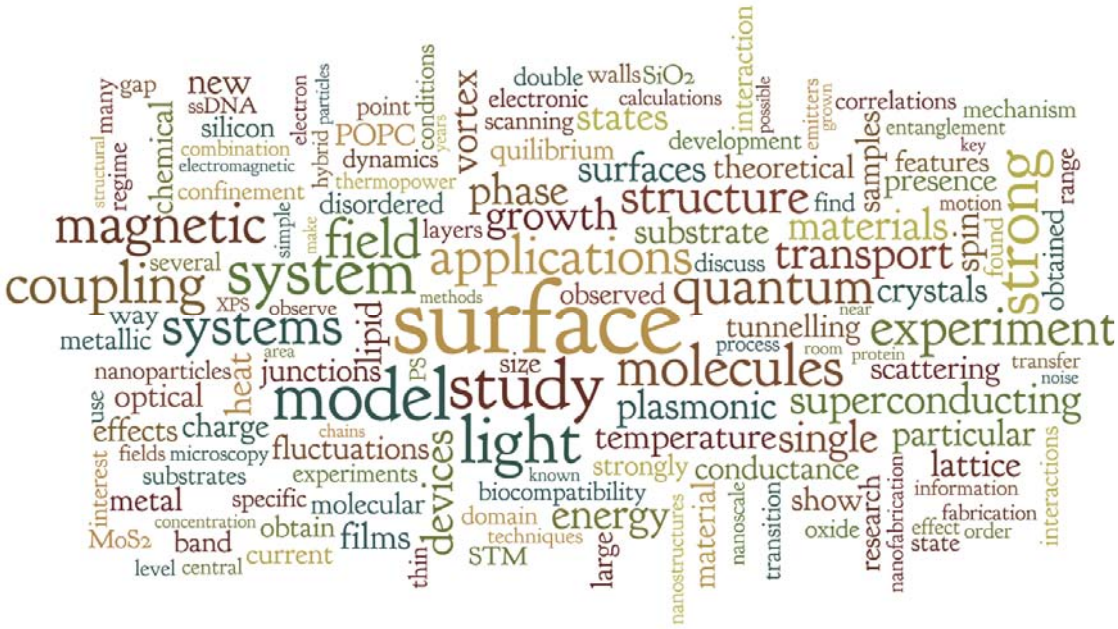
Instituto Universitario de Ciencia de Materiales Nicolás Cabrera

XVII JORNADA DE JÓVENES CIENTÍFICOS DEL INSTITUTO DE CIENCIA DE MATERIALES NICOLÁS CABRERA



19 de Diciembre de 2014

Residencia La Cristalera, UAM

Miraflores de la Sierra, MADRID

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FACULTAD DE CIENCIAS

TABLE OF CONTENTS

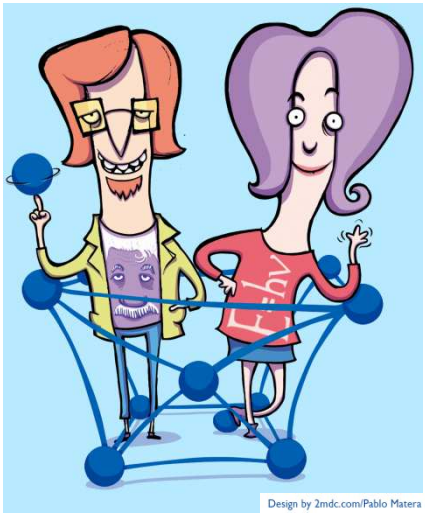
Cover figure: statistics on most common words in this booklet.

Dear members of the Nicolas Cabrera Institute:

The other day, I was browsing on the internet and I found a paper entitled "Disruption by Design". The author proposes that "design innovation—not technological innovation—is what disrupts businesses and industries.". If he is right, then we must shift our focus from "technological innovation to design innovation". He continues setting his argument by showing different examples and ends up, of course, with Apple. "By doing what it does, Apple disrupts. Again, and again, and again.". The point is relevant for us. How can we write highly cited papers and develop instruments and methods used by many scientists, again, and again and again?

The author then defines "Design thinking": "Design thinking is not focused on making things look attractive or trendy. Rather, it is focused on gaining an understanding of an area of human experience and then developing a product, service, or process that improves that area of experience for many people, often empowering people in new ways…New technologies can expand the universe of possible design solutions, but it is empathy with people in their actual daily lives that is essential to great design and disruptive innovation."

We can translate this into our "business", Physics: "Design thinking is focused on understanding an area of Physics and then writing a paper or developing a method or an instrument that improves that area of Physics for *many scientists*, often empowering scientists in new ways. New technologies can expand our possibilities to make Physics, but it *is empathy with our peers*, our colleagues within our Campus and our colleagues elsewhere, that is essential to great Physics and disruptive innovation.



During past years, in the Nicolás Cabrera Institute, we have promoted empathic relationships among us and with our peers abroad using different methods, as our Summer School, which will be held in July and is likely to be very successful again, our colloquia, prizes for young peers (two of which are talking today), video-making with our students and workshops. We have counted on the generous support of the FBBVA foundation for the Summer School and the colloquia, and with the help of UAM Vicerrectorates (Research and Science policy) for the rest of the activities. We deeply acknowledge in particular FBBVA. They represent the support from outside science, from the society, to our activities—this is fundamental to us.

In the Nicolás Cabrera Institute, we also promote the development of new services and infrastructures—new technologies, which could empower us in new ways. These

services and infrastructures are being managed by different organizations within our Campus. It is their responsibility to create empathic relationships, *in particular with the scientists having highest impact.*

When I was an early teenager, during the early eighties, I promenaded with my parents on nice forests during my vacations in Germany. I had to look up on Allied jets flying a few hundred meters above our heads, training for the worst case. It was fascinating to see these machines, but it was also frightening and I asked myself what was the point of all this noise. Managers, directors and coordinators in science are also making lots of noise now. They speak about technological issues, come up with analytical accounting and praise the importance of following norms and procedures. As fascinating as these creations may seem, their point is unclear to me. They don't use our metrics, the ISI web of knowledge and related services, in their accounting system, and they don't use our norms—which simply consist on gaining recognition from our peers through peer review—in setting up procedures. When applied to science and technological innovation, industrial management methods useful for production have been bound with failure, and are bound for failure.

The jets above Germany stopped at some point, a few years after Nena raised 99 red balloons against captain Kirk. What shall *we* do now to provide researchers with means to write papers and develop methods and instruments used by many scientists, again, and again and again? I think that we have to examine our managing methods, and understand how to put scientific excellence on the forefront. Establishing an empathic relationship with the best researchers, *giving priority to their projects*, asking them for ideas and hearing to their needs, is a reasonable first step. This starts by talking with our colleagues. Not only our Institute, but also IFIMAC, should be much more integrated in all discussions about our infrastructures and our services.

I would like to invite young scientists of our Institute to use this day to talk with each other. At the same time, I would like to invite everybody to think on the future, in particular of new infrastructures and services, and show the youngest that we have ideas which will help them to build the future.

Many of you have read your PhD in 2014 and are now going into the competitive procedure of obtaining grants within the European system. We wish you the greatest success and hope to see you coming back as scientific leaders.

Hermann Suderow

Director of the Nicolás Cabrera Institute

PROGRAM

9:30 **Openning** session of the XVII Young Researchers Meeting of the INC

Session I.

Chair of the session: Hermann Suderow

09:40 **INC Young Researchers First Prize in Materials Science 2014**: *"Low-temperature specific heat of amber: An insight on the universal properties of glasses"*
Tomás Pérez Castañeda (Dpto. de Física de la Materia Condensada)

10:10 **INC Young Researchers Second Prize in Materials Science 2014***: "Blue second harmonic generation enhancement by Ag nanocubes on nonlinear ferroelectric crystals"*
Laura Sánchez-García (Dpto. de Física de Materiales)

10:30 **Invited talk***: "Micro and Nanofabrication at the CEI UAM+CSIC"*
Daniel Granados (IMDEA)

11:00 – 11:20 **Cofee Break**

Session II.

Chair of the session: Mariola Ramirez

11:20 *"Biosensing platforms based on the plasmon resonance of gallium nanodroplets"*
Antonio García Marín (Dpto. de Física Aplicada)

11:40 "Non-stationary and noise properties of molecular junctions in the polaronic regime"
Ruben Seoane (Dpto. de Física Teórica de la Materia Condensada)

12:00 *"Effect of long-range spatial correlations on the lifetime statistics of an emitter in a two-dimensional disordered lattice"*
Nuno de Sousa (Dpto. de Física de la Materia Condensada)

12:20 "*Channel waveguide fabrication technique in $KY(WO_4)_2$ combining liquid-phase-epitaxy and beam-multiplexed fs-laser writing*"
Jon Martinez (Dpto. de Física de Materiales)

12:40 "*Porous silicon: from biological functionalization to optoelectronic nanocomposites*"
Darío Gallach Pérez (Dpto. de Física Aplicada)

13:00 – 14:15 **Poster Session**

14:15 – 15:30 **Lunch**

Session III.

Chair of the session: Isabel Guillamón

15:30 *"Entanglement detection in coupled particle plasmons"*
Javier del Pino (Dpto. de Física Teórica de la Materia Condensada)

15:50 *"Interaction between localized surface plasmons and rare-earth ion based solid-state gain media"*
Eduardo Yraola (Dpto. de Física de Materiales)

16:10 *"Study of the growth and interaction of Co oxides on oxide substrates"*
Daniel Díaz Fernández (Dpto. de Física Aplicada)

16:30 *"Superconducting properties and vortex lattice in β-Bi_2Pd"*
Edwin Herrera (Dpto. de Física Aplicada)

16:50 **Closing** session of the XVII Young Researchers Meeting of the INC

Session I.

Chair of the session: Hermann Suderow

09:40 **INC Young Researchers First Prize in Materials Science 2014:** "Low-temperature specific heat of amber: An insight on the universal properties of glasses"
Tomás Pérez Castañeda Dpto. de Física de la Materia Condensada

Low-temperature specific heat of amber: An insight on the universal properties of glasses

Tomás Pérez Castañeda[1], Rafael J Jiménez-Riobóo[2] and Miguel Ángel Ramos[1]

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Amber has been appreciated by mankind for its colour and natural beauty since the Neolithic Era. It also has a well-known paleontological significance, being a unique preservational system where ancient bio-inclusions of animal and plant materials were stuck in the viscous resin and then fossilized for million years[1,2]. However, amber can also be a gemstone for physics and chemistry research on glasses, including the glass transition problem[3-5], and the long-standing debate about the anomalous low-temperature properties of glasses or amorphous solids[6-8]. In this talk I will show that the two most prominent and ubiquitous features of glasses at low temperatures, namely the presence of tunnelling two-level systems[6,7] and the so-called boson peak[8] in the reduced vibrational density of states, persist essentially unchanged in highly stabilized glasses, contrary to what was usually envisaged. Specifically, we have studied 110 million-year-old amber samples from El Soplao (Northern Spain)[9]. Specific heat C_p measurements of pristine, partially- and fully-rejuvenated samples were conducted in the temperature range 0.07K < T < 30 K, as well as around its glass-transition temperature $T_g \approx 150$ºC. A modest increase of the boson-peak height (in C_p / T^3) with increasing rejuvenation was observed, that can be related to a corresponding increase of the Debye coefficient. The amount of two-level systems, assessed at the lowest temperatures, was however found to be exactly the same for the pristine hyperaged amber as for the subsequently rejuvenated samples.

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10:10 **INC Young Researchers Second Prize in Materials Science 2014:** "Blue second harmonic generation enhancement by Ag nanocubes on nonlinear ferroelectric crystals"

Laura Sánchez-García Dpto. de Física de Materiales

Blue second harmonic generation enhancement by Ag nanocubes on nonlinear ferroelectric crystals

L. Sánchez-García[1], P. Molina[1], M. O Ramírez[1], F. Gallego-Gómez[1], J.J. Carvajal[2], M. Aguiló[2], F.Díaz[2], C. de las Heras[1] and L.E. Bausá[1]

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Metallic nanoparticles are of enormous interest for a wide range of scientific and technologic applications such as chemical and biological sensors, surface-enhanced spectroscopies, photodetection, light harvesting and optical nanodevices [1]. In these systems, the resonant excitation of local surface plasmons (LSP) can lead to a strong confinement of the electromagnetic field at the nanoparticle surface providing a means to significantly enhance the optical interactions at subwavelength scales. The plasmon-resonance conditions depend on both size and geometry of the nanoparticles, which justifies the growing interest in the fabrication and control of metal nanoparticle of different morphologies. Well-shaped nanoparticles with narrow size distributions are highly desirable for specific applications [2].

Here, we show the ability of deposition of silver nanocubes exhibiting low (~10%) size dispersion by a simple photochemical method on the polar surface of the $RbTiOPO_4$ (RTP) ferroelectric crystal.

Due to its relatively large nonlinear coefficients, RTP has shown to be an interesting system for efficient blue light generation by means of quadratic frequency conversion processes. In this work, we demonstrate that the plasmonic properties of the photo-deposited silver nanocubes on the polar surface of RTP can be used to further enhance the performance of the nonlinear frequency conversion in the blue spectral region [3]. An enhancement by a factor of 3 is obtained, which is susceptible to be further improved by optimized nanoparticle distributions.
Additionally, it is important to mention that, in our system, the nonlinear frequency conversion takes place at nanometric interfaces (the ferroelectric domain walls), which is of technological interest in the context of the development of nonlinear photonic nanodevices.

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10:30 **Invited talk:** *"Micro and Nanofabrication at the CEI UAM+CSIC"*
Daniel Granados IMDEA

Micro and Nanofabrication at the CEI UAM+CSIC

Daniel Granados[1], Manuel Rodriguez[1], Ramón Bernardo-Gavito[1,2], Rodolfo Miranda[1,2,3]

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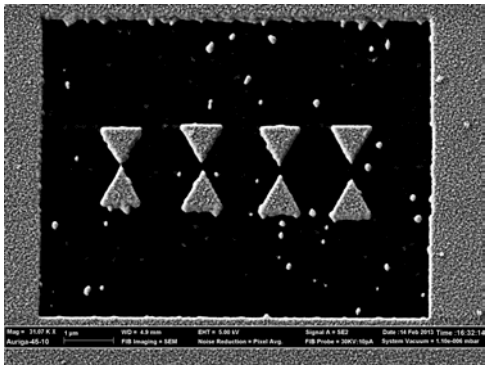
The Centre of Nanofabrication is a joint proposal between the IMDEA-Nanoscience and campus of excellence UAM-CSIC to create a facility of excellence for the micro and nanofabrication of structures and devices based on a wide range of nanosciences such as 2D materials, nano-optics, photonics, radiation detectors, nano-magnetism, bio-chemistry, micro-fluidics, nems&mems, or nanostructured organic semiconductors; among others. After 5 years of hard work, this centre has been recently finished and since September 2014 is fully operational. In this presentation i will present a brief summary of the micro and nanofabrication available resources and some examples of the ongoing research on several topics.

The fabrication of such nanostructures and devices is crucial for fundamental research, but also for the development of prospective nanotechnologies with commercial applications. The Centre for Nanofabrication plays a key role for the development of the strategic plan of IMDEA-Nanoscience as well as of the Campus of excellence UAM-CSIC. The Centre of Nanofabrication is hosted at the IMDEA-Nanoscience premises in a latest generation clean room, with more than 200m^2 of clean room surface The latest available state of the art micro and nanofabrication technologies, such as FIB Lithography, e-Beam Lithography, NanoImprint and hot embossing Lithogrpahy, ICP-Atomic Layer Deposition, UHR FE-SEM and STEM, cryo ICP-Reactive Ion Etching, etc, will be on hand for the fabrication and manipulation of metallic, semiconducting and organic nanostructures and nanoscience-based devices.

The Centre of Nanofabrication will empower the research groups in the framework of the Campus of Excellence project with an efficient access to the state of the art nanofabrication resources.



Bow-Tie Antennas fabricated by direct milling of 100nm Au on Soda-Lime Glass by Focused Ion Beam Lithography

Session II.

Chair of the session: Mariola Ramirez

11:20 *"Biosensing platforms based on the plasmon resonance of gallium nanodroplets"*
Antonio García Marín Dpto. de Física Aplicada

Biosensing platforms based on the plasmon resonance of gallium nanodroplets

A. García Marín[1], M. J. Hernández[1], E. Ruiz[1], José M. Abad[2], E. Lorenzo[2], J. Piqueras[1], J. L. Pau[1]

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In the field of refractive index sensing, many research groups have focussed on plasmon line shape tuning in order to narrow down the line widths, which results in a higher figure-of-merit (FOM = (dλ/dn)/fwhm), which makes it possible to reach lower detection limits.[1] One path to reach this goal is to look at Fano interference, a characteristic asymmetric line shape observed under certain conditions in scattering, transmission and reflection spectra. In periodic arrays of localized plasmon resonators, the origin of this interference is attributed to the coupling of different plasmonic modes which have been applied successfully for refractive index sensing applications.

In the present work, we investigate the resonance in self-assembled Ga nanodroplets (GaNDs) by spectroscopic ellipsometry. They present strong localized surface plamon resonance in the resulting spectra with two characteristic oscillation modes, whose energy position depends on the droplet diameter.[2] For diameters ranged between 240-280 nm (Figure 1A), we observe strong Fano interference between different plasmon modes, whose intensity is strongly dependent on the incident angle (Figure 1B).

The resonance is employed to develop an immunosensor capable of detecting small molecules, such as glutathione (GSH) in external reflection ellipsometry by using antibodies as recognition elements. The sensing characteristics of this architecture are demonstrated in immunoassays performed under increasing concentrations of L-reduced GSH (analyte).

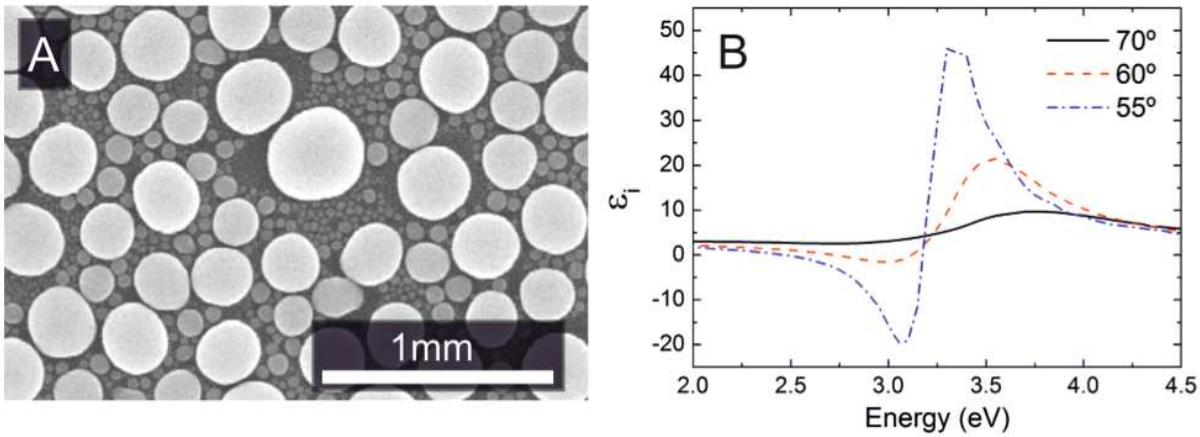

Figure 1: (A) GaNDs deposited on the Si(100) substrate; (B) Ellipsometric spectra of the GaNDs at different incident angles.

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11:40 "Non-stationary and noise properties of molecular junctions in the polaronic regime"

Ruben Seoane Souto Dpto. de Física Teórica de la Materia Condensada

Non-stationary and noise properties of molecular junctions in the polaronic regime

Rubén Seoane Souto, Rosa Carmina Monreal, Álvaro Martín Rodero and Alfredo Levy-Yeyati

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Localized vibrations (phonons) may have an important impact in the transport properties of nanoscale conductors [1]. Such effects have been observed in many different systems such as atomic chains, semiconducting quantum dots, carbon nanotubes and other molecular junctions. In spite of this variety, from a theoretical point of view all these situations can be qualitatively described by the rather simple Anderson-Holstein model. This model considers a single resonant level coupled to fermionic reservoirs and to a localized phonon mode. The exact solution for this model has not been found, except for some limiting cases.

In this work we focus in the so called polaronic regime, where the coupling between electrons and phonons is strong, compared with the coupling of the level to the electrodes. We present a new approach to the problem based on a resummation of the dominant Feynman diagrams from the perturbation expansion in the coupling to the leads [2]. This approximation eliminates the main pathologies found in the simple analytical approaches for this regime. With this scheme we are able to investigate the stationary transport properties, not only the average current but also the current fluctuations.

While the stationary properties of this model have been extensively analyzed, by many approximations, the way the system reaches the steady-state is not yet well understood. Using the approximation described before, we are able to analyze the evolution of the average current and the level population. We compare the results with numerical exact results obtained from path-integral Monte Carlo [3], showing a good agreement for different range of parameters and initials preparations of the system. It still remains open the question about the dynamical evolution of the current fluctuations.

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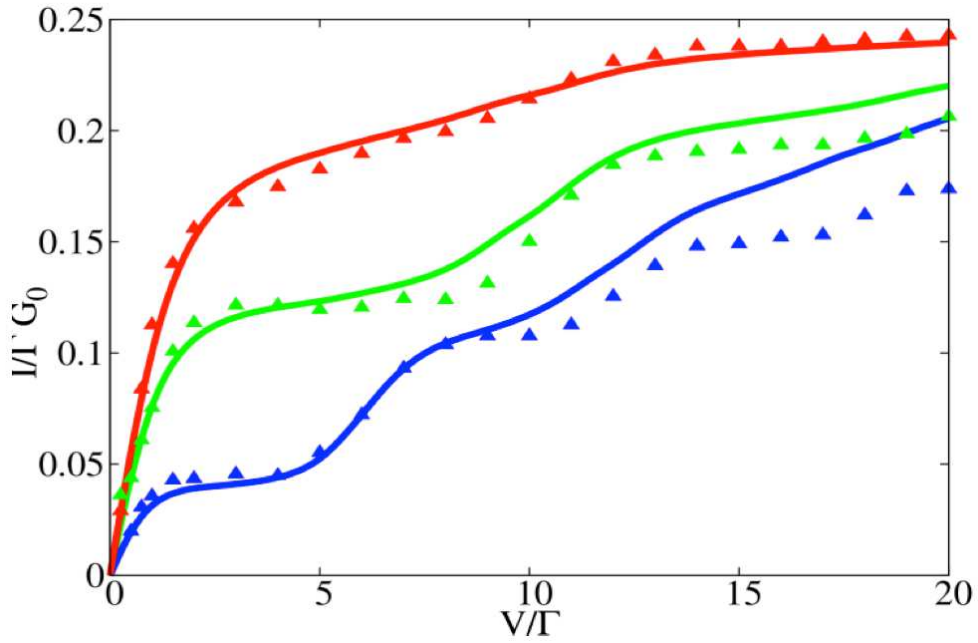

Figure 1: Evolution of the current with the bias voltage, for weak (red), intermediate (green) and strong (blue) electron phonon coupling. The dots correspond to the numerical Monte Carlo results shown in [4]

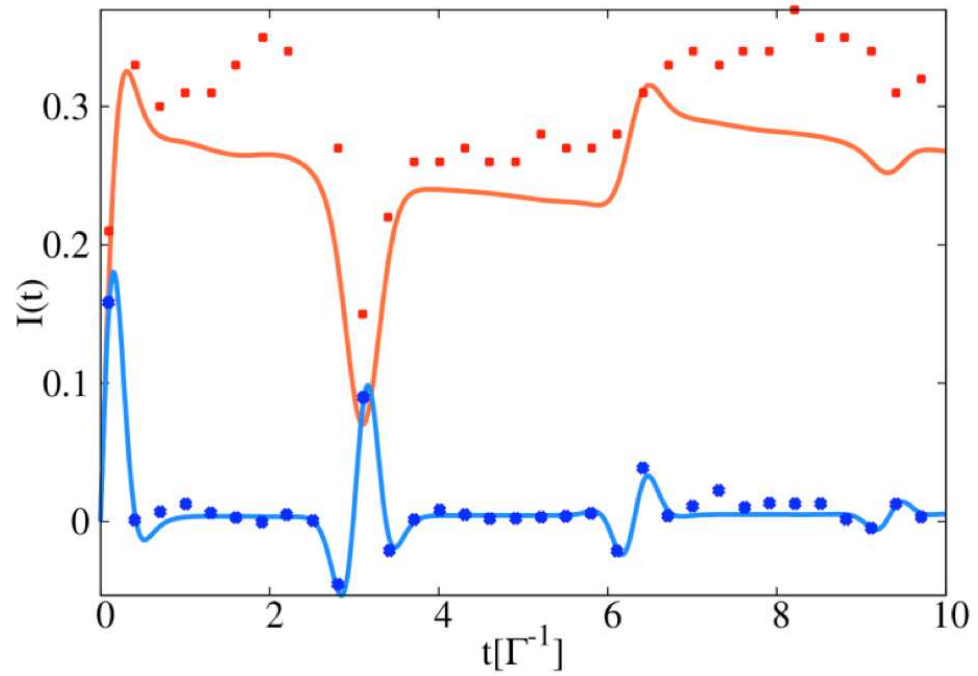

Figure 2: Time dependent evolution of the current for two initial preparations: Level initially empty (red) and initially full occupied (blue). The dots correspond with the numerical monte Carlo results presented in ref [3]

12:00 *"Effect of long-range spatial correlations on the lifetime statistics of an emitter in a two-dimensional disordered lattice"*

Nuno de Sousa Dpto. de Física de la Materia Condensada

Effect of long-range spatial correlations on the lifetime statistics of an emitter in a two-dimensional disordered lattice

N. de Sousa,[1] J. J. Sáenz,[1, 2, 3] A. García-Martín,[4] L. S. Froufe-Pérez,[5] and M. I. Marqués[2, 6]

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The statistical properties of light transport and emission in disordered media has been a matter of intense research during the last century. Being the basis of coherent multiple scattering of waves well known, the phenomenon itself is not yet fully explored and understood. These multiple wave scattering effects are at the heart of emerging behaviours like Anderson localisation of light and electrons, band structure in crystalline solids or photonic crystals (PhC), among many others. Although the limits of perfectly ordered systems on the one hand, and uncorrelated and relatively weakly scattering systems on the other hand, are quite well understood. Between these limits there is a gap largely unexplored. In particular, it has been shown in many different situations that disordered systems exhibiting certain structural correlations can share properties of both crystalline and fully disordered systems. For instance, the conductivity of liquid metals [1] or the cornea transparency [2] can be understood in the same footing: a disordered but correlated system can present spectral regions of high transparency for electron or light transport.

The effects of disorder in an initially ordered structure, such as a PhC, might lead to strong Anderson localisation, as the scattering mean free path can be severely reduced in the band edges [3]. Also, strongly correlated charged colloids can scatter light in such a way that the transport mean free path presents a strong chromatic dispersion [4]. Even in the absence of practically any long range correlations, the structure of the scatterers itself can be used to modify the light

emission and trans- port properties of a disordered system in such a way that transport parameters [5, 6], or even the threshold of a random laser [7], can present resonances which can be tuned in advance. The effect of correlations in a disordered structure regarding light emission properties of single fluorescent emitter has been a matter of much less intense research efforts. It is clear that the structure surrounding a single emitter can largely alter its emission dynamics [8]. In the last years, several groups considered such effects in a statistical way suitable for the description of disordered systems [8–10]. In particular, in ref.[10] it was shown that several structural properties near a phase transition can be accessed via fluorescence intensity fluctuations. Is has been theoretically and experimentally proven that near field scattering in random systems alters fluorescence dynamics in such a way that microscopic information about the surroundings of a single emitter can be obtained from lifetime fluctuations or from the shape of the statistical distribution tails [11–13].

In this presentation we show the effect of spatial correlations on the Purcell effect in a bidimensional dispersion of resonant nanoparticles. We perform extensive calculations on the fluorescence decay rate of a point emitter embedded in a system of nanoparticles statistically distributed according to a simple 2D lattice-gas model near the critical point. For short-range correlations (high temperature thermalisation) the Purcell factors present a long-tailed statistic that evolves towards a bimodal distribution when approaching the critical point where the spatial correlation length diverges. Our results suggest long-range correlations as a possible origin of the large fluctuations of experimental decay rates in disordered metal films.

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12:20 *"Channel waveguide fabrication technique in $KY(WO_4)_2$ combining liquid-phase-epitaxy and beam-multiplexed fs-laser writing"*

Jon Martinez Dpto. de Física de Materiales

Channel waveguide fabrication in $KY(WO_4)_2$ combining liquid-phase-epitaxy and beam-multiplexed fs-laser writing

J. Martínez de Mendívil[1], J. Hoyo[2], J. Solís[2], M.C. Pujol[3], M. Aguiló[3], F. Díaz[3] and G. Lifante[1]

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In the present work we propose a channel waveguide fabrication process based on the cladding microstructuration of a planar waveguide by fs-laser writing. The core of the waveguide is formed by a layer of $KY:Gd:Lu(WO_4)_2$ epitaxially grown over a $KY(WO_4)_2$ substrate by means of Liquid Phase Epitaxy (LPE) [1]. A cladding of $KY(WO_4)_2$ is then grown by LPE over the core waveguide. To obtain lateral light confinement, the cladding is then micromachined using the beam multiplexed femtosecond laser writing technique [2], forming thus a ridge structure. Channel waveguides fabricated following this approach have been characterized in terms of their mode sizes and propagation losses at 0.98 μm and 1.64 μm, which are close to the wavelengths of interest in lasers/amplifiers based on the Er^{3+}/Yb^{3+} system. Experimental results are compared with simulation analysis based on the Effective Index Method and the Beam Propagation Method [3], showing a good accordance between experimental and theoretical data.

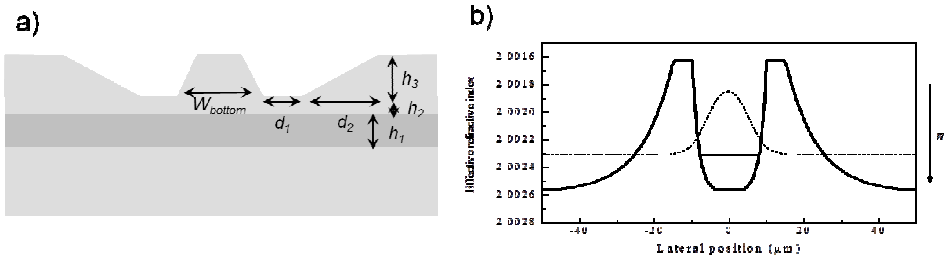

Figure 1: a) Cross-section scheme of the proposed waveguide structure. b) Effective refractive index for the fundamental mode at λ = 1.55 μm (thick line) and mode profile (dashed line) for a given structure.

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12:40 *"Porous silicon: from biological functionalization to optoelectronic nanocomposites"*
Darío Gallach Pérez Departamento de Física Aplicada

Porous silicon: from biological functionalization to optoelectronic nanocomposites

D. Gallach[1], A. Muñoz-Noval[2], V.Torres-Costa[1], M. Manso-Silván[1]

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It was in 1990 when L. Canham discovered porous silicon (PS): a new form of silicon with very special properties [1]. The most relevant property of this material is its efficient photoluminescence at room temperature caused by quantum confinement, but not less attractive are its biocompatibility and its high surface to volume ratio (about 500 $m^2 \cdot cm^{-3}$). All these properties make this material especially suitable for biomedical and optoelectronic applications. The present study aims at deepening in PS conditioning for biomedical and optoelectronic applications.

On the one hand, the functionalization of PS particles has been studied for possible biomedical applications by two different ways [2]: silanization (using 3-Aminopropyltriethoxysilane or APTS) and pegilation (using polyethylene glycol or PEG). Both molecules have attractive properties: the former has amino ($-NH_2$) capping groups capable of linking specialized molecules such proteins or ADN to the particles while the latter (with two alcohol (-OH) ending groups), makes the particles more soluble. It has been observed that the functionalization also protects the particles from oxidation, preserving their luminescence for longer time with respect to pristine PS particles.

On the other hand, new applications of PS are envisaged from a proper combination with zinc oxide (ZnO) to produce ZOPS nanocomposites [3]. The combination of the strong red luminescence from PS caused by the quantum confinement and the green and blue emissions from intrinsic defects of ZnO nanocrystals allowed us producing white light-emitting devices. Changes in the properties of ZOPS composites with processing temperature will be discussed.

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Session III.

Chair of the session: Isabel Guillamón

15:30 *"Entanglement detection in coupled particle plasmons"*
Javier del Pino Dpto. de Física Teórica de la Materia Condensada

Entanglement detection in coupled particle plasmons

Javier Del Pino[1,2], Johannes Feist[1], Francisco J. García-Vidal[1] and Juan José García-Ripoll[2]

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Surface plasmons are hybrid light-matter excitations confined at the interface between a metal and a dielectric. Due to their small mode volume and strong electromagnetic fields, surface plasmons interact very strongly with quantum optical emitters. This, together with their broadband nature, small size and their inherent quantum properties make them a promising platform for future integrated quantum information technologies. So far, several experiments have demonstrated that coupling pho- tons in and out of plasmonic resonances preserves quantum features such as anti-bunching and squeezing.

We present a plasmonic setup that intrinsically exhibits many-body entanglement and provide a recipe for characterizing it experimentally. Our results build on a quantum mechanical model for a 1D or a 2D array of coupled nanoparticles that includes the dipole-dipole interaction between particle plasmons, the losses in each nanoparticle and the possibility of injecting energy via coherent or incoherent light. This model allows us to make predictions not only on the dynamics of the dipoles (i.e., absorption or transport of excitations through the plasmonic band) but also about their correlations and the resulting entanglement.

Finally, we focus on the experimental observables that can detect the presence of entanglement in the plasmonic array, the so-called entanglement witnesses, formally proving that the presence of squeezing in the light with opposite momenta is a signature of entanglement [cf. Fig. 1]. From an experimental point of view, this implies that by refocusing the far-field light emitted from the structure and studying its quantum fluctuations [cf. Fig. 2], the amount of entanglement that

is present in the plasmonic array can be quantified. All this work is covered in more detail and also more references are given in a recent publication in Physical Review Letters [1].

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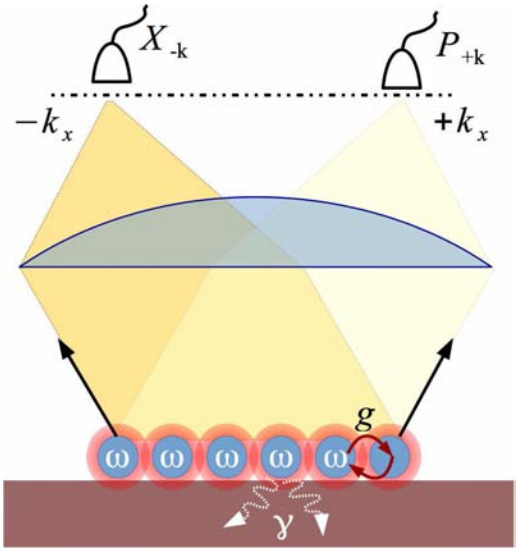

Figure 1: Entanglement witness in momentum space as a function of the coupling g and dissipation γ rates, where ω is the single-particle plasmon frequency. Values smaller than zero signify entangled states.

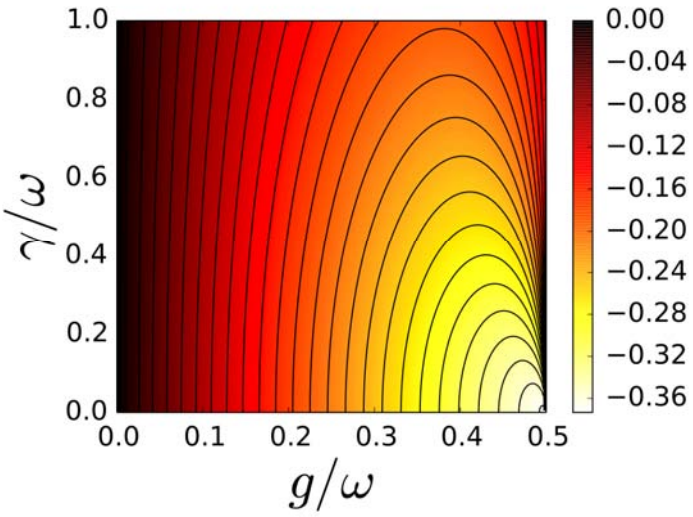

Figure 2: An array of interacting nanoparticles gives rise to a set of coupled plasmonic modes. The far-field emission of these modes is collected by a lens. By correlating the properties of the light at different points in the focal plane k_x, we get information about the multipartite entanglement.

15:50 *"Interaction between localized surface plasmons and rare-earth ion based solid-state gain media"*
Eduardo Yraola Dpto. de Física de Materiales

Interaction between localized surface plasmons and rare-earth ion based solid-state gain media

E. Yraola[1], P. Molina[1], M. O Ramírez[1] and L.E. Bausá[1]

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Noble metal nanostructures offer a promising perspective for the development of new photonic devices due to their ability to manipulate light in the nanoscale. Their extraordinary capability to couple light with collective oscillations of their conduction-band electrons results in a strong confinement of the electromagnetic energy in the surroundings of the metallic nanostructures [1,2]. This feature can be used to enhance the interactions between the far-field light and optical emitters placed in close proximity to the metallic nanostructures.

In this work chains of Ag nanoparticles (Nps) are photochemically assembled on the ferroelectric domain walls of Nd^{3+} doped periodically poled $LiNbO_3$ laser crystals[3]. A selective intensification of specific Nd^{3+} Stark transitions is observed when exciting the radiative modes of the Ag Nps chains with light polarized parallel to their axis [4].

These results are crucial to ultimate the appropriate design of hybrid metal/solid state gain media based on rare earth ions and constitute a needed step for subwavelength confinement and an active control of coherent light at nanoscale dimensions.

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16:10 *"Study of the growth and interaction of Co oxides on oxide substrates"*
Daniel Díaz Fernández Dpto. de Física Aplicada

Study of the growth and properties of Cobalt oxide ultra-thin films on different oxide substrates

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Ultrathin oxide films have shown unprecedented intrinsic chemical-physical properties [1], and it is widely known that the structural and chemical properties of the support influences the properties of the layers grown on them, giving rise to new phenomena and important applications [2]. In this work, we have studied the growth, size and interface effects and chemical stability of ultra-thin CoO films grown on different oxide substrates, namely SiO_2, Al_2O_3 and MgO, using x-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) as main characterization techniques. The XPS measurements were performed in situ in an UHV system consisting of a preparation chamber attached to an XPS spectrometer. The samples have been grown by thermal evaporation of metallic cobalt in an oxygen atmosphere ($P_{O_2}=2x10^{-5}$ mbar) at room temperature.

The study of the chemistry of the growth by XPS reveals a majority of CoO for coverages under 40 ML, and the growth of Co_3O_4 for larger coverages. The morphology of the growth on these substrates reveals two different morphologies for the first stages of the growth: Volmer-Weber way of growth (islands) for SiO_2 and Frank-Van Der Merwe (layer by layer) for Al_2O_3 and MgO. This has been rationalized in terms of the structural properties of the deposited CoO and the substrates. Also, size and support effects have been studied using theoretical cluster calculations of the Co $2p_{3/2}$ XPS spectra as starting point. The results show that the covalent/ionic character of the bonding of the substrates does not affect the properties of the deposited layers, in turn the results suggest that they are more affected by the structural properties of the substrates. These results are relevant, since past studies on other transition metal oxide layers on the same set of oxide substrates showed that the electronic properties of the support influenced the covalence of the oxide overlayers [3,4]. MgO has been found to be the most suitable substrate to obtain stable CoO ultra-thin layers.

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16:30 *"Superconducting properties and vortex lattice in β-Bi_2Pd"*
Edwin Herrera Dpto. de Física Aplicada

Superconducting properties and vortex lattice in β-Bi_2Pd

Edwin Herrera Vasco[1]

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I will discuss scanning tunneling microscopy (STM) experiments on single crystalline samples of the superconductor β-Bi_2Pd. We have obtained large high quality single crystals of this layered material using solution growth. The crystals can be easily exfoliated using scotch. We measure at 100 mK and find surfaces showing the square atomic lattice and spatially homogeneous tunneling conductance following single gap s-wave BCS theory. Under magnetic fields we find multiband features in the tunneling conductance. The orientation of the hexagonal vortex lattice, when the field is perpendicular to the surface, is locked to the square crystalline lattice. We conclude that the mixed phase of this superconductor is largely influenced by multiband features of the Fermi surface. Furthermore, we have studied in detail the vortex lattice in tilted magnetic fields. We observe vortex lattices with many different patterns, from square to distorted hexagons.

Poster Session.

13:00 – 14:15

K. N. L. Acharya Dpto. de Física de la Materia Condensada

Anisotropic Excitons in 2D materials : Application to Phosphorene

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Few layers of Black phosphorus has been a material of interest in graphene based two dimensional systems. Apart from having a finite band gap which can be tuned with manipulation of number of layers in the system, phosphorene is highly anisotropic which leads to high asymmetry of electronic band gap.These peculiar anisotropic nature of the band gap makes phoshorene an interesting material to investigate the effect of anisotropy on excitons . In this work we study the effect of anisotropic exictons in 2D materials using effective mass theory with an application to phosphorene.

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José Benito LLorens Dpto. de Física de la Materia Condensada

Tracking individual vortices under a magnetic field ramp

José Benito LLorens [1], I.Guillamón [1,2], J.Sesé [3,4], R.Córdoba [3,4], J.M. de Teresa [5,4], M.R. Ibarra [3,5,4], S.Vieira [1,2], H.Suderow [1,2]

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[3] *Instituto de Nanociencia de Aragón, Universidad de Zaragoza, Zaragoza, 50018, Spain*

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We present the development of numerical tools to identify individual vortex positions in scanning tunnelling microscopy (STM) images and to follow their trajectories along a long series of subsequent vortex lattice images taken through STM at 100 mK. We Delaunay triangulate the vortex positions, and identify defects and stress on the vortex lattice induced by linear surface features in the topography. We produce vortex motion by increasing the magnetic field in very small steps. Using our analysis tools, we identify rearrangements which we discuss in this presentation. We find that at some magnetic fields, dislocations appear in an otherwise ordered vortex lattice. By making statistics of vortex motion around dislocations, we observe that vortices around a dislocation travel longer distances than those in the hexagonal lattice.

In parallel, we have worked in the development of a very high magnetic field STM to be operated at UAM using a superconducting coil up to 17 T. The STM is made of Ti with all components free from magnetic materials. We have worked to minimize the mechanical vibrations at high magnetic fields by tightening the wiring and rigidly fixing the superconducting coil to the cryostat. Here I will discuss advantages of the STM design, methods used to damp mechanical vibrations and features of a new ultra-low noise electronics.

Juan Pedro Cascales Dpto. de Física de la Materia Condensada

Controlling shot noise in double barrier epitaxial magnetic tunnel junctions

J.P. Cascales[1], D.Herranz[1], F.G. Aliev[1], T. Szczepanski[2], V. Dugaev[2], J. Barnas[3]
A. Dulluard[4], M. Hehn[4], C. Tiusan[4]

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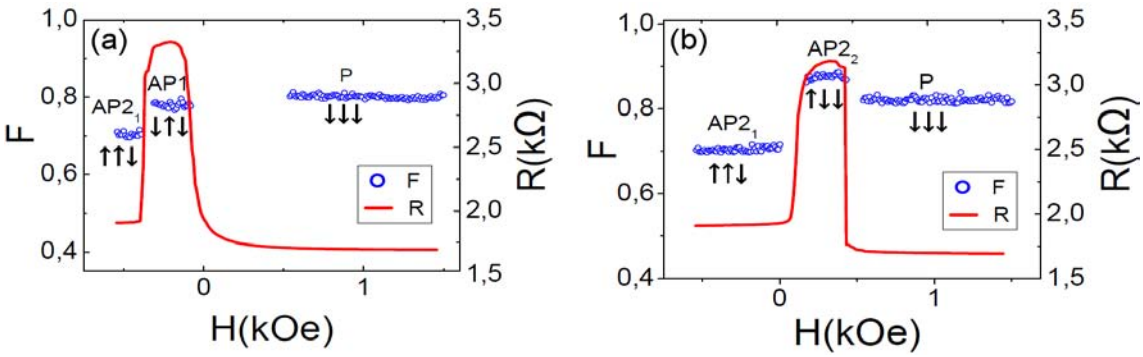
We have recently shown that shot noise is an effective tool to study the statistics of electron tunnelling in single and double barrier magnetic tunnel junctions [1-2]. This talk discusses our recent results on the magnetic control over shot noise in epitaxial double barrier magnetic tunnel junctions [3-4]. We demonstrate that shot noise in Fe/MgO/Fe/MgO/Fe double barrier magnetic tunnel junctions is determined by the asymmetry between both tunnel barriers, the relative magnetic configuration and is influenced by quantum well states in the central layer. The proposed theoretical model of sequential tunnelling through the system, with spin relaxation taken into account, successfully accounts for the experimental observations for all four different magnetic states in the applied bias range, for which the influence of tunnelling through barrier defects and resonant states inside the central electrode is negligible. These results open up a new perspective to engineer fundamental, out of equilibrium, noise mechanisms utilizing hybrid spintronic structures.



Shot noise and resistance at a fixed current during a magnetic field sweep at T=0.3K (a) from positive to negative values and (b) from the AP21 at negative fields back to positive fields

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Jorge Cayao Instituto de Ciencias de Materiales de Madrid

SNS junctions in nanowires with spin-orbit coupling: role of confinement and helicity on the sub-gap spectrum

Jorge Cayao[1], Elsa Prada[2], Pablo San-Jose[1], Ramon Aguado[1]

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We study normal transport and the sub-gap spectrum of superconductor-normal-superconductor (SNS) junctions made of semiconducting nanowires with strong Rashba spin-orbit coupling. We focus, in particular, on the role of confinement effects in long ballistic junctions. In the normal regime, scattering at the two contacts gives rise to two distinct features in conductance, Fabry-Perot resonances and Fano dips. The latter arise in the presence of a strong Zeeman field B that removes a spin sector in the leads (*helical* leads), but not in the central region. Conversely, a helical central region between non-helical leads exhibits helical gaps of half-quantum conductance, with superimposed helical Fabry-Perot oscillations. These normal features translate into distinct subgap states when the leads become superconducting. In particular, Fabry-Perot resonances within the helical gap become parity-protected zero-energy states (parity crossings), well below the critical field B_c at which the superconducting leads become topological. As a function of Zeeman field or Fermi energy, these zero-modes oscillate around zero energy, forming characteristic loops, which evolve continuously into Majorana bound states as B exceeds B_c. The relation with the physics of parity crossings of Yu-Shiba-Rusinov bound states is discussed.

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Rosalía Delgado Carrascón Dpto. de Física de la Materia Condensada

Biocompatibility of zinc titanate sol-gel thin films

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Both zinc and titanium stand among the most biocompatible transition metals. However, physicochemical variables such as specific composition and synthesis process are to be taken into account in the biocompatibility assignments. In this project, the biocompatibility of sol-gel processed zinc titanate thin films has been assayed. In particular, we aimed at obtaining the perovskite $ZnTiO_3$ phase. These films were obtained from titanium isopropoxide (TIPT) and zinc acetate (ZnAc). In addition, the yielding spin cast thin films were annealed at temperatures from 150ºC to 800ºC to study the evolution of the microstructure and composition at each temperature. The results prove that the composition and structure of these materials evolves with annealing temperatures. In particular, from the analysis of dried and grinded xerogels it is known that organic and ionic byproducts are lost at T>300ºC according to FTIR results. This temperature is also key from the microstructural point of view since a transformation of the amorphous materials into polycrystalline is activated. Although deviations from aimed powder composition were revealed by XRD, thin films contained exclusively $ZnTiO_3$. The biocompatibility of $ZnTiO_3$ thin films supports was assayed by culturing human bone progenitor cells. By using immunofluorescence, images of actin cytoskeleton and Ki67 proliferation were obtained. It was proved that these cells adhere on $ZnTiO_3$ films irrespective of their amorphous or crystalline nature, which gives a validation to the short term biocompatibility of this material and improves the biocompatibility of analogue ZnO films.

Victoria Doldán Martelli Dpto. de Física de la Materia Condensada

A Mathematical Model for Chimeric Ligand Design in Selective Drug Treatments

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Chimeric drugs with selective potential toward specific cell types constitute one of the most promising forefronts of modern Pharmacology. We present a mathematical model to test and optimize these synthetic constructs, as an alternative to conventional empirical design. We take as a case study a chimeric construct [1] composed of epidermal growth factor (EGF) linked to different mutants of interferon (IFN). Our model quantitatively reproduces all the experimental results, illustrating how chimeras using mutants of IFN with reduced affinity exhibit enhanced selectivity against cell overexpressing EGF receptor. We also explore the mechanism of interaction between chimeras when given in combination, within cells populations. For that purpose, we developed a population model where two cell populations expressing different levels of the target receptor are treated with different combinations of chimeric drugs. Chimeric drugs appeared to be synergistic in nature, so that the concentration that maximizes the selective potential in a population is reduced when using drug combinations, when compared to the concentration using a single drug treatment.

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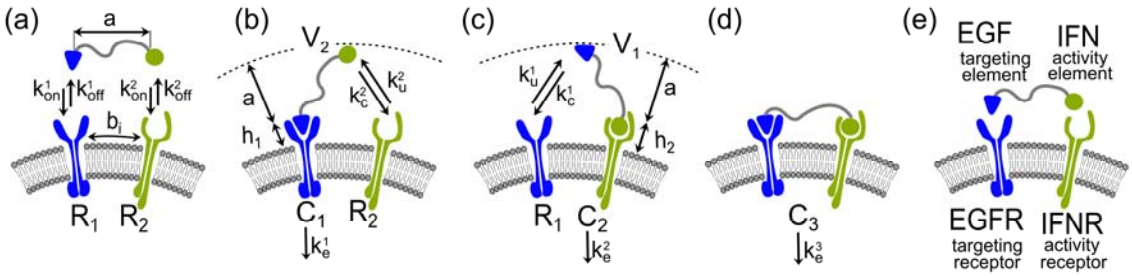

Figure 1. (a-d) Scheme of the chimeric ligand/receptor interaction. (e) Chimera IFNα-2a-EGF and their corresponding receptors.

Antón Fente Dpto. de Física de la Materia Condensada

Millikelvin scanning tunneling spectroscopy on non-reconstructed surfaces of the superconductor $Ca(Fe_{0.965}Co_{0.035})_2As_2$

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The ground state of the iron pnictide $CaFe_2As_2$ can be stabilized to an antiferromagnetic/orthorhombic or a non-magnetic collapsed tetragonal phase. Superconductivity appears with Co doping, with a Tc up to 15 K [1,2]. The ground state can be modified by applying pressure and by thermal post-growth treatments. The same phase diagram can be obtained using both methods (pressure and annealing) [1]. This opens the possibility to study the fine tuning of superconducting properties at ambient pressure using scanning tunnelling microscopy.

We first grew crystals of $CaFe_2As_2$ with different Co dopings and annealed them to obtain slightly different superconducting properties. We then measured our samples with millikelvin scanning tunnelling spectroscopy. We cleave samples *in situ* in cryogenic ultra-high vacuum to obtain clean and atomically flat surfaces. We make images from hundreds of thousands of conductance vs bias voltage curves (during several days long experiments at 100 mK), to obtain the electron dispersion relation through surface electronic wave scattering.

First we discuss results in $Ca(Fe_{0.965}Co_{0.035})_2As_2$. As in previous work, we find reconstructed surfaces [3]. Here we show that the electron dispersion relation measured at these surfaces give a hole-like band with an effective mass larger in superconducting than in non-superconducting samples. We have been systematically searching for unreconstructed surfaces with the square As lattice, and found them for the first time in these compounds. In these surfaces we find an electron and a hole band, as well as incoherent variations of the superconducting tunnelling conductance due to pair breaking. We find a four-fold pattern in the superconducting tunnelling conductance, which could be related to the superconducting gap anisotropy. Then, we briefly discuss results in $Ca(Fe_{0.97}Co_{0.03})_2As_2$, where we identify slightly different bandstructure and also observe the superconducting gap.

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Radiative heat transfer through nanometer-size gaps

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One of the central open problems in nanoscience is the study of the heat transport in nanoscale devices, which has remained largely unexplored due to experimental challenges. In this context, a key issue is the understanding of the heat transfer via thermal radiation between systems separated by nanometer-size gaps. In this extreme regime, the electromagnetic near-field is expected to give rise to a dramatic enhancement of the radiative heat transfer, something that has only be quantitatively verified for gaps on the order of 20-30 nm [1]. In this work, we present a combined experimental and theoretical study of the radiative heat transfer in the extreme near-field regime (gaps of 1-10 nm). From the experimental side, we performed systematic studies using AFM-based scanning probes with integrated nanoscale thermocouples [2], which were coated with dielectrics (SiO_2 or SiN_x). Our experiments of heat transport between the scanning probes and a flat substrate coated with dielectrics, performed in an ultra-high vacuum environment, confirm that heat transport is dramatically enhanced in the near-field. To understand our experimental results, we investigated these near-field enhancements within the framework of the theory of fluctuational electrodynamics [3]. To be precise, we performed extensive numerical simulations making use of a combination of a fluctuating-surface-current formulation of radiative heat transfer with the boundary element method [4,5]. Such a combination allows us describing realistic geometries for our tip-sample setups. Our theoretical results are in good agreement with the measured heat flows between both dielectric and metallic surfaces, which establishes the validity of fluctuational electrodynamics in modeling near-field heat transport all the way to nanometer-size separations.

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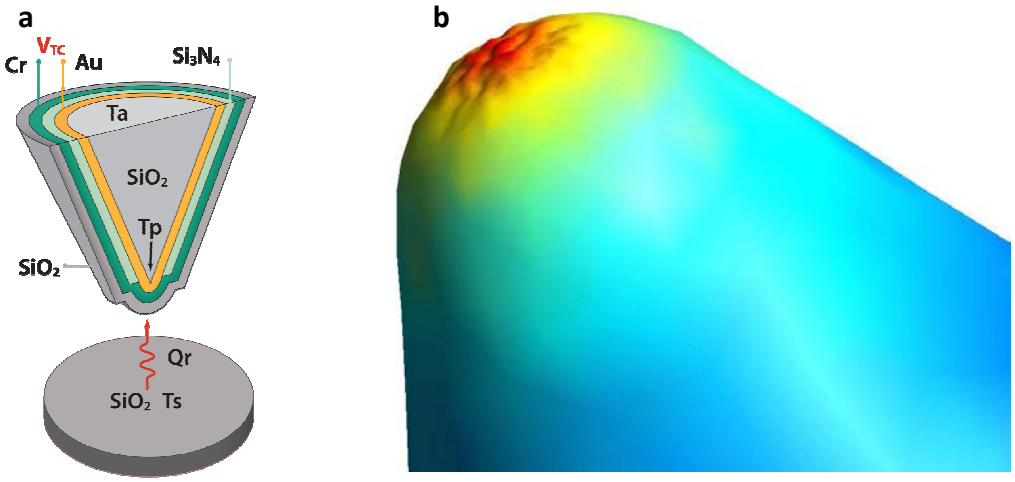

a Schematic diagram of the experimental setup. The AFM probes incorporate a thermocouple, made by a spherical Au/Cr junction with a diameter of 200 nm. **b** Numerical simulation of the spatially resolved heat transfer between a tip and a plate made of silica and separated by a distance of 1 nm. The radius of the tip is 225 nm. The color scale is logarithmic, showing the radiative heat transfer enhancement in the extreme near-field.

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Ab initio calculations of strongly coupled molecule-cavity systems

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When coherent energy exchange between an electromagnetic field mode (such as a cavity mode) and quantum emitters is faster than the decay and decoherence of either constituent, the system enters into the strong coupling regime. The elementary system excitations then become hybrid states with mixed light-matter character which display Vacuum Rabi Splitting, i.e., an energy splitting caused solely by the vacuum EM field. Cavity strong coupling and the associated resulting hybrid states have been extensively studied due to their many potential applications, such as room temperature Bose-Einstein condensates and ultra-low threshold lasers. One particularly interesting realization of strong coupling uses organic molecules as the quantum emitters, allowing Rabi splittings of up to 1 eV. Pionee-ring experimental studies show that even chemical structure and reactions could be modified and controlled using strong coupling [1].

In most theoretical descriptions, the quantum emitters are modelled as simple two-level systems, which can be appropriate for atoms or quantum dots, however, organic molecules possess a comp-lex internal structure due to nuclear motion. This internal structure due to coupling to rovibrational states is often described phenomeno-logically in a master equation description, which can not describe chemical modifications. Additionally, it is not a priori obvious if the underlying approximations are still valid in the strong coupling regime. In this contribution, we thus investigate an ab initio model in which both electronic and nuclear motion in the molecule are taken into account fully, allowing the description of chemical dynamics within a single unified framework. This is achieved using a model molecule with only one electronic and one nuclear degree of freedom.

We study the applicability of different approximations to obtain observables such as the absorption spectrum by comparing to the full ab initio results. In particular, we will discuss how the introduction of a new timescale due to strong coupling affects the validity of the Born-Oppenheimer approximation, which is typically used in molecular physics to separate the slow vibrational and fast electronic degrees of freedom. As for large enough Rabi splittings, the energy exchange with the EM field takes place exactly on an intermediate time scale between vibrational and electronic motion, it could potentially form a “bridge” between the two and affect the validity of the Born-Oppenheimer approximation.

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SiO_2 nanowires via the active oxidation of silicon

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Nowadays, a number of applications are being investigated for silica nanowires (SiO_2 NWs), including intensive blue light emitters in integrated optics, biological and chemical nanosensors or energy storage devices, in particular as active material for the anode of lithium-ion batteries. The vapor-liquid-solid (VLS) mechanism is one of the most accepted and employed methods for the growth of these nanostructures. By this mechanism, silicon whiskers grow from the vapor by the use of a metal impurity. The role of the impurity is to provide a preferential site for the nucleation, supersaturation and subsequent growth of the nanowires from the gaseous species ($SiCl_4$, SiH_4) used in the process. Currently, several efforts are being made in order to avoid the use of these unsafe and highly flammable vapor-phase silicon precursors during the synthesis, by the use of a solid silicon source. However, in such processes the mechanism by which silicon arrives to the catalyst for starting the nanowires growth is far from obvious.

In the present work, the active oxidation of the solid silicon wafer is postulated as the main responsible mechanism of the SiO_2 NWs growth. In order to prove it, a series of the SiO_2 NWs synthesis were performed varying the substrate and the sample configuration on the oven, but maintaining the same synthesis conditions. Details of the procedure have been previously reported in other works [1].

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Modelling the interplay between protein and lipid aggregation in supported membranes

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We present a theoretical model that deals with the complex interplay between lipid segregation and the self-aggregation of lipid-attached proteins. The model, in contrast to previous models that consider proteins only as passive elements affecting the lipid distribution, describes the system including dynamic interactions between protein monomers, the interactions between lipid components, and also a mixed term considering both protein-lipid interactions.

This model is an extension of a previous one [1,2] used to study the dynamics of the self-aggregating cytoskeletal protein FtsZ, and has been expanded to explain experimental results performed on a well-defined system that includes two elements: FtsZ proteins and a lipid bilayer with two lipid components. The model can reproduce the observed differences defined by the orientation of the filaments on the surface, indicating that all contributions to filament formation, including the interplay between torsion and an specific anchoring, are needed to account for the observations. Furthermore, it points out that lipid segregation can affect the length and curvature of protein filaments and that the dynamic behaviour of the lipids and proteins might have different time scales, giving rise to "memory effects".

This simple model that considers a dynamic protein assembly on a fluid and active lipid surface can be easily extended to other biologically relevant situations in which the interplay between protein and lipid aggregation are both needed to fully describe the system.

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Spin waves along topological domain walls

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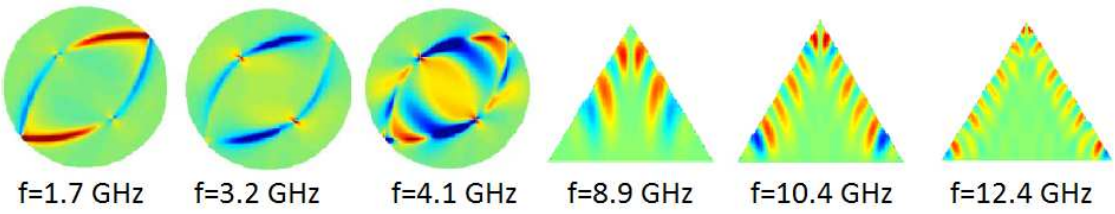
Spintronics, an information technology in which digital data is represented by the spin orientation of electrons. Magnonics is an emerging field dedicated to low dissipation information transmission using spin waves (i.e. without electron motion between components).

We have studied the propagation of spin waves along domain walls inside micron size magnetic permalloy dots. The dot shape and size, and the external magnetic field determines the dot magnetic structure, in which domain walls can be present.

In the case of circular dots, a metastable double vortex state can be achieved, with domain walls connecting the vortices with edge half antivortices, whereas in triangular dots domain walls can appear at the triangle edges, confining the spin waves to the edges.

Waves of discrete frequencies can be propagated through these domain walls, allowing for several future applications in spintronics. Logic devices could be easily designed with edge spin waves, indicating a potentially strong transformational impact on information technology in the long run.



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Charge fluctuations and unconventional superconductivity in quasi-one-dimensional superconductors.

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Paring mechanisms in high critical temperature superconductors are often related with the exchange of spin and charge fluctuations. Charge fluctuations have come into play recently, due to the advent of experimental techniques as inelastic X-ray scattering (RIXS) [1], and the observation of charge ordering near the superconducting region in cuprates [2]. We study the charge ordering transition in a multiorbital and quasi-one dimensional Hubbard model at quarter filling by Random Phase Approximation (RPA). The pairing vertex is calculated considering charge and spin fluctuations as pairing mechanisms within RPA. We adapt a methodology, intensively used for Fe-pnictides [3], to study the quasi-one dimensional and low-temperature superconductor [4] $Li_{0.9}Mo_6O_{17}$, which may be near a charge ordering transition [5]. We found that charge collective modes induced by Coulomb repulsion favour the superconductivity both in the singlet and triplet channels. s-wave superconductivity is favoured as the charge ordering transition of the model is approached by tuning the interaction. We discuss our results in terms of the anomalies of the normal phase of $Li_{0.9}Mo_6O_{17}$ which has been characterized as a quantum critical metal [6].

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Hydration Properties of Single-Stranded DNA Films

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In recent years, motivated by prominent biomedical applications, microcantilever-based biosensing devices have received a great deal of attention[1]. In this work, we focused on those biosensors that are able to detect the DNA hybridization process. Many experiments and theories[1] have been developed related to this mechanism, attempting to explain not only how the interaction between the single-stranded DNA (ssDNA) probed on a cantilever results in a given surface stress change of the cantilever, but also how this interaction changes when the ssDNA strands are joined with their complementary sequence. Nevertheless, the physical processes involved on the surface stress changes are not yet well understood[1]. Moreover, it has been showed that these changes strongly depend on a manifold of factors, such as the sequence of the ssDNA and the grafting density[1].

An example of such kind of applications is a device built by Mertens et al.[2] The key element of this device is a self-assembled-monolayer (SAM) of ssDNA molecules, and how it responds as one varies the hydration conditions of the SAM. With this device, they are able to detect mutations on a DNA sequence of a single base. This biosensor with unprecedented sensitivity, motivates the investigation of the hydration process of a SAM composed by ssDNA strands, attempting to explain the observed surface stress changes of the cantilever. For this purpose, we have performed *state of the art* atomistic molecular dynamics simulations using AMBER's force fields[3]. We have built up monolayers composed by hundreds of ssDNA and analyzed their behavior for different hydration levels. Two different cases have been studied: a SAM restrained to a fixed substrate and a SAM restrained to a movable substrate.

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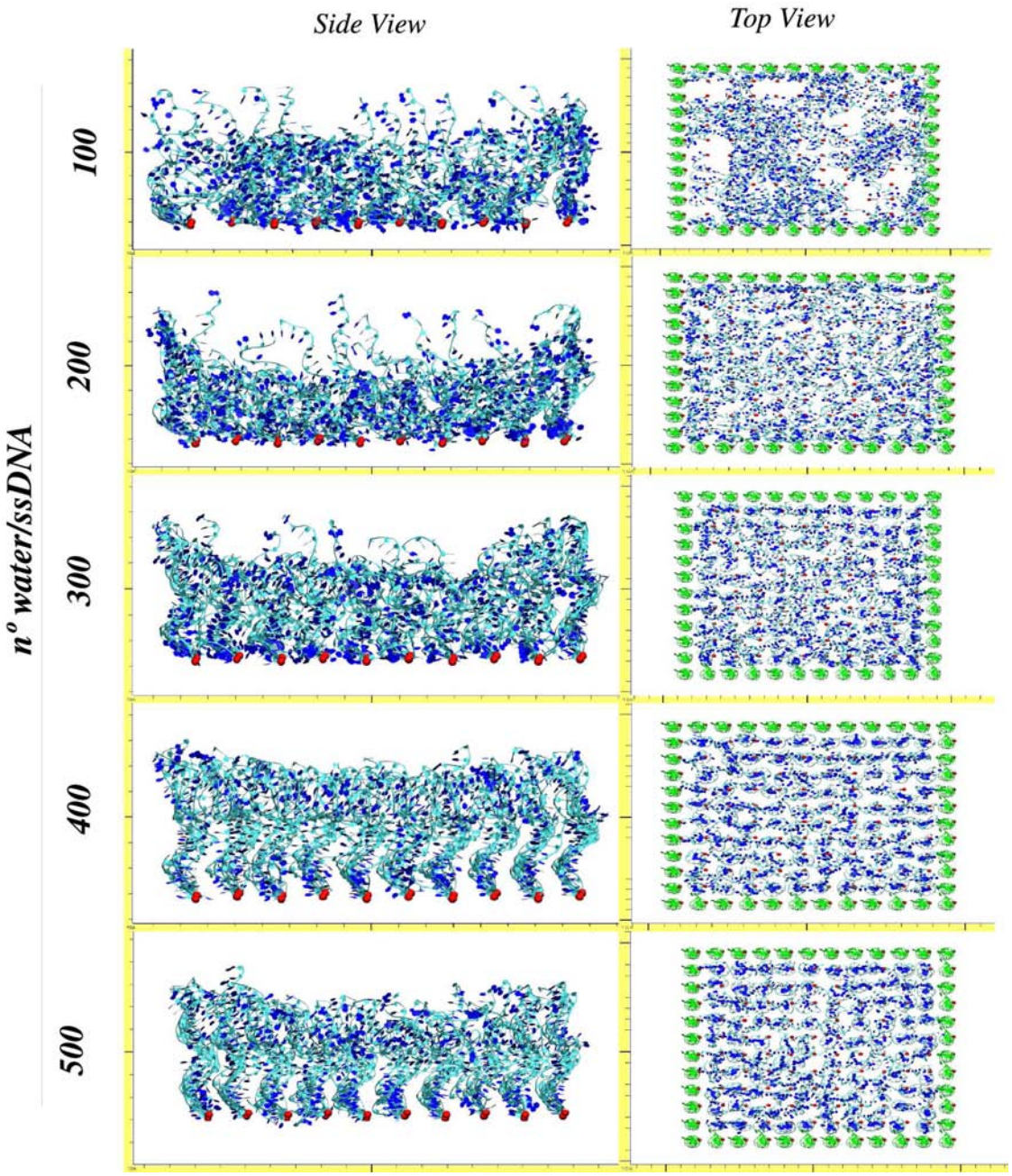

Fig. Side (left) and Top (right) view of a SAM conformed by 144 ssDNA. The first configuration (at the top) is the initial configuration of the SAM. The other five configurations represented are the final configurations of the SAM after 20 ns of simulation for five different hydration levels (from top to bottom): 100 water per ssDNA, 200 water per ssDNA, 300 water per ssDNA, 400 water per ssDNA and 500 water per ssDNA. The ssDNAs at the edges are kept fixed (green ones), to avoid interaction with periodic images. The last atom of each ssDNA is also fixed (red), to simulate a fixed substrate.

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Molecular Dynamics Study of a Lipid Membrane

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Pulmonary surfactant plays two principal roles: Defensive mechanism and surface activity. Concerning the latter, as pulmonary alveoli are spherical, they obey Laplace's law and, as a result, connected alveoli having different radii present a difference in pressure. Due to this difference, small alveoli would collapse into larger alveoli producing asphyxia. However this non-favorable scenario does not occur since phopholipids move to the air-liquid interface of alveoli, lowering surface tension and keeping the system pressure constant [1].

In this work we focus on lipid membranes made of two phospholipids, DPPC and POPC. Using Molecular Dynamic simulations, we study both thermodynamic and dynamic properties, such as lipids per area, bending energy and diffusion coefficient, as a function of the concentration of POPC molecules. Due to the double bond in one of the POPC chains, we expect that POPC molecules will cause molecular packing in the system to decrease, in such a way that the area per lipid will increase, while the bending energy will decrease, both as a function of POPC concentration. Furthermore, the diffusion of DPPC molecules is expected to be faster than that of POPC molecules since the POPC double bond makes them to be less fluid. Moreover, we study phase separation in DPPC membranes in the presence of a third specie, DAPC, as well as in presence of POPC molecules. We do not observe phase separation in DPPC/POPC mixture at any concentration. However, we do observe phase separation in a wide range of concentrations in the DPPC/DAPC mixture. We argue that this feature may be related to the presence of double bonds in the chains of both component [2],[3] [4].

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Local analysis of adsorption kinetics through devices based on plasmonic enhanced Au cavity arrays.

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Nowadays, there is a growing interest in plasmonics since it has allowed analytical progress in food and environmental safety, medical diagnostics and therapeutics [1]. A lot of studies have dealt with nanostructured plasmonic surfaces as biological or chemical sensors, coupling investigation of binding and detection of selected and specific targets with improved nanofabrication techniques, in order to obtain miniaturized devices with increased sensitivity and reliability [2]. In particular, nanofabrication techniques based on colloidal lithography have been intensively studied due to their ability to obtain low cost production of large area nanostructured surfaces [3, 4].

In this work we report a class of high-performance plasmonic sensors allowing both kinetic studies as well as spatially resolved information ideal for the detection of binding events taking place at the surface. The analytical surface consists of gold/polymer 2D plasmonic crystals obtained by a fabrication technique based on plasma processes and colloidal lithography. These systems consist of a hexagonal lattice of polymeric pillars embedded in an optically thick gold film on a glass substrate. Results for the optical characterization showed that the geometrical parameters at the nanometer scale strongly affect the optical response and sensitivity of the device [5].These samples are proved to work as extremely sensitive platforms for different applications [6], such as detection of diagnostic markers in plasma. The possible use of microstructured antifouling layers on the plasmonic sensor surfaces evidences the potential for selective area analysis, allowing an improved multiplexed kinetic recognition of target-analyte interaction in a microarray format. A further investigation of these surfaces is a subject of research in the framework of the ITN project “THINFACE”.

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W. S. Paz Dpto. de Física de la Materia Condensada

A Theoretical study fo the electrical contact between the 1T and 2H phases in monolayer MoS_2

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The presence of a finite bandgap and excellent electrostatic gate coupling in ultrathin two-dimensional materials such as molybdenum disulphide (MoS_2) make them interesting for electronics based on the current complementary metal oxide semiconductor (CMOS) paradigm[1-3].

We present a theoretical study of the electrical contact between the two known phases of MoS_2 monolayer crystals. While the 2H phase is the most common one and it is seminconducting, the 1T phase is metallic. The experimentally reported possibility for MoS_2 to present both phases in the same crystal opens a new venue for low-resistance current injection into the semiconducting phase, thus avoiding the problems associated with the direct contact between standard metals and the semiconductor. Here we present tight-binding and density functional theory calculations of the electrical transport properties of such interfaces. Advantages associated to both the natural edge-contact geometry and the similar chemistry of the metal and the semiconductor are evident from our conductance calculations in nanoribbon heterojunctions.

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MoS_2 roughness and friction quenching by interaction with atomically flat substrates.

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Atomically thin MoS_2 crystals are among the most widely investigated two-dimensional materials, showing a large intrinsic bandgap of 1.8 eV (698 nm), well-suited for electronics and optoelectronics [1, 2].

Due to their inherent large surface-to-volume ratio, the chemical, optical and electrical properties of atomically thin materials can be strongly modified by their interaction with the substrate where they are deposited [3].

In this work [4] we study MoS_2 monolayers transferred on amorphous SiO_2, as well as on two different atomically flat crystals – mica and hexagonal BN – using a combination of micromechanical cleavage and a recently reported deterministic transfer technique. Atomic force microscopy and friction force microscopy measurements reveal that both the roughness and sliding friction of MoS_2 monolayers are strongly influenced by the underlying substrate. Specifically, we find that the use of atomically flat mica or h-BN crystals as substrates leads to a remarkable reduction of single-layer MoS_2 surface roughness, sliding friction, and local inhomogeneities.

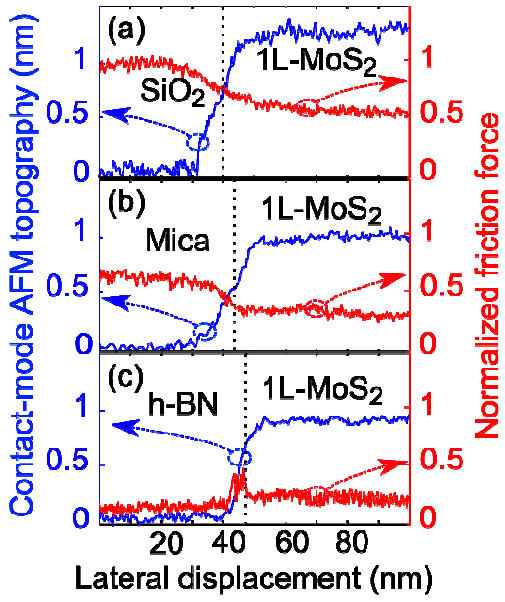

Figure - AFM topography (blue, left axis) and friction force (red, right axis) profiles, as a function of tip lateral displacement, across regions comprising both the bare substrate of SiO_2 (g), mica (h) or h-BN (i) and a single-layer MoS_2 flake laying on the substrate. The differences in surface roughness (sliding friction) can be observed in the topography (friction) profile for the MoS_2 monolayer on the various substrates.

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Mechanically tunable thermopower of single-molecule junctions

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The study of the thermoelectric properties of materials is of great interest for the development of thermoelectric devices that would allow an efficient conversion of thermal loses into utilizable current. In the last years, the experiments performed with different techniques on molecular junctions have shown promising results because of the high values of the thermopower [1][2][3][4]. In this context, I will present the unexpected results found when studying the thermopower of endohedral fullerene junctions, namely $Sc_3N@C_{80}$ molecules. We have used a recently-developed experimental technique that enables us to measure both conductance and thermopower simultaneously in truly single molecules and in ambient conditions using a scanning tunneling microscope (STM) [4]. The $Sc_3N@C_{80}$ molecules, as other fullerenes, show a large value of the thermopower and, interestingly, we have observed a novel effect: the molecules show different sign of the thermopower depending on their coupling with the gold surface and hence their behaviour can be changed by interacting mechanically with the molecules. Our results are the first to confirm the relation between the sign of the thermopower and the position of the Fermi energy with respect to the molecular levels.

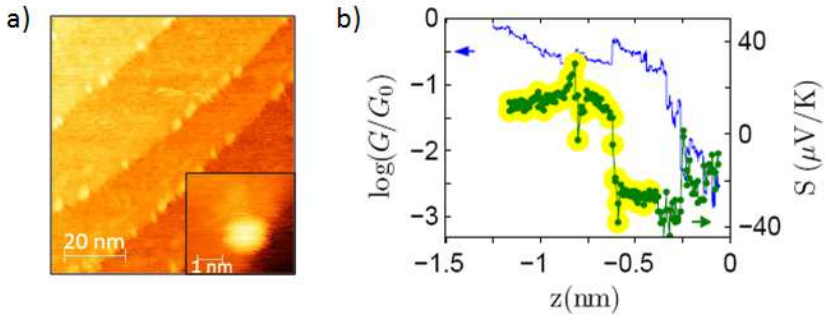

Figure: a) STM topographic images of $Sc_3N@C_{80}$ molecules deposited on a gold surface; **b)** Simultaneous conductance, G, and thermopower, S, measurements (in blue and green, respectively) as a function of the tip displacement, z, during the approach of the Au tip to a single molecule. G_0 is the conductance quantum. The thermopower measured while touching the molecule is marked in yellow.

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Atomic-scale Manipulation by means of Equilibrium and Nonequilibrium Forces

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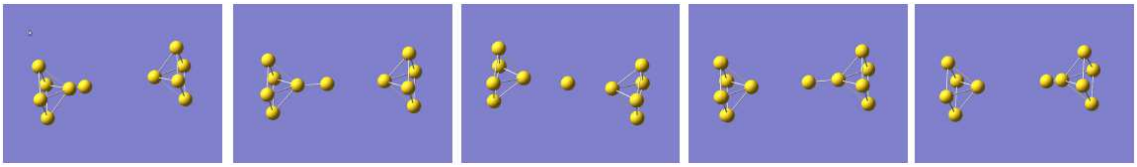
In recent years Nonequilibrium Electron Transport through metallic contacts at the nanoscale has been studied theoretically and with experiments. However, not only Nonequilibrium Transport, but mechanical phenomena appear in such devices due to nonequilibrium electrochemical conditions, as is the case of Electromigration. Nonequilibrium Forces appear because of the particular DOS of the materials, i.e. the quantum-chemical nature of the material. We studied how the nonequilibrium density and charge affect the forces induced on atoms forming this kind of junctions. This allows us to explain the transfer of atoms between metallic electrodes mediated by an applied bias voltage[1].

We used ab-initio calculations based on DFT methods and the Nonequilibrium Green's FunctionFormalism[2,3] to simulate such systems. To introduce nonequilibrium conditions, we apply an external bias voltage at which electrons are injected.



1. Simulation of Gold atom electromigration between two electrodes under applied bias.

Among the simulated systems, there are contacts from different metals. Non-voltage-symmetric charge distributions and current-voltage characteristics emerge of our calculations. This is a result of the absence of electron-hole symmetry. The distinctive DOS corresponding to each of the metals is determinant in the nonequilibrium charging effects and the induced forces[2].

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Adriana L. Sanz Dpto. de Física de la Materia Condensada

Drug treatment efficiency is governed by nonlinear interactions in celular signaling pathways: the AKT signaling pathway as a model.

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Biological networks bear self-regulatory motifs responsible for the non-linear dynamics in the transduction of signals [1]. One of the most studied non-linear network is th AKT-pathway. Deregulation of the AKT signaling pathway has a central role in human pathologies related to aging, such as cancer and diabetes. Small molecule inhibitors have significant potential as treatment for these diseases. However, the presence of positive and negative feedback loops in AKT regulation generate unpredictable responses during drug treatment.

Our experimental data show a bistable dose-response to reversible inhibitors targeting the AKT-pathway. Through mathematical analysis, we predict possible interactions that lead those kind of responses and we design a combinatorial treatment that supresses bistability and improves drug efficacy. Besides the biochemical properties, we demonstrate that the topology of the pathway strongly affects the efficiency of inhibitors. Hence the characterization of the interaction network is a key aspect to design more effective treatments [2].

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Humidity effects at the organic/porous silicon sensor interface

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Biosensing technology is a rapidly advancing field that benefits from the possibility to use the properties of functional advanced materials to analyse biological systems. Particularly, thin hybrid interface microstructures based on porous silicon (PSi) are currently in progress as optical ADMA sensors. Indeed, owing to its high surface area, the well-established fabrication methods, and its biocompatibility, PSi constitutes an ideal substrate for developing new chemistries. An optical (interferometric) transducing structure is considered for such sensor.

In this work, we will start by reviewing the processes for the surface functionalization of PSi in order to trigger its sensitivity as biosensing platform. Secondly, we will describe current approaches based upon modification by self-assembled silane monolayers, which critically depend on the type of process for the activation of PSi. Depending on the molecular structure of the monolayers, the surface will present hydrophobic/hydrophilic properties, what will allow a molecular selectivity, and, consequently, a local control of the biomolecular interactions. The surface of the functionalized material will then be biologically activated for the detection of specific species applying surface immobilization techniques. Preliminary results will be shown regarding the biosensing of ADMA.

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