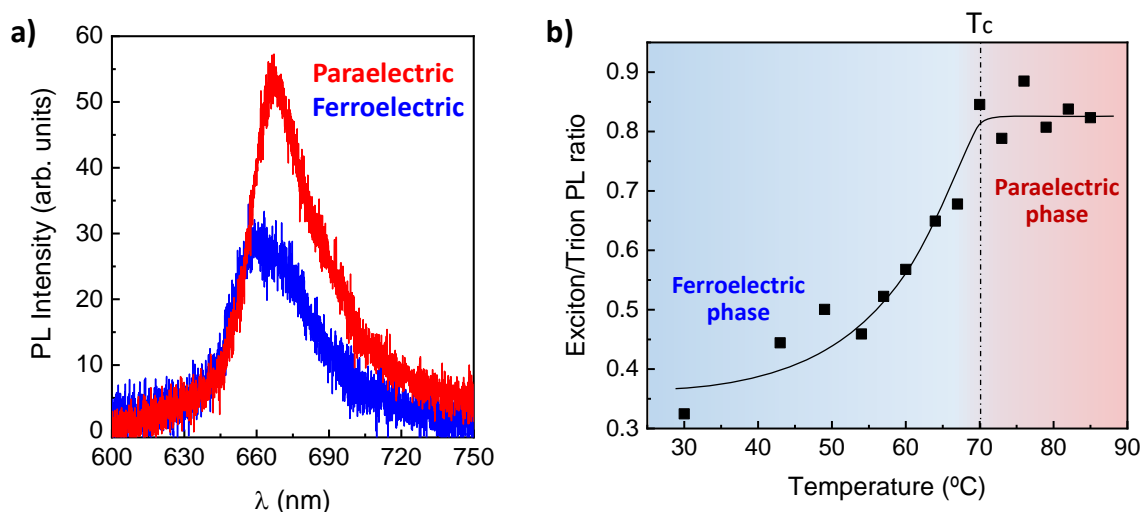


Figure 1. a) MoS<sub>2</sub> PL at the ferro- (blue) and paraelectric (red) phases. b) Evolution of the exciton/trion PL ratio along the relaxor phase transition of the SBN substrate.

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