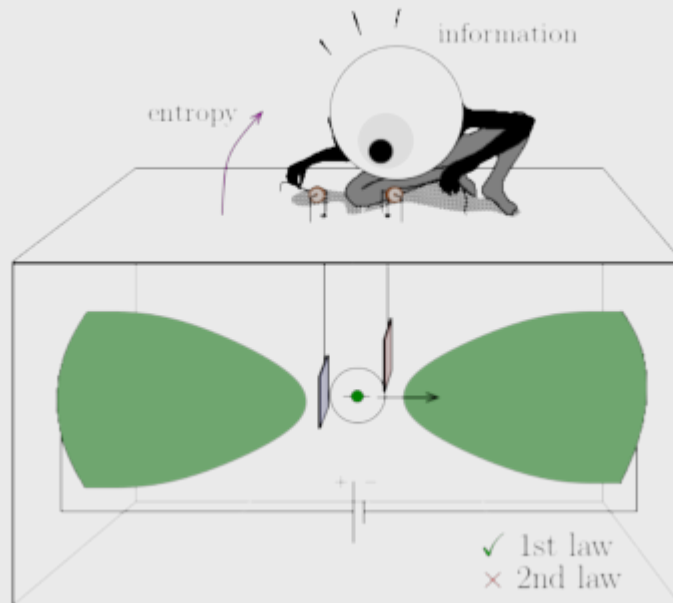


## Non-equilibrium Autonomous Maxwell (or not) Demons



Article: published in [Physical Review Letters](#) by [Rafael Sánchez](#), IFIMAC researcher and member of the Theoretical Condensed Matter Physics Department.

**T**he second law of thermodynamics dictates that a heat engine can generate power provided that it absorbs heat from its environment. Soon after its formulation, Maxwell protested against this claim by arguing that a microscopic “demon” could produce the same effect by selectively controlling the system based on the detailed knowledge of its state. The system hence produces work without changing neither its energy nor the number of its particles.

In a paper published in [Physical Review Letters](#) we show that a non-equilibrium distribution generates a paradoxical effect similar to a “Maxwell demon”: it raises the apparent paradox of reducing another system’s entropy at no cost, thereby suggesting that perpetual motion is possible. We call this a “N-demon” (with the “N” for non-equilibrium). Bennett showed that the paradox of the Maxwell demon was resolved by treating information as a thermodynamic resource like heat or work. Similarly, we resolve the paradox of the N-demon by treating “non-equilibrium” as a thermodynamic resource, which is used up as it reduces another system’s entropy. This forbids the building of a perpetual motion machine, but does allow us to propose devices that use such resources (in particular non-equilibrium distributions of electrons or photons) to generate more useful energy than is conventionally believed possible. Non-equilibrium distributions of states are all around us, and are often generated as an unwanted by-product of some physical process, so it is very appealing to think that we might be able to take such a distribution as a resource, and recycle it into useful energy.

In another work, published in [Physical Review Research](#), we consider an autonomous implementation of Maxwell’s demon based on quantum dots. Via capacitive couplings,

two quantum dots are able to measure and perform feedback on the system conductor where electric power is generated. This setup allows for comparing different descriptions based on information flows to a more conventional thermoelectric approach. It further allows us to investigate the entropic cost of breaking detailed balance as well as fluctuation theorems describing information to work conversion. In particular, we derive a fluctuation relation using a novel kind of time-reversal on the single-particle level for the system alone. [[Full article - PRL](#)][[Full article - PRR](#)]

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## Francisco J. Garcia-Vidal included in Clarivate 2019 Compilation of Most Influential Authors

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J. García-Vidal – IFIMAC Director.

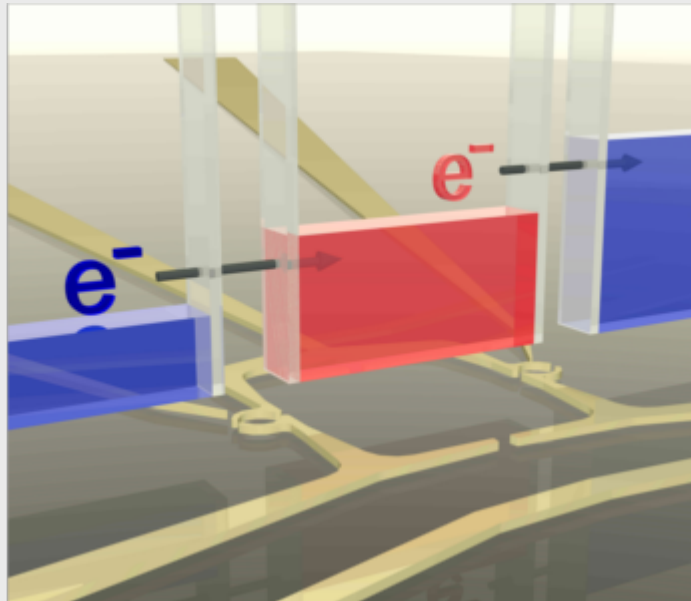
**H**ighly Cited Researchers from Clarivate Analytics is an annual list recognizing leading researchers in the sciences and social sciences from around the world. Researchers are selected for their exceptional performance in one or more of 21 fields (those used in Clarivate Analytics Essential Science Indicators, or ESI) or across several fields. Approximately 6,000 researchers are named [Highly Cited Researchers in 2019](#) – some 4,000 in specific fields and about 2,000 for cross-field performance. This is the first year that researchers with cross-field impact are identified. The number of researchers selected in each field is based on the square root of the population of authors listed on the field's highly cited papers. The number of those with cross-field influence is determined by finding those who have influence equivalent to those identified in the 21 fields.

In the list of Physics, in which [Prof. Garcia-Vidal](#) has been selected, only four researchers working in Spanish institutions have been included. [Clarivate 2019 compilation of researchers list](#).

We congratulate [Prof. Francisco J. Garcia-Vidal](#).

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## Experimental Realization of a Quantum Dot Energy Harvester

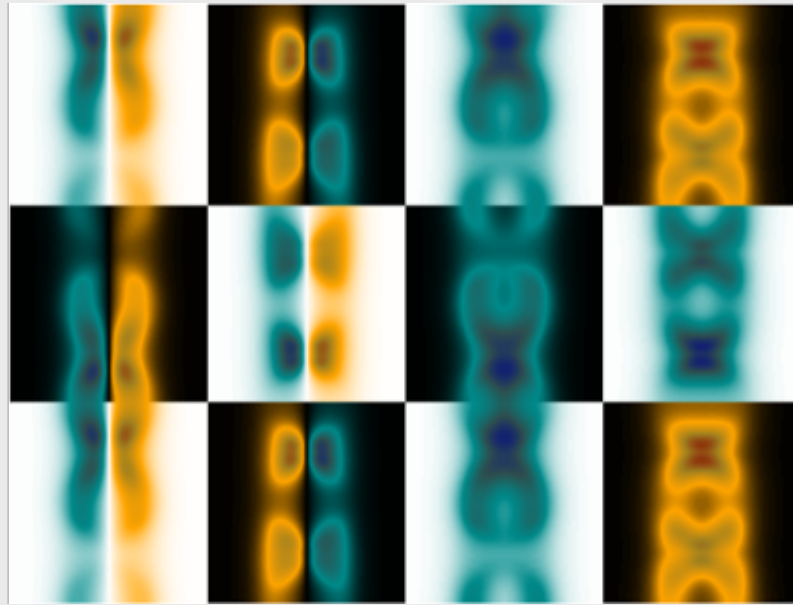


Article: published in [Physical Review Letters](#) by [Rafael Sánchez](#), IFIMAC researcher and member of Department of Theoretical Condensed Matter Physics.

**W**e demonstrate experimentally an autonomous nanoscale energy harvester that utilizes the physics of resonant tunneling quantum dots. Gate-defined quantum dots on GaAs/AlGaAs high-electron-mobility transistors are placed on either side of a hot-electron reservoir. The discrete energy levels of the quantum dots are tuned to be aligned with low energy electrons on one side and high energy electrons on the other side of the hot reservoir. The quantum dots thus act as energy filters and allow for the conversion of heat from the cavity into electrical power. Our energy harvester, measured at an estimated base temperature of 75 mK in a He3/He4 dilution refrigerator, can generate a thermal power of 0.13 fW for a temperature difference across each dot of about 67 mK. [[Full article](#)]

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## Reversible Thermal Diode and Energy Harvester with a Superconducting Quantum Interference Single-electron Transistor



Articles: published in [Applied Physics Letters](#) by [Rafael Sánchez](#), IFIMAC researcher and member of Department of Theoretical Condensed Matter Physics.

**T**he density of states of proximitized normal nanowires interrupting superconducting rings can be tuned by the magnetic flux piercing the loop. Using these as the contacts of a single-electron transistor allows us to control the energetic mirror asymmetry of the conductor, thus introducing rectification properties. In particular, we show that the system works as a diode that rectifies both charge and heat currents and whose polarity can be reversed by the magnetic field and a gate voltage. We emphasize the role of dissipation at the island. The coupling to substrate phonons enhances the effect and furthermore introduces a channel for phase tunable conversion of heat exchanged with the environment into electrical current.

We thank discussions and comments from A. Levy Yeyati, C. Urbina, and F. Giazotto. This work was supported by the Spanish Ministerio de Economía, Industria y Competitividad (MINECO) via the Ramón y Cajal Program No. RYC-2016-20778 and the “María de Maeztu” Programme for Units of Excellence in R&D (No. MDM-2014-0377). We also acknowledge the Université Paris-Saclay international grants, the EU Erasmus program. [\[Full article\]](#)

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[A Protein-based Junction Serves as a Current Switch](#)

Articles: published in [Angewandte Chemie](#) by [Juan Carlos Cuevas](#) and Linda A. Zotti, [IFIMAC](#) researchers and members of Department of Theoretical Condensed Matter Physics.

**P**roteins are key biological molecules that are responsible for numerous energy conversion processes such as photosynthesis or respiration. In recent years, proteins have been investigated in a new setting, namely in solid-state electronic junctions, with the goal of understanding the charge transfer mechanisms in these biomolecules, but also with the hope of developing a new generation of bio-inspired nanoscale electronic devices. Now, a new step towards this goal has been reported in a piece of work published in [Angewandte Chemie](#) by a collaboration between the group of [David Cahen](#) in the [Weizmann Institute of Science](#) (Israel) and the IFIMAC researchers Carlos Romero-Muñiz, Juan Carlos Cuevas, and Linda A. Zotti. In this work, these researchers show that a redox protein, cytochrome C, can behave as an electrically driven switch when incorporated in a solid-state junction with gold electrodes. By changing the external bias voltage in the junction, it was shown that the relevant molecular orbitals of the protein can be brought in and out of resonance with the chemical potential of the electrodes, which leads to the current-switch behavior. Showing transition from off- to on- resonance can be very challenging and this is the first time it has been achieved for proteins within the same working junction. Extensive ab initio DFT calculations revealed that the charge transport proceeds through the heme unit in these proteins and that the coupling between the protein's frontier orbitals and the electrodes is sufficiently weak to prevent Fermi level pinning. The on-off change in the electrical current was shown to persist up to room temperature, demonstrating reversible, bias-controlled switching of a protein ensemble, which provides a realistic path to protein-based bioelectronics. [[Angewandte Chemie - full article](#)]

References

A Solid-State Protein Junction Serves as a Bias-Induced Current Switch, Jerry A. Fereiro, Ben Kayser, Carlos Romero-Muñiz, Ayelet Vilan, Dmitry A. Dolgikh, Rita V. Chertkova, Juan Carlos Cuevas, Linda A. Zotti, Israel Pecht, Mordechai Sheves, David Cahen. Published in *Angewandte Chemie International Edition*, Volume 58, Issue 34, Pages 11852-11859, August 19 (2019). [[URL](#)]

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Promotional video: [Theoretical Condensed Matter Physics \(UAM\)](#)



In the Department of Theoretical Condensed Matter Physics at the Universidad Autónoma de Madrid, we focus on understanding and predicting the behaviour of condensed systems, which are ubiquitous in the world around us.

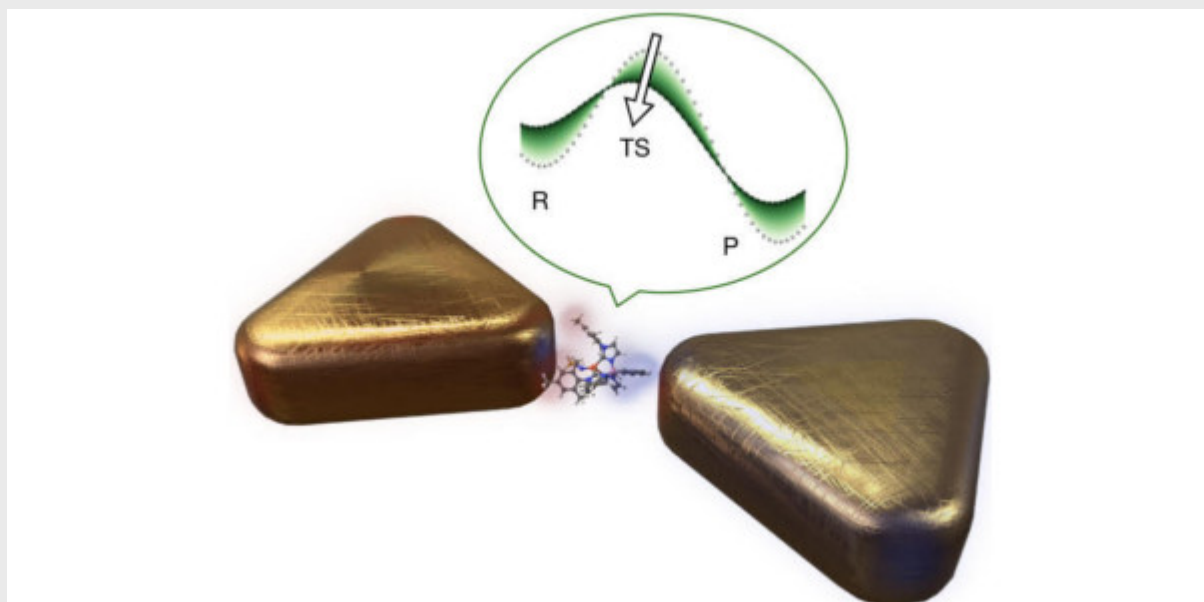
We are interested in problems in areas such as nanotechnology, biophysics, nanophotonics or material science. We employ a wide range of theoretical approaches to gain insight into diverse physical systems, from living matter to the atom itself. We work in optics, quantum mechanics, biophysics, fluid dynamics or material physics. We carry out creative research, which requires imagination and creativity. We work with fundamental equations, we study them, analyse them in different contexts, we take them to places they have never been and return with new and surprising information. Our findings reveal how simple rules can give rise to complex phenomena, which is helping us to understand and develop new material platforms for the implementation of the technology of the future.

Fundamentally, this is research with which we need your help.

Long version.

Short version.

## Nanocavity-modified Ground State Chemistry



Articles: published in [Angewandte Chemie](#) and [Physical Review X](#) by Javier Galego, Clàudia Climent Biescas, [Johannes Feist](#) and [Francisco J. García-Vidal](#), IFIMAC researchers and members of Department of Theoretical Condensed Matter Physics.

Over the past few years it has become clear that strong electromagnetic coupling between a molecule and light confined in a nanoscale cavity can lead to significant modifications of the electromagnetic response of the hybrid system as well as the internal molecular properties. This has already been exploited to manipulate the fate of photochemical reactions, however, up to now there has been no general theory on how these interactions affect the chemical reactivity of a molecule in its ground state without any external input of energy.

In a theoretical study published in [Physical Review X](#), a group of researchers from the [Departamento de Física Teórica de la Materia Condensada](#) and the [Condensed Matter Physics Center](#) (IFIMAC) at the [Universidad Autónoma de Madrid](#) have developed a theoretical framework that combines quantum electrodynamics and the quantum theory of chemical reactivity. The authors implemented this approach for a simple model molecule that can be solved without approximations. This allowed to explore the general properties of cavity-induced ground-state chemical reactivity changes and develop a simplified theoretical model that can be applied to more complex molecules. They found that the induced changes on the molecular potential energy surfaces do



not depend on any resonance condition between molecular transitions (such as vibrational or electronic excitations) and cavity modes, with the relevant interactions closely related to well-known electrostatic forces on the molecule due to other molecules or larger material bodies. In particular, the largest contribution to the modification of the energy landscape is typically determined by the change of the permanent dipole moment of the molecule between its equilibrium and transition state configuration. They have also shown that experimentally available nanocavities can induce changes in reaction rates by an order of magnitude in a single molecule, while for the case of many molecules, this effect becomes significant only if all the molecules are aligned.

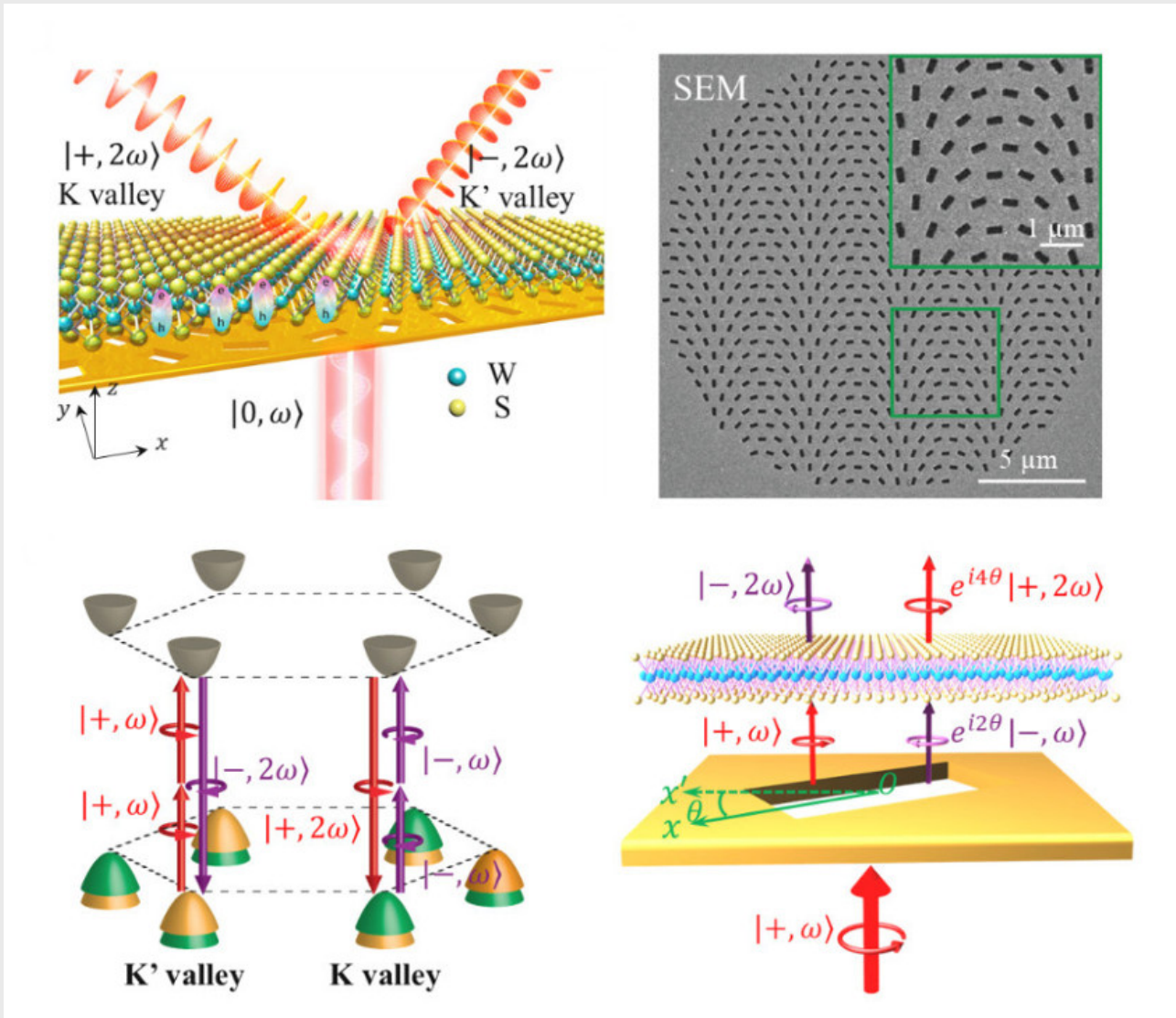
In a second paper published in [Angewandte Chemie](#), the same authors have combined this theory with quantum chemistry calculations and have shown how plasmonic nanocavities can enable self-induced electrostatic catalysis of typical organic reactions, without any external driving, due to the interaction of the molecular permanent and fluctuating dipole moments with the plasmonic cavity modes. They have also exploited this interaction between molecules and electromagnetic modes to predict cavity-induced changes in the transition temperature of spin-crossover transition metal complexes, the prime example of molecular switches.

These studies contribute to the fundamental understanding of how nanoscale cavities can be used to manipulate chemical reactions of single molecules and open the path towards ground-state catalysis with plasmonic nanocavities. They also provide an example on how the interaction with plasmonic modes may be ultimately exploited to manipulate material properties. [[Angewandte Chemie - full article](#)] [[Physical Review X - full article](#)]

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[Steering of Chiral Valley Photons in Transition Metal Dichalcogenides](#)





Article: published in [Nature Photonics](#) by [Francisco J. Garcia-Vidal](#), IFIMAC researcher and member of the Department of Theoretical Condensed Matter Physics.

Two-dimensional transition metal dichalcogenides (TMDCs) present extraordinary nonlinearities and direct bandgaps at the K and K' valleys. These valleys can be optically manipulated through, for example, plasmon-valley-exciton coupling with spin dependent photoluminescence. However, the weak coherence between the pumping and emission makes exploring nonlinear valleytronic devices based on TMDCs challenging. In a collaboration between IFIMAC member [Francisco J. Garcia-Vidal](#) and two experimental groups based in Singapore and China, it has been demonstrated that a metasurface (a gold film drilled with rectangular nanoholes arranged in a hexagonal lattice but with different local rotation angles), which entangles the phase and spin of light, can simultaneously enhance and manipulate nonlinear valley-locked chiral emission in monolayer tungsten disulfide at room temperature. The second-harmonic valley photons, accessed and coherently pumped by light, acquire a spin related geometric phase provided by the gold metasurface and are separated and routed to predetermined directions in free space. In addition, the nonlinear photons with the same spin as the incident light are steered owing to the critical spin-valley locked nonlinear selection rule of monolayer tungsten disulfide in the designed metasurface.

This work opens a new avenue to utilize plasmonic metalsurfaces in order to build-up advanced room-temperature and free-space nonlinear, quantum and valleytronic nanodevices. [[Full article](#)]

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## The Inclusion of the Gender Perspective in Scientific Research



**Inclusión de la perspectiva de género en la investigación científica**  
Curso teórico-practico dirigido a estudiantes de master y doctorado

**Programa**  
10h00-11h00 "Género y programas europeos" **Cristina Sánchez**  
11h00-11h30 Debate  
11h30-12h00 Café  
12h00-13h00 "Género e investigación", **Yolanda Guerrero**  
13h00-13h50 Debate  
13h50-14h00 Conclusiones

**Viernes 5 de Abril, 10:00-14:00**  
**Sala de seminarios, Módulo 3, 5ª planta**  
**Facultad de Ciencias**  
**UAM**

**IFiMaC** **iUEM** Instituto Universitario de Estudios de la MUJER



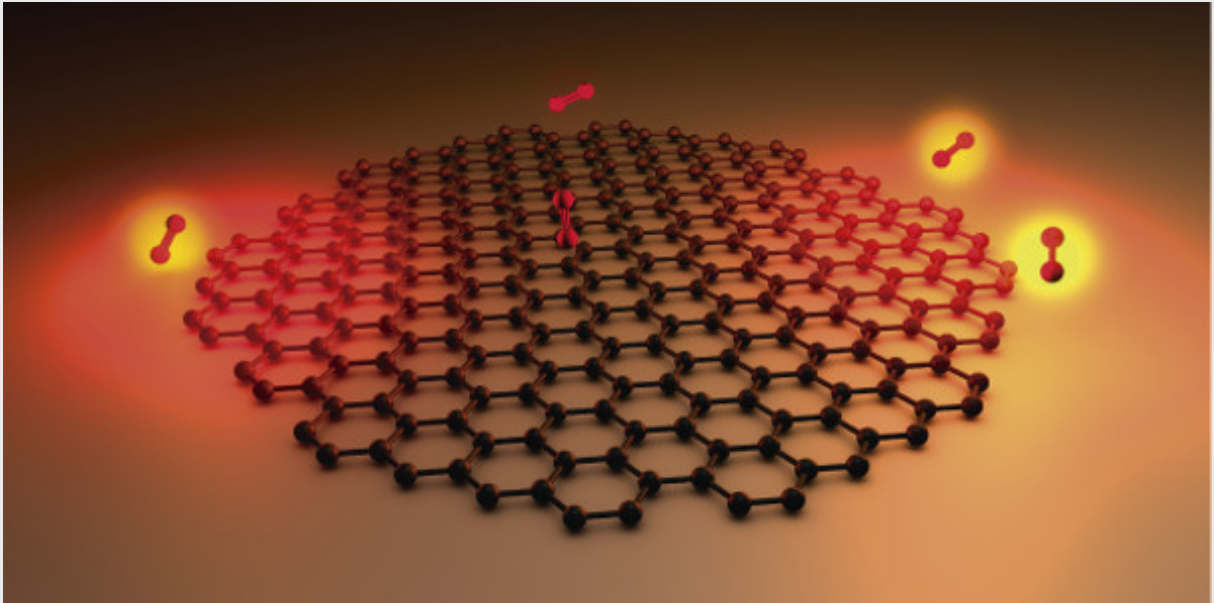
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Friday the 5<sup>th</sup> of April 2019, it has been organised a course about the inclusion of the gender perspective in scientific research. The course is primarily directed to Master and PhD students in Physics, as well as Post-Docs. The theoretical/practical course will be delivered by Prof. Yolanda Guerrero, professor of medieval history at the UAM and Prof. Cristina Sánchez, professor in philosophy of law at UAM. Both professors have been in charge of the UAM “[Instituto Universitario de Estudios de la Mujer](#)” and have already successfully taught this course in within other doctoral programs in science and, in particular, in Physics.

The course will last three hours with a coffee break in between. We ask you to confirm assistance by sending an email to Manuela Moreno at [manuela.moreno@uam.es](mailto:manuela.moreno@uam.es) no later than Wednesday April the 3<sup>rd</sup>, in order to organize the coffee break. You can find more information in the attached program.

This course is organized within the framework of the [Master in Physics of Condensed Matter and Biological Systems](#).

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Title: Metallic Nanostructures and Quantum Emitters.

When: Wednesday, April 03, (2019), 12:00.

Place: Department of Theoretical Condensed Matter Physics, Faculty of Sciences, Module 5, Seminar Room (5th Floor).

Speaker: Alejandro Manjavacas, University of New Mexico, USA.

**T**he optical response of quantum emitters, such as atoms, molecules, or quantum dots, is strongly modified by their interaction with the near-field of metallic nanostructures that support plasmon resonances. In this talk, we will discuss recent results showing how different metallic nanostructures, ranging from 3D gold elements to 2D graphene systems, can enhance the rates of dipole-forbidden transitions. Furthermore, we will analyze the fundamental limits of the local density of photonic states, a magnitude that quantifies the interaction of a quantum emitter with the local electromagnetic field, through the study of a sum rule that establishes an upper bound to this quantity. Finally, if time permits, we will discuss the response of arrays with multi-particle unit cells using an analytical approach based on plasmon hybridization, which provides a simple and efficient way to design structures with engineered properties.

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