Instituto Universitario de Ciencia de Materiales Nicolás Cabrera

XXIII YOUNG RESEARCHERS MEETING

28 January 2021

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13:30 **Closing** of the XXIII Young Researchers Meeting of the INC

Session I

Chair of the session: Pilar Prieto Recio

9:30 *"Performing deep-tissue photodynamic therapy with rare-earth-doped nanoparticles and Eosin Y"*

Gabriel López Peña Dpto. de Física Aplicada

Performing deep-tissue photodynamic therapy with rare-earth-doped nanoparticles and Eosin Y

Gabriel López-Peña[1], **Laura Ortiz-Rojano**[2], **Dirk H. Ortgies**[3, 4], **María Ribagorda**[2], **Francisco Sanz-Rodríguez**[4, 6], **Emma Martín Rodríguez**[1,4]

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Photodynamic therapy (PDT) consists in the generation of cytotoxic reactive oxygen species (ROS) by means of a photosensitizer (PS) and light [1] in order to cause cancer cell death. PDT is a commonly used technique to treat cancer because of advantageous properties like being easy, selective and having fewer side effects than other techniques. However, working *in vivo* presents difficulties due to the attenuation that the light suffers when penetrating the organism due to components like the skin or blood among others. This limitation is the main reasons why PDT is only used to treat small tumors on the skin or on the lining of internal organs or cavities.

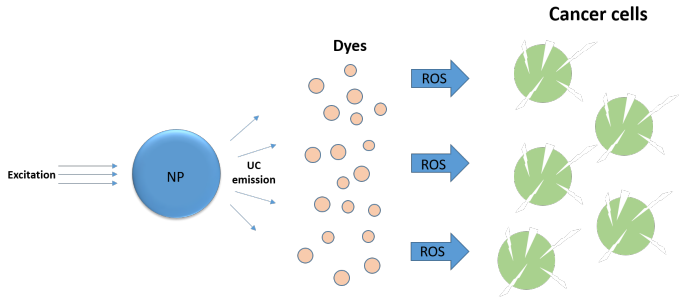

Fig. 1. Schematic process of ROS generation using the up-conversion emission of the NP's under NIR excitation

Eosin Y is going to be used as PS, because of having absorption and emission bands located in the visible region of the electromagnetic spectrum, and under the right excitation they generate ROS. However, their biological applications are limited because they are not able to enter living cells and can only pass through partially broken cell membranes (fixed cells). In order to solve this problem, we have attached eosin Y to $NaGdF_4$: Nd^{3+}, Yb^{3+}, Tm^{3+} nanoparticles via polyethylene glycol chains (PEG). These rare-earth-doped nanoparticles present both visible and NIR emissions when illuminated with light of 808 nm, being the visible one generated by upconversion processes. We expect that our NP-dye structures are capable of penetrating living cells and then performing PDT inside them. In addition, the NIR emissions of these NP's are located precisely in the biological windows (regions of the spectrum where the attenuation coefficient is low [2], allowing us to detect the emissions), which can be used for bioimaging applications.

We have shown that once NP and Eosin Y are linked, the resulting structure is able to bind to living cells and generate ROS, resulting in the death of cancer cells.

[1] B. del Rosal et al., Advanced Functional Materials **28**, 1803733, (2018).
[2] Eva Hemmer et al., Nanoscale **5**, 11339, (2013).

9:45 *"Nanojet trapping of a single sub-10 nm upconverting nanoparticle in the full liquid water temperature range"*

Dasheng Lu Dpto. de Física de Materiales

Nanojet trapping of a single sub-10 nm upconverting nanoparticle in the full liquid water temperature range

Dasheng Lu[1], Marco Pedroni[1], Lucía Labrador-Páez[2], Manuel I. Marqués[3], Daniel Jaque[1], Patricia Haro-González[1]*

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Upconverting nanoparticles (UCNPs) have been used as optical probes in a great variety of scenarios ranging from cells to animal models [1, 2]. When optically trapped, a single UCNP can be remotely manipulated making possible, for instance, thermal scanning in the surroundings of a living cell [3]. When conventional optics are used, the stability of an optically trapped UCNP is very limited. Its reduced size leads to optical potentials comparable to thermal energy and, up to know, stable optical trapping of a UCNP has been demonstrated only close to room temperature [4, 5]. This fact limits their use above room temperature, for instance, the use to investigate protein denaturalization that occurs in the 40-50 ºC range. In this work, we have demonstrated stable optical trapping of a single UCNP in the 20-90 ºC by using a photonic nanojet [6]. The use of an optically trapped microsphere makes possible to overcome the diffraction limit producing another optical trap of smaller size and enhanced strength. This simple strategy leads not only to an improvement in the thermal stability of the optical trap but also to an enhancement of the emission intensity generated by the optically trapped UCNP.

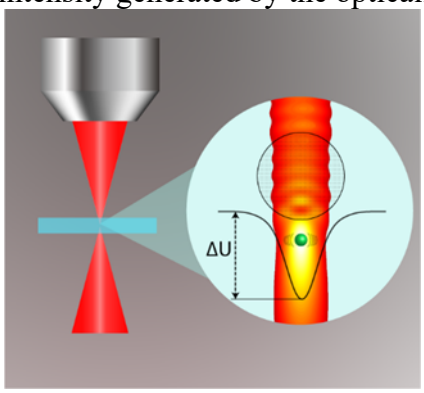

Figure 1. The schematic of a photonic nanojet, a sub wavelength beam that results from the constructive interference of the optical field and is generated on the shadow side of the microsphere

[1] D. Jaque, and F. Vetrone. Nanoscale **4**, 4301 (2012).
[2] B. Zhou, et al., Nat. Nanotech. **10**, 924 (2015).
[3] P. Rodriguez-Sevilla, et al., Adv. Mater. **28**, 2421 (2016).
[4] P. Rodríguez-Sevilla, et al., Journal of Materials Chemistry B **5**, 9085 (2017).
[5] Y. C. Li, et al., Light Sci. Appl. **5**, e16176 (2016).
[6] A. Heifetz, et al., J. Comput. Theor. Nanosci. **6**, 1979 (2009).

10:00 *"Plasmonic Heating and Luminescence Thermometry: Developing an Optical Thermal Probe to Perform in Biological Environments"*
Marta Quintanilla Dpto. de Física de Materiales

Plasmonic Heating and Luminescence Thermometry: Developing an Optical Thermal Probe to Perform in Biological Environments

M. Quintanilla,[1,2] I. García,[1] R. López-Méndez, [1,2] M. Henriksen-Lacey,[1] E. Cantelar,[2] L.M. Liz-Marzán[1]

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There is a growing interest in remote sensing of temperature at the nanoscale, largely because in biological environments localized thermal information allows to understand the physiological status of individual cells. If accompanied by localized heating, an option for monitored hyperthermal treatment arises. In principle, the thermometer task can be done using luminescent nanomaterials if neither emission nor excitation light are extinguished along the way through the tissue. However, several additional hurdles related to the heterogeneous nature of biological tissues and its interaction with both, the nanoparticles and light, can compromise the accuracy of the thermal reading. Based on a system that uses lanthanide doped nanoparticles (CaF_2:Nd^{3+},Y^{3+}) to measure temperature and plasmonic nanoparticles to activate heating, we aim to discuss the problems and the different ways we found to improve thermal control, including intensity optimization of Nd^{3+} emission and experimental protocols that allow in situ calibration of the thermometers.

10:15 *"Hybrid nanostructures for applications in photonics: photovoltaic and light-sensing devices"*
Rehab Ramadan Dpto. de Física Aplicada

Hybrid nanostructures for applications in photonics: photovoltaic and light-sensing devices

Rehab Ramadan[1,2,3]
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Sub-wavelength nanostructures are receiving increasing attention for potential photovoltaic and microelectronic devices [1]. Our work presents the design, development and characterization of three different hybrid nanostructures aiming at enhancing the optoelectronic properties of photonic devices based on silicon. (1) We grew nanostructured porous silicon (PSi) and hybrid nanostructures of PSi combined with Ag metallic nanoparticles (PSi+AgNPs) onto silicon substrates. PSi layers with different porosity were electrochemical etched and AgNPs were subsequently infiltrated by electrodeposition processes. In particular, the size, morphology and surface density of the AgNPs grown into PS were studied as a function of the electrolyte pH value and the infiltration current density [2]. Furthermore, the optical properties of the hybrid PSi+AgNPs structures were analyzed. The reflection and absorption characteristics as functions of the wavelength, angle of incidence, and polarization state of incident light were studied for PSi and the hybrid nanostructures. The experimental results show a broadband optical absorption characteristic of the hybrid layers, which will be useful in light-harvesting devices [3]. Accordingly, Metal-insulator-semiconductor (MIS) Schottky-junction solar cells with the basic structure Al/Si/TiO_2/Au were fabricated. This structure was modified by the addition of nanostructured PSi layers and AgNPs, resulting in devices with the following structures: Al/Si/PSi/TiO_2/Au and Al/Si/PSi+AgNPs/TiO_2/Au. The experimental results show a remarkable enhancement in the overall performance of the solar cells upon the addition of PSi and AgNPs layers to the basic structure [4]. The electrical properties of photovoltaic devices are of utmost importance to predict and optimize their overall optoelectronic performance. Within this context, the alternating current (AC) and direct current (DC) electrical characteristics of our MIS Schottky barrier diodes were studied [5]. (2) The luminescent properties of zinc oxide (ZnO) and nanostructured PSi make these materials very appealing for photoemission applications. For that, hybrid ZnO and PSi composite micropattern were grown on silicon substrates for the future development of LEDs. The experimental photoluminescence (PL) results show that the ZnO layers have blue emission broadbands, while the PSi layers show a red band emission. Therefore, the PL properties of the composite ZnO + PSi micropatterns are equivalent to those featuring the addition of PSi layers and ZnO thin films. Accordingly, broadband optical emissions are expected to arise from a combination between the ZnO layer (blue band) and PSi (red band) [6]. (3) Hybrid organic-inorganic self-powered photodetectors with three different configurations were fabricated and their optoelectronic performance was determined. The basic photodetector structure under study is Au/PEDOT:PSS/Si/Al. The performance of the device was greatly improved by modifying the structure of the active layer to be Si+PSi micro-arrays instead of single PSi layers or flat Si layers. This improved photonic behavior is associated to the combined effect of an effective reduction of the reflectance due to the presence of PSi and an improvement of the electrical conduction given by the presence of heavily-doped Si regions.

[1] F. Priolo, T. Gregorkiewicz, M. Galli, T.F. Krauss, Nat. Nanotech. **9, 19** (2014).
[2] R. Ramadan, R.J. Martín-Palma, Journal of Nanophotonics **14**, 040501 (2020).
[3] R.J. Martín-Palma, P.D. McAtee, R. Ramadan, A. Lakhtakia, Scientific reports **9**, 1 (2019).

[4] R. Ramadan, M. Manso-Silván, R.J. Martín-Palma, J. of Materials Science **55**, 5458 (2020).
[5] R. Ramadan, R.J. Martín-Palma, Energies **13**, 2165 (2020).
[6] R. Ramadan, V. Torres-Costa, R.J. Martín-Palma, Coatings **10**, 529 (2020)

Session I I

Chair of the session: Laura Rodríguez Arriaga

10:30 *"Tunable proximity effects and topological superconductivity in semiconductor superconductor/ferromagnetic hybrid nanowires"*
Samuel Díaz Escribano Dpto. de Física Teórica de la Materia Condensada

Tunable proximity effects and topological superconductivity in semiconductor/superconductor/ferromagnetic hybrid nanowires

Samuel Díaz Escribano[1]

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Hybrid semiconducting nanowire devices combining epitaxial superconductor and ferromagnetic insulator layers have been recently explored experimentally as an alternative platform for topological superconductivity at zero applied magnetic field. In this proof-of-principle work we show that the topological regime can be reached in actual devices depending on some geometrical constraints. To this end, we perform numerical simulations of InAs wires in which we explicitly include the superconducting Al and magnetic EuS shells, as well as the interaction with the electrostatic environment at a self-consistent mean-field level. Our calculations show that both the magnetic and the superconducting proximity effects on the nanowire can be tuned by nearby gates thanks to their ability to move the wavefunction across the wire section. We find that the topological phase is achieved in significant portions of the phase diagram only in configurations where the Al and EuS layers overlap on some wire facet, due to the rather local direct induced spin polarization and the appearance of an extra indirect exchange field through the superconductor. While of obvious relevance for the explanation of recent experiments, tunable proximity effects are of interest in the broader field of superconducting spintronics.

10:45 *"Topological phases induced by interactions and spin-orbit coupling in decorated honeycomb lattices"*
Manuel Fernández López Dpto. de Física Teórica de la Materia Condensada

Topological phases induced by interactions and spin-orbit coupling in decorated honeycomb lattices

Manuel Fernández López[1]

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The decorated honeycomb lattice (DHL) is a playground to study non-interacting topological states of matter such as the quantum spin Hall (QSH) insulator due to its peculiar band structure containing flat bands, Dirac and quadratic band touching points. In the search of novel interacting topological states we have analyzed the interplay of spin-orbit coupling (SOC) and on-site Coulomb interaction based on a Kane-Mele-Hubbard model on the DHL. For weak Coulomb repulsion a transition from a QSH insulator to a non-trivial semimetal with a non-quantized spin Hall conductivity occurs as SOC is increased.

In the strong interacting limit, SOC induces a transition from a resonance valence bond (RVB) spin liquid state to a magnetic insulator consisting of antiferromagnetically ordered S=3/2 localized moments on the honeycomb lattice. Our results are discussed in the context of organometallic compounds realizing the DHL.

11:00 *"Superconducting STM tip functionalized with a magnetic impurity to probe the transition from Yu-Shiba-Rusinov States to Kondo Screening"*
Cosme González Ayani Dpto. de Física de la Materia Condensada

Superconducting STM tip functionalized with a magnetic impurity to probe the transition from Yu-Shiba-Rusinov States to Kondo Screening

C. G. Ayani*[1,2], Fabian Calleja[2], Ivan. M. Ibarburu[1,2], Pablo Casado[1,2], J. Ripoll Sau[1,2], M. Garnica[2], Amadeo L. Vázquez de Parga[1,2], Rodolfo Miranda[1,2]

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One of the main fields of research in condensed matter physics is the interaction of magnetic impurities with non-magnetic metallic hosts. The scattering potential of the impurities in these systems give rise to interesting many body effects. Two of the most renown are: the Kondo effect in the case of a metallic host and the appearance on Yu-Shiba-Rusinov (YSR) bound states whenever a magnetic impurity is placed in a superconducting host.

In this work we explore the transition from YSR bound states to Kondo screening by employing the magnetic field of a commercial JT-STM. A superconducting Nb STM tip, Fig.1(a), is functionalized with a TCNQ molecule that upon being vertically manipulated from the substrate, gr/Ir(111), onto the STM tip develops a magnetic moment. This results in two bias-symmetric intra gap states in STS that are assigned to a pair of YSR bound states Fig.1(b) [1]. Although the initial magnetic ground state is determined by the absorption configuration of the molecule on the tip apex, we are able to change the coupling by altering the force exerted over the molecule (by changing tip-sample distance) [2]. Finally, we can observe the transition from YSR bound states to Kondo screening by ramping the magnetic field up to 1.5 T where the superconductivity of the tip is quenched Fig.1(c). The Kondo nature of the resulting feature is demonstrated by studying its thermal evolution.

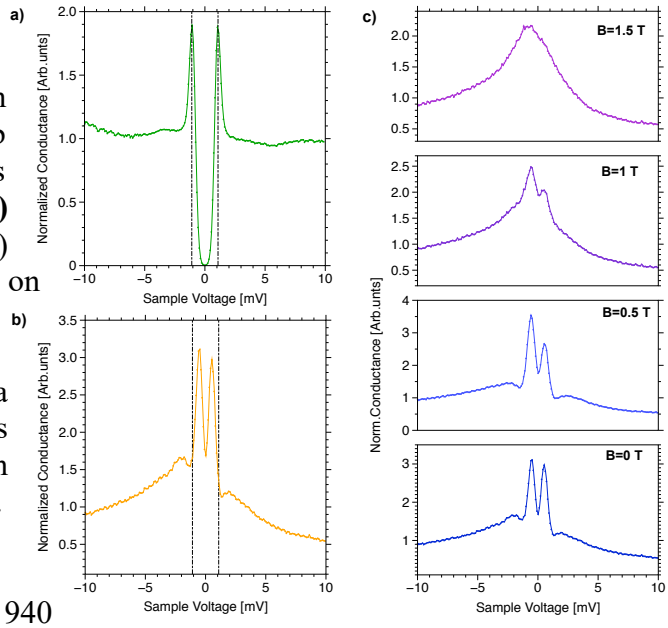

Figure 1. **(a)** dI/dV spectrum recorded on gr/Ir(111) exhibiting the SC gap of the Nb tip at T=1.2K. The tunnelling gap was stabilized at 15mV, 1nA, 100uV$_{mod}$. **(b)** Scanning tunnelling spectroscopy (STS) after a molecule is vertically manipulated on to the apex of the STM Nb tip, T=1.2K. Stabilization parameters: 15mV, 500pA, and 150uV$_{mod}$. **(c)** Set of four spectra recorded at different magnetic field values from B=0T to B=1.5T. Stabilization parameters: 15mV, 500pA and 150uV$_{mod}$.

[1] K. J. Franke et al., Science **332**, 940 (2011).
[2] L. Malavolti et al., Nano Lett. **18**, 7955 (2018).

11:15 *"Simultaneous conductance and thermopower measurements in single-molecule junctions using a scanning tunnelling microscope"*
Laura Rincón García Dpto. de Física de la Materia Condensada

Simultaneous conductance and thermopower measurements in single-molecule junctions using a scanning tunnelling microscope

L. Rincón-García[1], J. Hurtado-Gallego[1], C. Evangeli[1,2], E. Leary[3], M. T. González[3], G. Rubio-Bollinger[1,4] and N. Agraït [1,3,4]

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[3]*Madrid Institute of Advanced Research in Nanoscience IMDEA-Nanoscience, Madrid, Spain*
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The idea of using molecules as electronic components in functional devices has impelled an intensive experimental and theoretical research about charge transport through single-molecule junctions, that is, single molecules connected between two metallic electrodes [1]. Thermoelectric properties of these systems result especially interesting due to potential applications in waste heat recovery, energy harvesting or local cooling, and because they provide complementary insights about the charge transport mechanisms, not accessible characterizing only the electrical conductance. During the last fifteen years, a lot of effort has been done to investigate the effect on the thermoelectric response of different factors such as molecular length, anchor groups, electrode material or conjugated *versus* nonconjugated bridging units [2]. In this talk I will present the results obtained on the simultaneous characterization of conductance and thermopower of a series of single-molecule junctions, performed in ambient conditions and at room temperature with a home-made scanning tunnelling microscope (STM) adapted to apply voltage and temperature differences across the junctions [3-5]. The combination of these measurements (conductance and thermopower) has become an essential characterization tool for these systems and offers valuable information about their transport properties, as it is going to be shown for different molecules investigated.
/

Figure 1. Equivalent circuit of the STM junction in the presence of a voltage difference V_{bias} and a temperature difference between the tip (heated at T_h) and the substrate (at room temperature or $T_c<T_h$). G and S are the conductance and thermopower of the molecular junction, respectively. Examples of these systems are depicted on the left, where schematic representations of single-molecule junctions are shown.

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[2] L. Rincón-García et al., Chem. Soc. Rev., **45**(15), 4285 (2016)
[3] C. Evangeli et al., Nano Lett., **13**(5), 2141 (2013)
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[5] I. M. Grace et al., Nanoscale, **12**, 14682 (2020)

Session III

Chair of the session: Laura Rodríguez Arriaga

12:00 **Invited talk:** "*Toroids, Active Nematics and Topological Defects*"

Alberto Fernandez-Nieves Universidad de Barcelona & ICREA

Toroids, Active Nematics and Topological Defects

Alberto Fernandez-Nieves

Department of Condensed Matter Physics, University of Barcelona ICREA – Institució Catalana de Recerca i Estudis Avançats
Barcelona, Spain

We will discuss recent results with active nematics confined to either toroidal space. We will first review how we make and stabilize non-spherical droplets and describe how curvature affects defect arrangement on tori. We will show that despite the intrinsic activity and out-of-equilibrium character of the system, there are still remnants of the expected curvature-induced defect unbinding predicted for nematics in their ground state. Activity, however, augments the behavior leading to unexpected defect distributions. We will then focus on defect orientation and show that on flat space, there is short-range orientational correlations without long-range orientational order.

Session IV

Chair of the session: Miguel Ángel Ramos

13:00 Research awards for Physics students 2020 flash-talks

Transporte termoeléctrico en puntos cuánticos

Miguel Calvo Carrera

Se han simulado las corrientes eléctrica y térmica a través de punto cuántico. El punto modelizado consta de un nivel a una energía ajustable mediante un voltaje externo, no considera el espín, y se acopla a dos electrodos metálicos. Se ha utilizado un análisis perturbativo para distintas condiciones de simulación, y se ha comprobado su bondad con la solución analítica del formalismo de Landauer.

Pulsed photon correlations under strong light-matter coupling in nanoplasmonic cavities

Federico Martín Lucas

Single photon sources, which emit antibunched light, are very important in quantum information and technology. In this context, plasmonic nanocavities offer the potential to provide ultrafast sources which operate on femtosecond timescales. We investigate the ability of a coupled emitter-nanocavity system to serve as an ultrafast single-photon source, triggered through illumination by an ultrashort pulse. In such a setup, the relevant observable is not the 'conventional' photon correlation $g^{(2)}$ in the steady-state under continuous driving, but the 'pulsed' $g^{(2)}$ which determines the fidelity of emitting a single-photon wave packet triggered by the driving pulse. We study the differences and commonalities between continuous and short-pulse illumination in this system. It is shown that the pulsed $g^{(2)}$ can be approximated as a weighted convolution of $g^{(2)}(\tau)$ for long pulses, but significantly deviates from this approximation for short pulses due to the associated large frequency bandwidth. This implies that the pulsed $g^{(2)}$ has to be explicitly calculated for the specific driving pulse chosen, and the optimal design parameters differ from those found for continuous-wave illumination. An optimization process is performed to find the parameters where the pulsed $g^{(2)}$ is minimal, conditions to create antibunched light sources.

Topological Invariants in Disordered and Amorphous Systems from Neural Networks

Daniel Molpeceres Mingo

A number of topological invariants have been proposed over the past few years to characterize different topological phases in periodic systems (Chern number, Z2, etc). Some of these invariants are recently being extended to non-periodic systems (alloys, strongly disordered, or even amorphous materials), properly defined through local quantities [1-3]. At the same time (supervised) neural networks are gaining popularity as tools to identify these phases when the parameter phase space is large [2,4]. In this project, we carry out numerical simulations of the electronic structure and get acquainted with the use of supervised neural networks to identify non-trivial topological phases in non-periodic systems. We focus on electronic systems defined through simple tight-binding parametrizations on top of disordered lattices.

[1] Huaqing Huang and Feng Liu, Phys. Rev. B 98, 125130 (2018); Huaqing Huang and Feng Liu, Phys. Rev. Lett. 121, 126401 (2018).
[2] D. Carvalho et al., Phys. Rev. B 97, 115453 (2018).
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Transporte electrónico a través de impurezas magnéticas acopladas a superconductores

Gonzalo Morrás Gutiérrez

En este proyecto se ha realizado un estudio teorico de la corriente Josephson a través de una y dos impurezas magneticas acopladas a electrodos superconductores. Se ha estudiado como la corriente se transmite a través estados de Yu-Shiba-Rusinov, obteniendo predicciones que pueden ser testadas en microscopios de efecto túnel actuales. Este tipo de sistemas son de gran interés ya que muestran la competición entre dos fenómenos fisicos contrarios, el magnetismo y la superconductividad.

Espectroscopia resuelta en tiempo en nanoestructuras semiconductoras

Ignacio Robles López

La interacción radiación-materia es la conclusión lógica a la pregunta de cómo podemos hacer interactuar a los fotones entre sí y de esta forma usar sus propiedades para la circuitería. Los polaritones, sistemas formados por la interacción entre fotones y electrones en semiconductores, poseen unas propiedades excepcionales para este cometido y es así como en este trabajo veremos cómo su dinámica influye en la forma en que los estudiamos.

Modelling the transformation of zinc nitride metastable layers

Andrea Ropero Real

Zinc nitride (Zn_3N_2) is a semiconductor with remarkable electronic properties such as a high mobility, a high carrier concentration, and a low resistivity. Due to these excellent features, it has been already applied for sensors, thin film transistors, and flexible electronics. However, in ambient conditions Zn_3N_2 experiences oxidation that results in a severe transformation of the structural, optical and electrical characteristics, mainly due to the air humidity. In this work we have studied the transformation of Zn_3N_2 upon humidity by means of in-situ monitoring of the electrical conductivity and ex-situ spectroscopic ellipsometry and scanning electron microscopy. Our results demonstrate that Zn_3N_2 exhibits an important swelling effect when oxidized. This behavior can be well modelled with a progressive top-down transformation of the layer, which leads to a logistic variation of the overall resistance. Thanks to this mechanism we have successfully applied this material for corporal hydration sensors combined with IoT technology.

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