

Instituto Universitario de Ciencia de  
Materiales Nicolás Cabrera  
**XXV YOUNG RESEARCHERS MEETING**



16 de Diciembre de 2022  
Residencia La Cristalera, UAM  
Miraflores de la Sierra, Madrid  
<http://www.inc.es>

## PROGRAM

### 9:30 – 9:45 Welcoming session

### 9:45 – 10:15 Session I (Chair: Celia Tavares)

9:45 – 10:15 *Invited speaker*: Andrés Castellanos, “Integrating van der Waals materials on paper-electronics”, ICM – CSIC

### 10:15 – 11:10 “Chema Gómez-Rodríguez” awards to the best paper

10:20 – 10:45 Ruth Pulido Venegas, “Experimental and DFT study of the Li<sup>+</sup> desorption in spinel/layered lithium manganese oxide nanocomposites using HCl” Chem. Eng. J. 2022, 441, 136019.

10:45 – 11:10 O Francisco Matute Fernández-Cañadas, “Signatures of interactions in the Andreev spectrum of nanowire Josephson junctions”. Physical Review Letters 2022, 128, 197702.

### 11:10 – 11:20 “Research awards for physics students”

### 11:20 – 12:20 Coffee Break + Poster Session A

### 12:20 – 13:40 Session II (Chair: Mariola Ramírez)

12:20 Francisco J. Fernández Alonso, “High precision low – cost spectrophotometer for agricultural applications”

12:40 Elena Salagre Rubio, “Electronic Band Structure of Li<sub>x</sub>CoO<sub>2</sub> during the Insulator to Metal transition”

13:00 Jinan Hussein Al Shuaib, “Sensitized lanthanide emission in doped BaZrS<sub>3</sub> perovskite semiconductor”

13:20 Alejandro Vivas Viaña, “Two-photon dressing of quantum emitters for cavity-assisted generation of steady-state entanglement”

### 13:40 – 15:00 Lunch

### 15:00 – 16:00 Session III (Chair: Pablo Ares)

15:00 Klara Strobl Bardo, “Tuning the microenvironment of crowded proteins inside viral capsids”

15:20 Cosme González Ayani, “Kondo lattice development in a TaS<sub>2</sub> van der Waals heterostructure”

15:40 Juan José García Esteban, “Tunable thermal emission of subwavelength silica ribbons”

### 16:00 – 17:00 Coffee Break + Poster Session B

### 17:00 – 18:00 Session IV (Chair: Carlos Sánchez Muñoz)

17:00 Tamara Muñoz Ortiz, “Plasmonic nanoparticles for inflammation targeting in atherosclerosis”

17:20 Paula Magrinya, “Tribological motion of rotating vesicles”

17:40 Lucía Martín Pérez, “Direct magnetic evidence, functionalization and low-temperature magneto-electron transport in liquid-phase exfoliated FePS<sub>3</sub>”

### 18:00 Wrap up and closing

## Session I - Chair of the session: Celia Tavares

Invited speaker:

9:45 “Integrating van der Waals materials on paper-electronics”

Andrés Castellanos

ICMM – CSIC

### “Integrating van der Waals materials on paper-electronics”

Andres Castellanos-Gomez

Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain

[Andres.castellanos@csic.es](mailto:Andres.castellanos@csic.es)

A big chunk of the price tag of electronic components is due to the cost of silicon wafer substrates. Although silicon is a highly abundant and cheap element, the transformation and processing from the raw material into high quality silicon wafers results very costly. In fact, the cost of silicon substrates constitutes  $\sim 1/3$ rd of the total cost of a memory chip and about  $\sim 1/10$ th of the cost of a high-end state of the art micro-processor. The societal, industrial and technological demands of ultra-low-cost electronic components has spurred the quests towards lower cost substrates. This has motivated a surge of works on paper-based electronics in the last years. In fact, paper substrates cost ( $\sim 0.1$  €/m<sup>2</sup>) is orders of magnitude lower than that of polymer substrates (PET  $\sim 2$  €/m<sup>2</sup> and PI  $\sim 30$  €/m<sup>2</sup>) and crystalline silicon ( $\sim 1000$  €/m<sup>2</sup>).

Despite the promises of paper-based electronics, there are several challenges to be solved. One of the major challenges is that the rough, fiber-based structure of paper makes it impossible to fabricate devices using conventional lithographic techniques. In this talk I will discuss our last works to integrate different van der Waals materials onto standard paper substrates [1-4].

#### References

- [1] J Azpeitia et al. Materials Advances (2021)
- [2] W Zhang et al. Applied Materials Today (2021) 23, 101012
- [3] M Lee et al. Nanoscale (2020) 12 (43), 22091-22096
- [4] A Mazaheri et al. Nanoscale (2020) 12 (37), 19068-19074

#### Figures



**Figure 1:** Picture of several paper-electronic devices fabricated by integrating different van der Waals semiconductors on standard copy paper substrates.

## Chema Gómez-Rodríguez awards to the best paper

10:20 “Experimental and DFT study of the Li<sup>+</sup> desorption in spinel/layered lithium manganese oxide nanocomposites using HCl”

Ruth Pulido

Física Aplicada

# Experimental and density functional theory study of the Li<sup>+</sup> desorption in spinel/layered lithium manganese oxide nanocomposites using HCl

Ruth Pulido <sup>a,b,\*</sup>, Nelson Naveas <sup>a,b</sup>, Raúl J. Martín-Palma <sup>a</sup>, Teófilo Graber <sup>b</sup>, Iván Brito <sup>c</sup>, Jacobo Hernández-Montelongo <sup>d</sup>, Miguel Manso Silván <sup>a,e</sup>

<sup>a</sup> Departamento de Física Aplicada and Instituto Universitario de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>b</sup> Departamento de Ingeniería Química y Procesos de Minerales, Universidad de Antofagasta, Avenida Angamos 601, Antofagasta, Chile

<sup>c</sup> Departamento de Química, Universidad de Antofagasta, Avda. Universidad de Antofagasta 02800, 1240000 Antofagasta, Chile

<sup>d</sup> Departamento de Ciencias Matemáticas y Físicas, UC Temuco, 4813302 Temuco, Chile

<sup>e</sup> Centro de Microanálisis de Materiales, Universidad Autónoma de Madrid, Campus de Cantoblanco, 28049 Madrid, Spain

Lithium manganese oxides (LMO) are the most popular lithium-ion sieves (LIS) precursor materials. Despite being the critical step in forming LIS, the “Li<sup>+</sup> Desorption” process from the crystalline lattice of the LMO has been less explored than its counterpart, “Li<sup>+</sup> Adsorption”. Thus, there is a technological gap in the desorption optimization of materials such as the layered-type lithium-rich LMO that negatively impacts its application in chemical processes. In this study, we investigated the lithium desorption behaviour of different LMO nanocomposites in an acidic medium (HCl). LMO with different Li/Mn ratios were synthesized by promoting the lithium-rich layered phase (Li<sub>2</sub>MnO<sub>3</sub>) by hydrothermal synthesis. The morphology, size, crystallinity, chemical composition, and surface properties of LMO nanocomposites and their delithiated products, obtained after lithium desorption from LMO precursor materials, were studied. In addition, theoretical calculations were carried out to understand the lithium desorption behaviour of the different crystalline phases of LMO. Our study reported that there is a lithium desorption behaviour that depends on the Li/Mn ratio of the LMO nanocomposite. To release lithium efficiently from lithium-rich LMO, it is necessary to increase the temperature of the desorption process. While for LMO with a lower layered phase ratio, it is not. In parallel, by means of a computational study, we have shown that the transport of lithium ions within each compound can explain the differences in the release efficiency. Thus, overall, our results indicate that the lithium release process in acidic media is easier to achieve for an LMO with a “spinel” crystalline phase than with a “layered” phase. Our findings suggest that a thorough characterization of LIS precursor materials is necessary in order to select a desorption process suitable for each LMO crystalline phase. Thus, we emphasize that, if the differences are not taken into account in the design of the release process of LMO nanocomposites, it could have negative consequences for the practical application of these materials. For example, destabilization of the crystal structure in spinel-type LMO and/or reduced adsorption capacity in lithium-rich LMO due to unsuccessful desorption of lithium from the LMO. Therefore, we are confident that the findings of this publication will lead to the development of new strategies for the use of lithium adsorbent materials based on LMO as a precursor material (Figure 1).

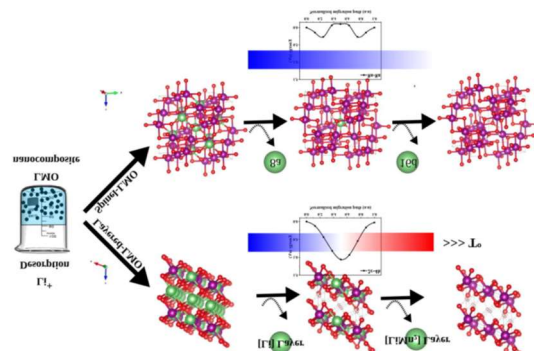


Figure 1: Schematic picture of lithium desorption behaviour from the crystalline structure present in LMO nanocomposites in acidic media.

## Chema Gómez-Rodríguez awards to the best paper

10:45 “Signatures of interactions in the Andreev spectrum of nanowire Josephson junctions”

Francisco J. Matute-Cañadas

Física Teórica de la Materia Condensada

# Signatures of interactions in the Andreev spectrum of nanowire Josephson junctions

**F. J. Matute-Cañadas<sup>1</sup>, C. Metzger<sup>2</sup>, Sunghun Park<sup>1</sup>, L. Tosi<sup>3</sup>, P. Krogstrup<sup>4</sup>, J. Nygård<sup>4</sup>,  
M. F. Goffman<sup>2</sup>, C. Urbina<sup>2</sup>, H. Pothier<sup>2</sup> and A. Levy Yeyati<sup>1</sup>**

<sup>1</sup>*Departamento de Física Teórica de la Materia Condensada, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Spain*

<sup>2</sup>*Quantronics group, Service de Physique de l'État Condensé (CNRS, UMR 3680), IRAMIS, CEA-Saclay, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*

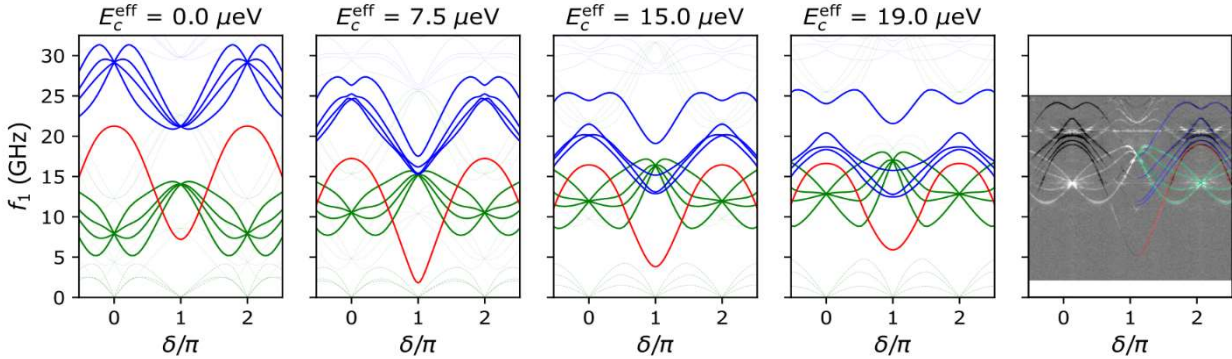
<sup>3</sup>*Centro Atómico Bariloche and Instituto Balseiro, CNEA, CONICET, 8400 San Carlos de Bariloche, Río Negro, Argentina*

<sup>4</sup>*Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark*

*Universitetsparken 5,*

Email: francisco.matute@uam.es

The Andreev states in a nanowire Josephson junction comprise a rich set of discrete, localized levels. This is analogous to an atom, except here the superconducting gap of the leads is playing the role of the confining potential. Microwave spectroscopy has revealed the transitions between Andreev states and has evidenced their fine structure owing to spin-orbit coupling [1]. However, while some of the observed transition lines could be explained in terms of non-interacting models [1,2], other expected lines from these models could not be clearly identified, and some other experimental features remained unexplained.



In this work [3] we show that the inclusion of electron-electron interactions in the normal region of the junction is necessary to account for these unexplained features, which consist in the splitting of certain degeneracies expected in the non-interacting models. The relevance of these interactions is further confirmed through their interplay with an external magnetic field [4].

Figure 1. Evolution of the transitions with the effective charging energy  $E_c^{\text{eff}}$  of the normal region and the phase difference  $\delta$  between the superconducting leads. The rightmost panel is an experimental spectrum.

- [1] L. Tosi, C. Metzger, M. F. Goffman, C. Urbina, H. Pothier, Sunghun Park, A. Levy Yeyati, J. Nygård and P. Krogstrup, *Phys. Rev. X* **9**, 011010 (2019)
- [2] C. Metzger, Sunghun Park, L. Tosi, C. Janvier, A. A. Reynoso, M. F. Goffman, C. Urbina, A. Levy Yeyati and H. Pothier, *Phys. Rev. Research* **3**, 013036 (2021)
- [3] F. J. Matute-Cañadas, C. Metzger, Sunghun Park, L. Tosi, P. Krogstrup, J. Nygård, M. F. Goffman, C. Urbina, H. Pothier and A. Levy Yeyati, *Phys. Rev. Lett.* **128**, 197702 (2022)
- [4] J. J. Wesdorp, F. J. Matute-Cañadas, A. Vaartjes, L. Grünhaupt, T. Laeven, S. Roelofs, L. J. Splitthoff, M. Pita-Vidal, A. Bargerbos, D. J. van Woerkom, P. Krogstrup, L. P. Kouwenhoven, C. K. Andersen, A. Levy Yeyati, B. van Heck and G. de Lange, arXiv:2208.11198

## Session II - Chair of the session: Mariola Ramírez

12:20 "High precision low – cost spectrophotometer for agricultural applications"

Francisco J. Fernández Alonso

Física Aplicada

### High precision low – cost spectrophotometer for agricultural applications

**F.J. Fernández – Alonso<sup>1</sup>, L. García – Pelayo<sup>1</sup>, Z. Hernández<sup>2</sup> and V. Torres – Costa<sup>1</sup>**

<sup>1</sup> Department of Applied Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>2</sup> Department of Geography, Universidad Autónoma de Madrid, 28049 Madrid, Spain

Email: [franciscoj.fernandez05@estudiante.uam.es](mailto:franciscoj.fernandez05@estudiante.uam.es)

Reflectance spectroscopy has been widely used as a rapid and non-invasive evaluation technique for plant physiological state monitoring and quality control of fruits and vegetables [1, 2]. The objective of this work was to design a low-cost seven-band reflectance spectrophotometer for agricultural applications based on the Arduino platform. Seven LEDs whose bands covered from blue to infrared, as well as a photodiode were used. It was possible to measure the reflection in the different bands with an average accuracy of 0.8 % full scale. In addition, a repeatability of 0.6 % was obtained, more than three times better than that corresponding to commercial devices available in the market. The applicability of the device to monitor the physiological status of plants and the fruit ripening process was verified, observing changes in the reflection spectrum and vegetation indexes of plants and fruits before these changes were visible to the naked eye. This was possible due to the high accuracy and precision of our device, as well as because of the geometry in which it was implemented. These changes could not be observed with the commercial devices until they were visible to the naked eye.

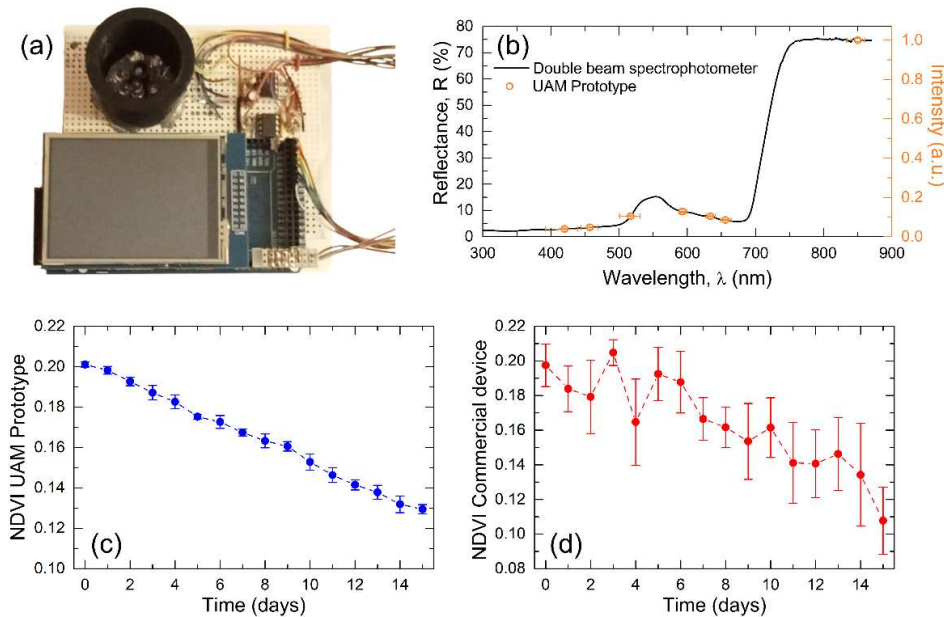


Figure 1. (a) Photograph of the implemented device. (b) Reflectance spectrum of a leaf obtained using both a commercial double beam spectrophotometer and our prototype, for the seven bands considered. (c,d) Evolution of the NDVI vegetation index of a conference pear as a function of ripening measured with (c) our prototype and (d) the commercial device *NDVI FieldScout CM 1000 NDVI Meter*. The vertical error bars represent the deviation between the various measurements made.

The bill of materials for this device is less than €65, which is between 10 and 100 times less than the price of devices available in the market for similar applications. This favors the possibility of accessing this technology in developing countries, promoting the fulfillment of the UN Sustainable Development Goals.

[1] B. Li. et al., *Plants*, **7**(1), 3166 (2018)

[2] C. Liu et al., *PLoS ONE*, **9**(2), e87818 (2014)

**Note:** Part of this work has been awarded by the Autonomous University of Madrid as the best Bachelor Thesis in the "II Convocatoria de Premios a la Investigación en el Ámbito de la Agenda 2030 de la UAM".



12:40 “Electronic Band Structure of  $\text{Li}_x\text{CoO}_2$  during the Insulator to Metal transition”**Elena Salagre Rubio**

Física de la Materia Condensada

## Electronic Band Structure of $\text{Li}_x\text{CoO}_2$ during the Insulator to Metal Transition

**E. Salagre<sup>1</sup>, P. Segovia<sup>1,2</sup>, M.A. González-Barrio<sup>3</sup>, J. Pearson<sup>4</sup>, I. Takeuchi<sup>4</sup>,  
E.J. Fuller<sup>5</sup>, A.A. Talin<sup>5</sup>, M. Jugovac<sup>6</sup>, P. Moras<sup>6</sup>, A. Mascaraque<sup>3</sup> and E.G. Michel<sup>1,2</sup>**

*1. Dto Física Materia Condensada, Univ. Autónoma de Madrid, Spain*

*2. IFIMAC (Condensed Matter Physics Center), Univ. Autónoma de Madrid, Spain*

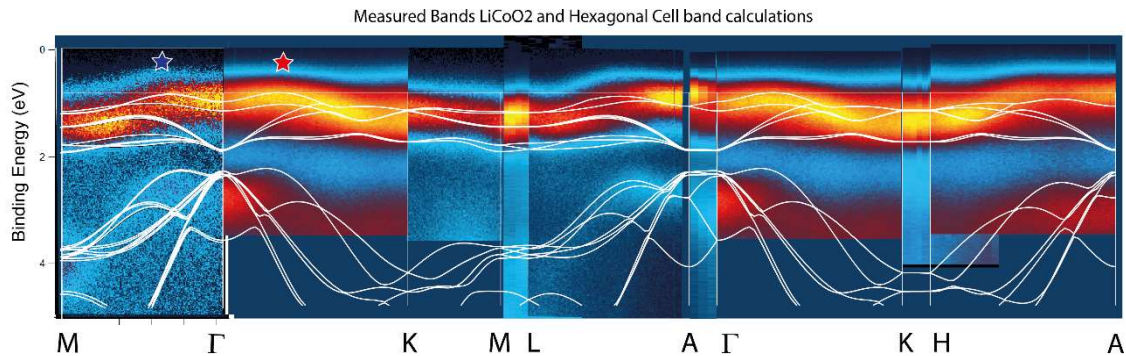
*3. Dto. Física de Materiales, Fac. Ciencias Físicas, Univ. Complutense de Madrid, Spain*

*4. Materials Science and Engineering, Univ. of Maryland, College Park (MD), USA*

*5. Sandia National Laboratories, Livermore (CA), USA.*

*6. Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy*

We report here a detailed study of the valence band structure of  $\text{Li}_x\text{CoO}_2$  (LCO) for a range of Li molar fractions that allows the observation of changes induced by the insulator to metal transition that takes place at  $x=0.95$  and that determines the behavior of the material in the  $0.75 < x < 0.95$  molar fraction range. LCO has been used as Li-ion battery cathode for decades owing to its energy density and cycle life [1]. Despite many studies on the properties and applications of LCO, some unknowns still remain due to the rich physico-chemical behavior and the relevance of several fundamental phenomena. The stoichiometric material,  $x=1$ , is a band insulator. However, upon small Li removal ( $x=0.95$ ), LCO undergoes an insulator to metal transition, still not fully understood [2]. In terms of the band occupation, this transition is explained by hole doping of the Co  $t_{2g}$  band [3], which has an important contribution to the density of states. In the range  $0.75 < x < 0.95$ , the metallic ( $x=0.75$ ) and the insulating ( $x=0.95$ ) phases coexists and LCO exhibits metallic character. The Li deintercalation generates subtle changes of the lattice parameters for each phase. Li deintercalation is usually done via electrochemical or chemical reactions. This makes it impossible to perform reliable electronic structure studies. We have used epitaxial LCO thin films grown by pulsed laser deposition on Nb-doped  $\text{SrTiO}_3$  substrates, combined with a fully physical delithiation method to obtain high resolution ARPES, XPS and XAS of for different Li molar fractions of the material. The results have been compared with previously reported data and calculations for the electronic band structure of stoichiometric LCO. The changes observed upon metallization are interpreted in this context [4][5][6]. Information of the chemical and structural changes are combined to give a full picture of the phase evolution. The full 3D reciprocal space mapping of stoichiometric and understoichiometric samples is presented, giving a direct visualization of the effects of the insulator – to – metal transition.



- [1] N. Nitta *et al*, *Mat. Today* **18**, 252 (2015).
- [2] C.A. Marianetti *et al*, *Nat. Mat.* **3**, 627 (2004); A. Milewska *et al*, *Sol. State. Ion* **263**, 110 (2014)
- [3] T. Mizokawa *et al*, *PRL* **111**, 056404 (2013)
- [4] Y. Okamoto *et al*, *Phys. Rev. B.* **96**, 125147 (2017).
- [5] K. Miyoshi *et al*, *Phys. Rev. B* **98**, 195106 (2018).
- [6] Kumar Radha *et al.*, *SciPost Phys* **10**, 57 (2021).

13:00 "Sensitized lanthanide emission in doped BaZrS<sub>3</sub> perovskite semiconductor"

Jinan Hussein Al Shuaib

Física de Materiales

## Sensitized lanthanide emission in doped BaZrS<sub>3</sub> perovskite semiconductor

Jinan H. Al Shuhaib<sup>1</sup>, Isabel J. Ferrer<sup>1,2</sup>, José R. Ares<sup>1</sup>, Antonio Polimeni<sup>3</sup>, Antonio Benayas<sup>4,5</sup>,  
Riccardo Marin<sup>4,5</sup> Fabrice Leardini<sup>1,2</sup>

<sup>1</sup> Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

<sup>2</sup> Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

<sup>3</sup> Dipartimento di Fisica, Sapienza Università di Roma, I-00185, Rome (Italy)

<sup>4</sup> Nanomaterials for Bioimaging Group (NanoBIG), Universidad Autónoma de Madrid, Madrid 28049, Spain

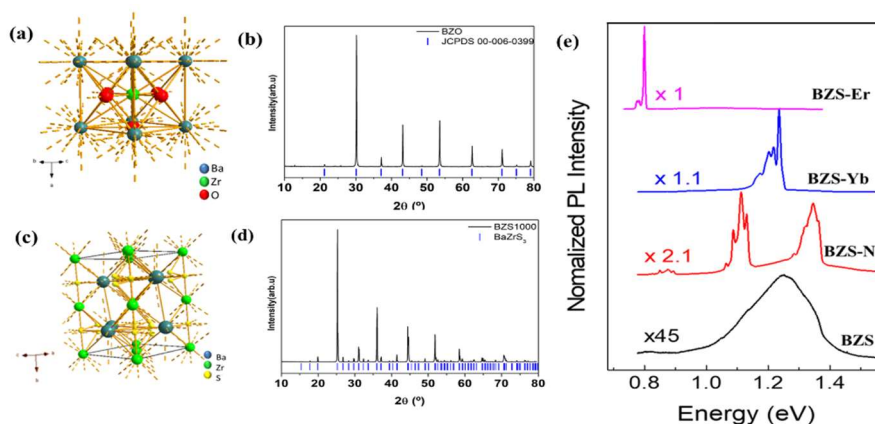
<sup>5</sup> Institute for Advanced Research in Chemistry (IAdChem), Campus de Cantoblanco, 28049 Madrid, Spain

E-mail: jinan.awadh@estudiante.uam.es

Nowadays there is a great interest in using semiconductors as host materials for photoluminescent lanthanide ions (Ln<sup>3+</sup>). In such a material, the poor light absorption intrinsically featured by lanthanides is compensated by the semiconductor moiety, which harvests the optical energy and funnel it to the luminescent metal center [1]. However, incorporating Ln<sup>3+</sup> in semiconductors is difficult to achieve because Ln<sup>3+</sup> prefer to occupy sites in the crystal lattice with high coordination number, such as octahedral sites [2], whereas most semiconductors offer cationic sites with tetrahedral coordination.

In this vein, inorganic chalcogenide perovskites can offer a solution. These materials are semiconductors with general formula ABX<sub>3</sub>, with A being a group II cation (*i.e.*, Ca<sup>2+</sup>, Sr<sup>2+</sup>, or Ba<sup>2+</sup>), B a group IV transition metal (*i.e.*, Ti<sup>4+</sup>, Zr<sup>4+</sup>, or Hf<sup>4+</sup>), and X a chalcogen anion (S<sup>2-</sup> or Se<sup>2-</sup>) [3]. The B site features an octahedral coordination environment ideal for embedding Ln<sup>3+</sup>.

Moving from these considerations, here we present the synthesis and characterization of BaZrS<sub>3</sub> perovskites doped with Ln<sup>3+</sup> (Yb<sup>3+</sup>, Er<sup>3+</sup>, Nd<sup>3+</sup>). Samples were prepared by sulfurization of Ln<sup>3+</sup>-doped BaZrO<sub>3</sub> powders, which were in turn prepared via a microwave-assisted hydrothermal method. The morphology, chemical composition and crystalline structure of the samples were characterized by scanning electron microscopy coupled to energy dispersive x-ray analysis, Raman spectroscopy and x-ray powder diffraction (XRPD). Optical band gaps were determined by diffuse optical reflectance measurements. Preliminary photoluminescence studies confirm the occurrence of effective energy transfer from the semiconductor host material to the dopant Ln<sup>3+</sup> (see Figure 1e).



**Figure 1.** Schematic crystal structure (a) and XRPD pattern (b) of BaZrO<sub>3</sub>. Schematic crystal structure (c) XRPD pattern of chalcogenide perovskite BaZrS<sub>3</sub>. (e) Photoluminescence emission spectra of pure and Ln<sup>3+</sup>-doped BaZrS<sub>3</sub> powders, recorded under illumination with  $\lambda_{ex}$  = 405 nm at T=10 K.

[1] R. Marin, D. Jaque, *Chem. Rev.* 121, 1425–1462 (2021)

[2] W. Mir *et al.*, *NPG Asia Mater* 12, 9 (2020)

[3] Y. Sun *et al.*, *Nano Letters*, 15, 581–585 (2015)



13:20 “Two-photon dressing of quantum emitters for cavity-assisted generation of steady-state entanglement”

**Alejandro Vivas Viaña**

Física Teórica de la Materia Condensada

## Two-photon dressing of quantum emitters for cavity-assisted generation of steady-state entanglement

**A. Vivas-Viaña<sup>1</sup>, D. Martín-Cano<sup>1</sup> and C. Sánchez Muñoz<sup>1</sup>**

<sup>1</sup>*Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, 28049, Spain*

Email: (alejandro.vivas@uam.es)

In this work we show how driving the two-photon resonance of a system of interacting quantum emitters can be exploited for the generation of cavity-assisted steady state entanglement. The fact that two interacting emitters can be coherently driven via two-photon processes has been exploited, e.g., to estimate interaction strengths and inter-molecular distances at the nanometer scale [1]. It has also been shown that, under a strong two-photon drive, the emitters can be dressed with photon pairs from the drive, developing a rich family of energy levels that translate into a complex structure in the spectrum of resonance fluorescence [2].

By coupling the dressed system to a cavity in the bad cavity limit, new processes among the two-photon dressed energy levels can be engineered. We show that, by placing particular dressed-state transitions in resonance with the cavity, these novel decay processes can stabilize the system into a highly entangled state. Since the energy of the dressed states can be tuned through the Rabi frequency of the drive, the system can be optically tuned in and out of these resonances. We also show that the stabilization of entanglement translates into particular features in the quantum optical properties of the light emitted by the system at frequencies that are well detuned from the drive, allowing to isolate the optical signatures of entanglement by simple spectral filtering.

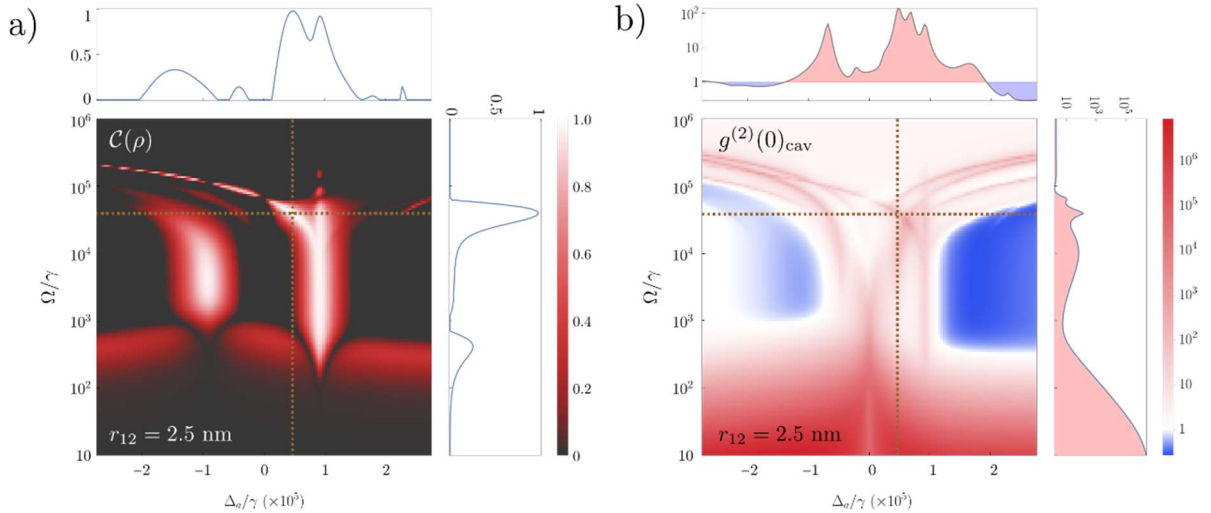


Figure 1. (a) Concurrence of the two-interacting quantum emitters. (b) Second-order correlation function of the photons emitted by the cavity. In both panels the corresponding quantity is described in terms of the cavity detuning and the laser driving strength along with transversal cuts at the maximum value of the concurrence.

[1] C. Hettich *et al.*, *Nanometer resolution and coherent optical dipole coupling of two individual molecules*, Science 298, 385 (2002).

[2] A. Vivas-Viana and C. Sánchez Muñoz, *Two-photon resonance fluorescence of two interacting nonidentical quantum emitters*, Physical Review Research 3, 33136 (2021).

## Session III - Chair of the session: Pablo Ares

---

15:00 “Tuning the microenvironment of crowded proteins inside viral capsids”

**Klara Strobl Bardo**

Física de la Materia Condensada

---

### Tuning the microenvironment of crowded proteins inside viral capsids

**K. Strobl<sup>1</sup>, E. Selivanovitch<sup>2</sup>, P. Ibañez-Freire<sup>1</sup>, F. Moreno-Madrid<sup>1</sup>,  
I. Schaap<sup>3</sup>, R. Delgado-Buscalioni<sup>1</sup>, T. Douglas<sup>2</sup> and P. J. de Pablo<sup>1</sup>**

<sup>1</sup> *Universidad Autónoma de Madrid, Madrid, Spain*

<sup>2</sup> *Indiana University, Bloomington, USA*

<sup>3</sup> *Hensoldt Optronics GmbH, Wetzlar, Germany*

Email: klara.strobl@uam.es

The use of viral capsids for packing biomolecules has opened new possibilities for studying their function in confined environments. They not only mimic the highly crowded conditions in nature, but also allow their exquisite manipulation at the nanoscale for technological applications.

Here, we pack green fluorescent proteins in virus like particles derived from P22 bacteriophage procapsids at high packing fractions and use their emission signal to monitor molecular functionality by Total Internal Reflection Fluorescence Microscopy (TIRFM) while changing the microenvironment of individual capsids with the stylus of an Atomic Force Microscope.

With this simultaneous correlative microscopy at the nanoscale, we could identify two phenomena: a) a mechanical quenching of ~10 %, b) an additional electronic quenching of ~10 % when metallic probes were used. Although fluorescence quenches and recovers after the conductive tip releases the capsid regardless of its structural integrity, in the insulator tip's case quenching happens only if the capsid keeps the local organization of the packed protein. Electronic quenching is associated with the coupling of the protein fluorescence emission with the tip surface plasmon resonance while the mechanical quenching is a consequence of the unfolding of aggregated proteins during the mechanical disruption of the capsid.

15:20 "Kondo lattice development in a TaS<sub>2</sub> van der Waals heterostructure"

Cosme González Ayani

Física de la Materia Condensada

**Kondo lattice development in a TaS<sub>2</sub> van der Waals heterostructure****Cosme G. Ayani<sup>1,2</sup>, Michele Pisarra, Iván Martínez<sup>1,2</sup>, Manuela Garnica<sup>1</sup>, Rodolfo Miranda<sup>1,2,3</sup>, Fabián Calleja<sup>1</sup>, Fernando Martín, Amadeo L. Vázquez de Parga<sup>1,2,3</sup>**<sup>1</sup>Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain<sup>2</sup>IMDEA Nanociencia, Calle Faraday 9, Cantoblanco 28049, Madrid, Spain<sup>3</sup>IFIMAC, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain[Cosme.gonzalez@uam.es](mailto:Cosme.gonzalez@uam.es)

Kondo screening occurs when a magnetic impurity is embedded in a metal, below a given temperature, known as the Kondo temperature, a singlet state forms between the spin of the impurity and the spins of the conduction electrons [1]. When the distance between the magnetic impurities is small enough the physics of the system is expected to be modified [2]. The first experimental evidence was obtained in the 1970s in systems containing rare earths [3]. By means of scanning tunneling microscopy (STM) and spectroscopy (STS) at low temperatures we explore a van der Waals heterostructure consisting in a single layer of 1T-TaS<sub>2</sub> on a 2H-TaS<sub>2</sub> crystal. The 1T-TaS<sub>2</sub> layer presents a ( $\sqrt{13} \times \sqrt{13}$ )R13.9° charge density wave (CDW) with a localized electron at the center of every unit cell of the CDW. For temperatures below 28K the spatially resolved STS shows the presence of a Kondo resonance in the Mott-Hubbard gap. For temperatures below 11K the system develops a quantum coherent state called Kondo lattice.

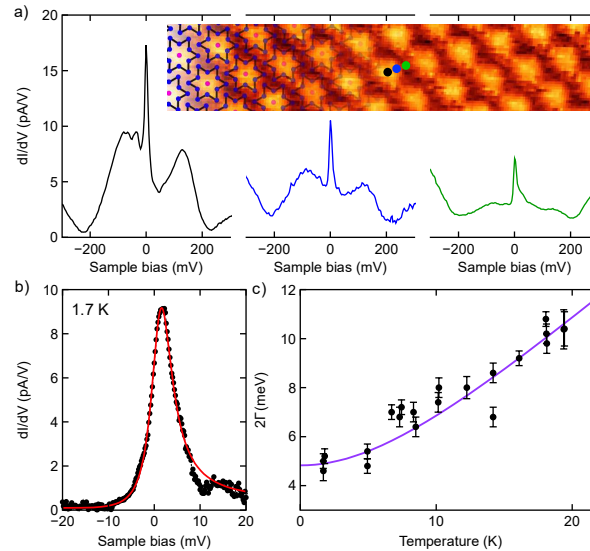


Figure 1 a) Single point STS taken on different locations along the CDW unit cell showing the modulation of the intensity of the zero bias Kondo peak. The Kondo resonance is more intense at the center of the CDW unit cell (black spectrum) and decays very fast away from the center (blue and green spectra). STS parameters: 500 mV, 500 pA,  $V_{mod}=5$  mV. The inset shows the area of the sample where the spectra were measured, with the STS locations colored accordingly. Image parameters: 500 mV, 90 pA, 20 nm x 4 nm. b) Individual spectrum belonging to the temperature series of the panel c), in this case the spectrum is taken at  $T=1.7$  K and fitted with a Fano function considering the broadening produced by temperature and the lock-in modulation. c) Plot showing the dependence with temperature of the intrinsic full width at half maximum (FWHM) of the Kondo resonance, and corresponding fit to the expected behavior according to the Fermi liquid theory, giving a Kondo temperature of  $T_K=27$  K.

[1] J. Kondo, Prog. Theor. Phys. 32 (1961) 41

[2] P. Nozieres, Ann. Phys. 10 (1985), 19

[3] W.R. Johanson, et al Phys. Rev. Lett. 46 (1981) 504

15:40 “Tunable thermal emission of subwavelength silica ribbons”

**Juan José García Esteban**

Física Teórica de la Materia Condensada

## Tunable thermal emission of subwavelength silica ribbons

**J. J. García-Esteban<sup>1</sup>, J. Bravo-Abad<sup>1</sup> and J.C. Cuevas<sup>1</sup>**

<sup>1</sup>*Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC),  
Universidad Autónoma de Madrid, Madrid, Spain*

Email: juanjose.garciae@uam.es

The thermal properties of individual subwavelength objects, which defy Planck’s law, are attracting significant fundamental and applied interest in a variety of different research areas. Special attention has been devoted to anisotropic structures made of polar dielectrics featuring thicknesses smaller than both the thermal wavelength and the skin depth. Recently a novel experimental technique [1] has enabled the measurement of the thermal emissivity of anisotropic SiO<sub>2</sub> nanoribbons (with thicknesses on the order of 100 nm), demonstrating that their emission properties can be largely tuned by adjusting their dimensions. However, despite the great interest of these results, their rigorous theoretical analysis has remained elusive due to the computational challenges arising from the vast difference in the length scales involved in the problem. In this work, we present a systematic theoretical analysis of the thermal emission properties of these dielectric nanoribbons based on simulations within the framework of fluctuational electrodynamics carried out with the boundary element method implemented in the SCUFF-EM code. In agreement with the experiments, we show that the emissivity of these subwavelength structures can be largely tuned and enhanced over the thin film limit. We elucidate that the peculiar emissivity of these nanoribbons is due to a very anisotropic thermal emission that originates from the phonon polaritons of this material and the properties of the waveguide modes sustained by these dielectric structures. Our work illustrates the rich thermal properties of subwavelength objects, as well as the need for rigorous theoretical methods able to unveil the complex thermal emission phenomena emerging in this class of systems.

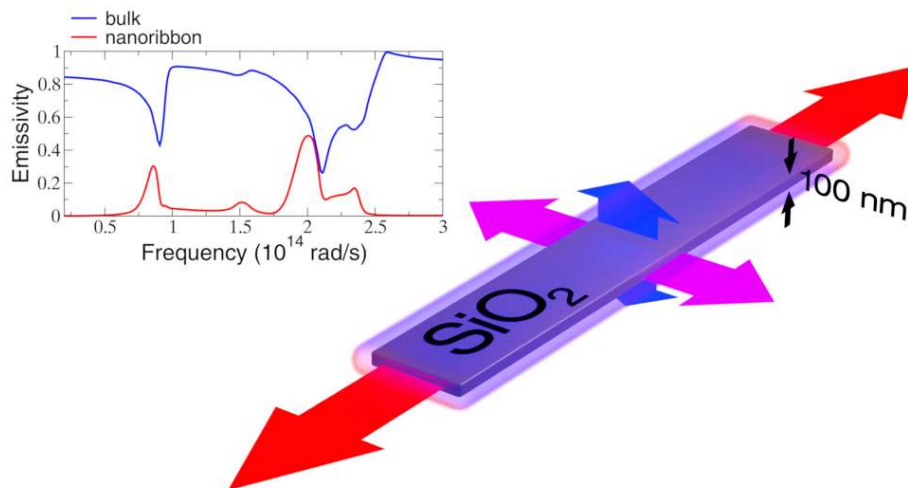


Figure 1. Schematic representation of the studied silica ribbons, with the subwavelength dimension of 100 nm highlighted for clarity. Inset: emissivity spectra of the ribbon compared to bulk silica. [2]

[1] S. Shin et al., Nat. Commun., **10**, 1377 (2019)

[2] J.J. García-Esteban et al., ACS Photonics, **9**, 11, 3679-3684 (2022)

## Session IV - Chair of the session: Carlos Sánchez Muñoz

17:00 "Plasmonic nanoparticles for inflammation targeting in atherosclerosis"

Tamara Muñoz Ortiz

Física de Materiales

### Plasmonic nanoparticles for inflammation targeting in atherosclerosis

T Muñoz-Ortiz<sup>1,2</sup>, M. C. Iglesias-de la Cruz<sup>1</sup>, F. Sanz-Rodríguez<sup>1</sup>, M. Granado<sup>1</sup>, M. J. Marín<sup>3</sup>, F. Rivero<sup>4</sup>, D. H. Ortigies<sup>1</sup>, R. Aguilar Torres<sup>4</sup>, F. Alfonso<sup>4</sup>, D. Jaque<sup>1</sup>, E. Martín Rodríguez<sup>1,2</sup> and J. García-Solé<sup>1,2</sup>

<sup>1</sup>Nanomaterials for Bioimaging Group, Universidad Autónoma de Madrid, Madrid, Spain.

<sup>2</sup>Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain.

<sup>3</sup>School of Chemistry, University of East Anglia, Norwich, United Kingdom

<sup>4</sup>Cardiology Department, Hospital Universitario de la Princesa, Universidad Autónoma de Madrid, Madrid, Spain.

Email: tamara.munnoz@estudiante.uam.es

Cardiovascular optical coherence tomography (CV-OCT) is a pure-optical imaging technique used for the clinical diagnosis of atherosclerosis; a cardiovascular disease based on the formation of plaques in the arterial walls that can pose a severe risk of the patient's health. Despite the high sensitivity and spatial resolution of CV-OCT, the disease is diagnosed after the appearance of plaques in a late stage of development. For this reason, there is an urgent need for contrast agents to promote the diagnose of atherosclerosis in its early stages, characterized by the inflammation of the arterial walls and subsequent overexpression of several molecules [1].

For this reason, we propose to combine CV-OCT with functionalized plasmonic gold nanoparticles to obtain information about the presence of inflammation-related molecules in the walls of the arteries (endothelium). Among the commercial possibilities, core/shell gold nanoparticles (gold nanoshells, GNSs) provide the strongest signal in CV-OCT [2] thanks to their scattering properties, while having reduced cytotoxicity.

In this work, we study in detail the specific targeting of inflamed endothelial cells using peptide-functionalized GNSs (Figure 1(a)). Targeting is evaluated with CV-OCT and dark field optical microscopy, and was achieved both under static and dynamic conditions, as shown in Figure 1(b).

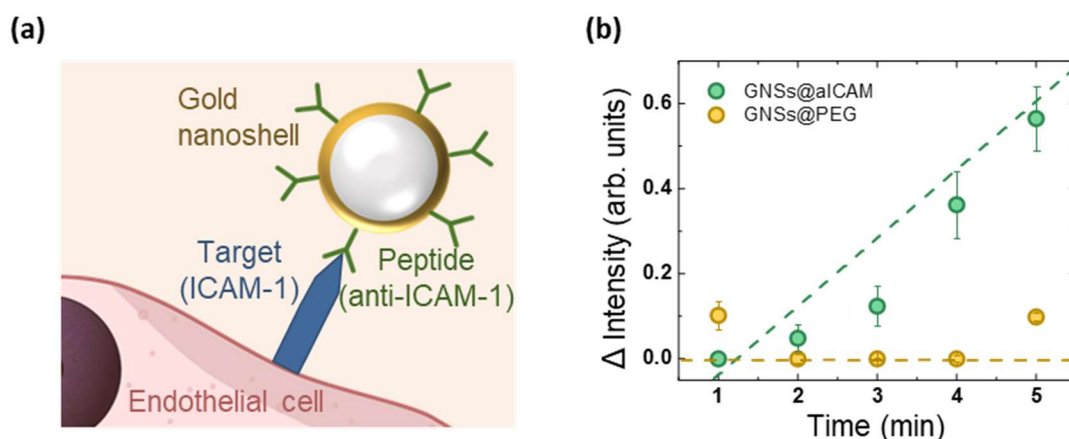


Figure 1. (a) Representation of the targeting process. (b) Increase in the intensity of microscopy images due to the attachment of functionalized GNSs (GNSs@alCAM) to inflamed endothelial cells as a function of the circulation time of the GNSs. Non-functionalized GNSs (GNS@PEG) have been used as a control.

[1] J. Sanz et al., Nature, **451**, 953 (2008)

[2] J. Hu et al., Journal of Biophotonics, **5**, 674 (2017)

[5] Puebla, S., D'Agosta, R., Sanchez-Santolino, G. et al. npj 2D Mater Appl 5, 37 (2021).



17:20 "Tribological motion of rotating vesicles"

Paula Magrinya

Física Teórica de la Materia Condensada

## Tribological motion of rotating vesicles

**Paula Magrinya<sup>1,2</sup>, Alfredo Alexander-Katz<sup>3</sup>, Laura R. Arriaga<sup>1,2,4</sup>, Juan L. Aragonés<sup>1,2,4</sup>.**

<sup>1</sup> Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup> Instituto de Ciencias de Materiales Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain

<sup>3</sup> Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

<sup>4</sup> Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

Email: paula.magrinya@uam.es

Cellular lipid membranes support important biological processes such as sensing, trafficking and motility, often interacting mechanically with the extracellular matrix. Cell motility is mainly driven by friction, understood as dynamical adhesive iterations between the cell membrane and the substrate. However, because its dynamic nature, a physical description of cell motion accounting for friction remains elusive. Therefore, we fabricate a minimal cell model, using droplet-microfluidics [1], to measure and study the tribological properties of cell membranes. The model consists of vesicles with different membrane compositions and thus different mechanical properties encapsulating each a single ferromagnetic microparticle within their cores, as shown in Figure 1. Using this system, we study the dynamics of the rotating magnetic particle confined within the vesicle under the actuation of an external rotating magnetic field. We show that the confined flows generated by the rotating particle determine the particle and vesicle dynamics. Moreover, the hydrodynamic coupling between the particle and the vesicle with the substrate results into translation of the vesicle. Finally, we show that the vesicle translation velocity is controlled by the membrane mechanical properties and degree of confinement. This system opens a new venue to study how protein receptors within the membrane may result in directed motion along gradients in the mechanical properties or ligand concentration of the substrate [2].

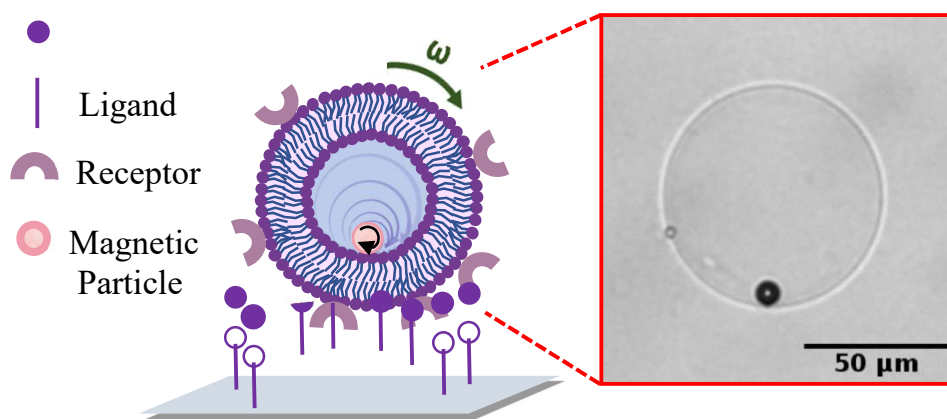


Figure 1: Schematic illustration of our experimental system together with a bright field image of a lipidic giant unilamellar vesicle with an encapsulated ferromagnetic particle.

[1] Arriaga LR, Datta SS et al., *Small*, 10, 950(2014).

[2] Steimel JP, Aragonés JL, Alexander-Katz A, *Phys. Rev. Lett.*, 113, 178101(2014)

17:40 “Direct magnetic evidence, functionalization and low-temperature  
magneto-electron transport in liquid-phase exfoliated FePS<sub>3</sub>”

Lucía Martín Pérez

IMDEA

## Direct magnetic evidence, functionalization and low-temperature magneto-electron transport in liquid-phase exfoliated FePS<sub>3</sub>

Lucía Martín-Pérez<sup>1</sup>, Samara Medina Rivero<sup>1</sup>, Manuel Vázquez-Sulleiro<sup>1</sup>, Alicia Naranjo<sup>1</sup>, I. Jéniffer Gómez<sup>2</sup>, Luisa Ruiz-Gonzalez<sup>3</sup>, Andres Castellanos-Gomez<sup>4</sup>, Mar García-Hernández<sup>4\*</sup>, Emilio M. Pérez<sup>1\*</sup> and Enrique Burzuri<sup>1,5\*</sup>

<sup>1</sup>IMDEA Nanociencia C/Faraday 9, Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain

<sup>2</sup>Department of Condensed Matter Physics, Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic

<sup>3</sup>Departamento de Química Inorgánica, Universidad Complutense de Madrid, Madrid, Spain

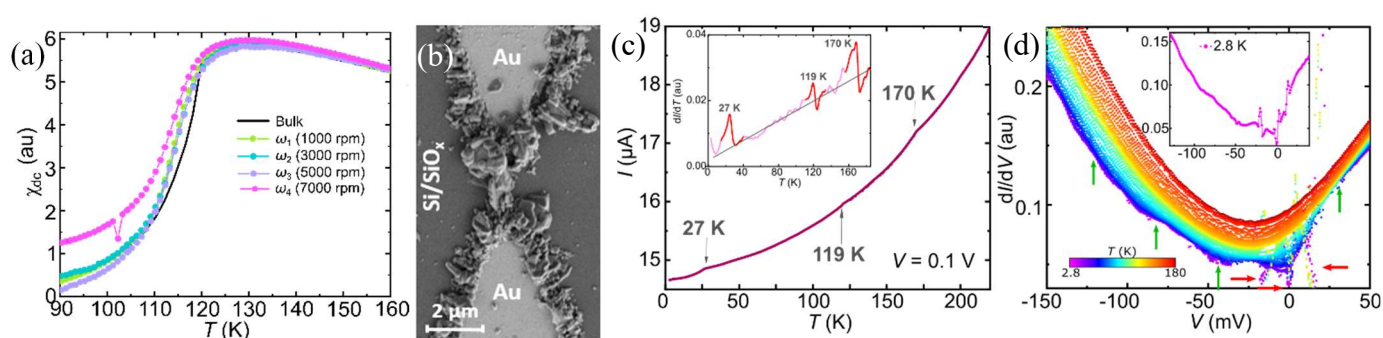
<sup>4</sup>2D Foundry, Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049 Madrid, Spain

<sup>5</sup>Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

[lucia.martin@imdea.org](mailto:lucia.martin@imdea.org)

Magnetism and the existence of magnetic order in a material is determined by its dimensionality. In this regard, the recent emergence of magnetic layered van der Waals (vdW) materials provides a unique playground to explore the exotic magnetism arising in the two-dimensional (2D) limit. The magnetism of 2D flakes has been commonly studied by indirect methods like Raman spectroscopy. Here, taking advantage of liquid-phase exfoliation (LPE) method, we show a first direct magnetic evidence of the antiferromagnetic transition in FePS<sub>3</sub> few-layer flakes, performed with a SQUID magnetometer (Figure 1a). It is concomitant with a clear reduction of the Néel temperatures with the flake thickness, in contrast with previous Raman reports.[1]

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



**Figure 1:** (a) First derivative of magnetic susceptibility ( $\chi$ ) measured as a function of temperature in a bulk reference sample and exfoliated samples  $\omega_1$ ,  $\omega_2$ ,  $\omega_3$  and  $\omega_4$ . (b) Scanning Electron Microscopy (SEM) image of a representative electrode pair containing LPE FePS<sub>3</sub> flakes ( $\omega_1$ ) trapped by DEP. (c) Current  $I$  – Temperature  $T$  characteristics measured on a FePS<sub>3</sub> device at a fixed  $V = 0.1$  V and its first derivative ( $dI/dT$ ) (inset). (d) First derivative ( $dI/dV$ ) of the Current  $I$  – Voltage  $V$  characteristic at different  $T$ .

- [1] Lee, J.-U. et al., *Nano Lett.*, **16** (12), 7433–7438 (2016)
- [2] Burzurí, E. et al., *Nanoscale*, **10** (17), 7966–7970 (2018)
- [3] Klein, D. R. et al., *Science*, **360** (6394), 1218–1222 (2018)
- [4] Vázquez Sulleiro, M. et al., *Nat. Chem.*, **14** (6), 695–700 (2022)

## Poster Session

11:20 – 12:20 Poster Session A

16:00 – 17:00 Poster Session B

### List of Posters:

1. **Águeda, Miguel:** Tunneling spectroscopy in thin films of EuS and Nb
2. **Aldaz Caballero, Leyre:** Pressure nanosensors based on CuInS<sub>2</sub>
3. **Andrino Gómez, Alberto:** Preparation and study of potential Bi-Sb amorphous topological superconductors
4. **Bastante, Pablo:** Engineering Transport Orbitals in Single Molecule Junctions
5. **Bernabeu Gómez, Joan:** Phonon-Mediated Hydrodynamic Transport in Weyl Semimetals
6. **Blanco Peces, Alejandro:** Developing atomically tailored networks of quasi-zero dimensional alloys
7. **Bravo Tapia, Ely Anira:** Non-invasive monitoring of cholestasis rat model by near-infrared autofluorescence
8. **Bueno, Jaime:** Modelling and optimization of perovskite/perovskite tandem solar cells through plasmonic effects
9. **Campusano, Richard:** Swimming motility of E. coli in the presence of magnetic rotating obstacles
10. **Cantero Reviejo, Miguel:** Lemon and salt: Mechanical interplay between low pH and halophilic virus HCIV-1
11. **Carrasco, Roberto:** Control at the nanoscale of graphene superconductivity
12. **Díez Martínez, Alejandro:** Nanomechanical characterization of individual TMV particles with AFM
13. **Escobar Ortiz, Arin:** Transport of Active Colloids in Structured Environments
14. **Esteve Paredes, Juanjo:** Bulk photovoltaic effect in 2D materials from density functional theory and real-time dynamics
15. **Caso, Diego:** Dynamics and reversible control of the vortex Bloch point domain wall in short cylindrical magnetic nanowires
16. **Fernández de la Pradilla, Diego:** Vacuum-field-induced state mixings
17. **Fernández Martínez, Javier:** Silver nanoparticles chains as waveguides for ultra-long range fluorescence transport
18. **Fernández-Lomana Gómez-Guillamón, Marta:** Vortex lattice at high magnetic fields and charge density wave in KCaFe<sub>4</sub>As<sub>4</sub> and CaK(Fe<sub>0.988</sub>Mn<sub>0.012</sub>)
19. **Galindo Sanz, Arturo:** Functional Optimization of PVD-LiCoO<sub>2</sub> Cathodes for Li-Ion Batteries
20. **Gallego Fuente, Daniel:** Development of a technological AFM microscope for operation in UHV
21. **García García, Jorge:** Optical interferometry as an efficient tool to characterize STM head vibrations
22. **García González, Asier:** Efecto de la integración de nanopartículas magnéticas en electrodos de baterías de ion litio
23. **García Herreros, Sergio:** Neural networks for simultaneous quantum parameter estimation
24. **García Rodríguez, Tomás:** Hydrogenated amorphous silicon thin film as electrode for lithium-ion batteries

25. **García, Pablo:** Characterization of FeSe<sub>0.7</sub>S<sub>0.3</sub> with Scanning Tunneling Microscopy
26. **Geva Galor:** Collective behaviour in driven colloidal crystals
27. **González Sánchez, Celia:** Towards hybrid van der Waals Josephson junctions based on NbSe<sub>2</sub>
28. **González-Ruano Iriarte, César:** Superconducting spintronics in epitaxial Fe/MgO/V junctions with spin-orbit interaction
29. **Hernandez Pinilla, David:** Q-switched plasmonic solid-state nanolasers assisted by 2D transition metal dichalcogenides
30. **Inglés Cerrillo, Julia:** Study of the plasmonic resonance of nanoparticles based on liquid metals with a high degree of ordering
31. **Jiménez Arévalo, Nuria:** Highly defective MoS<sub>2</sub> ultrathin nanoflakes for electrolytic hydrogen production
32. **Köhler Ruiz, Elena:** Growth and characterization of Sr<sub>1-x</sub>TiS<sub>3-y</sub> perovskite thin films
33. **Lednev, Maksim:** Cavity mediated energy transfer driven by a photochemical reaction
34. **López Peña, Gabriel:** Bovine serum albumin and Rose Bengal decorated gold nanoparticles for photodynamic therapy applications
35. **Manzanares Negro, Yolanda:** Low resistance contacts to few layered MoS<sub>2</sub> by local pressurization
36. **Ming, Liyan:** Thermal reading in brain phantom under microwave radiation
37. **Moratalla Martín, Manuel:** Specific heat of ultrastable glasses at low temperatures
38. **Moreno, Jose Antonio:** Electronic band structure inside the superconducting gap from Yu-Shiba-Rusinov states in quasi two-dimensional 2H-NbSe<sub>2</sub>-xS<sub>x</sub>
39. **Ortiz Rivero, Elisa:** Local temperature and viscosity sensing by a rotating upconverting microparticle
40. **Osuna Bris, Eva:** Nano-scale conductivity of Ni<sub>3</sub>(HITP)<sub>2</sub> Metal-Organic Framework
41. **Palacios Alonso, Pablo:** Modelling AC hysteresis loops of ferromagnetic nanoparticles
42. **Pérez Picazo, Elena:** Monitorization of H-absorption/desorption process in metallic films via optical measurements
43. **Ramirez Peral, M<sup>a</sup> Jesús:** Study of Oxide Equilibrium in Pulsed Laser Deposited LiCoO<sub>2</sub> for Li-Ion Batteries
44. **Rincón Arroyo, Esther:** Manipulation of aqueous micro-droplets containing particles and bio-species by photovoltaic tweezers
45. **Ripoll Sau, Joan:** Phase engineering of two-dimensional Transition Metal Ditungstenides
46. **Rodríguez Espinosa, M<sup>a</sup> Jesús:** N-terminal conformation of the coat protein modulates RNA cargo retention of human picobirnavirus
47. **Ronquillo Tutiven, Joan Javier:** Electrostatic doping of monolayer MoS<sub>2</sub> deposited on hexagonal ferroelectric domains
48. **Szewczyk, Daria:** Comparative studies of thermal properties: the case of detonated nanodiamond ceramics
49. **Tamargo, André I.:** Two-dimensional Fermi polarons, same problem different realisations: doped TMD monolayers & ultracold atomic Fermi gases
50. **Vega Martín, Jorge:** Proton Transport through Peptide Nanotubes
51. **Vida García, Jaime:** Study of colloidal systems in lattice obstacles
52. **Viña Bausa, Beatriz:** Superconductivity and Coulomb Correlations in nanosized Pb islands
53. **Yang, Youhuang:** Study of Two-Mode Interference in Quantum Light-Matter Interactions

- 54. **Yue, Senlin:** Inverse Design applied to Schrödinger Equation: Tailored Potential Wells for Exciton Trapping
- 55. **Zambudio Sepúlveda, Aitor:** Defects as a key to control friction on monolayer MoS<sub>2</sub>
- 56. **Zhang, Fengchan:** Plasmon-assisted simultaneous enhancement of single upconverting nanoparticle luminescence and trapping force



## Tunneling spectroscopy in thin films of EuS and Nb

**Miguel Águeda<sup>1</sup>, Beilun Wu<sup>1</sup>, Hisa Matsuki<sup>2</sup>, Isabel Guillamón<sup>1</sup>, Edwin Herrera<sup>1</sup>, Jason W. Robinson<sup>2</sup> and Hermann Suderow<sup>1</sup>**

*<sup>1</sup> Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos,*

*Departamento de Física de la Materia Condensada,*

*Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC),*

*Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

*<sup>2</sup> Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom*

Email: miguel.agueda@estudiante.uam.es

Magnetism with large spin orbit coupling can be combined with superconductivity in hybrid structures consisting of thin films of a magnetic and a superconducting compound. This leads to situations that have sparked much interest, as the Zeeman effect, spin orbit coupling and superconductivity can lead to unconventional states close to the interface between the superconductor and the magnet, such as Majorana modes. There are few studies of the superconducting density of states of such hybrid systems and even less studies performed with a Scanning Tunneling Microscope (STM). The STM measures the spatial dependence of the tunneling density of states and is particularly interesting to identify new features due to the combination of magnetism and superconductivity. Here we present successful millikelvin scanning tunneling microscopy and spectroscopy (STM) experiments in Nb thin films covered with Au. We present the spatial dependence of the superconducting gap and the vortex lattice. We then discuss results obtained in a hybrid EuS-Nb-Au structure. We discuss the modification of the superconducting density of states induced by EuS.

## Pressure nanosensors based on CuInS<sub>2</sub>

Leyre Aldaz-Caballero<sup>1</sup>, Ulises R. Rodríguez-Mendoza<sup>2</sup>, Víctor Lavín<sup>2</sup>, Antonio Benayas<sup>1,3</sup> and Riccardo Marin<sup>1</sup>

<sup>1</sup> Nanomaterials for Bioimaging Group (nanoBIG) Dpto. Física de Materiales, Universidad Autónoma de Madrid, 28049, Spain.

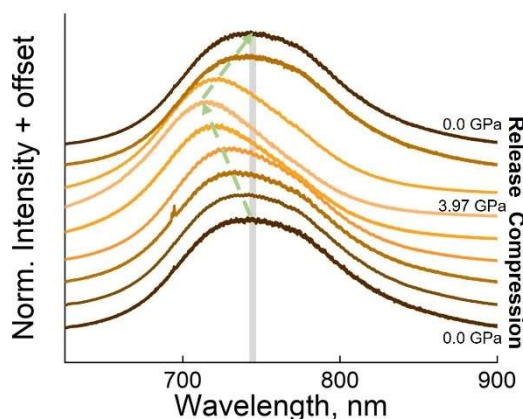
<sup>2</sup> Universidad de La Laguna, MALTA-Consolider Team, IMN and IUdEA, Departamento de Física, Apdo. Correos 456, E-38200, San Cristóbal de La Laguna, Santa Cruz de Tenerife, Spain

<sup>3</sup> Nanomaterials for Bioimaging Group (nanoBIG), Instituto Ramón y Cajal de Investigación Sanitaria, Ctra. Colmenar Viejo, Km. 9,100, 28034 Madrid, Spain

Email: [leyre.aldaz@estudiante.uam.es](mailto:leyre.aldaz@estudiante.uam.es)

Pressures in the range of 0-3 KPa are involved in several biological processes, such as tumor progression.<sup>1</sup> Knowledge of the magnitude of these mechanical forces at the cellular level could hence guide/inform the diagnosis and treatment of diseases with marked impact on our well-being. Nanoparticles with mechanical pressure-dependent luminescence are ideal nano-probes to afford a minimally invasive readout of forces at the (sub)cellular level.

Semiconductor QDs have attracted attention in the pressure sensing field due to the dependence of the photoluminescence peak position with the applied pressure and their nanoscale size.<sup>2</sup> One of the best candidates as pressure sensor probes are copper indium sulfide (CuInS<sub>2</sub>) QDs due to their visible emission and nanometric size, being ideal for pressure sensing at a cellular level purpose. In this work, we studied the response to stress of CuInS<sub>2</sub> QDs while exploring how the size and the stoichiometry play a role in the stress-sensitivity. While applying different loading pressure, the QDs exhibit a blueshift in the peak position of the emission spectrum, and while this pressure is unloaded, the original peak position is recovered. This recovery behavior implies that the studied QDs are operating in the elastic regime. This pressure sensors could be used into dynamic systems, such as the analysis of mechanical forces at cellular level. This could suppose a big step into the understanding of the processes that take place at pathological level.



**Figure 1.** CuInS<sub>2</sub> compression and release photoluminescence spectra. The emission peak position exhibits a blueshift while applying pressure and recovers the original position when the applied pressure is removed.  $\lambda_{ex} = 532$  nm.

[1] Kai et al., Trends in Cell Biology., **26** (2016)

[2] Wang et al., ACS Applied Nano Materials., **5** (2022)

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

A. Andrino<sup>1,2,3</sup>, N. Gordillo<sup>2,3,4</sup> and M. A. Ramos<sup>1,3,4</sup>

<sup>1</sup>Laboratorio de Bajas Temperaturas, Dpto. Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup>Laboratorio de Microelectrónica, Dpto. Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>3</sup>Centro de Micro-Análisis de Materiales (CMAM), Universidad Autónoma de Madrid, Madrid, Spain

<sup>4</sup>Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain

Email: [alberto.andrinog@estudiante.uam.es](mailto:alberto.andrinog@estudiante.uam.es)

One of the most promising paths to make quantum computation a reality is based on topological superconductivity, which can provide quantum devices protection against external noise [1,2]. However, no one has yet experimentally come up with a stable topological superconductor. Good candidates have been proposed to be bismuth (Bi) and its alloys (particularly, bismuth-antimony, Bi-Sb), which are the most studied topological insulators and which, in a metastable amorphous state, become superconductors below a critical temperature close to 6 K [3].

The aim of this work is to grow  $\text{Bi}_x\text{Sb}_{100-x}$  alloys and try to amorphize them by ion beam irradiation to achieve a significant damage in depth that avoids recrystallization [4]. The resulting material will be morphological and structurally characterized, and its electrical behavior will also be studied in a wide range of temperatures. From these results, we will check whether our hypothesis is true and, therefore, if we are able to fabricate these potential amorphous topological superconductors.

[1] C. Beenakker and L. Kouwenhoven, *Nature Physics*, **12**(7), 618-621 (2016)

[2] R. Aguado and L. Kouwenhoven, *Physics Today*, **73**(6), 44-50 (2020)

[3] J. S. Shier and D. M. Ginsberg, *Physical Review* **147**(1), 384 (1966)

[4] J. Barzola-Quiquia et al., *Superconductor Science and Technology*, **30**(1), 015013 (2016)

# Engineering Transport Orbitals in Single Molecule Junctions

P. Bastante<sup>1</sup> and N. Agraït<sup>1,2,3</sup>

<sup>1</sup>*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

<sup>2</sup>*Condensed Matter Physics Center (IFIMAC) and Instituto Universitario de Ciencia de Materiales “Nicolás Cabrera” (INC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

<sup>3</sup>*Instituto Madrileño de Estudios Avanzados en Nanociencia IMDEA-Nanociencia, E-28049 Madrid, Spain*

Email: [pablo.bastante@uam.es](mailto:pablo.bastante@uam.es)

Molecular-scale electronics provides an ideal strategy towards miniaturization of electronic components, as molecular design enables the integration of electronic functions at the smallest level [1]. Charge transport can be tuned using electron-donating substituents, just like traditional semiconductors [2]. In this work, single-molecule junctions of tolane model compounds **1-3** (the parent tolane structure **1**, with either electron withdrawing nitro-groups in **2** or electron donating dimethylamino groups in **3** introduced) decorated with either thiol (-SAC) in **a** compounds or methylsulfanyl (-SMe) in **b** compounds anchor groups are fabricated and characterized using the STM-break junction technique in a home-built STM. Measuring the conductance and the thermopower we find that the dimethylamino groups have a limited influence in the charge transport properties while the nitro-groups shift the energy levels to the LUMO orbitals (Figure 1b) and enhance conductance as shown in the LC histograms in Figure 1c. This demonstrates how withdrawing side groups can be used to tune energy levels of transport orbitals and create additional charge transport channels for the enhancement of charge transport properties.

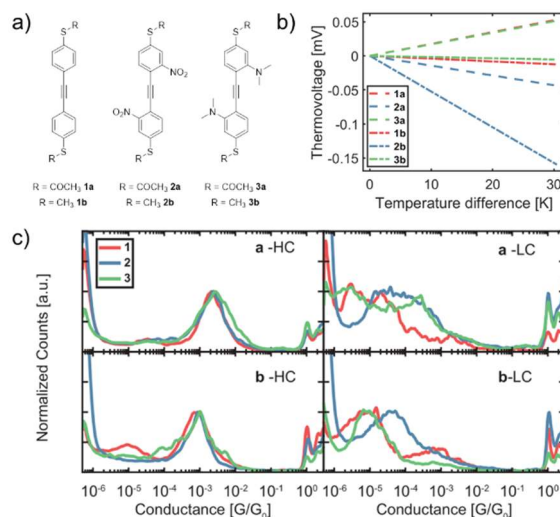


Figure 1: (a) Schematic view of compounds **1-3** with -SAC (**a**) and -SMe (**b**) anchor groups. (b) Linear fit of all the temperature difference dependent thermovoltage values for all the compounds to obtain the thermopower, combined for comparison. (c) 1D-conductance histograms of the HC (left) and LC (right) peaks as obtained from clustering, separated by anchoring group (top: -SAC, bottom: -SMe). Measurements have been normalized by peak height to make the peak position and shape directly comparable across the different molecules

- [1] D. Xiang et al., Chem. Rev. Lett., **116**, 4318 (2016)
- [2] L. Venkataraman et al., Nano Lett., **7**, 502 (2007)
- [3] A. Daaoub et al., J. Phys. Chem. Lett., **13**, 9156 (2022)

# Phonon-mediated Hydrodynamics in a Weyl SM

J. Bernabeu<sup>1</sup> and A. Cortijo<sup>1,2</sup>

<sup>1</sup>*Departamento de Física de la Materia Condensada*

*Universidad Autónoma de Madrid, Cantoblanco, Madrid, Spain*

<sup>2</sup>*Condensed Matter Physics Center (IFIMAC), Cantoblanco, Madrid, Spain*

Email: [joan.bernabeu@uam.es](mailto:joan.bernabeu@uam.es)

In light of recent experimental and numerical analyses [1-3], we study through a simple microscopic model the role that electron-electron interactions mediated by virtual phonons can play in inducing a hydrodynamic regime in Weyl semimetals. The electric and thermal conductivities are obtained, and similarly to interactions with real phonons, they display a different scaling with temperature ( $T$ ) depending on whether  $T$  lies above or below the Bloch-Grüneisen temperature  $T_{BG}$ . For  $T > T_{BG}$  the virtual phonons act on-shell and the standard results with real phonons are recovered. At low temperatures  $T < T_{BG}$ , a  $T^2$  behavior is obtained for the electric and thermal scattering times. In addition, it is seen that chirality-violating interactions play a crucial role in inducing electric current relaxation through Baber scattering. We find in that in our simple model the electron-phonon interaction needs to be abnormally large for momentum-conserving electron-electron interactions to dominate over phonon emission and absorption at low temperatures [4].

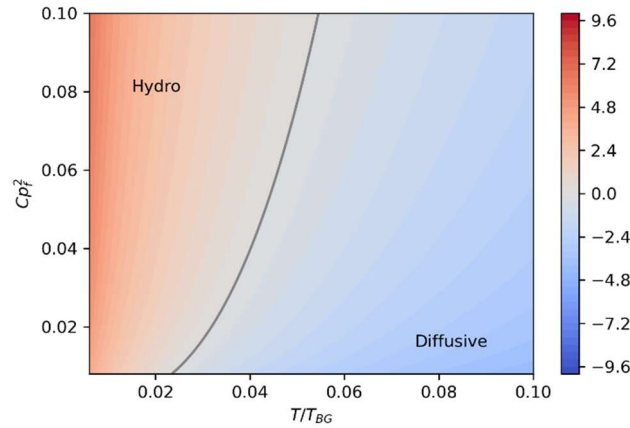


Figure 1. Plot of  $\tau_{e-e}^{-1} / \tau_{e-ph}^{-1}$ , i.e. the quotient between the electron-electron and electron-phonon inverse relaxation times for the electric conductivity at low temperatures. The region where electron-electron interactions dominate (are dominated by) electron-phonon interactions is labeled as “Hydro” (“Diffusive”).

- [1] J. Gooth et al., Nature Communications, 9, 1 (2018)
- [2] A. Jaoui et al., npj Quantum Materials, 3, 1 (2018)
- [3] U. Vool et al., Nature Physics, 17, 1216 (2021)
- [4] J. Bernabeu et al., to be announced



# INC Research awards for Physics students 2022

Blanco Peces, Alejandro

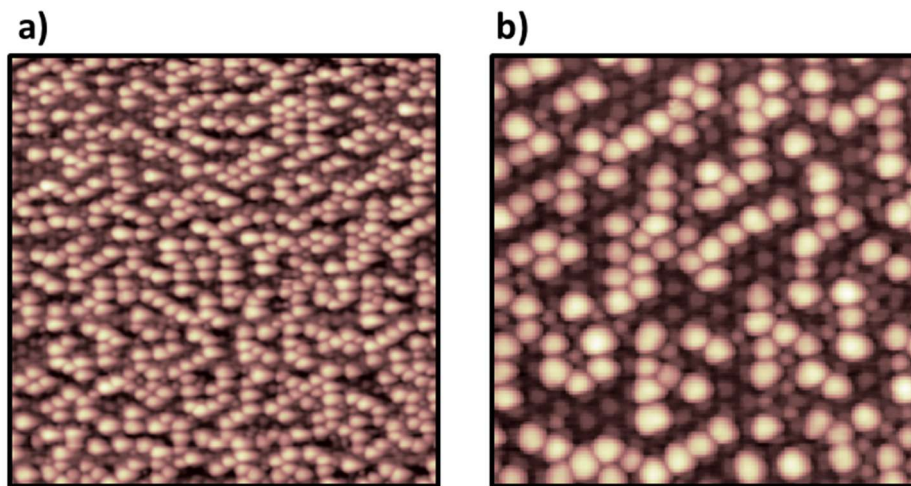
Física de Materiales

## Developing atomically tailored networks of quasi-zero dimensional alloys

A. Blanco-Peces<sup>1,2</sup> and A. J. Martínez-Galera<sup>1,2</sup><sup>1</sup>Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain<sup>2</sup>Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, SpainEmail: [alejandro.blancop@estudiante.uam.es](mailto:alejandro.blancop@estudiante.uam.es)

During the earliest stages of research in heterogeneous catalysis, the knowledge of the processes taking place on the catalysts was rather poor. It was mainly due the reduced control in the synthesis of the nanoparticles achievable at that time. When nanotechnology became a prime research area, different approaches offering a better control in the composition, shape and size of nanoparticles, were developed [1-5]. Nevertheless, given that, today, around 90% of the industrial production is based on catalytic processes, a more accurate control in the synthesis of the nanocatalysts is still currently a major challenge, which will be mandatory to achieve in a near future, to keep the development level of current civilization.

In this work, we have tailored with atomic precision a nanocatalysts system, consisting in a network of quasi-zero dimensional Si-Ir binary alloys, grown on a one-atom thick 2D material. Nanoalloys growth and characterization was carried out *in situ*, in an ultra-high vacuum (UHV) system. The main characterization technique employed was scanning tunneling microscopy (STM). Both the relative Si-Ir composition and the nanoparticle size were controlled, with nearly atomic accuracy, by setting the amounts of the two elements deposited over the 2D material surface. As a next step, we intend to employ these nanocatalysts as a model system to study different reactions of current relevance for green energy production from hydrogen.



**Figure 1.** STM images showing a network of quasi-zero dimensional Si-Ir alloys grown over a graphene/Ru(0001) nanotemplate. Tunneling parameters:  $V_s = -2.5$  V,  $I_T = 40$  pA. Size: **a)**  $100 \times 100$  nm<sup>2</sup>, **b)**  $50 \times 50$  nm<sup>2</sup>.

- [1] G. Ertl, *Angew. Chem. Int. Ed.*, **47**, 3524–3535 (2008).
- [2] B. Roldan Cuenya, *Thin Solid Films*, **518**, 3127–3150 (2010)
- [3] A. J. Martínez-Galera *et al.*, *Nanoscale*, **11**, 2317 (2019)
- [4] J. Díez-Albar *et al.*, *J. Phys. Chem. C*, **123**, 5525–5530 (2019)
- [5] A. J. Martínez-Galera *et al.*, *Nano Res.*, **15**, 6969–6976 (2022)
- [1] J. Sanz *et al.*, *Nature*, **451**, 953 (2008)
- [2] J. Hu *et al.*, *Journal of Biophotonics*, **5**, 674 (2017)

# Non-invasive monitoring of cholestasis rat model by near-infrared autofluorescence

Ely Bravo\*<sup>1</sup>, Hernán Martín Salido<sup>1</sup>, Dirk H. Ortgies<sup>1</sup>, Nuria Fernández<sup>2</sup>, M<sup>a</sup> Isabel Prieto-Nieto<sup>3</sup>, Javier Blanco-Rivero<sup>4</sup>, Luis Monge<sup>2</sup>

<sup>1</sup> Nanomaterials for Bioimaging Group, Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain.

<sup>2</sup> Nanomaterials for Bioimaging Group, Departamento de Fisiología, Facultad de Medicina, Universidad Autónoma de Madrid, Madrid, Spain,

<sup>3</sup> Departamento de Cirugía General y Digestiva, Hospital Universitario la Paz, Madrid, Spain.

<sup>4</sup> Departamento de Fisiología, Facultad de Medicina, Universidad Autónoma de Madrid, Madrid, Spain,

\*[ely.bravo@estudiante.uam.es](mailto:ely.bravo@estudiante.uam.es)

A new cost and time effective alternative to conventional medical imaging technologies due to its simple setup is based on the use of non-harmful near-infrared (NIR) light with high imaging/sensing resolution. One of the benefits of NIR autofluorescence is that it can be used to detect the presence of endogenous fluorescent compounds. In the liver the principal autofluorescence emissions between 680 – 950 nm stems from bilirubin [1]. The disease cholestasis is characterized by an increase of bilirubin in the bloodstream, and we proposed to trace it through NIR imaging. Furthermore, studies have reported good effects of probiotics in cirrhotic liver (a consequence of cholestasis) by counteracting hepatic hemodynamic and circulatory dysfunction [2]. Therefore, the goal of this project was evaluating cholestasis and its response to the administration of probiotics by NIR. We confirmed, that using this symbiotic product resulted in improvements by observing a lower emission intensity of bilirubin which is correlated with a positive result from the implementation of the probiotic. Additionally, we probed the integrity of the blood brain barrier (BBB, highly selective semipermeable border that prevents solutes crossing into the central nervous system) which can be affected by cholestasis. This analysis was performed with Ag<sub>2</sub>S nanoparticles with an emission at 1200 nm, hence, comparing a healthy rat with a sick one, we obtained a peak at 1200 nm from the cholestasis rat brain, demonstrating a bigger permeability and transportation across the BBB of nanoparticles. In summary, we correlate the organ status in a liver disease by the emission of endogenous fluorophore with the effect of probiotics on the liver and investigated its effect on the BBB helped by nanoparticles, demonstrating how endogenous and exogenous fluorophores can advance the diagnosis of diseases.

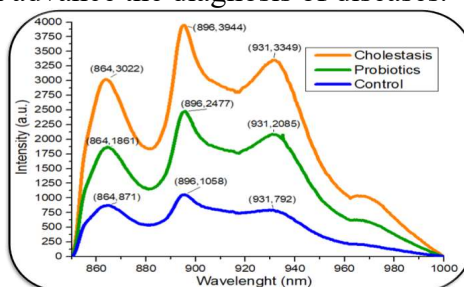


Figure 1. Autofluorescence rat liver with an Ex 800 nm & Em > 900nm. (Orange) Emission of rat liver with cholestasis. (Green) Emission of rat liver with cholestasis and administration of probiotics. (Blue) Control healthy rat.

## References

- [1] J. Lifante, Y. Shen, E. Ximendes and e. al., "The role of tissue fluorescence in in vivo optical bioimaging," *Journal of Applied Physics*, vol. 128, pp. 171100-171117, 2020.
- [2] Di Wu, Dingwei Xue, Jing Zhou, Yifan Wang, Zhe Feng, Junjie Xu, Hui Lin, Jun Qian and Xiujun, "Extrahepatic cholangiography in near-infrared II window with the clinically approved fluorescence agent indocyanine green: a promising imaging technology for intraoperative diagnosis," *Theranostics*, vol. 10, no. 8, pp. 3636-3651, 2020.

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

Jaime Bueno<sup>1</sup>, Sol Carretero-Palacios<sup>1</sup> and Miguel Anaya<sup>2</sup>

<sup>1</sup> Dpt. Física de Materiales, Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049-Madrid, Spain.

<sup>2</sup> Department of Chemical Engineering & Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK

Email: jaime.buenob@estudiante.uam.es

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

In this talk, we introduce how nanoplasmonic spheres embedded in lowgap perovskite films have the potential to dramatically boost the efficiency of perovskite tandem solar cells. Taking advantage of Kramers-Kronig consistent refractive indices, we perform advanced FDTD based calculations to evaluate the Pb/Sn perovskite absorption enhancement induced by both scattering and near field effects produced due to the presence of the nanospheres. An example of this is shown in Figure 1, where it is plotted a map of the electric field inside the lowgap perovskite. We screen a multiparametric space including different types of metals (e.g. Ag, Au, Al, etc.), particle sizes and positions inside the perovskite and volume filling fraction with the aim of maximising light harvesting while minimising parasitic absorption. We show how a fine balance between the perovskite properties and the near field plasmonic effects results in dramatic increases in the calculated matched photocurrent. This fact allows the use of thinner layers, which not only facilitates charge carrier extraction but also reduces the use of material. This novel approach promises unprecedented perovskite/perovskite tandem efficiencies surpassing 30%, opening avenues for the realisation of next generation, affordable PV.

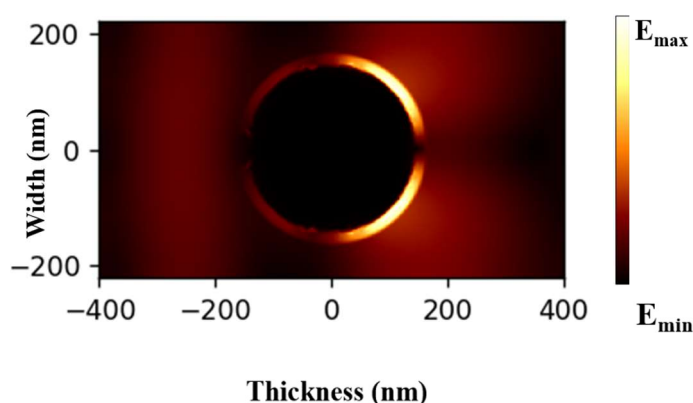


Figure 1. Map of the electric field inside a perovskite with an embedded silver nanosphere when a plane wave is incident from the left.

### References

- [1] Shockley, W., Queisser, H., *Journal of Applied Physics*, **32**, 510-519 (1961).
- [2] Anaya, M., Lozano, G., et al., *Joule*, **1**, 769-793 (2017).
- [3] Lin, R., Xu, J., Wei, M. et al., *Nature*, **603**, 73-78 (2022).

# Swimming motility of *E. coli* in the presence of magnetic rotating obstacles

Richard A. Campusano<sup>1</sup>, Pablo Llombart<sup>1</sup>, Paula Magrinya<sup>1</sup>, Berta Tinao<sup>1</sup>, Laura R. Arriaga<sup>1,2</sup> and Juan L. Aragones<sup>1,2</sup>

<sup>1</sup> Department of Theoretical Condensed Matter Physics, <sup>2</sup> Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

Email: [richard.campusano@inv.uam.es](mailto:richard.campusano@inv.uam.es)

Bacteria have developed a swimming strategy to outrun diffusion, which is required to find food or colonize surfaces. *E. coli* swimming strategy is based on the paradigmatic run and tumbling protocol in which the bacteria alternate periods of swimming in straight lines at constant speed with tumbling that randomizes its swimming direction [1]. The swimming motion of *E. coli* is sensitive to the presence of different substrates and respond to external stimuli such as chemical gradients or shear flows, which affect their swimming dynamics [2]. In this work, we analyze the swimming dynamics of *E. coli* in the presence of magnetic rotating obstacles, which generates local rotational flows. We observe that *E. coli* exhibit close circular trajectories due to the presence of the planar substrate they are settled on. In the presence of obstacles *E. coli* tend to increase the frequency of tumbling events. The presence of local rotational flows does not modify the *E. coli*'s average swimming velocity but reduces their rotational relaxation time.

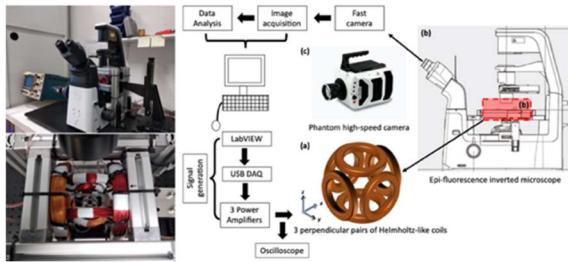


Figure 1. Experimental setup for the generation of homogeneous rotating magnetic fields.

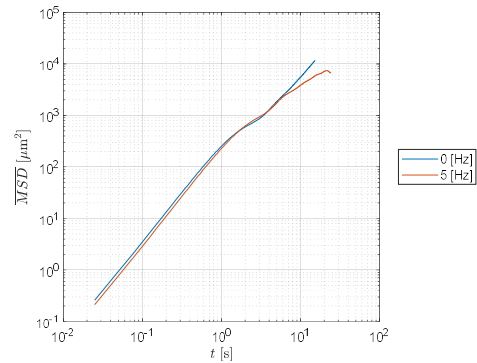


Figure 2. Comparison of  $MSD_{avg}$  between bacteria with and without external rotating magnetic field.

[1] H.C. Berg, *E. coli in Motion*, Springer-Verlag: New York Inc., USA (2004).

[2] S. Makarchuk *et al.*, *Nature Comm.*, **10**, 4110-4121 (2019).

# Lemon and salt: Mechanical interplay between low pH and halophilic virus HCIV-1

M. Cantero<sup>1</sup>, K. Eskelin<sup>2</sup>, N. Abrescia<sup>3</sup>, H. Oksanen<sup>2</sup> and P. de Pablo<sup>1</sup>

<sup>1</sup>Condensed PhysicsMatter Department, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup>Department of Biosciences and Institute of Biotechnology, PO Box 56, University of Helsinki, 00014 Helsinki, Finland.

<sup>3</sup> Molecular recognition and host-pathogen interactions programme, CIC bioGUNE, CIBERehd, Derio, Spain.

Email: miguel.cantero@uam.es

Viruses are complex machines that can be found in many different niches where cells are. In fact, they can also be found in extreme environments such as hot springs or salty lakes. HCIV-1 is an archaeal halophilic virus that can thrive in a wide concentration of salts, ranging from millimolar up to 5M. Cryo-EM structure of HCIV-1 and genetic studies proved the structural similarity with other members of the *Sphaerolipoviridae* family that comprises other halophilic archaea viruses such as PH1 or HHIV-1 and extremophilic bacteriophages such as P23-77. This family is characterized for having an internal membrane protecting the genome that interacts with an external icosahedral protein capsid. The similarities in the capsid structure despite inhabiting different niches led into the study of biophysical determinants for the virion stability. Using AFM and AF4 we have characterized the mechanical behavior of HCIV-1 particles under native and acidic stress and also monitored the structural effect of acidic environment to both the capsid and the inner membrane vesicle.

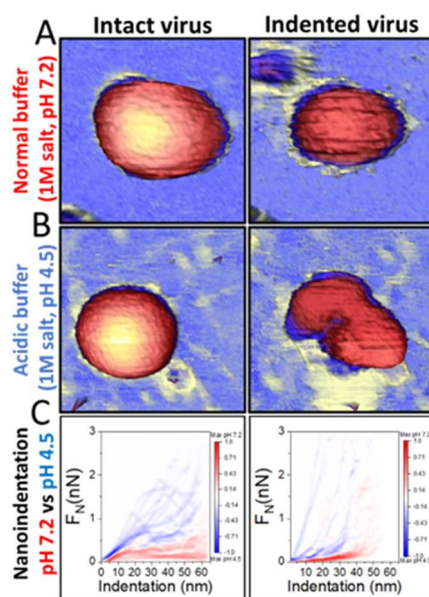


Figure 1. Mechanical and topographical effect of acidification in HCIV1 virus. A. Topography of HCIV1 virus at pH 7.2 previous to indentation (left) and after the indentation (right). B. Topography of HCIV1 virus at pH 4.5 previous to indentation (left) and after the indentation (right). C. Comparison between nanoindentation for intact (left) and indented (right) viral particles.

- [1] Abrescia, N.G.A., Bamford, D.H., Grimes, J.M., Stuart, D.I., Annual Review of Biochemistry 81, 795–822 (2012)
- [2] Atanasova, N.S., Oksanen, H.M., Bamford, D.H., Current Opinion in Microbiology 25, 40–48 (2015)
- [3] Horcas, I., Fernández, R., Gómez-Rodríguez, J.M., Colchero, J., Gómez-Herrero, J., Baro, A.M., Review of Scientific Instruments 78. (2007)
- [4] de Pablo, P.J., Carrión-Vázquez, M., Cold Spring Harbor Protocols 2014, 167–177 (2014)



## Control at the nanoscale of graphene superconductivity.

Eva Cortés-del Río<sup>1</sup>, Roberto Carrasco<sup>1</sup>, Jose Luis Lado<sup>2</sup>, Vladimir Cherkov<sup>3,4</sup>, Pierre Mallet<sup>3,4</sup>, Jean-Yves Veuillen<sup>3,4</sup>, Juan Carlos Cuevas<sup>5,6</sup>, José María Gómez-Rodríguez<sup>1,6,7</sup>, Joaquín Fernández-Rossier<sup>8,9</sup> and Iván Brihuega<sup>1,6,7</sup>.

<sup>1</sup>*Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid E-28049, Spain*

<sup>2</sup>*Department of Applied Physics, Aalto University, Espoo 02150, Finland*

<sup>3</sup>*Université Grenoble Alpes, Grenoble 38000, France*

<sup>4</sup>*CNRS, Institut Neel, Grenoble F-38042, France*

<sup>5</sup>*Departamento Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid E-28049, Spain*

<sup>6</sup>*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid E-28049, Spain*

<sup>7</sup>*Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid E-28049, Spain*

<sup>8</sup>*QuantaLab, International Iberian Nanotechnology Laboratory (INL), Avenida Mestre José Veiga, Braga 4715-310, Portugal*

<sup>9</sup>*Departamento de Física Aplicada, Universidad de Alicante, San Vicente del Raspeig, Alicante 03690, Spain*

Email: roberto.carrasco@uam.es

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.

[1] H. Hasai et al. *The Oxford Handbook of Small Superconductors*. Ed. by A. V. Narlikar. Oxford University Press, 2017.

[2] Eva Cortés-del Río et al. "Observation of Yu-Shiba-Rusinov States in Superconducting Graphene". *Advanced Materials* 33.22 (2021), p. 2008113. DOI: 10.1002/adma.202008113.

## Biomechanics of tobacco mosaic virus: from cutting tubes to undressing nucleic acids

A. Díez<sup>1</sup>, A. Bittner<sup>2</sup>, A. Eleta<sup>2</sup> and P. J. de Pablo<sup>1</sup>

<sup>1</sup>Department of Condensed Matter Physics, Universidad Autónoma de Madrid, Spain

<sup>2</sup>CIC nanoGUNE Consolider, 20018 Donostia-San Sebastián, Spain.

Email: (alejandro.diez@uam.es)

Tobacco Mosaic Virus (TMV) is the main reference virus model in plant virology due to its robustness, its simple structure and its importance as a tool for other research fields in biology. Here we used Atomic Force Microscopy (AFM) to characterize the mechanical properties of individual TMV particles through nanoindentations and mechanical fatigue in order to mimic the disassembly process of the protein capsid structure of the virus during infection. Results show that the mechanical disassembly induces and propagates cracks which is governed by aging. This process begins with the appearance of rifts throughout the entire viral structure but correlated in time with each other. At the same time, we have observed a tendency of the virions to disassemble into two different phases, especially at low forces, due the distribution of the mechanical stress is cushioned by the central hollow cavity, protecting the bottom half of the virion until the upper half has almost disappeared. Interestingly, mechanical disassembly also induces the gradual externalization of the viral genome in real time.

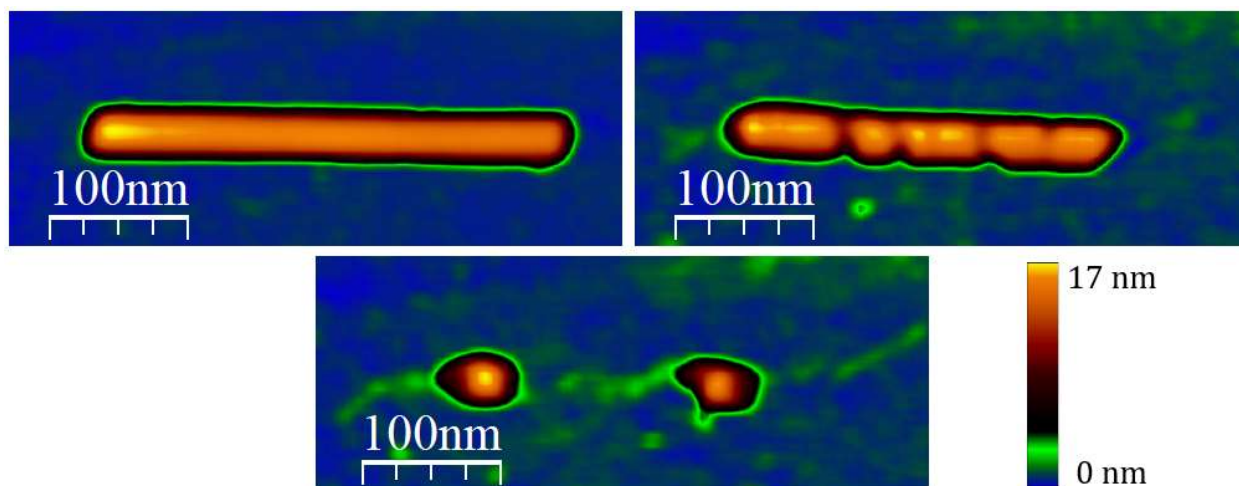


Figure 1. TMV fatigue sequence at 200pN. (A) Initial state of the virion. (B) Rifts appearances along the virion at frame sixty. (C) Final degradation stage where the release of the RNA can be appreciated (green horizontal line) after the disassembly of the protein capsid.

- [1] Bruinsma, R. F., Wuite, G. J. L., & Roos, W. H. (2021). Physics of viral dynamics. *Nature Reviews Physics*, 3(2), 76-91.
- [2] I. Horcas, R. Fernández, J.M. Gómez-Rodríguez, J. Colchero, J. Gómez-Herrero and A.M. Baró. *Review of Scientific Instruments* 78, 013705 (2007).
- [3] Scholthof, K. B. G. (2004). TOBACCO MOSAIC VIRUS: A Model System. *Annu. Rev. Phyto-pathol*, 42, 13-34.
- [4] Zhao, Y., Ge, Z., & Fang, J. (2008). Elastic modulus of viral nanotubes. *Physical Review E*, 78(3), 031914.

## Transport of active colloids in structured environments

Arin Escobar Ortiz<sup>1</sup>, Galor Geva<sup>1</sup>, Jose V. Alvarez<sup>1,2</sup>, Laura R. Arriaga<sup>1,2</sup> and Juan L. Aragonés<sup>1,2</sup>

<sup>1</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup>IFIMAC, Universidad Autónoma de Madrid, Madrid, Spain

Email: arin.escobar@uam.es

Transport of active or driven particles plays a crucial role in a multitude of processes ranging from biological systems to electrons in solids. In all these systems, transport is controlled by the structure and properties of the environment. Therefore, we are studying the physical principles that control the transport of active particles in structured environments to eventually be able to program their transport depending on their dynamics and environment structure.

Specifically, we study the two-dimensional transport of active rotating particles, or spinners, on a substrate containing arrays of fixed obstacles. In the absence of obstacles, the spinners just rotate in place [1]; however, in the presence of one or more fixed obstacles, the spinner translates due to the hydrodynamic coupling with the obstacles. We study the transport properties of spinners within different obstacles arrays. Contrary to the behavior of passive Brownian-diffusive colloids [2], we observe that the transport of spinners is enhanced in the presence of disorder on the positions of the obstacles. While the spinner is trapped at two different steady-state trajectories in square and triangular obstacle's lattices, spinner's transport is achieved even at small amounts of disorder on the obstacle's lattice positions. Thus, we analyze the role of disorder on the transport properties of spinners on these structured environments.

The disorder-induced transport mechanism here described is robust, and similar physical principles might be relevant to understand non-thermal transport processes in biological systems. Moreover, our model system is the first step in the design of a smart material for controlled transport and separation of colloidal particles based on their physicochemical properties, which will find applications in microfluidics and soft robotics.

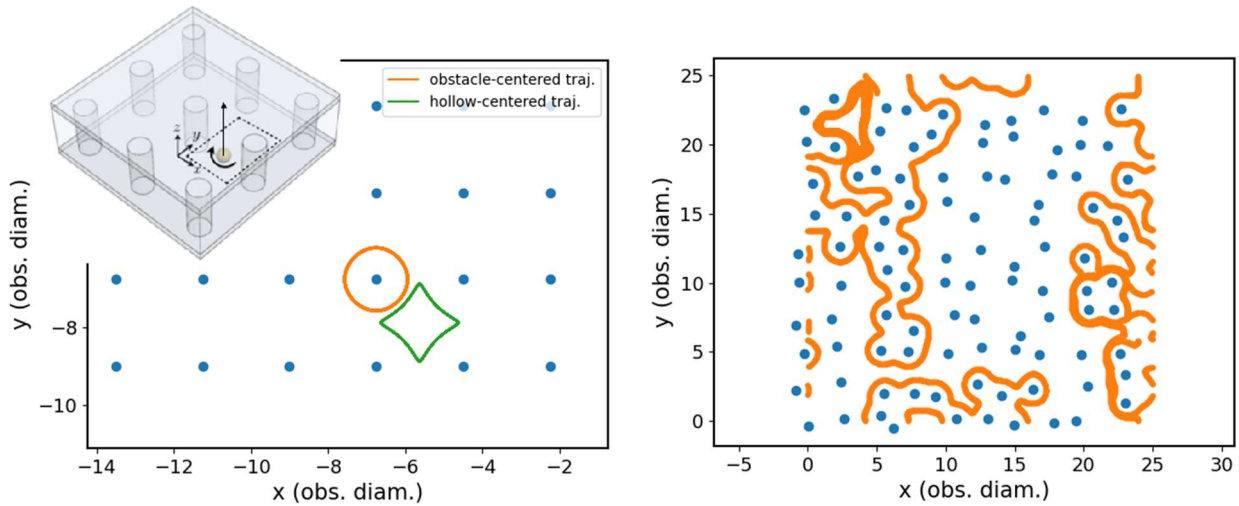


Figure 1: Left, upper-left corner: a simple diagram of the system. The colloidal particle rotates in place and moves between fixed obstacles in the XY plane. Left: the two possible steady-state trajectories in an ordered square lattice. Right: a trajectory in a square array where obstacles have undergone random Gaussian displacements in their positions, showing that disorder opens up the path for a wider range of spinner behaviours.

- [1] Aragonés, J. L., Steimel, J. P., & Alexander-Katz, A. (2016). Elasticity-induced force reversal between active spinning particles in dense passive media. *Nature Communications*, 7, 11325
- [2] Chakraborty, I., & Roichman, Y. (2020). Disorder-induced Fickian, yet non-Gaussian diffusion in heterogeneous media. *Physical Review Research*, 2(2).

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

J.J. Esteve-Paredes<sup>1</sup>, M. Malakhov<sup>2</sup>, A. Uría<sup>2</sup>, G. Cistaro<sup>2</sup>, A. Picón<sup>2</sup> and J.J. Palacios<sup>1,3</sup>

<sup>1</sup>*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain.*

<sup>2</sup>*Departamento de Química, Universidad Autónoma de Madrid, Madrid, Spain.*

<sup>3</sup>*Instituto Nicolás Cabrera (INC) and Condensed Matter Physics Center (IFIMAC).*

Email: [juan.esteve@uam.es](mailto:juan.esteve@uam.es)

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

### References:

- [1] G. Cistaro et al, "A theoretical approach for electron dynamics and ultrafast spectroscopy", arXiv:2207.00249 (Submitted - in revision, 2022).
- [2] J.J Esteve and J.J. Palacios, "A comprehensive study of the velocity, momentum and position matrix elements for Bloch states: application to a local orbital basis", arXiv:2201.12290 (In press, 2022).

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

Diego Caso<sup>1</sup>, Pablo Tuero<sup>1</sup>, Javier García<sup>1</sup>, Konstantin Y. Guslienko<sup>2,3,4</sup>, Farkhad G. Aliev<sup>1,5</sup>

<sup>1</sup>Departamento Física de la Materia Condensada C03, Universidad Autónoma de Madrid, Madrid 28049, Spain.

<sup>2</sup>Departamento Polímeros y Materiales Avanzados: Física, Química y Tecnología, Universidad del País Vasco, UPV/EHU, 20018 San Sebastián, Spain.

<sup>3</sup>EHU Quantum Center, University of the Basque Country, UPV/EHU, 48940 Leioa, Spain.

<sup>4</sup>IKERBASQUE, the Basque Foundation for Science, 48009 Bilbao, Spain.

<sup>5</sup>IFIMAC and INC, Universidad Autónoma de Madrid, Madrid 28049, Spain

Email: (diego.caso@uam.es)

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

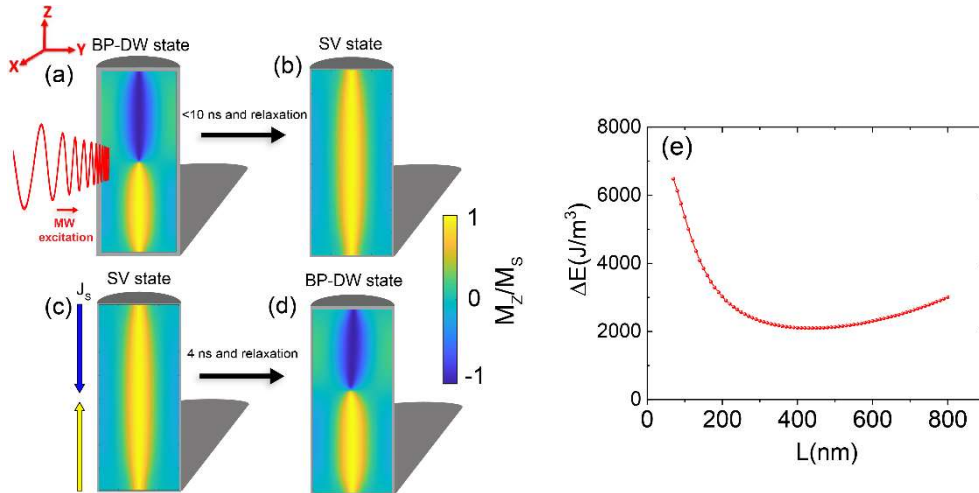


Figure 1. Cross section sequence of the  $m_z$  magnetization component of a 250 nm long NW, showing the used method to destroy the BP-DW state via a frequency-tuned mw field (a,b) and its posterior restoration using spin currents, (c,d). (e) Energy difference between the SV and BP-DW states against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

[1] F. G. Aliev et al., *Phys. Rev. B*, **79**, 174433 (2009).

[2] F. Tejo et al., *Sci. Rep.*, **11**, 21714 (2021).

# Vacuum-field-induced state mixing

D. Fernández de la Pradilla<sup>1,2</sup>, E. Moreno<sup>2</sup> and J. Feist<sup>2</sup>

*<sup>1</sup>Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC),  
Universidad Autónoma de Madrid, Madrid, Spain*

Email: (diego.fernandez@uam.es)

The properties of atoms and molecules undergo modifications due the electromagnetic vacuum, as described by the spontaneous decay rate and the Lamb shift. Through the presence of macroscopic bodies, the electromagnetic vacuum is altered, and the spontaneous decay and energy shifts can be changed [1]. Usually, this change is studied for each atomic state independently. However, when the size of the vacuum-induced perturbation becomes comparable to the bare atomic energy differences, an off-diagonal, environment-induced interaction between different states appears. Within the framework of macroscopic quantum electrodynamics [2], we develop a Lindblad master equation based on [3] that allows us to treat these interactions and use it to describe a hydrogen atom next to a dielectric nanoparticle. In this system, we explore the consequences of the off-diagonal terms regarding the effective atomic energies, decay rates and eigenstates. We observe strong modifications in both the atomic energies and decay rates, compared to the dynamics obtained with the usual diagonal model, and even behavior that contradicts the expected Purcell enhancement of the decay rates. As for the eigenstates, the original atomic states become now superposed to form the effective eigenstates. To quantify the amount of mixing, we use the so-called participation ratio. The large values we obtain indicate that the atomic structure at atom-nanoparticle separations of the order of 50 nm is no longer reminiscent of the bare hydrogen atom, and the effects we incorporate are crucial to properly describe the dynamics of the atom.

- [1] C.-H. Chang et al., ACS Photonics, **4**, 3098 (2017)
- [2] S. Scheel et al., Acta Physica Slovaca, **58**, 5 (2008)
- [3] G. McCauley et al., npj Quantum Information, **6**, 74 (2020)



# Silver nanoparticles chains as waveguides for ultra-long range fluorescence transport

Javier Fernández-Martínez<sup>1,3</sup>, Sol Carretero-Palacios<sup>1</sup>, Pablo Molina<sup>1</sup>, Jorge Bravo-Abad<sup>2,3</sup>, Mariola O Ramírez<sup>1,3</sup> and Luisa E. Bausá<sup>1,3</sup>

<sup>1</sup>*Dept. de Física de Materiales and Instituto de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049-Madrid, Spain*

<sup>2</sup>*Dept. de Física Teórica de la Materia Condensada Universidad Autónoma de Madrid, 28049-Madrid, Spain*

<sup>3</sup>*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049-Madrid, Spain*

Email: [javier.fernandezm@uam.es](mailto:javier.fernandezm@uam.es)

The manipulation and control of the emission properties of Rare Earth (RE) ions is nowadays a field of intense research due to the applicability of these emitters in a variety of technological fields such as sensing, green energy, bioimaging or quantum technologies [1, 2]. In this context, combining plasmonic nanostructures with RE-doped crystals has been revealed as an interesting approach, offering robust and integrable solid-state platforms with emergent functionalities at subwavelength scales. Among others, dual wavelength laser operation enabled by disordered plasmonic nanostructures in RE-doped crystals and plasmon-induced spatial coherence in Nd<sup>3+</sup> emitters have been recently demonstrated [3,4].

In this work, the association of plasmonic arrangements with RE ions is further exploited to demonstrate the possibility of guiding the fluorescence of Nd<sup>3+</sup> ions at ultra-long distances in the sub-wavelength regime by means of plasmonic chains of silver nanoparticles (NPs). Such nanostructures exhibit a spectrally broad longitudinal plasmonic mode with low ohmic losses, which extends from the VIS to the NIR region, overlapping most of the spectral regions in which Nd<sup>3+</sup> transitions occur.

The fluorescence guiding along the silver chains is monitored by means of a novel dual confocal fluorescence microscopy that enables the spatial separation of the excitation and emission beams. The possibility of sub-wavelength fluorescence propagation is demonstrated over tens of microns in the NIR spectral region in which Nd<sup>3+</sup> ions emit. Numerical simulations, based on the finite-difference time-domain method, are used to analyze the response of the plasmonic chain when excited by an oscillating dipole representing the Nd<sup>3+</sup> ion. The results are explained considering the near field coupling of the Nd<sup>3+</sup> emitting ions with the collective plasmon modes of the Ag NP chains.

The observed propagation range exceeds by an order of magnitude that of previous reports on electromagnetic energy transport using plasmonic NP chains, and holds promise for potential rare earth based optical circuits for quantum technologies and sensing applications

- [1] D. Serrano et al., Nature **603**, 241 (2022)
- [2] M. O Ramírez et al., Adv. Mater. **31**, 1901428 (2019)
- [3] L. Sánchez-García et al., Light Sci. Appl. **8**, 14 (2019)
- [4] J. Fernández-Martínez et al., Opt. Express **29**, 26244 (2021)

**Fernández-Lomana Gómez-Guillamón,  
Marta**

Física de la Materia Condensada

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

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

*<sup>1</sup> Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos,*

*Departamento de Física de la Materia Condensada,*

*Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC),*

*Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.*

*<sup>2</sup>Institute for Theoretical Physics, Goethe University Frankfurt,*

*Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany.*

*<sup>3</sup>Department of Physics & Astronomy, Iowa State University, Ames, IA 50011*

The  $1144 \text{ CaKFe}_4\text{As}_4$  compound is a pnictide superconducting material showing optimal superconducting critical temperature with  $T_c$  as large as 38 K [1,2]. There are no signatures of nematic, structural or magnetic transitions. Doping with Ni and Mn induces a decrease in  $T_c$  and the appearance of magnetism. Instead of the stripe like spin density wave (SSDW) antiferromagnetic order present in the 122 systems, Ni and Mn-doped  $\text{CaKFe}_4\text{As}_4$  shows a spin vortex (or hedgehog) magnetic order [3,4]. This is due to the lack of glide symmetry in the FeAs plane of the crystalline structure of the 1144 compounds. Here we present scanning tunneling microscopy experiments in pure, Ni-doped and Mn-doped  $\text{CaKFe}_4\text{As}_4$ . We have determined the superconducting density of states and observed the vortex lattice at very high magnetic fields up to 20 T. Atomic scale measurements show the appearance of a charge density wave order (CDW) induced by the magnetic field in  $\text{CaKFe}_4\text{As}_4$  above 10 T, which is also observed in the magnetic Ni and Mn-doped compounds at lower magnetic fields. The CDW has a periodicity of  $\sqrt{2} a_0 \times \sqrt{2} a_0$  where  $a_0$  is the lattice parameter. Our results suggest that Hedgehog magnetic order is accompanied by an asymmetric displacement of the of the As atoms giving rise to a CDW [5] and that the magnetic field reinforces Hedgehog antiferromagnetic correlations.

[1] K. Cho, A. Fente et al., Phys. Rev. B **95**, 100502(R) (2017).

[2] A. Fente et al., Phys. Rev. B **97**, 134501 (2018).

[3] W.R. Meier et al., npj Quantum Materials **3**, 5 (2018).

[4] M. Xu, P. C. Canfield et al., Phys. Rev. B **105**, 214526 (2022)

[5] W. Richard Meier. Growth, properties and magnetism of  $\text{CaKFe}_4\text{As}_4$ . PhD Tesis (Iowa State University Ames, Iowa, (2018).

# Functional Optimization of PVD-LiCoO<sub>2</sub> Cathodes for Li-Ion Batteries

Arturo Galindo<sup>1,2</sup>, María J. Ramirez-Peral<sup>1,3,4</sup>, Jesús Díaz-Sánchez<sup>3</sup>, Íñigo Salazar<sup>2</sup>, Herko van der Meulen<sup>4,5</sup>, Celia Polop<sup>3,4,6</sup>, Carmen Morant<sup>2,4</sup> and Enrique Vasco<sup>1</sup>

<sup>1</sup> Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Madrid, Spain

<sup>2</sup> Departamento de Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>3</sup> Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>4</sup> Instituto Universitario de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain

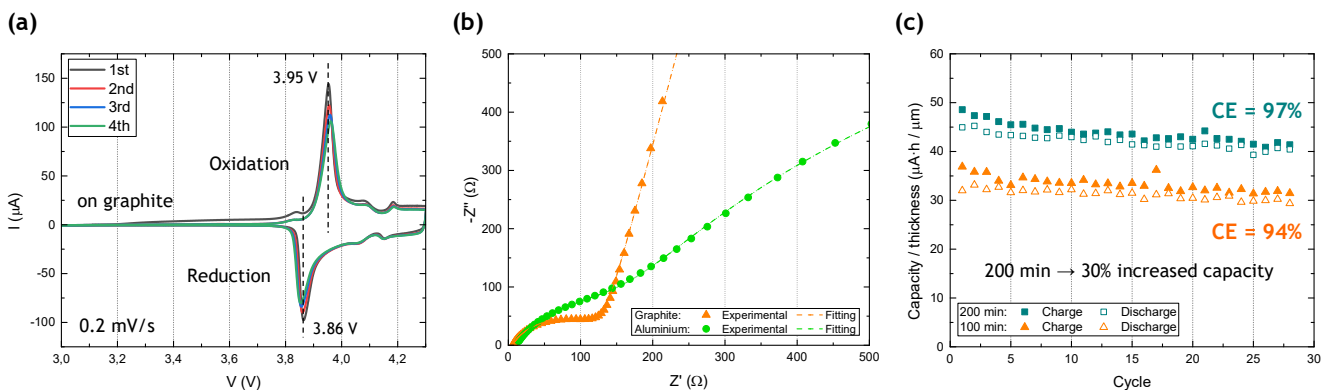
<sup>5</sup> Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain

<sup>6</sup> Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

Email: arturo.galindo.sanz@csic.es

In the context of limited resources and the increase in energy consumption, in addition to the high levels of pollution, the use and development of renewable energy sources becomes increasingly necessary. Many of these new technologies take advantage of intermittent and seasonal sources, such as the photovoltaic or wind industry, and therefore depend heavily on energy storage to be able to supply current consumption levels on a continuous basis. In this aspect, lithium-ion batteries (LIB) are nowadays one of the main options to fulfil this purpose and thus be part of a sustainable future [1]. The objective of this work is the optimization of the functional properties of thin film LiCoO<sub>2</sub> (LCO) cathodes prepared by Physical Vapor Deposition (PVD). LCO is a Li intercalation material with a high chemical potential introduced in 1991 by John B. Goodenough (Nobel Prize in Chemistry in 2019) and constitutes the first and the most commercially successful form of layered transition metal oxide cathodes [2]. In recent years, LCO cathodes have become especially attractive for the development of high-capacity solid-state LIBs, where electrodes with negligible chemical expansion coefficients are required to minimize the internal stresses that appear during the Li massive intercalation/deintercalation. Such stresses accumulate during charge/discharge loops and are responsible of the early degradation of these devices. From this perspective, the use of composite cathodes incorporating LCO, which is the only cathode material with a negative chemical expansion coefficient, provides an optimal solution [3].

The optimization is performed by correlating the functional properties of the films with its microstructure and composition. We prepare thin-film LCO cathodes by Pulsed Laser Deposition (PLD), a PVD technique, on graphite and aluminium foils. The deposition parameters are systematically modified to explore different growth temperatures, substrate materials, and film thickness. The deposited thin films are characterized in terms of microstructure and composition by Scanning Electron Microscopy (SEM) and micro-Raman Spectroscopy (Micro-RS), respectively. The LCO films deposited on the conductive foils are inserted into coin cell batteries operating in semi-cell configuration with metal Li as anode for their electrochemical characterization. Such a characterization comprises: Cyclic Voltammetry (CV) to identify the redox couple reaction (Fig.1.a), Electrochemical Impedance Spectroscopy (EIS) to study the transport mechanisms (Fig.1.b) and Cyclic Charge-Discharge (CCD) to test the cathode capacity (Fig.1.c). Finally, the functional parameters of the coin cell are correlated with the microstructure and composition of the LCO films in order to address how these affect battery performance. It is observed that the battery assembled from LCO grown on graphite foil with the highest thickness exhibits the better performance (charge capacity of 48.6  $\mu\text{A}\cdot\text{h}/\mu\text{m}$ , CE of  $97 \pm 1\%$ , and good electrochemical reversibility). These properties are related to an improvement in the proportion of the LCO phase in relation to the non-electrochemical active spinel Co<sub>3</sub>O<sub>4</sub> phase that results from Li losses in LCO during PLD.



**Fig. 1.** (a) CV curves of the first four cycles of the batteries assembled using LCO cathodes deposited on graphite, (b) EIS curves of the batteries assembled from LCO cathodes deposited on graphite and aluminium foils together with the fitting curves, and (c) CCD specific capacity as a function of cycles of the batteries assembled from LCO cathodes deposited for 100 minutes and 200 minutes on graphite.

- [1] D. CHOI et al., *Li-ion battery technology for grid application*, Journal of Power Sources, 511, 230419 (2021)
- [2] F. NING, S. LI, B. XU, C. OUYANG, *Strain tuned Li diffusion in LiCoO<sub>2</sub> material for Li ion batteries: A first principles study*, Solid State Ionics, 263, 46–48 (2014)
- [3] R. KOERVER et al., *Chemo-mechanical expansion of lithium electrode materials – on the route to mechanically optimized all-solid-state batteries*, Energy Environ. Sci., 11, 2142 (2018)

# Development of a technological AFM microscope for operation in UHV

D Gallego-Fuente<sup>1,\*</sup>, P Ares<sup>1,2</sup>, J Gomez-Herrero<sup>1,2</sup>

<sup>1</sup>*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain.* <sup>2</sup>*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain*

\*e-mail: daniel.gallego@uam.es

Atomic Force Microscopy (AFM) is a key tool for the study of nanoscopic systems. Since its invention in 1986[1], AFM research and development has been continuously in progress, including new measurement methods, new features and adapting to different environments in which to operate.

The majority of AFMs that operate in Ultra High Vacuum (UHV) are focused on the study of atomically resolved systems. However, they lack the versatility of more standard AFMs under ambient conditions. Here, we are tackling the development of a technological AFM operating in UHV but based on the same operation principles of standard AFMs, combining all their capabilities with those of standard UHV technology. Our setup will include advanced measuring modes, sample manipulation and lithography, as well as optical sample location.

To perform lithography, indentations, and general sample manipulation, a long-range XYZ scanner will be employed along with the beam deflection method for the force detection. Ultra-clean electrical nano-circuits will be fabricated by deposition and manipulation of gold nanowires under UHV conditions. Furthermore, the electrical characterization of such circuits will be possible under different contact schemes. On top of that, the combination with optical characterization approaches will allow the precise multidisciplinary study of nanoscopic defects in 2D materials.

In conclusion, this instrument will be a complementary and useful tool in relation with the existing systems, as well as being a stepping stone in the development of UHV-compatible SPM microscopy. Its simplicity in use and broad range of applicability will help to bridge the gap in the understanding of electrical, mechanical and optical properties at the nanoscale.

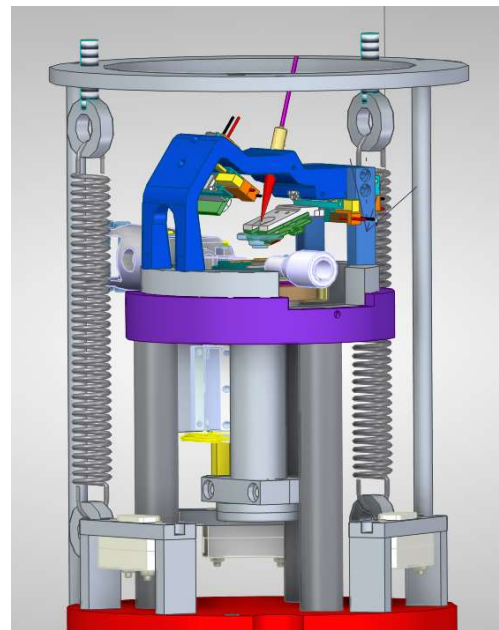


Figure 1. Technological AFM design with spring damping, including a long-range piezotube XYZ scanner, laser focuser and photodiode.

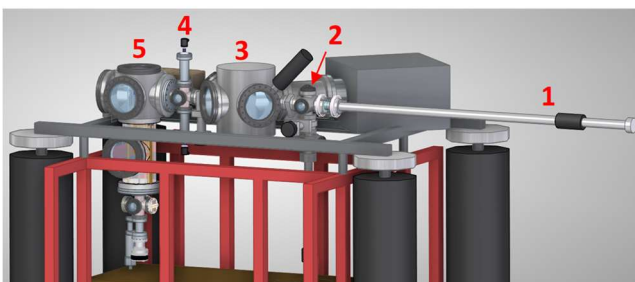


Figure 2. UHV system consisting (from right to left) of a transfer stage (1), insertion (2), preparation (3), multi tip and sample storage (4) and AFM (5) chambers.

[1] Binnig, G., Quate, C. F., & Gerber, C., *Physical Review Letters* **56**, 930 (1986).

# INC Research awards for Physics students 2022

García García, Jorge

Física de la Materia Condensada

## Optical interferometry as an efficient tool to characterize STM head vibrations

J. García García<sup>1,2</sup>, D. Expósito<sup>1</sup>, I. Brihuega<sup>1,2,3</sup><sup>1</sup>Departamento Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.<sup>2</sup>Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain<sup>3</sup>Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

Email: Jorge.garciagarcia02@estudiante.uam.es

Science and technology have evolved together in recent years. In this way, technological progress has allowed, among other things, the development of fundamental science. A clear example can be found in the invention of Scanning Tunnelling Microscopy (STM), a powerful experimental technique that can be considered as the first experimental realization of nanotechnology. Since the very early days, the UAM has been one of the key actors in the development of the STM, with the first STM existing outside of the IBM laboratories in Zurich, where it was invented in 1981 [1], being placed at the UAM. Here, the first scientific results were already achieved in 1985 [2], one year before the inventors of STM were awarded with the Nobel Prize by their instrumental development.

The main contribution of STM resides in its capability to visualize the properties of surfaces with atomic resolution. This is possible thanks to the quantum tunnelling effect between the tip of the microscope and the sample to be studied, which is the working principle of STM. This great resolution comes with a prize, one must be able to construct a microscope which is able to maintain a fixed tip-sample distance with picometer precision.

This makes necessary to attenuate all the vibrations from the micrometer scale noise coming from the floor, to the final picometer one, which implies an attenuation of 6 orders of magnitude. To achieve this, the STMs are designed with different damping stages, being the last one the head of the STM itself.

In this work, I present a new approach to efficiently optimize the design of STM heads, by the rapid evaluation of the vibrations attenuation taking place in this crucial last stage, by means of optical interferometry. This is currently being applied in our lab, to design a new STM head that incorporates an inertial sample stage with a 5x5mm<sup>2</sup> X/Y motion capability, with a reproducibility in the nanometer range.

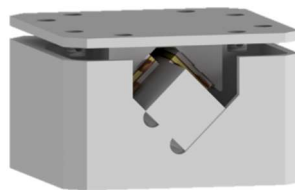


Figure 1. 3D drawing of the new design of the inertial X/Y sample stage

[1] Binning, G, et al Helv. Phys Acta 55, 726 (1982)

[2] A.M. Baró et al, Nature 315,253(1985)

# INC Research awards for Physics students 2022

García González, Asier

Física Aplicada

## Effect of the integration of magnetic nanoparticles in electrodes of lithium ion batteries.

A. García, E. Martín Rodríguez <sup>1</sup> and C. Morant<sup>1</sup>

*<sup>1</sup>Departamento de Física Aplicada, Universidad Autónoma de Madrid*

Email: [asier.garcia@estudiante.uam.es](mailto:asier.garcia@estudiante.uam.es)

In recent years, the search for new electrode materials for rechargeable lithium-ion batteries has undergone a drastic change thanks to nanomaterials. This is caused by the fact that nanometer-sized materials are much less limited by their ionic or electronic conductivities than bulk materials. Nanomaterials can also withstand much higher mechanical stress during charge/discharge cycles. In general, these favorable effects significantly broaden the variety of inorganic compounds that can be used as storage media for Li and Na ions.

In this work we have studied the effect of adding nanoparticles with magnetic properties, particularly iron oxides, to the electrodes of lithium-ion batteries. We have begun by learning methods used for the manufacture and characterization of lithium batteries and by synthesizing iron oxide nanoparticles by coprecipitation methods. Then we have prepared electrode composites by mixing FeOx nanoparticles with carbon nanotubes (CNTs), by vacuum filtration method. We have assembled Li-ion batteries and we have studied how the properties of the iron oxide nanoparticles affect the response of the battery.

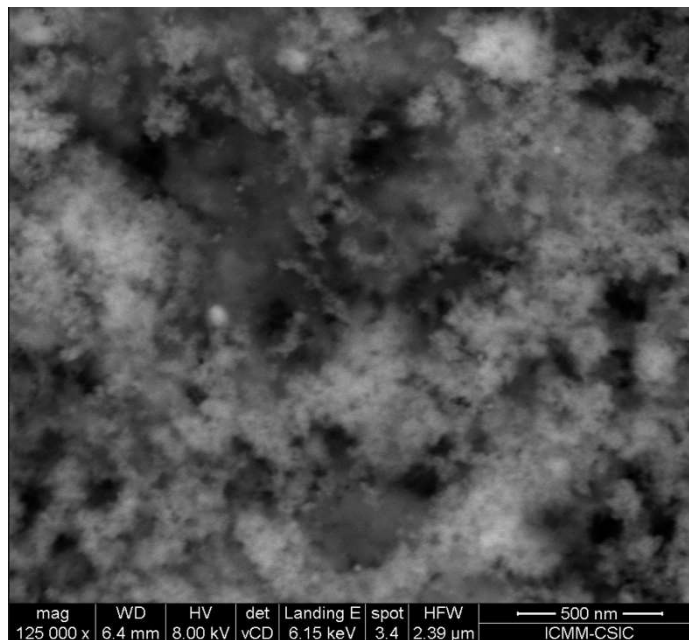


Figure 1. Surface SEM image of the FeOx-CNT composite electrode.

The electrodes synthesized in this work showed high specific capacity and durability, over 100 cycles at a current intensity of 500 mA/g, proving that iron oxides nanoparticles are a promising, inexpensive, ecofriendly alternative for Li ion battery electrodes



# INC Research awards for Physics students 2022

García Herreros, Sergio

Física Teórica de la Materia Condensada

## Neural networks for simultaneous quantum parameter estimation

Sergio García Herreros<sup>1,2</sup> and Carlos Sánchez Muñoz<sup>1,2</sup>.<sup>1</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049, Madrid, Spain.<sup>2</sup>Instituto Universitario de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049, Madrid, Spain.

Email: SERGIO.GARCIAH@ESTUDIANTE.UAM.ES

We have studied the implementation of a neural network for the simultaneous estimation of two quantum parameters. A driven-dissipative system based on Rabi-Oscillations was employed [1]. We generated photodetection registers using Monte Carlo methods in order to train and the test the neural network [1]. To asses the performance, that same data was analyzed using the Fisher information in order to set a benchmark [2]. The network estimations are reasonably good since they are close to that of the Fisher information.

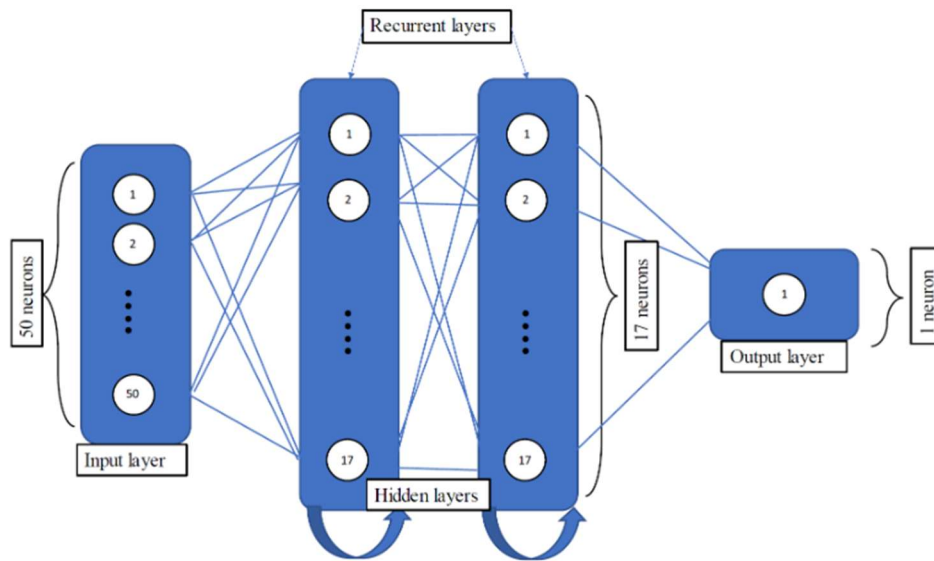


Figure 1. Recurrent neural network used.

[1] C. Gerry and P. Knight, *Introductory Quantum Optics*. Cambridge University Press (2004).[2] A. H. Kiilerich and K- Mølmer. *Estimation of atomic interaction parameters by photon counting*. Phys. Rev. A. **89**, 052119 (2014).

## Hydrogenated amorphous silicon thin film as electrode for lithium-ion batteries

Tomás García<sup>1</sup>, Carmen Morant<sup>1</sup>, Rocío Barrio<sup>2</sup> and Nieves González<sup>2</sup>

*<sup>1</sup>Department of Applied Matter Physics, Instituto de Ciencias de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid (UAM), Madrid, Spain*

*<sup>2</sup>Cento de Investigaciones Energéticas, Medioambientales y Tecnologías (CIEMAT), Madrid, Spain*

Email: ( [tomas.garcia@estudiante.uam.es](mailto:tomas.garcia@estudiante.uam.es) )

One of the keys to soften the impact of the current energy crisis we are facing is the improvement in the storage capacity and transport of electrical energy. Lithium-ion batteries (LIBs) are one of the most used and marketed devices for this purpose. Traditionally, LIBs have incorporated graphite anodes with a great stability but a maximum specific capacity around 370 mAh/g, which is lower than demanded. A sound alternative are thin film silicon anodes, which reach experimental capacities higher than 2000 mAh/g [1]. Nevertheless, the crystalline silicon (c-Si) degrades readily and exhibits loss of electrical contact and capacity due to the huge volumetric changes (greater than 300%) that it suffers during the battery charge and discharge. By comparison, it is thought that the amorphous nature of the hydrogenated amorphous silicon (a-Si:H) and its high porosity could avoid the enormous changes of volume during the lithiation in order to increase the life of the LIBs.

The aim of this project is to make an electrochemical characterization of LIBs with different thin film a-Si:H electrodes, grown by Plasma Assisted Chemical Vapour Deposition (PECVD) [2], in order to study how the thickness of the thin film and the hydrogen concentration affect to the anode degradation.

As a global result, the batteries studied with a-Si:H anodes have presented initial specific capacity values between 2,000 mAh/g and 3,500 mAh/g, which gradually decays with cycle number. About the thickness study, a tendency towards stability has been observed for greater thickness in a range between 0.5 and 1  $\mu\text{m}$ . Concerning hydrogen concentration, the analysis has shown that the anode stability decreases with increasing the poli-hydride concentration (hydrogen arranged as Si-H<sub>x</sub>) in a range between 0% and 26%. These tendencies encourage a more exhaustive study of the thickness and suggests limiting the poli-hydride presence during the material growth for future research.

[1] Mukanova, Aliya, et al. "A mini-review on the development of Si-based thin film anodes for Li-ion batteries." *Materials Today Energy* 9 (2018): 49-66.

[2] Rodríguez, José Domingo Santos. *Desarrollo y caracterización de dispositivos fotovoltaicos pin de silicio amorfo depositados por PECVD*. Diss. Universidad Complutense de Madrid, 2012.

# Characterization of $\text{FeSe}_{0.7}\text{S}_{0.3}$ with Scanning Tunneling Microscopy

**Pablo García<sup>1</sup>, Raquel Sanchez-Barquilla<sup>1</sup>, Francisco Martín Vega<sup>1</sup>, Edwin Herrera<sup>1,2</sup>, Hermann Suderow<sup>1,2</sup> and Isabel Guillamón<sup>1,2</sup>**

<sup>1</sup>*Laboratorio de Bajas Temperaturas, Departamento de Física de la Materia Condensada, Instituto de ciencia de Materiales Nicolás Cabrera, Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049*

<sup>2</sup>*Unidad Asociada de Bajas Temperaturas y Altos Campos Magnéticos, UAM, CSIC, Cantoblanco, E-28049 Madrid, Spain*

Email: pablo.garcia@estudiante.uam.es

Iron based superconductors show unconventional superconductivity, along with several ordered phases at low temperature, such as nematicity, where the rotational symmetry is broken, or an antiferromagnetic phase. Among these materials, FeSe is of particular interest since it does not display any magnetic order at ambient pressure and allows the study of both superconductivity and nematicity. FeSe undergoes a structural transition from tetragonal to orthorhombic at around 90 K, and becomes superconducting below 8.5 K. While the nematic phase in FeSe can be suppressed by applying pressure, an antiferromagnetic state also appears. However, by doping with S, the compound  $\text{FeSe}_{1-x}\text{S}_x$  has its nematic phase completely suppressed at  $x \approx 0.17$  at ambient pressure, with no emerging magnetic order. Here, we study the superconducting properties of  $\text{FeSe}_{1-x}\text{S}_x$  with a sulfur concentration of  $x=0.29$ , which places it in the tetragonal regime. We also applied several magnetic fields along the c axis of the unit cell, observed the vortex lattice of this material and measured the superconducting gap both in the core and outside the vortices.

- [1] Y. Mizuguchi, et al., Journal of the Physical Society of Japan, 78, 074712 (2009).
- [2] S. A. Moore, J. L. Curtis, C. Di Giorgio et al. Physical Review B 92, 235113 (2015)
- [3] T. Hanaguri, K. Iwaya, Y. Kohsaka et al. Science Advances, 4 (2018).
- [4] P. Wieck et al. Physical Review B, 98, 020507 (2018)
- [5] M. Bristow, P. Reiss, A. A. Haghighirad et al. Physical Review Research 2, 013309 (2020)
- [6] F. M. Vega, Ph.D. dissertation, (2021).

## Collective behavior in driven colloidal crystals

G. Geva<sup>1,2,3</sup>, N.C.X. Stuhlmüller<sup>4</sup>, J.L. Aragones<sup>1,2,3</sup>, L.R. Arriaga<sup>1,2,3</sup> and D. De Las Heras<sup>4</sup>

<sup>1</sup>*Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain*

<sup>2</sup>*Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain*

<sup>3</sup>*IFIMAC, Universidad Autónoma de Madrid, Madrid, Spain*

<sup>4</sup>*University of Bayreuth, , Germany*

Email: galor.geva@uam.es

Micron-size solid particles self-assemble into higher order structures when suspended in a fluid medium; this property makes them excellent model systems to mimic atoms or molecules and their interactions [1]. A prominent example is the formation of colloidal crystals, which have attracted considerable attention due to their potential applications in photonics [2]. The properties of these colloidal crystals at equilibrium have been intensively investigated; however, the properties of this material out of equilibrium are yet to be determined. Therefore, we are considering the properties and dynamical behaviors of colloidal crystal in which their constituents are active. Specifically, we study a system composed by superparamagnetic colloidal particles that rotate under the actuation of an external magnetic field. We observe that above critical rotational frequency of the magnetic field, the particles aggregate forming clusters of particles that grow in time. We study the structure and dynamics of these active crystals and analyze the emergent collective behaviors.

[<sup>1</sup>] de Gennes, P-G, Soft Matter (Nobel Lecture). *Angew. Chem. Int. Ed.* **31**, 842 (1992).

[<sup>1</sup>] Wang, Y. et al. Colloids with valence and specific directional bonding. *Nature* **490**, 51–55 (2013).

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

Celia González Sánchez<sup>1</sup>, J. Cuadra<sup>1</sup>, V. Barrena<sup>1</sup>, A. Spuri<sup>2</sup>, E. Scheer<sup>2</sup>, H. Suderow<sup>1</sup>, A. di Bernardo<sup>2</sup>, E. J. H. Lee<sup>1</sup>

<sup>1</sup> Condensed Matter Physics Department, Universidad Autónoma de Madrid, Spain.,

<sup>2</sup> Department of Physics, Universität Konstanz, Germany.

Email: celia.gonzalezs@uam.es

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 steps towards the fabrication of nanodevices based on NbSe<sub>2</sub>, including our first attempts to fabricate Josephson junctions with and without ferromagnetic and antiferromagnetic tunnel barriers

- [1] N. Yabuki et al., Nat. Commun., **7**, 10616 (2016)
- [2] S. Kezilebieke et al, Nature, **588**, 424–428 (2020)
- [3] H. Idzuchi et al., Nat. Commun., **12**, 5332 (2021)
- [4] K. Kang et al., arXiv: 2201.09185
- [5] L. Ai et al., Nat. Commun., **12**, 6580 (2021)
- [6] K. Kang et al., Nano Lett., **22**, 5510-5515 (2022)

Figure 1. (a) Temperature dependent PL spectrum of a GaP<sub>1-x</sub>N<sub>x</sub> layer with x = 0.012 grown at 550 °C. (b) PL peak energy as a function of temperature. The black line represents a fit to Pässler's equation and the red line the temperature dependent bandgap according to the BAC model taken C<sub>NM</sub> equal to 3.05 eV. (c) Integrated PL intensity as a function of 1/k<sub>B</sub>T. The blue line is a fit of eq.(1) to the experimental data. The fit yields activation energies of 13 and 63 meV.

# Superconducting spintronics in epitaxial Fe/MgO/V junctions with spin-orbit interaction.

César González-Ruano<sup>1</sup>, Diego Caso<sup>1</sup>, Pablo Tuero<sup>1</sup>, Coriolan Tiusan<sup>2</sup>, Chenghao Shen<sup>3</sup>, Jong Han<sup>3</sup>, Igor Zutic<sup>3</sup>, Jacob Linder<sup>4</sup>, Farkhad G. Aliev<sup>1</sup>.

<sup>1</sup>Departamento Física de la Materia Condensada C-III, Universidad Autónoma de Madrid, Madrid 28049, Spain.

<sup>2</sup>Center of Superconductivity Spintronics and Surface Science C4S, Technical University of Cluj-Napoca, Romania.

<sup>3</sup>State University of New York, Buffalo, New York 14260, USA

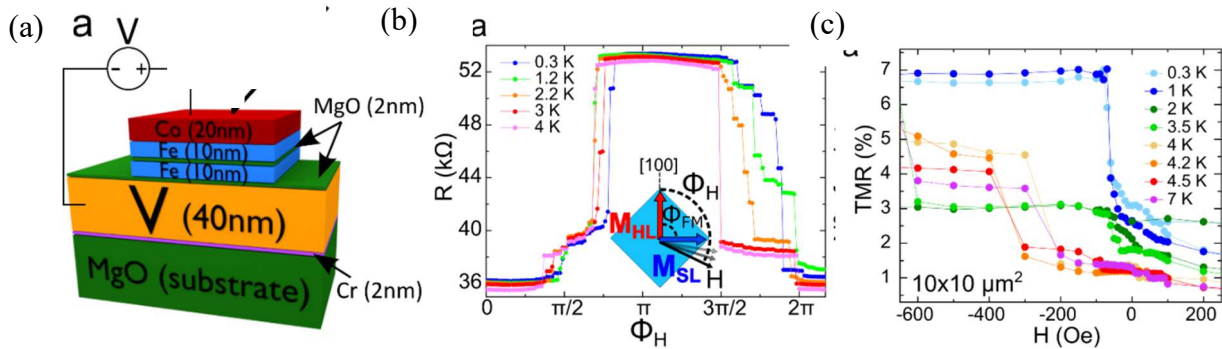
<sup>4</sup>Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Email: cesar.gonzalez-ruano@uam.es

Generation and control over long-range triplet (LRT) Cooper pairs is a key milestone for applications in superconducting spintronics. These proximity effects were thought to require complex ferromagnetic multilayers, non-collinear magnetization or half-metals. With our work, we propose a new platform compatible with commercial spintronics.

We have studied epitaxial V/MgO/Fe junctions with competing magnetic anisotropies and interfacial spin-orbit coupling. First, we demonstrated a 1000x increase in tunneling anisotropic magnetoresistance below the V critical temperature ( $T_C$ ), supporting magnetization-dependent LRT formation [1]. Then we studied the converse effect: the superconductivity-induced transformation of the magnetocrystalline anisotropies of Fe, with both the in-plane and out-of-plane anisotropies being modified in the superconducting state as a result of the free energy of Fe being affected by the magnetization-dependent generation of LRTs [2,3]. Further evidence for LRT generation comes from the below-gap noise signal of the junctions, which shows a giant increase in the Fano factor that can't be explained in a system with a single superconductor. This suggests the presence of a proximity-induced gap in the Fe layer that makes the system effectively behave as a Josephson junction. In addition, the TMR of the junctions shows a steady increase reaching record high values above 0.5 V, both at cryogenic and room temperatures [4].

Our findings, supported by theoretical and numerical modelling, offer the ability to control the transport and interaction between ferromagnets and superconductors, including the generation of triplet Cooper pairs - a key step in designing future cryogenic magnetic memories.



(a) sketch of the samples. (b) In-plane field rotations above and below  $T_C$  showing the superconductivity-induced magnetic states. (c) Out-of-plane TMR showing the spontaneous reorientation below  $T_C$ .

- [1] I. Martínez et al; Phys. Rev. Appl. **13**, 014030 (2020).
- [2] C. González-Ruano et al; Phys. Rev. B, **102**, 020405(R) (2020).
- [3] C. González-Ruano et al; Sci. Rep. **11**, 19041 (2021).
- [4] C. González-Ruano et al; Adv. Electronic Materials **8**, 2100805 (2021).



# Q-switched plasmonic solid-state nanolasers assisted by 2D transition metal dichalcogenides

D. Hernández-Pinilla<sup>1,4</sup>, P. Molina<sup>1,4</sup>, G. López-Polín<sup>1</sup>, J. H. Al Shuhaib<sup>1</sup>, F. Leardini<sup>1,4</sup>, H. Yan<sup>2</sup>, Y. Wang<sup>2</sup>, S. Sarkar<sup>2</sup>, M. Chhowalla<sup>2</sup>, P. Ares<sup>2,3,4,5</sup>, J. Gómez<sup>3,4,5</sup>, M. O Ramírez<sup>1,4,5</sup>, L. E. Bausá<sup>1,4,5</sup>

<sup>1</sup>Dept. Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup>Dept. of Materials Science & Metallurgy, University of Cambridge, Cambridge, UK

<sup>3</sup>Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>4</sup>Instituto de Ciencia de Materiales Nicolás Cabrera y <sup>5</sup>Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain

Email: david.hernandezp@uam.es

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

Here, we combine a solid-state gain media with plasmonic chains of metallic nanoparticles and with a two-dimensional (2D) transition metal dichalcogenide (TMD) to simultaneously achieve temporal and spatial confinement of the laser gain in a hybrid monolithic architecture (Fig 1). Namely, the hybrid system combines a Nd<sup>3+</sup>-doped solid-state crystal which provides laser gain in the NIR spectral region, plasmonic chains of Ag nanoparticles that enables subwavelength spatial confinement of laser radiation, and a 2D TMD acting as saturable absorber to achieve the temporal confinement of laser radiation by means of passive Q-switch. Different configurations are analyzed demonstrating stable laser pulse trains in the ns and  $\mu$ s temporal domain with subwavelength spatial confinement at room temperature. The results are relevant for applications such as photolithography for ultra-small motif size fabrication, ultra-compact integrated circuits or biodetection, with the added value of reduced energy consumption.

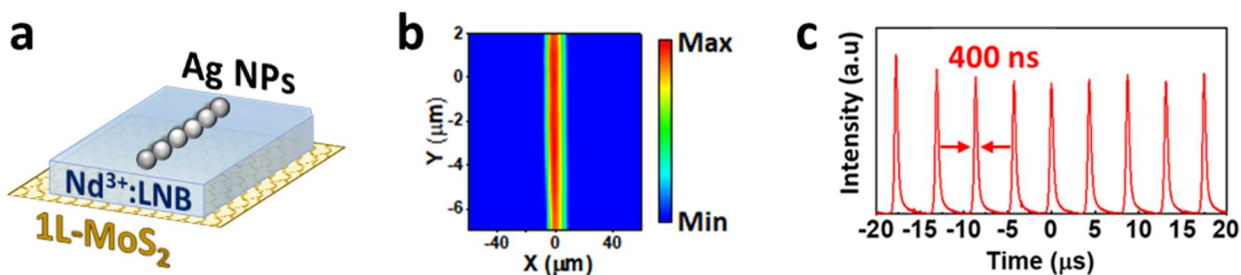


Figure 1. a) Schematics of the monolithic architecture for pulsed nanolasing. The hybrid system includes: Nd<sup>3+</sup>-doped LiNbO<sub>3</sub> as a gain media, plasmonic Ag nanoparticle chains for sub-wavelength spatial confinement, and 1-layer MoS<sub>2</sub> for temporal confinement of laser radiation. b) Spatial distribution of the laser emission confined in the vicinities of a single Ag nanoparticle chain. c) Temporal evolution of laser emission.

- [1] R-M. Ma, R. F. Oulton, Nature Nanotechnology, **14**, 12-22 (2019).
- [2] D. Hernández-Pinilla et al, ACS Photonics, **5**, 406-412 (2018).
- [3] M. O Ramírez et al., Advanced Materials, **31**, 1901428 (2019).

## INC Research awards for Physics students 2022

Inglés Cerrillo, Julia

Física Aplicada

---

### Study of the plasmonic resonance of nanoparticles based on liquid metals with a high degree of ordering

J. Inglés<sup>1,2</sup>, N. Gordillo<sup>1,2,3</sup>

<sup>1</sup> *Laboratorio de Microelectrónica, Dpto. Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain*

<sup>2</sup> *Centro de Micro-Análisis de Materiales (CMAM), Universidad Autónoma de Madrid, Madrid, Spain*

<sup>3</sup> *Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain*

*Email: julia.ingles@estudiante.uam.es*

Of the wide family of plasmonic materials currently available, metallic 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 such as In and Ga, evaporated on nanostructured patterns that allow the nanoparticles to be organized and produce uniform and adjustable sizes.

[1] N. Gordillo et al., *Nanotechnology* **30** 475705 (2019)

[2] S. Catalán-Gómez et al., 2018 *Nano Futures* **2** 041001(2018)

# Highly defective MoS<sub>2</sub> ultrathin nanoflakes for electrolytic hydrogen production

N. Jiménez-Arévalo<sup>1</sup>, J. Hussein Awadh Al Shuhaib<sup>1</sup>, R. Bautista Pacheco<sup>1</sup>, D. Marchiani<sup>2</sup>, M. M Saad Abdelnabi<sup>2</sup>, R. Frisenda<sup>2</sup>, M. Grazia Betti<sup>2</sup>, C. Mariani<sup>2</sup>, Y. Manzanares<sup>3</sup>, C. Gómez Navarro<sup>3,4</sup>, A. Martínez Galera<sup>1,4</sup>, J. Ramón Ares<sup>1</sup>, I. Jiménez Ferrer<sup>1,4</sup>, F. Leardini<sup>1,4</sup>

<sup>1</sup> Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup> Dipartimento di Fisica, Sapienza Università di Roma, Roma, Italy

<sup>3</sup> Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain.

<sup>4</sup> Instituto Nicolas Cabrera, Universidad Autónoma de Madrid, Madrid, Spain

Email: [nuria.jimenez@uam.es](mailto:nuria.jimenez@uam.es)

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 is the first to report the growth of highly homogeneous nanostructured MoS<sub>2</sub> over large area substrates (of about 1cm<sup>2</sup>). We have also shown that the introduction of a 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 other reported work [2].

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 possibility of growing homogeneous thin films, which brings applications closer.

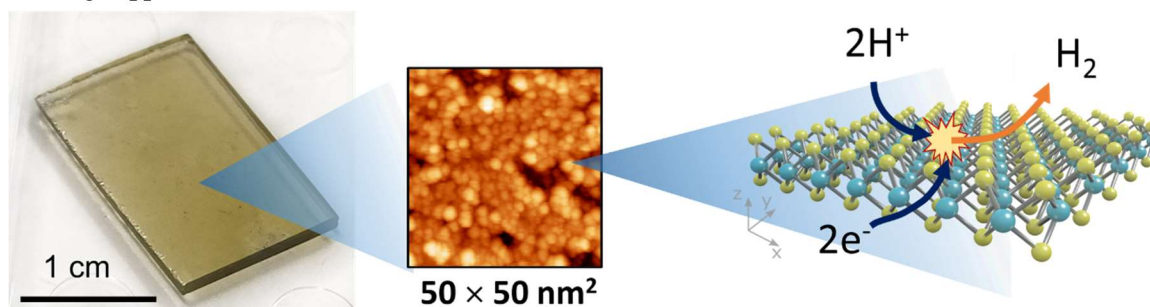


Figure 1. From left to right: Photograph of one MoS<sub>2</sub> layer grown on quartz that shows high homogeneity. STM image which evidences the nanoflake structure of our layers. Schematic of hydrogen production on the 2H-MoS<sub>2</sub>.

[1] J. Zhu, et al. "Boundary activated hydrogen evolution reaction on monolayer MoS<sub>2</sub>", Nature Communications, **10**, 1-7 (2019).

[2] H. Li, et al. "Activating and optimizing MoS<sub>2</sub> basal planes for hydrogen evolution through the formation of strained sulphur vacancies." Nature materials, **1**, 48-53 (2016)

# INC Research awards for Physics students 2022

Köhler Ruiz, Elena

Física de Materiales

## Growth and characterization of $\text{Sr}_{1+X}\text{TiS}_{3-Y}$ perovskite thin films

Elena Köhler<sup>1</sup>, Jinan H. Al Shuhaib<sup>1</sup>, J.J. Peinado-Pérez<sup>2</sup>, M.C. López-Escalante<sup>2</sup>, Isabel J. Ferrer<sup>1,3</sup>, Fabrice Leardini<sup>1,3</sup>

<sup>1</sup> Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

<sup>2</sup> Departamento de Ingeniería Química, Universidad de Málaga, E-29010 Málaga, Spain

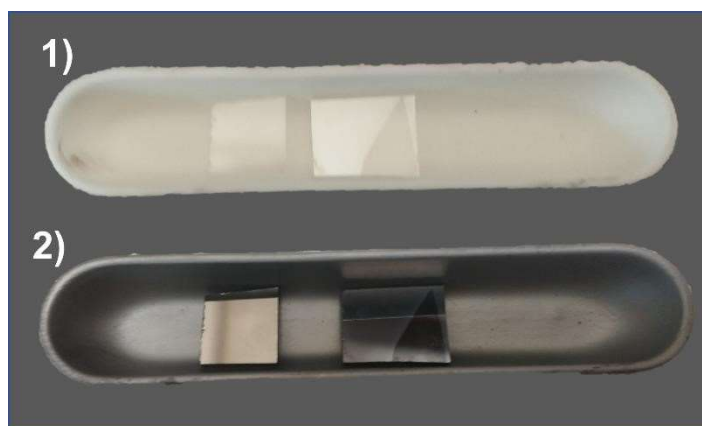
<sup>3</sup> Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain.

E-mail: [elena.kohler@estudiante.uam.es](mailto:elena.kohler@estudiante.uam.es)

Inorganic chalcogenide perovskites are semiconductors with the general formula  $\text{ABX}_3$ , with A being a group II cation (i.e.,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ , or  $\text{Ba}^{2+}$ ), B a group IV transition metal (i.e.,  $\text{Ti}^{4+}$ ,  $\text{Zr}^{4+}$ , or  $\text{Hf}^{4+}$ ), and X a chalcogen anion ( $\text{S}^{2-}$  or  $\text{Se}^{2-}$ ). These materials have recently attracted significant attention, due to their promising optoelectronic properties in the visible and infrared regions, with good thermal stability, composed of non-toxic and abundant elements. These unique properties make chalcogenide perovskites promising candidates for many applications, such as photonic, optoelectronic, and energy harvesting. Some of these compounds have been poorly investigated to date. For instance, only a few works deal with the synthesis and characterization of  $\text{Sr}_{X+1}\text{TiS}_{3-Y}$  (STS hereafter) powders. Here we present a novel synthesis procedure to obtain STS thin films.

STS films have been obtained by sulfurization of  $\text{SrTiO}_3$  (STO hereafter) layers prepared by Magnetron Sputtering onto quartz substrates. The sulfurization process has been carried out using two different methods. The first method consists of a reaction between  $\text{CS}_2$  and STO thin films inside a closed quartz ampoule. The second procedure has been accomplished in a tubular quartz reactor under  $\text{CS}_2$  flow. For this purpose, different flow lines and shut-off valves have been installed, which allow gases to flow through different conduits and purge the system in sections. An  $\text{Ar}/\text{H}_2$  mixture (95%-5%) has been used as the carrier gas by passing it through a bubbler containing  $\text{CS}_2$ . The small  $\text{H}_2$  concentration is used to detect possible leaks before starting the sulfurization process and as a reduction agent during the reaction.

The structure, chemical composition and morphology of the STS thin films have been analyzed using different techniques, such as glazing-angle x-ray diffraction, Raman spectroscopy and scanning electron microscopy coupled to energy-dispersive x-ray analysis. In addition, optical properties of the films have been characterized by transmittance and diffuse reflectance measurements. The results of these characterizations indicate that the obtained STS films present a semiconducting nature and can be of interest in renewable energy applications, in particular in photoelectrolytic water splitting for  $\text{H}_2$  production.



**Figure 1.** Pictures of a  $\text{SrTiO}_3$  thin film and a bare quartz substrate (to the left) inside an alumina crucible before (1) and after (2) the sulfurization process with a  $\text{CS}_2$  flow.

# Cavity mediated energy transfer driven by a photochemical reaction

A. Cargioli<sup>1,2</sup>, M. Lednev<sup>3</sup>, L. Persano<sup>1</sup>, F.J. García-Vidal<sup>3</sup>, J. Feist<sup>3</sup>, A. Tredicucci<sup>1,2</sup>

<sup>1</sup> NEST Lab., CNR—Istituto di Nanoscienze and Scuola Normale Superiore, Piazza San Silvestro 12, Pisa 56217, Italy

<sup>2</sup> Dipartimento di Fisica, Università di Pisa, Largo Pontecorvo 3, Pisa 56127, Italy

<sup>3</sup> Dep. de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Email: maksim.lednev@uam.es

Light-matter interaction between molecules and confined electromagnetic fields is of great interest because it allows the modification of fundamental properties of the coupled system. This effect has been exploited for several different applications, such as low-threshold Bose-Einstein condensation and lasing [1-3], cavity-modified photochemical reactivity [4], and (long-range) energy transfer between donor and acceptor molecules [5-8]. By placing a donor-acceptor pair in a microcavity, delocalized polariton states are formed if the strong coupling condition is met. In this case, the efficiency of resonant energy transfer from the donor to the acceptor is changed, as a result of the appearance of new relaxation channels.

Here we investigate how a photochemical reaction of donor molecules can affect the efficiency of the energy transfer process. We first demonstrate the strong coupling regime between the chromophores and the cavity mode. Using UV illumination, we drive a photochemical reaction of the donor molecules that allow us to modify the hybrid light-matter states. By tuning the time of UV illumination, we obtain a significant enhancement of the emission intensity from the acceptor excitonic reservoir as compared to the outside-cavity case. We also present a theoretical explanation of the physical mechanism behind this experimental finding and we discuss a new way to achieve controllable modification of cavity-mediated energy transfer based on this fundamental knowledge.

- [1] S. Kena-Cohen et al., Nat. Photonics, **4**, 371. (2010)
- [2] J. D. Plumhof et al., Nat. Mater., **13**, 247. (2013)
- [3] M. Ramezani et al., Optica, **4**, 31. (2017)
- [4] J. A. Hutchison et al., Angew. Chem. Int. Ed. **51**, 1592 (2012)
- [5] D. M. Coles et al., Nat. Materials, **13**(7), 712–719 (2014)
- [6] X. Zhong et al., Angew. Chem., Int. Ed., **56**, 9034–9038 (2017)
- [7] K. Georgiou et al., ACS Photonics, **5**(1), 258–266 (2018)
- [8] S. Satapathy et al., Science Adv. **7**, eabj0997 (2021)

## Bovine serum albumin and Rose Bengal decorated gold nanoparticles for photodynamic therapy applications

Gabriel López-Peña<sup>1</sup>, Tamara Muñoz-Ortiz<sup>2</sup>, Emma Martín Rodríguez<sup>1,3</sup> and María J. Marín<sup>4</sup>

<sup>1</sup>Dpto. Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain

<sup>2</sup>Instituto Investigación Sanitaria Princesa (IIS-IP), Universidad Autónoma de Madrid, Madrid, Spain

<sup>3</sup>Nanomaterials for Bioimaging Group, Universidad Autónoma de Madrid, Madrid, Spain

<sup>4</sup>School of Chemistry, University of East Anglia, Norwich Research Park, NR4 7TJ, Norwich, United Kingdom

Email: (gabriel.lopezp@uam.es)

Photodynamic therapy (PDT) is a well established treatment of cancer that consists of the activation of a photosensitizer drug with light of a specific wavelength to generate reactive oxygen species (ROS) capable of inducing cell death in areas where the drug is accumulated. Due to its simplicity and localized toxicity [1], PDT has been subject of research interest in the past decades, focusing on the different photosensitizers available and their properties or on improving their ability to target a specific type of tissue. In this work, we will use Rose Bengal (RB) as photosensitizer, an organic dye capable of generating ROS under the right conditions.

One of the main characteristics of tumors is their uncontrolled growth, so they need a large amount of oxygen and nutrients to allow it. For this reason, the tumor generates much larger and less polished blood vessels. Due to their size, nanoparticles (NPs) cannot enter the blood vessels of healthy tissues, but can enter those generated by tumors, causing most of them to passively accumulate inside these tumors – what is known as enhanced permeability and retention (EPR) effect [2]. Among the types of NPs that can be used to carry out this type of treatment, gold nanoparticles (AuNPs) stand out, since they present low toxicity and are chemically inert. Nanoparticles has been used in combination with photosensitiser drugs to achieve the targeted delivery to tumour tissues via the EPR effect. Furthermore, the surface of nanoparticles can be further functionalized with targeting agent to further the targeting ability of the nano-based delivery systems. Amongst the possible targeting agents reported in the literature, albumins have been described to interact with specific receptors overexpressed on tumour sides and can contribute to the targeted delivery of drugs.

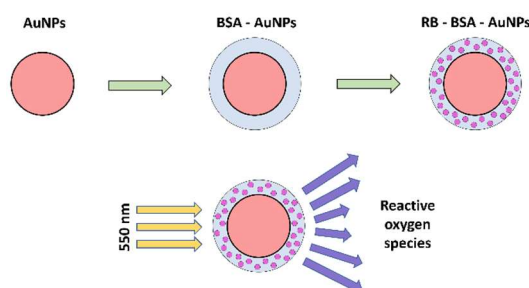


Figure 1. Schematic drawing of the different of the structures, starting from the AuNPs, then the BSA functionalized AuNPs, and finally the RB-BSA-AuNPs structures used in PDT.

The work here presented describes the synthesis and characterization of BSA-AuNPs and their use to encapsulate the photosensitizer Rose Bengal. The potential of these nanoconjugates as drug delivery systems for PDT will also be explored.

- [1] P. García Calavia et al., Photochemical & Photobiological Sciences, **17**, 281 (2018)
- [2] Z. Rachael Goddard et al., Chem. Soc. Rev., **49**, 8774-8789 (2020).
- [3] O. Penon et al., Journal of Colloid and Interface Science, Vol 496, 100-110 (2017)



# Low resistance contacts to few layered MoS<sub>2</sub> by local pressurization

Y. Manzanares-Negro<sup>1</sup>, J. Quan<sup>2</sup>, M. Rassekh<sup>1</sup>, M. Moaied<sup>1</sup>, X. Li<sup>2</sup>, P. Ares<sup>1,3</sup>, J. J. Palacios<sup>1,3</sup>, J. Gómez-Herrero<sup>1,3</sup> and C. Gómez-Navarro<sup>1,3</sup>

<sup>1</sup> Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Cantoblanco 28049, Spain

<sup>2</sup> Department of Physics, University of Texas at Austin, 78712, Austin, TX, U. S. A.

<sup>3</sup> Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Cantoblanco 28049, Spain

Email: yolanda.manzanares@uam.es

In semiconductor devices the output performance is dominated by both a change of resistance at the channel or at the contact junctions. Therefore, controlling the charge injection through the electrical contacts is as essential as controlling the semiconductor channel itself and the realization of well-controlled low resistance electrical contacts is one of the main challenges to overcome for emerging materials [1]. Up to date, mainly two strategies have succeeded in creating ohmic contact to MoS<sub>2</sub>: the first strategy involves the use of semimetals as electrical contacts [2]. The second strategy is based on chemical phase engineering through locally inducing metallic crystallographic 1T phase contacts [3].

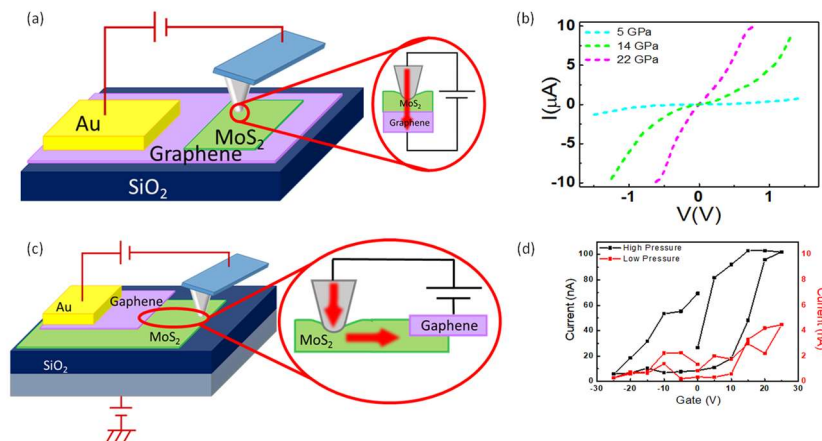


Figure 1. a) Schematic vertical configuration used to measure the conductivity of MoS<sub>2</sub> pressurized under the tip. b) I-V curves metallize when ultra-high pressure is applied to MoS<sub>2</sub>. c) Schematic horizontal device in FET configuration. It allows measuring the improvement on mobility and contact resistance of the devices. d) Transfer curve of a MoS<sub>2</sub> FET with normal contacts (red) and with one contact under ultra-high pressure (black).

Here, we report a strategy to reduce contact resistance to MoS<sub>2</sub> via local pressurization. We make electrical contacts using an Atomic Force Microscopy tip and apply variable pressure ranging from 0 to 25 GPa. By measuring transverse electronic transport properties, we show that MoS<sub>2</sub> under pressure undergoes a reversible semiconducting-metallic transition. Planar devices in field effect configuration with electrical contacts at pressures above ~15 GPa show an up to 30-fold reduced contact resistance and an up to 25-fold improved field-effect mobility when compared to those measured at low pressure.

- [1] A. Allain et al., Nature Mater., **14**(12), 1195-1205 (2015)
- [2] P. C. Shen et al., Nature, **593**(7858), 211-217 (2021)
- [3] R. Kappera et al., Nature Mater., **13**(12), 1128-1134 (2014)

## Thermal reading in brain phantom under microwave radiation

**Liyan Ming<sup>\*1</sup>, Erving Ximendes<sup>1,2</sup>, Riccardo Marin<sup>1</sup>, Paloma Rodriguez-Sevilla<sup>1,2</sup>, Daniel Jaque García<sup>1,2</sup>**

<sup>1</sup>*Nanomaterials for Bioimaging Group (NanoBIG), Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid 28049, Spain*

<sup>2</sup>*Nanomaterials for Bioimaging Group (NanoBIG), Instituto Ramón y Cajal de Investigación Sanitaria IRYCIS, Ctra Colmenar Km 9-100, Madrid, 28034, Spain*

<sup>\*</sup> [liyan.ming@estudiante.uam.es](mailto:liyan.ming@estudiante.uam.es)

Microwave (MW) electromagnetic radiation is increasingly used for electronic devices, networks, and wireless communications. Although regarded as safe, it can induce unwanted heating of human tissues and organs by heating the water contained in them.<sup>[1]</sup> Since brain is more than 70% water, it can easily experience thermal effects under MW exposure. This temperature elevation can induce changes in brain activity and even cerebral injuries, hence monitoring of MW-induced heating in brain is of utmost importance.<sup>[2]</sup> Given their invasiveness and size, traditional thermometers are not suitable for deep-tissue measurements. Luminescence nanothermometer presents thus itself as a valuable alternative for efficient thermal monitoring inside the brain.<sup>[3]</sup> More specifically, a suitable luminescent nanothermometer show absorb and emit in the near-infrared – given the greater penetration in tissues in this spectral range. In addition, recent studies have pointed at fluorescence lifetime as a reliable thermometric parameter, since it is not dependent, e.g., on variations in nanothermometer local concentration and fluctuations in the excitation power density.<sup>[4]</sup> Moving from these considerations, we developed a thermometric approach based on Ag<sub>2</sub>S nanothermometer with emission in the second near-infrared window (NIR-II, 1000-1350 nm) and temperature-dependent lifetime for remote thermal reading inside brain phantoms under MW irradiation (Figure 1a). The developed approach allows to monitor in real-time temperature changes within the phantom in a remote way (Figure 1b). The results indicate that MW irradiation of different frequencies and powers can induce significant heating within the phantom brain. This study opens the door to further investigations into the effect of MW on internal organs and accurate deep-tissue thermal monitoring more in general.

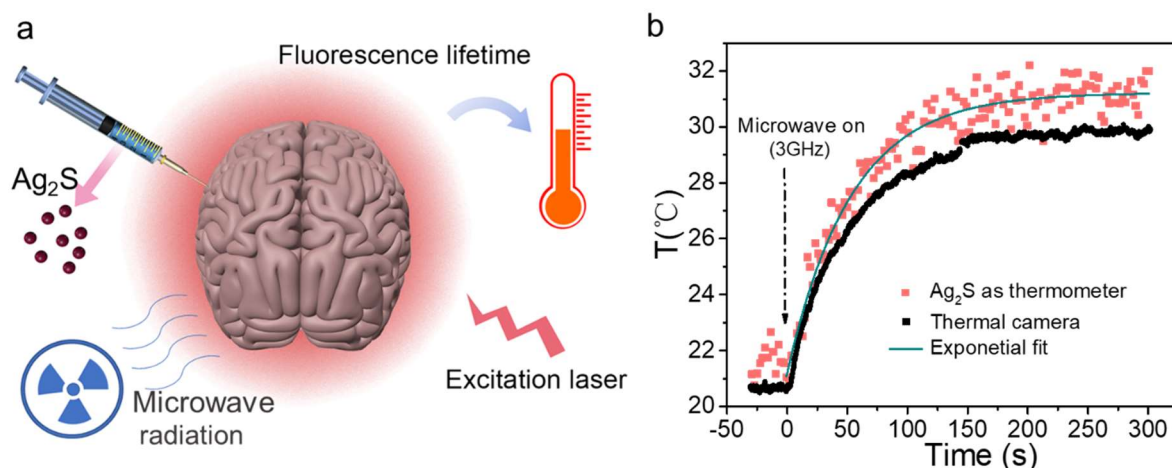


Figure 1. (a) Fluorescence lifetime-based thermometry in the phantom brain. (b) Thermal reading in the phantom brain under microwave (3 GHz) irradiation.

### References

- [1] Wongkasem, N., Electromagnetic pollution alert: Microwave radiation and absorption in human organs and tissues. *Electromagn Biol Med* 2021, 40 (2), 236-253.
- [2] Wang H, et. al., Brain temperature and its fundamental properties: a review for clinical neuroscientists. *Front Neurosci.* 2014, 00307.
- [3] del Rosal, B.; et. al., *In Vivo* Contactless Brain Nanothermometry. *Advanced Functional Materials* 2018, 28 (52).
- [4] Shen, Y.; et. al., In Vivo Spectral Distortions of Infrared Luminescent Nanothermometers Compromise Their Reliability. *ACS Nano* 2020, 14 (4), 4122-4133.

## Specific heat of ultrastable glasses at low temperatures

M. Moratalla<sup>1</sup>, R. Jiménez-Riobóo<sup>2</sup>, M. A. Ramos<sup>1,3</sup>

<sup>1</sup>*Laboratorio de Bajas Temperaturas, Dpto. Física de la Materia Condensada, and Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain*

<sup>2</sup>*Instituto de Ciencias de Materiales de Madrid (ICMM-CSIC), Campus de Cantoblanco, Madrid, Spain*

<sup>3</sup>*Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain*

Email: [manuel.moratalla@uam.es](mailto:manuel.moratalla@uam.es)

Glasses are well-known materials since long, which exhibit thermal and acoustic properties at low temperatures anomalously different from those found in crystalline solids, and with a remarkable degree of universality. Their specific heat is characterized by a linear term below 1 K, ascribed to quantum tunneling between two states (two-level systems, TLS) of similar energy [1, 2].

Here we present our low-temperature specific-heat experimental set-up, recently implemented, which permits us to reach 0.3 K and measure thin-film samples with masses of a few milligrams prepared by PVD (physical vapor deposition), and that also could be used for measuring other heavier samples.

Moreover, we also present our recent studies on ultrastable glasses employing this set-up: specific-heat measurements down to 1 K, as well as Brillouin Scattering results, in N,N-Diphenyl-N,N'-bis(methylphenyl) -1,1'-biphenyl-4,4'-diamines (TPD). Our objective has been to confirm the disappearance of TLS observed in indomethacin ultrastable glasses [3] and to shed light on the knowledge about ultrastable glasses, a topic with a high recent interest [4].

[1] W. A. Phillips, ed., *Amorphous Solids, Low-Temperature Properties*, Springer, 1981

[2] M. A. Ramos, ed., *Low-Temperature Thermal and Vibrational Properties of Disordered Solids*, World Scientific, 2022

[3] T. Pérez-Castañeda et al., *PNAS*, 111, 31, 11275-11280 (2014)

[4] C. Rodríguez-Tinoco et al., *Rivista del Nuovo Cimento*, 45, 325-406 (2022)

Moreno, Jose Antonio

Física de la Materia Condensada

# Electronic band structure inside the superconducting gap from Yu-Shiba-Rusinov states in quasi two-dimensional 2H-NbSe<sub>2-x</sub>S<sub>x</sub>

Jose A. Moreno<sup>1</sup>, Edwin Herrera<sup>1,2,3</sup>, Víctor Barrena<sup>1</sup>, Anita Smeets<sup>1</sup>, Samuel Mañas<sup>4</sup>, Eugenio Coronado<sup>4</sup>, José J. Baldoví<sup>4,5</sup>, Isabel Guillamón<sup>1</sup> and Hermann Suderow<sup>1</sup>

<sup>1</sup>Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

<sup>2</sup>Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia.

<sup>3</sup>Facultad de Ingeniería y Ciencias Básicas, Universidad Central, Bogotá, Colombia.

<sup>4</sup>Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Catedrático José Beltrán 2, 46980 Paterna, Spain

<sup>5</sup>Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, D-22761 Hamburg, Germany

Email: josea.moreno@uam.es

Yu-Shiba-Rusinov (YSR) states in s-wave superconductors due to magnetic impurities provide features in the subgap density of states whose spatial dependence pictures the electronic anisotropy. When YSR states extend over large distances, they provide subgap electronic excitations whose band structure contains an intrinsic electron hole anisotropy which is absent in the normal phase. This is particularly interesting in presence of multiple bands and a large anisotropy. However, viewing the full band structure requires YSR impurities with extremely well defined YSR peaks inside the small energy range of the superconducting gap. Here we show a considerable enhancement of the spatial extension of YSR states in superconducting 2H-NbSe<sub>2-x</sub>S<sub>x</sub> and identify features coming from the whole Fermi surface, including Se and Nb derived bands. These features are absent around Fe impurities in pure 2H-NbSe<sub>2</sub>. Density Functional calculations suggest that the two-dimensional electronic properties of S doped 2H-NbSe<sub>2</sub> enhance the YSR pattern over the whole Fermi surface. By investigating nanometric fields of view via Scanning Tunneling Microscopy (STM) with different Fe impurity density and different S dopings, we furthermore demonstrate that the cross-over between isolated YSR states and gapless Abrikosov-Gorkov superconductivity occurs at a very small Fe impurity concentration.

# Local temperature and viscosity sensing by a rotating upconverting microparticle

E. Ortiz-Rivero<sup>1</sup>, D. Jaque<sup>1</sup> and P. Haro-González<sup>1</sup>,

<sup>1</sup> Nanomaterials for bioimaging group, Departamento de Física de Materiales, UAM. 28049 Madrid, Spain

Email: elisa.ortiz@uam.es

The precise and non-invasive control over single particles is key for an array of physical and bio-medical applications, such as microfluidics and biophysics. In particular, the three-dimensional manipulation of single rare-earth-doped luminescent particles is of great interest due to their biocompatibility and the sensitivity of their luminescent properties to environmental conditions, which stand out among other dielectric luminescent particles. [1] The analysis of the damped rotation dynamics of an optically trapped microparticle is a powerful tool that allows not only the controlled and remote manipulation of the sensor, but also an improved characterization of the medium. [2]

Here, an optically trapped and rotated birefringent upconverting  $\beta$ -NaYF<sub>4</sub>: Yb<sup>3+</sup>, Er<sup>3+</sup> microparticle is presented as a local sensor. The microparticle shows an intense visible emission under 808 nm photoexcitation: The red emission ( $^4F_{9/2} \rightarrow ^4I_{15/2}$  transition of Er<sup>3+</sup> ions) is orientation-dependent, which is used to obtain the angular velocity of the microparticle and, therefore, the local viscosity of the medium. Moreover, the green emission ( $^2H_{11/2} \rightarrow ^4I_{15/2}$  and  $^4S_{3/2} \rightarrow ^4I_{15/2}$  transitions of Er<sup>3+</sup> ions) is temperature-dependent. [3,4] Therefore, the microparticle is used to characterize local temperature and viscosity of liquids of unknown viscosity while monitoring its temperature in the microscale.

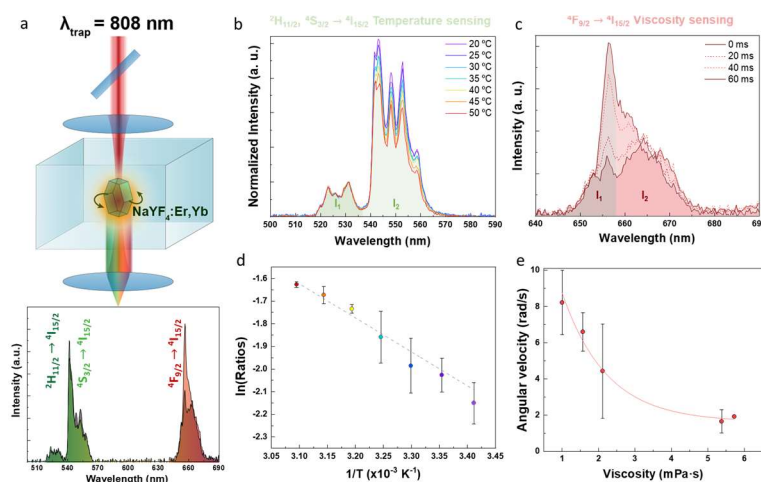


Figure. a) Schematic representation of a trapped and rotated upconverting microparticle in a liquid medium. b) Normalized intensity of the Er<sup>3+</sup> ions green bands,  $^2H_{11/2} \rightarrow ^4I_{15/2}$  (I<sub>1</sub>) and  $^4S_{3/2} \rightarrow ^4I_{15/2}$  transitions (I<sub>2</sub>), as a function of temperature. c) Intensity fluctuations of the Er<sup>3+</sup> ions red emission,  $^4F_{9/2} \rightarrow ^4I_{15/2}$ . c) Temperature calibration. c) Angular velocity obtained from c as a function of the medium viscosity.

This work was supported by the Ministerio de Ciencia e Innovación de España (PID2019-106211RB-I00 and PID2019-105195RA-I00) and by Universidad Autónoma de Madrid and Comunidad Autónoma de Madrid (SII/PJI/2019-00052).

- [1] E. Ortiz-Rivero et al., Front. Chem., **8**, 593398 (2020)
- [2] P. Rodríguez-Sevilla et al., Adv. Opt. Mater., **6** (12), 1800161 (2018)
- [3] E. Ortiz-Rivero et al., Small, 2103122 (2021)
- [4] E. Ortiz-Rivero, et al., Small, **15**, 1904154 (2019)

## Nano-scale conductivity of $\text{Ni}_3(\text{HITP})_2$ Metal-Organic Framework

E. Osuna<sup>1,2</sup>, A. Zambudio<sup>3</sup>, D. Rodríguez San-Miguel<sup>4</sup>, Y. Belce<sup>4</sup>, J. Gómez-Herrero<sup>1,2</sup>, C. Gómez-Navarro<sup>1,2</sup> and J. Puigmartí-Luis<sup>4,5</sup>

<sup>1</sup> Condensed Matter Physics Dept., Universidad Autónoma de Madrid, Madrid, E-28049, Spain.

<sup>2</sup> Condensed Matter Physics Center, Universidad Autónoma de Madrid, Madrid, E-28049, Spain.

<sup>3</sup> Optics and Nanophysics Research Center, Universidad de Murcia, E-30100, Murcia, Spain

<sup>4</sup> Departament de Ciència dels Materials i Química Física, Institut de Química Teòrica i Computacional, University of Barcelona (UB), 08028 Barcelona, Spain.

<sup>5</sup> Institució Catalana de Recerca i Estudis Avançats (ICREA), Pg. Lluis Companys 23, 08010 Barcelona, Spain

Email: eva.osunab@estudiante.uam.es

Metal-Organic Frameworks (MOFs) are compounds formed by metallic ions or clusters linked together by organic molecules forming one-dimensional, two-dimensional or three-dimensional structures. MOFs have attracted researchers' attention in recent years because they present the rare combination of being crystalline, electrically conductive and porous materials [1].

However, usual MOF preparation methods have poor control over the orientation, compactness, roughness profile and morphology of the MOF crystals, which can greatly impact their function and performance. Very recently, it has been shown that sample preparation using microfluidics to simulate microgravity conditions allows the control over these parameters and generates crack-free two-dimensional MOFs [2].

Here, we study the transport properties of 2D films of nanometric thickness of  $\text{Ni}_3(\text{HITP})_2$  grown in simulated microgravity conditions.  $\text{Ni}_3(\text{HITP})_2$  is a MOF which is considered the "analogue of graphene" in MOFs compounds and serves as a prototype material.

We present a suitable method for measuring the nano-scale conductivity of MOFs using Atomic Force Microscopy (AFM). We obtain resistance profiles as a function of the distance to the electrode and correlate them with the topography of the sample. From this data we estimate the inter-grain resistance and propose a simple model of the electrical behaviour of polycrystalline  $\text{Ni}_3(\text{HITP})_2$  thin films.

[1] R.W. Day, D. K. Bediako, M. Rezaee et al., ACS Cent. Sci. **5** 12, 1954-1964 (2019).

[2] N. Contreras-Pereda, D. Rodríguez San-Miguel et al., Adv. Mater. **33** (2021).



# Modelling AC hysteresis loops of ferromagnetic nanoparticles

P. Palacios-Alonso<sup>1</sup>, E. Sanz-de Diego<sup>1</sup>, Sedef Özel<sup>1</sup>, A. L. Cortajarena<sup>1,2,3</sup>, F. J. Teran<sup>1,4</sup>, Rafael Delgado-Buscalioni<sup>5</sup>

<sup>1</sup>*iMdea nanociencia, C. Faraday 9, Cantoblanco, 28049, Madrid Spain*

<sup>2</sup>*CIC biomaGUNE-BRTA. Paseo de Miramón 194, 20014, Donostia-San Sebastián, Spain.*

<sup>3</sup>*Ikerbasque, Basque Foundation for Science, Bilbao, Spain*

<sup>4</sup>*Nanobiotechnología (iMdea-Nanociencia), Unidad Asociada al Centro Nacional de Biotecnología (CSIC), 28049 Madrid, Spain*

<sup>5</sup>*Dpto de Física Teórica de la Materia Condensada, C. Francisco Tomás y Valiente 7, Universidad Autónoma de Madrid, 28049, Madrid, Spain*

Email: (pablo.palacios@imdea.org)

In recent years, magnetic nanoparticles (MNPs) have been extensively exploited in biomedical applications. There are a lot of actual research lines that are using magnetic nanoparticles in different fields as drug delivery, hyperthermia, biosensing... In particular, some recent works have shown that it is possible to detect the presence of a target biomolecule in a solution if we apply an AC field of radio frequency (10 kHz-100 kHz) to a system of MNP functionalized with a peptide that specifically recognizes the target biomolecule, looking at the magnetic area of the AC hysteresis cycles, M-H curves, (see Figure 1).

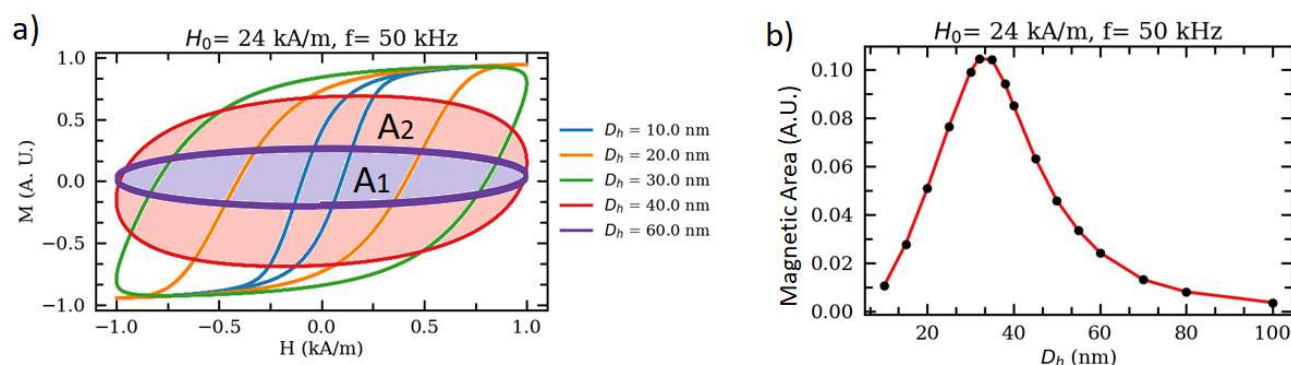


Figure 1. a) AC hysteresis loops of magnetic nanoparticles with different hydrodynamic sizes (shaded regions indicate the magnetic area of the cycles). b) Dependence of the magnetic area of the AC cycles on the hydrodynamic size of the MNP.

In this work we present a theoretical, computational and experimental study about how the magnetic area of the AC cycles of a system of ferromagnetic nanoparticles varies with the field conditions (field intensity and frequency) and the diffusion coefficient of the particles. We have studied the range of parameters in which we can find a master curve that describes the dependence of the normalized area of the cycles against the adimensional magnitudes of the problem, and the set of parameters that maximizes the magnetic area of the loops. This work can be very useful in order to find the optimal field conditions that should be used in order to detect a target biomolecule in a solution using AC magnetometry.

# Monitorization of H-absorption/desorption process in metallic films via optical measurements

E. Pérez-Picazo<sup>1</sup>, I. J. Ferrer<sup>1,2</sup>, F. Leardini<sup>1,2</sup> and J.R. Ares<sup>1</sup>

<sup>1</sup>MIRE, Dpto. de Física de Materiales, Facultad de Ciencias, UAM, 28049, Madrid, Spain

<sup>2</sup>Instituto Nicolás Cabrera, UAM, 28049 Madrid, Spain

Email: [elena.perezpicazo@estudiante.uam.es](mailto:elena.perezpicazo@estudiante.uam.es)

Hydrogen storage is a fundamental aspect of the hydrogen economy. Storing H<sub>2</sub> in the form of atomic hydrogen into a metal, *i.e.* forming so-called "metal hydride" [1] is a safe and efficient method. A detailed knowledge of the thermodynamic and kinetic properties of the hydride formation/decomposition reactions is compulsory to improve the hydrogen storage conditions. In this context, it is known that certain metals change drastically their optical properties under hydrogen. Therefore, this property seems attractive to investigate the hydrogenation/dehydrogenation mechanism of metals and further its plausible utilization as hydrogen sensors [2].

In this work, we present the thermodynamic and kinetic properties of the palladium-hydrogen system (Pd-H) obtained by using optical methods. To this aim, palladium thin films were deposited onto glass substrates. Films were structurally and morphologically characterized by x-ray diffraction and scanning electron microscopy, respectively. They were hydrogenated under different conditions of pressure and temperature. Optical transmittance was "in situ" recorded during the metal hydride formation and decomposition process (Fig.1). The obtained results indicate the suitability of this method for analysing different aspects of metal hydrogenation processes.

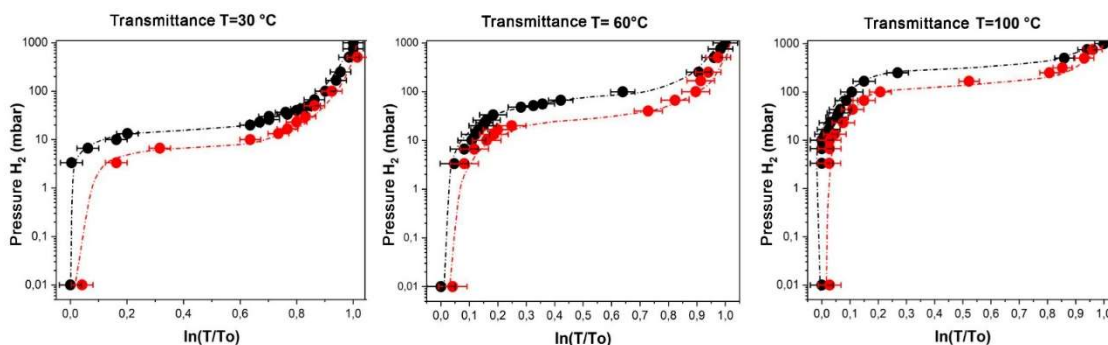


Figure 1. Optical-pressure-composition isotherms of the Pd-PdH<sub>x</sub> transformation. Curves have been obtained with Pd thin films (thickness of 45 nm) at different temperatures. In black, hydrogen absorption process ( $\alpha$  to  $\beta$  phase transformation). In red, hydrogen desorption process ( $\beta$  to  $\alpha$  phase transformation).

[1] A. Fernández, C. Sánchez, O. Friedrichs, J.R. Ares, F. Leardini, J. Bodega, J.F. Fernández, *Hidruros sólidos como acumuladores de hidrógeno*, RSEF, 24(1), 63-68 (2010)

[2] R. Gremaud, M. Slaman, H. Schreuders, *An optical method to determine the thermodynamics of hydrogen absorption and desorption in metals*, Appl. Phys. Lett. 91, 23916 (2007)

## *Study of Oxide Equilibrium in Pulsed Laser Deposited LiCoO<sub>2</sub> for Li-Ion Batteries*

María J. Ramirez-Peral<sup>1,2,3</sup>, Jesús Díaz-Sánchez<sup>1</sup>, Arturo Galindo<sup>3,4</sup>, I. Salazar<sup>4</sup>, H. van der Meulen<sup>2,5</sup>, Miguel Crespillo<sup>6</sup>, Carmen Morant<sup>2,4</sup>, Enrique Vasco<sup>3</sup> and Celia Polop<sup>1,2,7</sup>.

<sup>1</sup> Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain; <sup>2</sup> Instituto Universitario de Ciencia de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, Spain; <sup>3</sup> Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Spain; <sup>4</sup> Departamento de Física Aplicada, Universidad Autónoma de Madrid, Madrid, Spain; <sup>5</sup> Departamento de Física de Materiales, Universidad Autónoma de Madrid, Spain; <sup>6</sup> Centro de Micro-Análisis de Materiales, Universidad Autónoma de Madrid, Madrid, Spain; <sup>7</sup> Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain.

The sustainability of modern society while maintaining quality of life standards implies the use of new sources of renewable energy, as well as the development of systems for its efficient storage. These systems are required to alleviate the intermittent seasonal nature of renewable energy sources. In this context, it is crucial to study the materials used in lithium-ion batteries (LIB), one of the most used and promising energy storage devices today, to improve their functional properties and performance.

In this work, we focus on the study of LiCoO<sub>2</sub> (LCO), a widely used material as LIB cathode (CAT), in the form of thin film deposited by Pulsed Laser Deposition (PLD). LCO was the first CAT marketed by Sony in 1991, but soon was replaced by NCM and NCA (with Co being partially substituted by Ni and Mn or Al) due to its poor thermal stability. Recently, LCO has regained prominence in the design of "zero-strain" composite CATs since this is the only commercial CAT with a negative chemical expansion coefficient [1]. On the other hand, PLD is a physical vapor deposition technique extensively exploited for the stoichiometric preparation of multicationic oxides, and conformal interfaces with improved wetting and mechanical clamping between components [2]. Combining both solutions by using prepared "zero-strain" CATs forming a conformal interface with solid-state electrolyte is expected to improve the mechanical stability of solid-state LIBs, which is one of the crucial issues hindering the marketing of these devices. LCO is sensitive to Li stoichiometry, which is hard to achieve by PLD due to the interaction of the light species with the deposit atmosphere and the low sticking of Li metal. Losses of Li beyond 50% irreversibly give rise to the segregation of Co-oxide phases. Here, we study the dependence of the phase equilibrium of LCO-Co oxides on the PLD deposition parameters (temperature, oxygen pressure and film thickness). Four phases (hexagonal LCO [HT-LCO], cubic LCO [LT-LCO], spinel Co<sub>3</sub>O<sub>4</sub> and CoO) were identified, whose evolutions with the PLD parameters are investigated by  $\mu$ Raman spectroscopy, Confocal Raman, GIXRD, RBS-NRA and AFM. Raman and GIXRD reveal the two HT-LCO and Co<sub>3</sub>O<sub>4</sub> phases coexist in the films for the entire explored range of PLD parameters, while LT-LCO and CoO appear under low temperature conditions (CoO under 600°C and LT-LCO at room temperature and annealed at 600°C). HT-LCO/Co<sub>3</sub>O<sub>4</sub> ratio increases with deposition temperature, the oxygen pressure and film thickness. Combined NRA-RBS reveals that Li is depleted on the surface and at the interface with the substrate, suggesting that the sources of Li loss are the diffusion towards the substrate and Li reevaporation from the surface. AFM and Confocal Raman show two grain-sizes distributions, which can be related to the coexistence and competition between the phases. Finally, electrochemical tests show that the films with higher HT-LCO proportion are those exhibiting higher specific charge capacities.

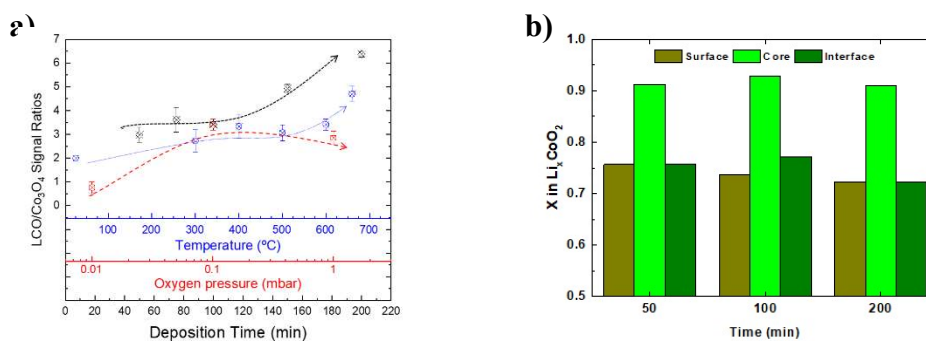


Fig. (a) HT-LCO/Co<sub>3</sub>O<sub>4</sub> Raman signal ratio and (b) analysis of the Li depth profiles by RBS-NRA.

[1] R. Koerver *et al.*, *Energy Environ. Sci.* **11**, 2142–2158 (2018)

[2] Li Z *et al.* Structural study of epitaxial LiCoO<sub>2</sub> films grown by pulsed laser deposition on single crystal SrTiO<sub>3</sub> substrates. *Thin Solid Films*. 2016;612:10.1016/j.tsf.2016.05.017. doi: 10.1016/j.tsf.2016.05.017. PMID: 32831417; PMCID: PMC7436253.

# Manipulation of aqueous micro-droplets containing particles and bio-species by photovoltaic tweezers

E. Rincón<sup>1</sup>, P. Camarero<sup>1</sup>, M. Quintanilla<sup>1,2</sup>, P. Haro-González<sup>1,2</sup>, M. Carrascosa<sup>1,2</sup>, Á. García-Cabañes<sup>1,2</sup>

<sup>1</sup>Departamento de Física de Materiales, Universidad Autónoma de Madrid, Madrid 28049, Spain

<sup>2</sup>Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid 28049, Spain

Email: esther.rincon@estudiante.uam.es

Photovoltaic optoelectronic tweezers (PVOT) have become a flexible tool to trap and pattern micro- and nanoparticles [1]. They are based on the light-induced electric fields generated in some ferroelectric crystals by the bulk photovoltaic effect, being particularly strong in  $\text{LiNbO}_3\text{:Fe}$ . Very recently, a method for manipulating aqueous solution micro-droplets by PVOT has been also demonstrated [2]. In this work we extend the capabilities of this method using the aqueous droplets as carriers containing different kind of objects such as particles or bio-species. Specifically, we have successfully transported polystyrene particles (diameter  $0.5\ \mu\text{m}$ ) in water droplets and cell spheroids (3D cell models,  $\sim 100\text{--}300\ \mu\text{m}$ ) inside cell culture medium droplets. In the first case, the droplet is a homogeneous suspension of particles whereas in the second one, the droplet constitutes a hybrid system with the spheroid clearly distinguishable as observed in figure 1. As it can be seen in that figure, the substrate is located in the bottom of a cuvette filled with paraffin oil. Droplets are deposited in the air-paraffin interphase. As the light is switch on and illuminates the ferroelectric substrate, an electric field is generated inside and outside it. This electric field acts on the two kinds of droplets manipulating them. Analysis of the different migration behaviors found, attraction to the illuminated region or repulsion from it, have been carried out. The results allow to characterize the charge state of the droplets. They show that droplets containing polystyrene particles were not appreciably charged. In turn, cell culture droplet is positively charge, but when the spheroid is included, it provides negative charge to the droplet.

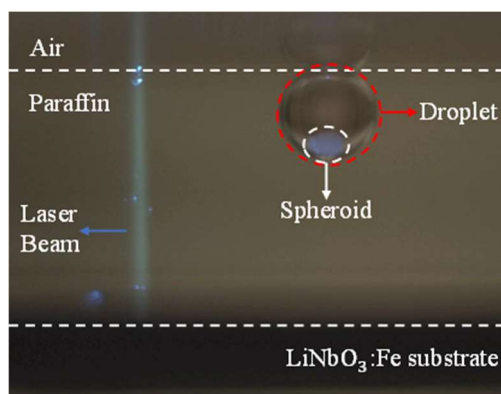


Figure 1. Schematics of the PV ferroelectric platform showing the hanging droplet containing the spheroid. The ferroelectric substrate is illuminated with a laser beam that generates a PV electric that manipulates the droplet

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

- [1] M. Carrascosa, A. García-Cabañes, M. Jubera, J. B. Ramiro, and F. Agulló-López, *Appl. Phys. Rev.* **2**, 040605 (2015)
- [2] A. Puerto, A. Méndez, L. Arizmendi, A. García-Cabañes, and M. Carrascosa, *Phys. Rev. Applied* **14**, 024046 (2020)



# Phase engineering of two-dimensional Transition Metal Ditellurides

Joan Ripoll-Sau<sup>1,2</sup>, I. Di Bernardo<sup>2</sup>, F. Calleja<sup>1</sup>, P. Casado Aguilar<sup>1,2</sup>, I.M. Ibarburu<sup>1,2</sup>, R. Miranda<sup>1,2,3,4</sup>, A.L. Vázquez de Parga<sup>1,2,3,4</sup>, M. Garnica<sup>1,3</sup>

<sup>1</sup>Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), 28049 Madrid, Spain

<sup>2</sup>Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>3</sup>Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>4</sup>Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Email: joan.ripoll@estudiante.uam.es

Phase engineering of two-dimensional transition metal ditellurides (2D-TMDTs) is a promising way to exploit their electronic properties in order to apply them in electronic devices such as photodetectors, LEDs, phototransistors, and solar cells [1]. 2D-TMDTs have a  $\text{MTe}_2$  stoichiometry, where M is a transition metal (groups IV-X). Interestingly, their properties change according to the transition metal, the crystallographic structure and number of layers. An interesting example is  $\text{MoTe}_2$ , which presents a semiconducting hexagonal phase showing an indirect bandgap in bulk (2H phase) or a direct bandgap at the monolayer (1H) [2] or the semimetallic distorted octahedral (1T') phase (unstable in bulk) predicted to exhibit quantum spin Hall (QSH) effect in the monolayer regime [3]. Another example is  $\text{TaTe}_2$ , which in bulk is only stable in the 1T' distorted octahedral phase [4] but is predicted to exhibit two additional metallic phases in the ML: one magnetic (1H) and the other non-magnetic (1T) [5]. Here, we report the growth of 2D islands of  $\text{MoTe}_2$  and  $\text{TaTe}_2$  via molecular beam epitaxy (MBE) on epitaxial graphene on Ir(111) (Fig. 1(a)). We show how by varying the growth parameters, such as substrate temperature (Fig. 1(b) and 1(e)) and precursor ratio, we can tune the relative coverage of different phases. Their structural and electronic characteristics are studied by means of scanning tunneling microscopy (STM).

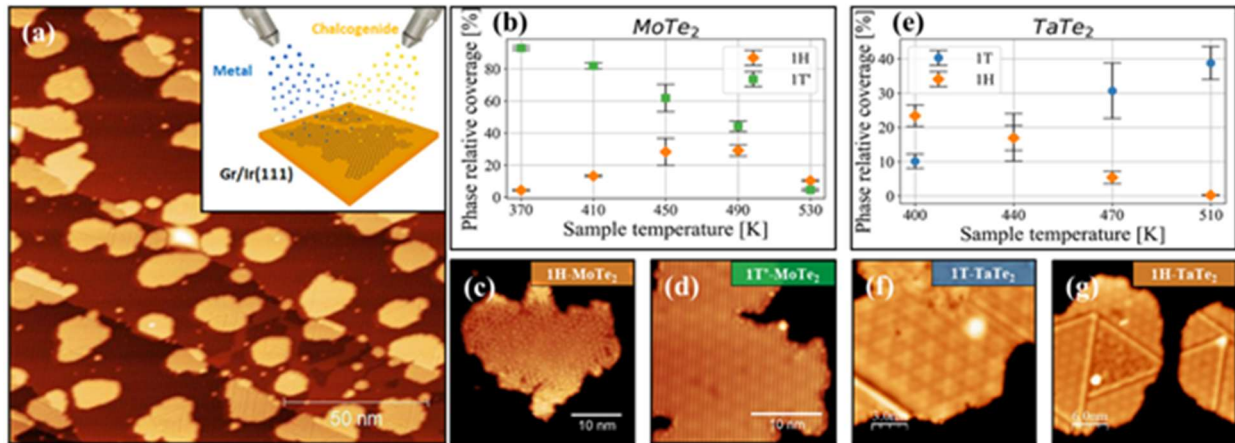


Figure 1. (a) Large STM image of  $\text{TaTe}_2$  islands on gr/Ir(111) ( $V = -1\text{V}$ ;  $I = 0.1\text{nA}$ ). Inset: sketch of the growth procedure. (b) Relative coverage of 1T' vs. 1H- $\text{MoTe}_2$  phases for different growth temperatures. STM images of (c) 1H- $\text{MoTe}_2$  ( $V = 0.5\text{V}$ ;  $I = 0.1\text{nA}$ ) and (d) 1T'- $\text{MoTe}_2$  islands ( $V = 1\text{V}$ ;  $I = 0.1\text{nA}$ ). (e) Relative coverage of 1T vs 1H- $\text{TaTe}_2$  phases for different growth temperatures. STM images of (f) 1T- $\text{TaTe}_2$  ( $V = 0.75\text{V}$ ;  $I = 0.2\text{nA}$ ) and (g) 1H- $\text{TaTe}_2$  islands ( $V = 1\text{V}$ ;  $I = 0.2\text{nA}$ ).

- [1] H. Li *et al.*, Advanced Functional Materials, **31**, 2010901 (2021).
- [2] I. Gutiérrez Lezama *et al.*, 2D Materials, **1**, 021002 (2014).
- [3] X. Qian *et al.*, Science, **346**, 1344 (2014).
- [4] I. El Baggari *et al.*, Physical Review Letters, **125**, 165302 (2020).
- [5] D. C. Miller *et al.* Physical Review B, **97**, 045133 (2018).

## N-terminal conformation of the coat protein modulates RNA cargo retention of human picobirnavirus

**María J Rodríguez-Espinosa<sup>1,2</sup>, Javier M Rodríguez<sup>2</sup>, Jose R Caston<sup>\*2</sup>, Pedro J de Pablo<sup>\*1</sup>**

<sup>1</sup>*Department of Condensed Matter Physics, Universidad Autónoma de Madrid, Spain*

<sup>2</sup>*Department of Macromolecular Structures, Centro Nacional de Biotecnología (CNB-CSIC), Madrid, Spain*

High resolution cryo-electron microscopy structures of nucleocapsids qualitatively indicate the interaction degree between single-stranded (ss) RNA and coat proteins (CPs) in viruses but lack the direct evaluation of its effects on the virus capsid. Here we study the mechanical uncoating of three variants of the human picobirnavirus (hPBV) virus-like particles (VLPs) which differ in the N-terminal of their CPs: (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 an N-terminal 36-residue tag that includes a 6-His segment. We used Atomic Force Microscopy (AFM) to induce and monitor mechanical disassembly of individual hPBV particles. First, whereas  $\Delta 45$ -CP particles that lack packaged ssRNA exhibited a fast post-breakage indentation, CP and Ht-CP particles that pack ssRNA showed a gradual behavior after being fractured. Second, mechanical fatigue experiments revealed that the increased length of N-terminal (Ht-CP) in 8% makes the virus particles to crumble  $\sim 10$  times slower than wild type N-terminal CP, indicating an enhanced RNA cargo retention after Ht-CP particles have been crack-opened. Our results indicate that the three differentiated N-terminal topologies of the capsid lumen result in distinct disassembly dynamics as a consequence of their particular interaction with the packaged RNA.

### References

- [1] Duquerroy et al. The EMBO journal, 28(11), 1655-1665 (2009).
- [2] De Pablo et al. Applied Physics Letters, 73(22), 3300-3302 (1998).
- [3] Llauró et al. Nanoscale, 8(17), 9328-9336 (2016).
- [4] Horcas et al. Review of Scientific Instruments, 78(1), 013705 (2007).



# INC Research awards for Physics students 2022

Ronquillo Tutiven, Joan Javier

Física de Materiales

## Electrostatic doping of monolayer MoS<sub>2</sub> deposited on hexagonal ferroelectric domains

**Joan J. Ronquillo<sup>1,3,\*</sup>, Javier Fernández-Martínez<sup>1,3</sup>, Daniel Gallego-Fuente<sup>2,3</sup>, Guillermo López-Polin<sup>1,3</sup>, Pablo Ares<sup>2,3,4</sup>, Julio Gómez-Herrero<sup>2,3,4</sup>, Mariola O. Ramírez<sup>1,3,4</sup>, and Luisa E. Bausá<sup>1,3,4</sup>**

<sup>1</sup> Dept. Física de Materiales, Universidad Autónoma de Madrid, 28049-Madrid, Spain

<sup>2</sup> Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049-Madrid, Spain

<sup>3</sup> Instituto de Materiales Nicolás Cabrera, Universidad Autónoma de Madrid, 28049-Madrid, Spain

<sup>4</sup> Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049-Madrid, Spain

\*email: joan.ronquillo@estudiante.uam.es

Two-dimensional (2D) Transition Metal Dichalcogenides (TMDs) are an interesting class of materials which offer unique properties for the next generation of electronic and optoelectronic devices [1-2]. Doping of 2D TMDs is needed for the development of the devices, which sometimes requires complex strategies. In fact, considerable efforts have been made to create ultra-thin p-n junctions either by vertical assembling p- and n-type 2D materials, leading to out of plane junctions, or by tuning their charge carrier concentration to form in plane lateral homojunctions.

Here, we exploit the atomic thickness nature of monolayer (1L) TMDs, which offers the opportunity to modulate the optoelectronic properties of 2D materials by means of the surrounding environment. We demonstrate substrate induced electrostatic doping of 1L MoS<sub>2</sub> when deposited on a ferroelectric crystal (LiNbO<sub>3</sub>) with hexagonal domains of alternating polarity.

By using spatially resolved high-resolution micro-fluorescence, we show that the spontaneous polarization of the substrate gives rise to p- and n-doped regions depending on the polarization of the ferroelectric domain [3]. The ferroelectrically driven spatial carrier modulation is revealed through the different contribution of the excitons and trions to the spectra. Figure 1 shows the optical image and the corresponding micro-luminescence map. The spectroscopic image shows that the spatial dominance of each quasiparticle is directly related with the different type of doping in the 1L MoS<sub>2</sub>. The photoluminescence (PL) behavior of the p- and n- doped regions is also analyzed when the excitation power is varied.

The results open new routes for the design of simple and cost-effective electronic and optoelectronic devices based on 2D TMDs.

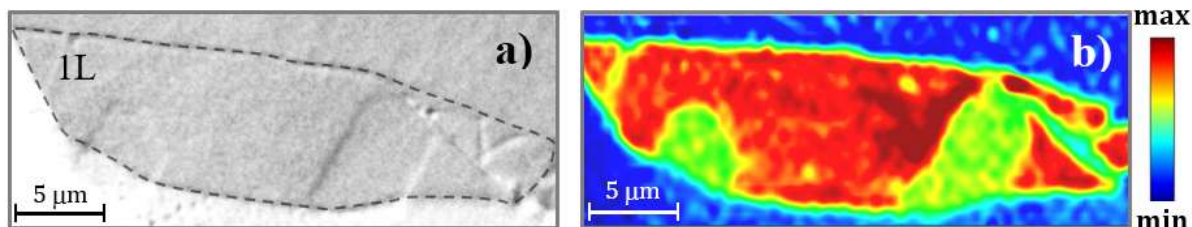


Figure 1. (a) Optical microscopy image of 1L MoS<sub>2</sub> deposited on hexagonal ferroelectric domains structure (LiNbO<sub>3</sub>). (b) PL intensity distribution showing the exciton-dominant region (p type, in red) and the trion-dominant region (n type, in green).

[1] J. W. Chen et al., Nat. Commun. **9**, 3143 (2018).

[2] W. Zhang et al., Adv. Mater. **25**, 3456 (2013).

[3] B. Wen et al., ACS Nano **13** (5), 5335 (2019).

## Comparative studies of thermal properties: the case of detonated nanodiamond ceramics

D. Szewczyk<sup>1,2</sup>, M. A. Ramos<sup>2,3</sup>

<sup>1</sup>*Institute of Low Temperature and Structure Research, Wroclaw, Poland*

<sup>2</sup>*Low Temperature Laboratory, Condensed Matter Physics Department, “Nicolás Cabrera” Institute, Universidad Autónoma de Madrid, Madrid, Spain*

<sup>3</sup>*Centro de Microanálisis de Materiales (CMAM), Universidad Autónoma de Madrid, Madrid, Spain*

Email: (d.szewczyk@intibs.pl)

Thermal properties of detonated nanodiamond ceramics were investigated by combining specially designed experimental systems: for thermal conductivity implementing the uniaxial stationary heat flow method and for heat capacity the thermal relaxation method. Additionally, studies on a commercial Physical Properties Measurement System, operating either in Thermal Transport Option or in Heat Capacity Option were performed to supplement the data. The need to use both experimental setups is emphasized. Two types of high-pressure (6–6.5 GPa) sintered samples were considered, differentiating both in sintering temperatures (either 1000°C or 1600°C) and sintering time (11–25 s). The effect of different sintering conditions on resulting thermal transport is examined. In thermal conductivity  $\kappa(T)$ , an improvement up to a factor of 3 of heat flow at room temperature is observed, while increasing both the sintering time and temperature. The temperature dependence of  $\kappa(T)$  exhibits a typical polycrystalline character due to hindered thermal transport stemming from the microstructure of ceramic material, but with values around 1–2 W/mK. At the lowest temperatures, the thermal conductivity is very low and increases only slightly faster than linear with temperature, once again resembling the significant contribution of the scattering due to multiple grain boundaries. The heat capacity data did not exhibit such a strong sensitivity toward the different sintering conditions of particular samples, as was the case of thermal conductivity studies. For both samples, an unexpected upturn at the lowest temperatures is observed connected to a low-T Schottky anomaly –reminiscent of the ceramics fabrication process. A linear contribution to the specific heat is also present, with a value of 20  $\mu\text{J/K}$ , one order of magnitude higher than in canonical glasses, but similar to some disordered crystals. The determined Debye temperature is 482 ( $\pm 6$ ) K of the order of other nanoscale diamond-type materials. The thermal transport considerations are supported by the phonon mean free path calculations.

### Acknowledgments:

D.S. was funded by the Bekker Programme of the Polish National Agency of Academic Exchange (Grant BPN/BEK/2021/1/00091). M.A.R. acknowledges financial support by the Ministerio de Ciencia e Innovación of Spain (Grant PID2021-127498NB-I00/AEI/FEDER/10.13039/501100011033), as well as from the Autonomous Community of Madrid through program S2018/NMT-4321 (NANOMAGCOST-CM).

# INC Research awards for Physics students 2022

Tamargo, Andrés

Física Teórica de la Materia Condensada

## Two-dimensional Fermi polarons, same problem different realisations: doped TMD monolayers & ultracold atomic Fermi gases

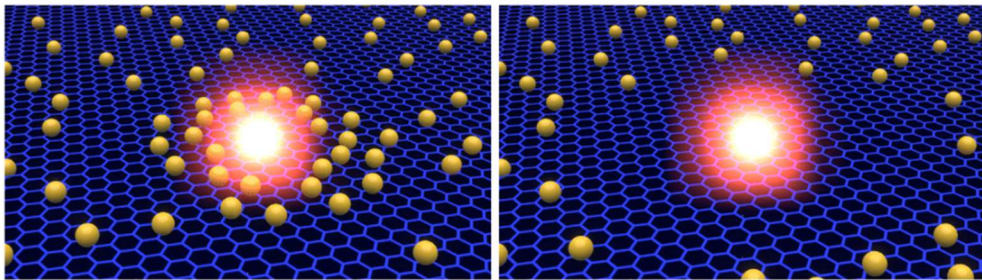
**A. Tamargo<sup>1</sup> and F. M. Marchetti<sup>1,2</sup>**

<sup>1</sup>Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid 28049, Spain

<sup>2</sup>Condensed Matter Physics Center (IFIMAC) & Instituto Nicolás Cabrera (INC) Universidad Autónoma de Madrid, Madrid 28049, Spain

Email: [andres.tamargo@estudiante.uam.es](mailto:andres.tamargo@estudiante.uam.es)

The objective of this project is to study the two-dimensional Fermi polaron problem and its realization in two very different experimental contexts: 2D doped or gated semiconductor transition metal dicalchogenide monolayers [1] and quasi-2D ultracold atomic Fermi gases with imbalanced spin population [2]. Even though the quantum impurity problem, i.e., an impurity surrounded by a quantum medium, was first introduced almost 90 years ago by Landau [3], it has ever since been generalized to a plethora of different systems and continues to attract noticeable interest. We will show that the very same Hamiltonian model can be used for describing both realizations. To solve the Fermi polaron problem, we will use a variational calculation, which includes quantum correlations by dressing the impurity with particle-hole excitations of the medium (Fig. 1). We will describe how to evaluate observables in both realizations, such as optical absorption in the semiconductor case and injection radiofrequency spectroscopy for the atomic gas case.



*Figure 1. Schematic representation of the strongly correlated Fermi polaron quasiparticle: an impurity (bright particle) surrounded by a Fermi sea (yellow particles) can either attract (left) or repel the Fermi gas, leading to a new quasiparticle dressed by quantum excitations of the medium (adapted from Ref. [4]).*

[1] M. Sidler, P. Back, O. Cotlet, A. Srivastava, T. Fink, M. Kroner, E. Demler, and A. Imamoglu, *Nature Physics* **13**, 255 (2017).

[2] Massignan, M. Zaccanti, and G. M. Bruun, *Rep. Prog. Phys.* **77**, 034401 (2014).

[3] L. D. Landau, *Phys. Z. Sowjetunion* **3**, 644 (1933).

[4] O. Cotlet, PhD thesis “Bose-Fermi mixtures with electrons and polaritons”, ETH Zürich (2019).

## Proton Transport through Peptide Nanotubes

Jorge Vega<sup>1</sup>, Jesús Mendieta<sup>2</sup>, Daniel G. Trabada<sup>1</sup>, Jesús I. Mendieta-Moreno<sup>1</sup>, Linda A. Zotti<sup>1</sup>, José Ortega<sup>1</sup>

<sup>1</sup> *Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Facultad de Ciencias, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*

<sup>2</sup> *Departamento de Biotecnología, Universidad Francisco de Vitoria, E-28223 Pozuelo de Alarcón, Madrid, Spain*

Email: jorge.vega@uam.es

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 both from the fundamental point of view and for the possible technological applications. They have been employed in biocompatible devices and as drug-delivery agents and are also 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 octa-peptides based on phenylalanine and functionalized with either lysine, arginine, or histidine [1] showed an-order-of-magnitude-larger proton conductivity for the lysine-containing nanotubes. Theoretical simulations there included ascribed this to the different flexibilities of the side chains. However, what the role of the surrounding water molecules is on the proton transport through these systems had not been clarified. Inspired by these results, therefore, we carried out molecular dynamics simulations on these systems in aqueous environment to try gaining an insight into how water molecules can mediate the proton flow. For that 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 seems a viable candidate to mediate proton transport through a Grotthuss-like mechanism.

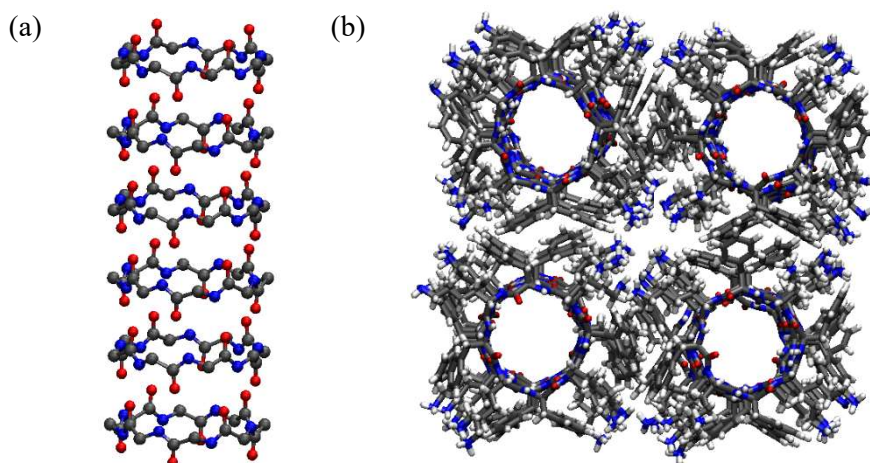


Figure 1. (a) Side view of a section of the peptide nanotube  $c(KF)_4$  (only the backbone is shown for clarity i.e., the lysine (K) and phenylalanine (F) side chains are not shown). Each peptide ring contains 4 K and 4 F amino acids in an alternate fashion. (b) Top view of a bundle of 4 nanotubes.

[1] S. Roy, L. Zheng, O. Silberbush, M. Engel, Y. Atsmon-Raz, Y. Miller, A. Migliore, D. N. Beratan, and Nurit Ashkenasy, *J. Phys. Chem. B*, **125**, **46**, 12741-12752 (2021)

# INC Research awards for Physics students 2022

Vida García, Jaime

Física de la Materia Condensada

## Study of colloidal systems in lattice obstacles

J. Vida <sup>1</sup>

<sup>1</sup>*UAM, Madrid, Spain*

Email: [jaime.garciav@estudiante.uam.es](mailto:jaime.garciav@estudiante.uam.es)

Currently I'm studying a macroscopical version of the experiment that is been done in INC by the group of J.L. Aragonés that consists in the study of colloidal systems in a grid of obstacles with an applied magnetic field. We record a video of the particle and with MATLAB we developed a program that finds particle position and orientation that allows us to measure some properties like trajectory, angular momentum, magnetic moment, etc. We can also change the fluid and what effects this has and also the study of inertial and viscous forces

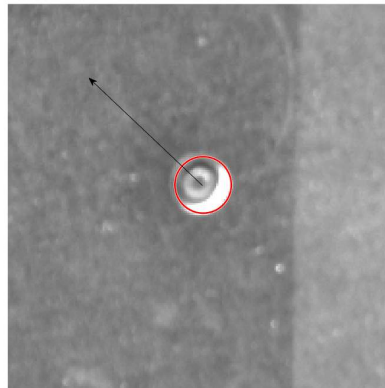


Figure 1. A frame of the video of the particle where the red ring represents its position and the arrow represents its magnetic moment.



# Superconductivity and Coulomb Correlations in nanosized Pb islands

**B. Vina-Bausa<sup>1,2</sup>, S. Trivini<sup>1</sup>, E. Cortes-del-Rio<sup>2</sup>, K. Vaxevani<sup>1</sup>, J. Ortuzar<sup>1</sup>, D. Longo<sup>1</sup>, V. Cherkez<sup>3</sup>, Pierre Mallet<sup>3</sup>, J-Y Veuillen<sup>3</sup>, J. C. Cuevas<sup>2</sup>, I. Brihuega<sup>2</sup>, J. I. Pascual<sup>1</sup>**

<sup>1</sup> CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain

<sup>2</sup> Universidad Autónoma de Madrid, 28049 Madrid, Spain

<sup>3</sup> Université Grenoble Alpes, CNRS, Institut Néel, Grenoble, France

Email: beatriz.vina@estudiante.uam.es

Quantum confinement modifies most solid state phenomena. Specifically, in superconductors, significant alterations from the bulk superconducting properties arise at the nanometer scale. When the energy level spacing that arises from quantum confinement ( $\delta$ ) is comparable to the bulk superconducting energy gap ( $\Delta$ ) the superconducting order is destabilized. In fact, repulsive Coulomb interactions near the Fermi level, acting against the superconducting electron pairing, may drive the system into a Coulomb-gapped, correlated state [1-3].

Here, we study the competition between Coulomb and superconducting correlations in Pb nanostructures grown on Graphene/SiC(000-1). The energy gap of nanosized Pb islands (Fig.1a) is probed by low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). An enhancement of the gap from its bulk value is observed as the lateral size of the Pb structures is reduced (Fig.1b). As confinement increases, electron repulsions may compete with the electron-phonon interactions responsible of the formation of Cooper pairs, leading to the opening of a Coulomb gap. Moreover, our results show the systematic presence of coherence peaks when approaching the critical size (islands < 100 nm), suggesting the coexistence of superconducting and Coulomb correlations. Such coherence peaks present a strong asymmetry evidencing a different tunneling behavior for quasiparticles and holes excitations.

Our work shows the importance of exploring superconducting properties at reduced length scales to understand the fundamental dimensional limits of superconductivity.

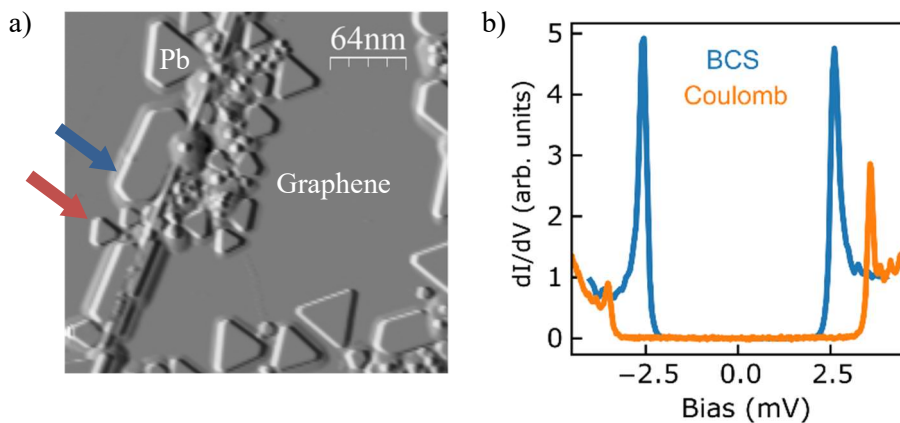


Figure 1. a) STM topography of Pb nano-islands on Graphene/SiC(000-1). b) STS differential conductance showing the density of states of the small and large islands highlighted in a).

- [1] S. C. Ganguli et al., Nano Letters **22**, 1845 (2022)
- [2] S. Bose and P. Ayyub, Rep. Prog. Phys. **77** 116503 (2014)
- [3] C. Brun et al. Phys. Rev. Lett. **108**, 126802 (2012)



# INC Research awards for Physics students 2022

Yang, Youhuang

Física Teórica de la Materia Condensada

---

## Study of Two-Mode Interference in Quantum Light-Matter Interactions

*Presenter: Youhuang Yang*

*Supervisor: Johannes Feist*

*Department: Theoretical Condensed Matter Physics*

The interaction of a single emitter with an arbitrary electromagnetic environment can be fully described by the local density of states of the environment at the emitter position, encoded in the so-called spectral density  $J(\omega)$ . It was recently shown that for a broad class of nanophotonic systems, the spectral density can be represented by few-mode quantum models characterized by a small number of interacting and decaying modes, leading to a compact Lindblad master equation for the dynamics of the emitter [1]. We exploit this formalism to study the spontaneous emission dynamics of an emitter coupled to an electromagnetic environment consisting of two interacting modes. Our particular interest lies in the cases where destructive interference between modes causes a sharp minimum in the spectral density exactly at the frequency of the emitter, which can lead to nonstandard behavior of the emitter decay rate as a function of the coupling strength.

[1] I. Medina, F. J. García-Vidal, A. I. Fernández-Domínguez, J. Feist, *Few-Mode Field Quantization of Arbitrary Electromagnetic Spectral Densities*, Phys. Rev. Lett. **126**, 093601 (2021)

# INC Research awards for Physics students 2022

Yue, Senlin

Física Teórica de la Materia Condensada

## Inverse Design applied to Schrödinger Equation: Tailored Potential Wells for Exciton Trapping.

Senlin Yue<sup>1\*</sup>, Antonio I. Fernández Domínguez<sup>1</sup><sup>1</sup>*Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28043 Madrid, Spain*

\*Email: senlin.yue@estudiante.uam.es

The advent of quantum technologies relies on the design and implementation of physical platforms able to support quantum states involving a large number of elemental quantum systems. Thus, the starting point and initial focus for quantum design must be these basic units, usually known as qubits. These are the quantum version of the classic binary state and their realization always involve some kind of confining potential able to trap material excitations (excitons) in space, which translates into a well-defined, discrete set of energetic levels [1]. Here, we devise potential wells with tailored properties, both in their spectrum of eigenenergies and in the spatial characteristics of their corresponding eigenfunctions. With that purpose, we have developed an inverse-design approach that combines both perturbation theory and exact Numerov solutions [2] of the Schrödinger Equation [3]. Starting from simple potentials such as the square well or the harmonic potential, the evolution of the wells under different optimization conditions are analyzed in order to obtain potentials with the desired properties.

[1] Kavokin A.V., Baumberg J. J., Malpuech G., Laussy, F. P. Microcavities [pages 133-153]. Oxford University Press, 2011.

[2] Numerov, Boris Vasilevich, Note on the numerical integration of  $d^2x/dt^2 = f(x,t)$ , *Astronomische Nachrichten*, 230, 359, 1927.

[3] Cohen-Tannoudji C., Diu B., Laloe F. Quantum Mechanics, Volume 2 [pages 1115-1129]. Wiley, 1986.

## Defects as a key to control friction on monolayer MoS<sub>2</sub>

A. Zambudio<sup>1,2</sup>, P. Ares<sup>1</sup>, G. López-Polín<sup>1</sup>, J. Colchero<sup>2</sup>, J. Gomez-Herrero<sup>1</sup> and C. Gómez-Navarro<sup>1</sup>

<sup>1</sup>University Autónoma of Madrid, Madrid, Spain

<sup>2</sup>University of Murcia, Murcia, Spain

Email: aitor.zambudio@uam.es

Friction plays an important role in the implementation of 2D materials on the large-scale production for different applications such as electronic devices. This singular characteristic is known to be highly influenced by any subtle structural modification hosted by those low-dimensional layers [1]. Additionally, MoS<sub>2</sub> is earning a growing interest in recent years thanks to its convenient electronic and optical properties to be an active part in the electronic semiconductors industry [2].

In this work, we study the friction using Atomic Force Microscopy (AFM) in air and under high vacuum conditions of single-layer MoS<sub>2</sub> with a controlled density of defects generated via ion irradiation. Thanks to a thorough technique, we are able to create a gradient of defects along a monolayer of MoS<sub>2</sub> and systematically study defect impact on friction and effective friction coefficient. We characterize the friction behavior of the individual vacancies and establish a method to estimate the concentration of atomic defects in a low density regime, far from Raman spectroscopy resolution.

As a result of this work, we can precisely obtain the friction coefficient of MoS<sub>2</sub> as a function of its vacancy density. It enhances our understanding of the relevance of atomic defects in the performance of this material, not restricted to tribological applications, but in any mechanical or electronic device where friction emerges as a fundamental factor.

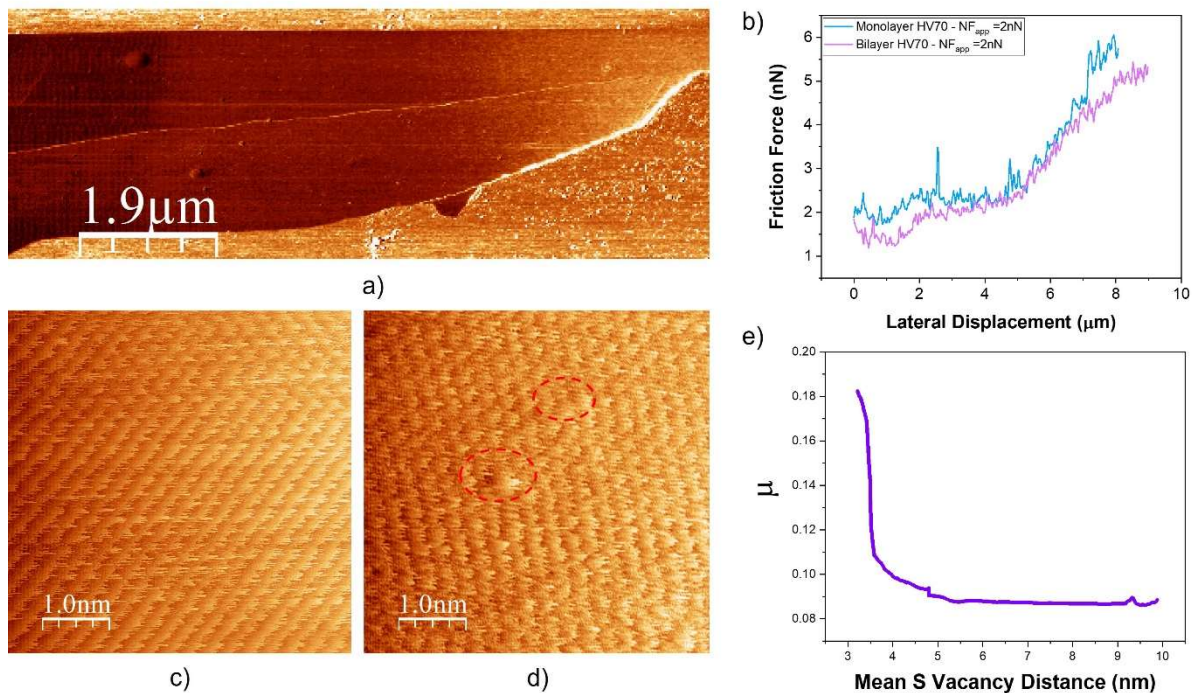


Figure 1. a) Lateral Force AFM image showing the region with generated defect gradient. b) Averaged friction profile along defect gradient region. c), d) Stick-slip images in a pristine and defective region, respectively. e)  $\mu$  vs mean sulfur vacancies density measured in MoS<sub>2</sub> monolayer.

[1] S. Zhang et al., Materials Today, **26**, 67-86 (2019)

[2] O. H. Wang et al., Nature Nanotechnology, **7**, 699-712 (2012)

# Plasmon-assisted simultaneous enhancement of single upconverting nanoparticle luminescence and trapping force

Fengchan Zhang<sup>1</sup>, Pedro Ramon Oiticica<sup>2</sup>, Marylyn Setsuko Arai<sup>2</sup>, Andrea S. S. de Camargo<sup>2</sup>, Daniel Jaque<sup>1</sup> and Patricia Haro González<sup>1</sup>

<sup>1</sup>Nanomaterials for Bioimaging Group, Departamento de Física de Materiales, Facultad de Ciencias, Universidad Autónoma de Madrid, Madrid 28049, Spain

<sup>2</sup>São Carlos Institute of Physics, University of São Paulo, Av. Trabalhador Saocarlense 400, São Carlos, SP, 13566-590, Brazil

Email: Fengchan.zhang@estudiante.uam.es

The lanthanide doped upconverting nanoparticles (UCNPs) are promising single particle imaging probes thanks to their unique luminescence properties [1]. However, there are some problems in dealing with single UCNP, such as weak brightness and low trapping stability. Surface plasmons (SPs) is an ideal approach to solve these problems. The upconverting efficiency can be improved by plasmon resonances [2]. The plasmonic traps provide the potential to break diffraction limit and enhance the trapping force [3]. Herein, we proposed the excitation of SPs to simultaneously enhance the luminescence intensity of a single UCNP and the trapping force acting on it. A 980 nm laser serves to optically trap, to excite luminescence, and to excite SPs. An Au-patterned substrate is used to generate SPs. A single NaYF<sub>4</sub>: 0.3%Tm<sup>3+</sup>, 25%Yb<sup>3+</sup> UCNP with bright visible emission is optically trapped (Figure 1a). The luminescence intensity and trapping force is measured when the trapped single UCNP is above the glass or Au-patterned substrates, respectively. Experimental results indicate that the luminescence intensity of a single UCNP is enhanced by using the Au-patterned substrate (Figure 1b). The laser power dependence of the optical trapping force shows a linear trend in both cases. The trapping force acting on a UCNP above the Au-patterned substrate shows a significant increase (Figure 1c). Such enhancement of luminescence and trapping force has a great potential in bio photonic applications and stable nanoscale manipulation.

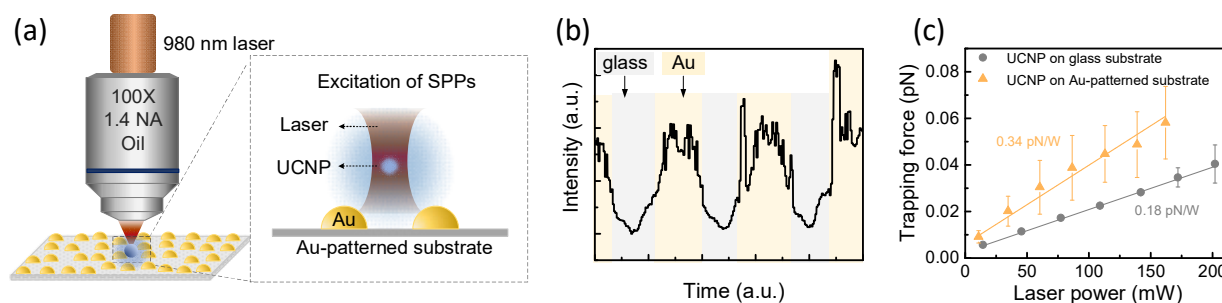


Figure 1. (a) Schematic of the trapped UCNP above the Au-patterned substrate. (b) Luminescence intensity variation of a trapped single UCNP it is moved between glass and Au-patterned substrates. (c) Laser power dependent optical trapping force acting on the single UCNP above glass and Au patterned substrates.

## References

- [1] P. Rodríguez Sevilla, L. Labrador Páez, P. Haro González. Upconverting materials for boosting the development of advanced optical microrheometric techniques. *Opt. Mater.* 2018, 84, 514-523.
- [2] D. M. Wu, A. García-Etxarri, A. Salleo, and J. A. Dionne. Plasmon-enhanced upconversion. *J. Phys. Chem. Lett.* 2014, 5, 4020-4031.
- [3] Y. Zhang, C. Min, X. Dou, X. Wang, H. Urbach, M. Somekh, X. Yuan. Plasmonic tweezers: for nanoscale optical trapping and beyond. *Light: Sci. Appl.* 2021, 10, 59.



## Organizing committee:

**Jaime Merino, Mercedes Hernando, Carmen Morant and Iván Brihuega**

### **Dirección del INC:**

**Director:** Miguel Angel Ramos.

**Deputy Director:** Isabel Jimenez Ferrer.

**Secretary:** Enrique Velasco.

**Admin. assistant:** Rocío Gómez-Argüello.

**Board:** Iván Brihuega, M<sup>a</sup> Dolores Martín, Carmen Morant and Jaime Merino.

Facultad de Ciencias - Módulo 08, 4ª Planta  
Calle Francisco Tomás y Valiente 7, 28049 Madrid  
Universidad Autónoma de Madrid  
Secretaría: Tel.: 91.497.4689. Fax: 91.497.8734. Email: [inc@uam.es](mailto:inc@uam.es)  
web: [www.inc.uam.es](http://www.inc.uam.es)

