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)


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


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)


12:40 Elena Salagrè Rubio, “Electronic Band Structure of LixCoO2 during the Insulator to Metal transition”

13:00 Jinan Hussein Al Shuaib, “Sensitized lanthanide emission in doped BaZrS3 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 TaS2 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 FePS3”

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

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

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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 ~1/3rd of the total cost of a memory chip and about ~1/10th 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 (~0.1 €/m²) is orders of magnitude lower than that of polymer substrates (PET ~2 €/m² and PI ~30 €/m²) and crystalline silicon (~1000 €/m²).

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**


**Figures**

Figure 1: Picture of several paper-electronic devices fabricated by integrating different van der Waals semiconductors on standard copy paper substrates.
Experimental and density functional theory study of the Li+ desorption in spinel/layered lithium manganese oxide nanocomposites using HCl

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Lithium manganese oxides (LMO) are the most popular lithium-ion sieves (LIS) precursor materials. Despite being the critical step in forming LIS, the "Li+ Desorption" process from the crystalline lattice of the LMO has been less explored than its counterpart, "Li+ 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 (Li2MnO3) 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.
Signatures of interactions in the Andreev spectrum of nanowire Josephson junctions


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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.

High precision low – cost spectrophotometer for agricultural applications

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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.


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".
We report here a detailed study of the valence band structure of Li$_x$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$) phases coexists and LCO exhibits metallic character. Li deintercalation generates subtle changes of the lattice parameters for each phase. Li deintercalation is usually done via electrochemical or chemical reactions. This makes it impossible to perform reliable electronic structure studies. We have used epitaxial LCO thin films grown by pulsed laser deposition on Nb-doped SrTiO$_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.

Sensitized lanthanide emission in doped BaZrS₃ perovskite semiconductor

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Nowadays there is a great interest in using semiconductors as host materials for photoluminescent lanthanide ions (Ln³⁺). 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 Ln³⁺ in semiconductors is difficult to achieve because Ln³⁺ 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 ABX₃, with A being a group II cation (i.e., Ca²⁺, Sr²⁺, or Ba²⁺), B a group IV transition metal (i.e., Ti⁴⁺, Zr⁴⁺, or Hf⁴⁺), and X a chalcogen anion (S²⁻ or Se²⁻) [3]. The B site features an octahedral coordination environment ideal for embedding Ln³⁺.

Moving from these considerations, here we present the synthesis and characterization of BaZrS₃ perovskites doped with Ln³⁺ (Yb³⁺, Er³⁺, Nd³⁺). Samples were prepared by sulfurization of Ln³⁺-doped BaZrO₃ 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 Ln³⁺ (see Figure 1e).

Figure 1. Schematic crystal structure (a) and XRPD pattern (b) of BaZrO₃. Schematic crystal structure (c) XRPD pattern of chalcogenide perovskite BaZrS₃. Photograph of chalcogenide perovskite BaZrS₃. (e) Photoluminescence emission spectra of pure and Ln³⁺-doped BaZrS₃ powders, recorded under illumination with λex= 405 nm at T=10 K.

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.


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

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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.
Kondo lattice development in a TaS$_2$ van der Waals heterostructure

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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$_2$ on a 2H-TaS$_2$ crystal. The 1T-TaS$_2$ 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.

Tunable thermal emission of subwavelength silica ribbons

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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 SiO₂ 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]

Plasmonic nanoparticles for inflammation targeting in atherosclerosis

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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 diagnosis of atherosclerosis in its early stages, characterized by the inflammation of the arterial walls and subsequent overexpression of several molecules \cite{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 \cite{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@aICAM) 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.](image)

\cite{1} J. Sanz et al., Nature, 451, 953 (2008)
\cite{2} J. Hu et al., Journal of Biophotonics, 5, 674 (2017)
17:20 “Tribological motion of rotating vesicles”

Paula Magrinya

Física Teórica de la Materia Condensada

Tribological motion of rotating vesicles

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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.](image)


Direct magnetic evidence, functionalization and low-temperature magneto-electron transport in liquid-phase exfoliated FePS$_3$


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Magnetism and the existence of magnetic order in a material is determined by its dimensionality. In this regard, the recent emergence of magnetic layered van der Waals (vdW) materials provides a unique playground to explore the exotic magnetism arising in the two-dimensional (2D) limit. The magnetism of 2D flakes has been commonly studied by indirect methods like Raman spectroscopy. Here, taking advantage of liquid-phase exfoliation (LPE) method, we show a first direct magnetic evidence of the antiferromagnetic transition in FePS$_3$ 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$_3$ 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$_3$ flakes ($\omega_1$) trapped by DEP. (c) Current $I$ – Temperature $T$ characteristics measured on a FePS$_3$ 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 $T$.

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 CuInS2
3. Andrino Gómez, Alberto: Preparation and study of potential Bi-Sb amorphous topological superconductors
5. Bernabeu Gómez, Joan: Phonon-Mediated Hydrodynamic Transport in Weyl Semimetals
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
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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$_2$

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Pressures in the range of 0-3 KPa are involved in several biological processes, such as tumor progression. 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. One of the best candidates as pressure sensor probes are copper indium sulfide (CuInS$_2$) 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$_2$ 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](image-url)

**Figure 1.** CuInS$_2$ 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.


Preparation and study of potential Bi-Sb amorphous topological superconductors

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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 Bi\textsubscript{x}Sb\textsubscript{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.

Engineering Transport Orbitals in Single Molecule Junctions

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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 theromopower, 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.

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”).

[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

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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$^2$, b) $50 \times 50$ nm$^2$.

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

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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 Ag2S 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


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

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

In this talk, we introduce how nanoplasmonic 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
Swimming motility of E. coli in the presence of magnetic rotating obstacles

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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 \cite{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 \cite{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.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Experimental setup for the generation of homogeneous rotating magnetic fields.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Comparison of MSD_{avg} between bacteria with and without external rotating magnetic field.}
\end{figure}

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

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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](image-url)

**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.

Control at the nanoscale of graphene superconductivity.

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

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

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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 to 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 dissipated. 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.

Transport of active colloids in structured environments

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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.


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

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

References:

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

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

Figure 1. Cross section sequence of the mz 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.

Vacuum-field-induced state mixing

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The properties of atoms and molecules undergo modifications due to 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.

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

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

The 1144 CaKFe$_4$As$_4$ compound is a pnictide superconducting material showing optimal superconducting critical temperature with Tc 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 Tc 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 CaKFe$_4$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 CaKFe$_4$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 CaKFe$_4$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.

Functional Optimization of PVD-LiCoO$_2$ Cathodes for Li-Ion Batteries

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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 fulfill 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$_2$: (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 μA·h/μm, CE of 97 ± 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$_3$O$_4$ 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)
Development of a technological AFM microscope for operation in UHV

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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 environments (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.

Optical interferometry as an efficient tool to characterize STM head vibrations

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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 5x5mm² 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

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

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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.

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.
Neural networks for simultaneous quantum parameter estimation

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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 \cite{1}. We generated photodetection registers using Monte Carlo methods in order to train and test the neural network \cite{1}. To assess the performance, that same data was analyzed using the Fisher information in order to set a benchmark \cite{2}. The network estimations are reasonably good since they are close to that of the Fisher information.

![Figure 1. Recurrent neural network used.](image)

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García Herreros, Sergio

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

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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 µm. Concerning hydrogen concentration, the analysis has shown that the anode stability decreases with increasing the poli-hydride concentration (hydrogen arranged as Si-Hₓ) 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.

García, Pablo
Física de la Materia Condensada

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

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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 FeSe$_{1-x}$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 FeSe$_{1-x}$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.

Collective behavior in driven colloidal crystals

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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.

Towards hybrid van der Waals Josephson junctions based on NbSe$_2$

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The emergence of van der Waals heterostructures has paved the way for a “designer” approach, in which novel devices and new physics can be obtained by combining the properties of distinct two-dimensional materials. Among the many possibilities in this context, heterostructures based on superconducting few-layer NbSe$_2$ 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$_2$ 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$_2$, including our first attempts to fabricate Josephson junctions with and without ferromagnetic and antiferromagnetic tunnel barriers


Figure 1. (a) Temperature dependent PL spectrum of a GaP$_{1-x}$N$_x$ layer with x = 0.012 grown at 550 ºC. (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 $C_{NM}$ equal to 3.05 eV. (c) Integrated PL intensity as a function of 1/kBT. 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.

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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 $T_C$.

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

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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$^{3+}$-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 μs 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](image)

Figure 1. a) Schematics of the monolithic architecture for pulsed nanolasing. The hybrid system includes: Nd$^{3+}$-doped LiNbO$_3$ as a gain media, plasmonic Ag nanoparticle chains for sub-wavelength spatial confinement, and 1-layer MoS$_2$ 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.

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Inglés Cerrillo, Julia

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

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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.

Highly defective MoS$_2$ ultrathin nanoflakes for electrolytic hydrogen production

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The rational design of advanced electrocatalysts for green hydrogen production by supplying electricity from renewable sources is a key issue to be addressed in order to reduce CO$_2$ emissions. Two-dimensional transition metal dichalcogenides, such as MoS$_2$, 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$_2$ over large area substrates (of about 1 cm$^2$). We have also shown that the introduction of a H$_2$ 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 ($A_{1g}$ and $E_{2g}$) characteristic of 2H-MoS$_2$.

Next, we tested our MoS$_2$ 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$_2$ through nanostructuring and defect engineering, playing with the growth conditions and the possibility of growing homogeneous thin films, which brings applications closer.

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Figure 1. From left to right: Photograph of one MoS2 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-MoS2.


Inorganic chalcogenide perovskites are semiconductors with the general formula ABX₃, with A being a group II cation (i.e., Ca²⁺, Sr²⁺, or Ba²⁺), B a group IV transition metal (i.e., Ti⁴⁺, Zr⁴⁺, or Hf⁴⁺), and X a chalcogen anion (S²⁻ or Se²⁻). 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 Sr₁⁺ₓTiS₃₋ₙthin films. Here we present a novel synthesis procedure to obtain STS thin films.

STS films have been obtained by sulfurization of SrTiO₃ (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 CS₂ and STO thin films inside a closed quartz ampoule. The second procedure has been accomplished in a tubular quartz reactor under CS₂ 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 Ar/H₂ mixture (95%-5%) has been used as the carrier gas by passing it through a bubbler containing CS₂. The small H₂ 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 H₂ production.

**Figure 1.** Pictures of a SrTiO₃ thin film and a bare quartz substrate (to the left) inside an allumina crucible before (1) and after (2) the sulfurization process with a CS₂ flow.
Cavity mediated energy transfer driven by a photochemical reaction

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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.

López Peña, Gabriel  
Física Aplicada

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

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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 photosensitizer 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.](image)

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.

Low resistance contacts to few layered MoS$_2$ by local pressurization

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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$_2$: 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$_2$ pressurized under the tip. b) I-V curves metallize when ultra-high pressure is applied to MoS$_2$. 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$_2$ 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$_2$ 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$_2$ 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.

Thermal reading in brain phantom under microwave radiation

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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.[1] 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.[2] 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.[3] 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. [4] Moving from these considerations, we developed a thermometric approach based on Ag2S 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
Specific heat of ultrastable glasses at low temperatures

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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].

Electronic band structure inside the superconducting gap from Yu-Shiba-Rusinov states in quasi two-dimensional 2H-NbSe$_2$-$x$S$_x$

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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$_2$-$x$S$_x$ 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$_2$. Density Functional calculations suggest that the two-dimensional electronic properties of S doped 2H-NbSe$_2$ 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

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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 β-NaYF₄: Yb³⁺, Er³⁺ microparticle is presented as a local sensor. The microparticle shows an intense visible emission under 808 nm photoexcitation: The red emission (⁴F₉/₂ → ⁴I₁₅/₂ transition of Er³⁺ 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 (²H₁₁/₂ → ⁴I₁₅/₂ and ⁴S₃/₂ → ⁴I₁₅/₂ transitions of Er³⁺ 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.

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Nano-scale conductivity of Hi3(HITP)2 Metal-Organic Framework

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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 Hi3(HITP)2 grown in simulated microgravity conditions. Hi3(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 Ni3(HITP)2 thin films.

Modelling AC hysteresis loops of ferromagnetic nanoparticles

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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 (shadowed 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

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Hydrogen storage is a fundamental aspect of the hydrogen economy. Storing H₂ 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.


Study of Oxide Equilibrium in Pulsed Laser Deposited LiCoO$_2$ for Li-Ion Batteries

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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$_2$ (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$_3$O$_4$ and CoO) were identified, whose evolutions with the PLD parameters are investigated by µRaman spectroscopy, Confocal Raman, GIXRD, RBS-NRA and AFM. Raman and GIXRD reveal the two HT-LCO and Co$_3$O$_4$ 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 600ºC and LT-LCO at room temperature and annealed at 600ºC). HT-LCO/Co$_3$O$_4$ 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 revaporation 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$_3$O$_4$ Raman signal ratio and (b) analysis of the Li depth profiles by RBS-NRA.](image-url)

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

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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 LiNbO₃: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 µm) in water droplets and cell spheroids (3D cell models, ~100-300 µm) 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-paraffine 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](image)

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Phase engineering of two-dimensional Transition Metal Ditellurides

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Phase engineering of two-dimensional transition metal ditellurides (2D-TMDTs) is a promising way to exploit their electronic properties in order to apply them in electronic devices such as photodetectors, LEDs, phototransistors, and solar cells [1]. 2D-TMDTs have a MT₂ 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 MoTe₂, 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 TaTe₂, 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 MoTe₂ and TaTe₂ 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 TaTe₂ islands on gr/Ir(111) (V = -1V; I = 0.1nA). Inset: sketch of the growth procedure. (b) Relative coverage of 1T’ vs. 1H-MoTe₂ phases for different growth temperatures. STM images of (c) 1H-MoTe₂ (V = 0.5V; I = 0.1nA) and (d) 1T’-MoTe₂ islands (V = 1V; I = 0.1nA). (e) Relative coverage of 1T vs 1H-TaTe₂ phases for different growth temperatures. STM images of (f) 1T-TaTe₂ (V = 0.75V; I = 0.2nA) and (g) 1H-TaTe₂ islands (V = 1V; I = 0.2nA).

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

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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 Δ45-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 Δ45-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 ~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
Electrostatic doping of monolayer MoS$_2$ deposited on hexagonal ferroelectric domains

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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$_2$ when deposited on a ferroelectric crystal (LiNbO$_3$) 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$_2$. 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.

![Image](image.png)

Figure 1. (a) Optical microscopy image of 1L MoS$_2$ deposited on hexagonal ferroelectric domains structure (LiNbO$_3$). (b) PL intensity distribution showing the exciton-dominant region (p type, in red) and the trion-dominant region (n type, in green).

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

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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 μJ/K, one order of magnitude higher than in canonical glasses, but similar to some disordered crystals. The determined Debye temperature is 482 (±6) K of the order of other nanoscale diamond-type materials. The thermal transport considerations are supported by the phonon mean free path calculations.

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

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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]).

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.

INC Research awards for Physics students 2022

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Study of colloidal systems in lattice obstacles

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Currently I’m studying a macroscopical version of the experiment that is been done in INC by the group of J.L. Aragones 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 MATAB 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

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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 \cite{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.

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.

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

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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.

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Defects as a key to control friction on monolayer MoS$_2$

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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$_2$ 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$_2$ 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$_2$ 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$_2$ 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$_2$ monolayer.

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

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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 NaYF₄: 0.3%Tm³⁺, 25%Yb³⁺ 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

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