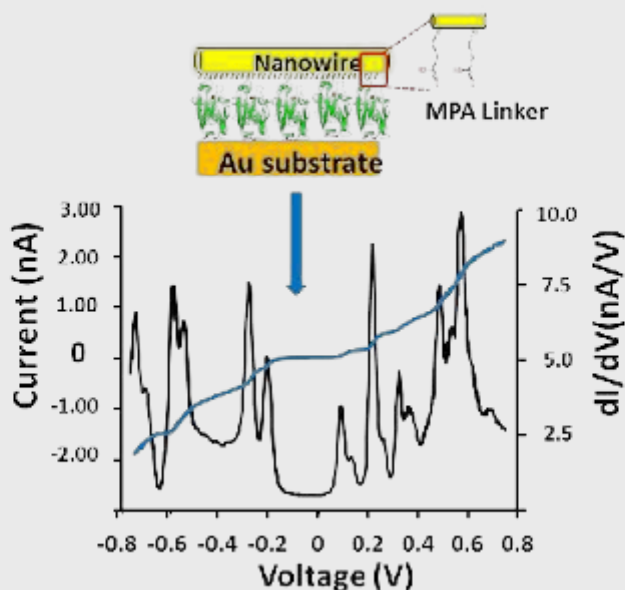


## Resonant Tunneling in Protein-based Junctions

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ling through an Azurin monolayer.

Article: published in [PNAS](#) by [Juan Carlos Cuevas](#), IFIMAC researcher and member of the Department of Theoretical Condensed Matter Physics.

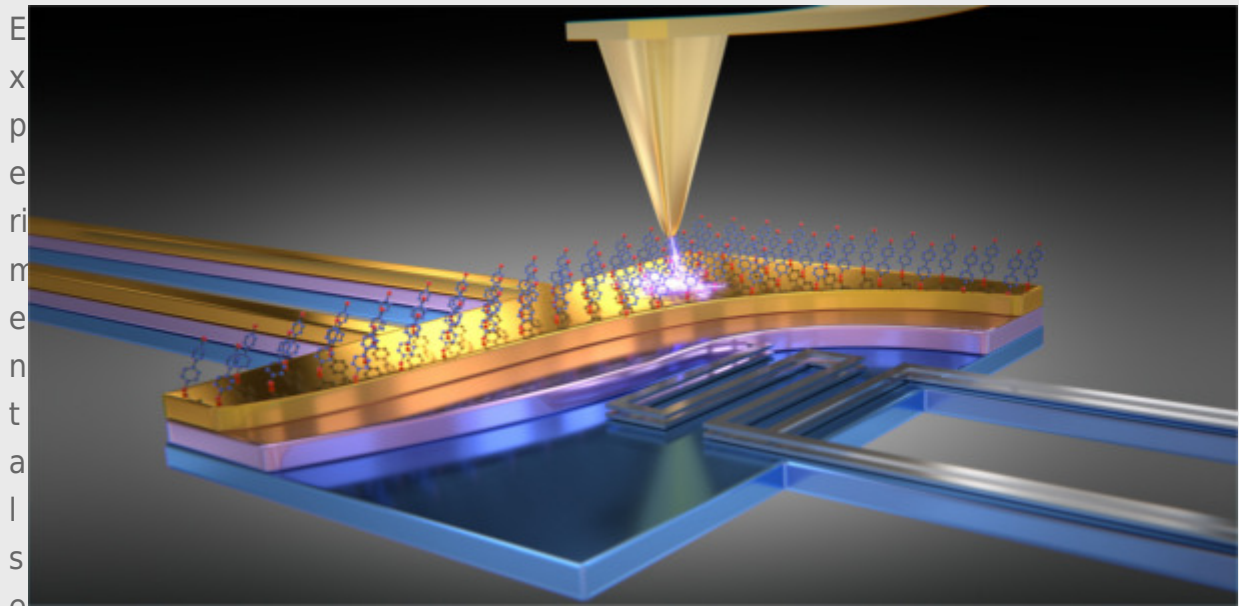
**P**roteins play a fundamental role in numerous biological energy conversion processes such as photosynthesis, respiration, and a wide variety of enzymatic reactions. In recent years, redox proteins containing transition metal ion centers have been integrated into solid-state electronic junctions. The goal is to shed new light on the electron transfer mechanisms in these biomolecules, but also to investigate the possibility of using proteins as active elements in novel, bio-inspired electronic devices. In this context, recent experiments have shown that the electron transport through proteins can be surprisingly efficient. However, the origin of this efficiency and, in general, the underlying transport mechanisms remain largely unknown.

New light on this fundamental problem has now been shed in a work published in the *Proceedings of the National Academy of Sciences of USA* (PNAS) by a collaboration between the group of [David Cahen](#) (Weizmann Institute of Science, Rehovot, Israel) and the IFIMAC researcher Juan Carlos Cuevas. In this work, these researchers report low-temperature (10 K) electron transport measurements via monolayer junction based on the blue copper protein Azurin that strongly suggest that quantum tunneling is the dominant charge transport mechanism. In particular, they show that weakening the protein-electrode coupling by introducing a spacer, one can switch the electron transport from off-resonant to resonant tunneling, which has never been reported before in protein-based junctions. Moreover, vibronic features of the Cu(II) coordination sphere were identified in the transport characteristics, which shows directly the active

role of the metal ion in the resonant tunneling. These results illustrate how quantum mechanical effects may dominate electron transport via protein-based junctions, which is clearly at variance with the common wisdom in the field of protein electron transfer in biological settings. [[Full article](#)]

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## Peltier Cooling in Molecular Junctions



Experimental setup for the measurement of Peltier cooling in molecular junctions.

Article: published in [Nature Nanotechnology](#) by Linda Angela Zotti, member of the Department of Theoretical Condensed Matter Physics and [Juan Carlos Cuevas](#), IFIMAC researcher and member of the Department of Theoretical Condensed Matter Physics.

**T**hermoelectric cooling is based on the Peltier effect that consists in the generation of a reversible heat flow in response to the passage of an electrical current. Thus, depending on the direction of the electrical current in a junction, one can cool down an electrode at the expense of heating up the other one. Thermoelectric or Peltier coolers have many applications, especially in electronics, and they possess several advantages over conventional vapor-compression refrigeration systems, although they are typically less efficient than these latter ones. In the context of nanoscale systems, a lot of attention has been devoted to the study of thermoelectricity in molecular junctions with the hope, in particular, to increase the efficiency of Peltier cooling. However, in spite of the fact that a lot of progress has been made in probing related phenomena such as the Seebeck effect (the conversion of a temperature difference into an electrical current), the observation of Peltier cooling in molecular junctions has

remained inaccessible thus far.

This fundamental problem has now been resolved in a work published in Nature Nanotechnology by a collaboration between the groups of Pramod Reddy and Edgar Meyhofer (University of Michigan) and the members of our department Linda Angela Zotti and Juan Carlos Cuevas. In this work, these researchers report for the first time the direct observation of Peltier cooling in molecular junctions. This observation was possible due to the use of a novel experimental platform that combines conducting-probe atomic force microscopy with home-built calorimetric micro-devices with picowatt resolution. This platform enables the simultaneous measurement of electrical, thermoelectric and energy dissipation characteristics of molecular junctions. Using this platform, molecular junctions formed with gold electrodes and a variety of organic molecules were investigated. Such studies revealed not only the possibility to achieve molecular-based refrigeration, but they also showed the close relationship between heating or cooling and the transmission characteristics of these junctions. In particular, it was shown that the Peltier cooling can be tuned and optimized by an appropriate choice of the molecular architecture, and all this in exquisite agreement with density-functional-theory-based calculations performed in the framework of the Landauer approach for quantum coherent transport.

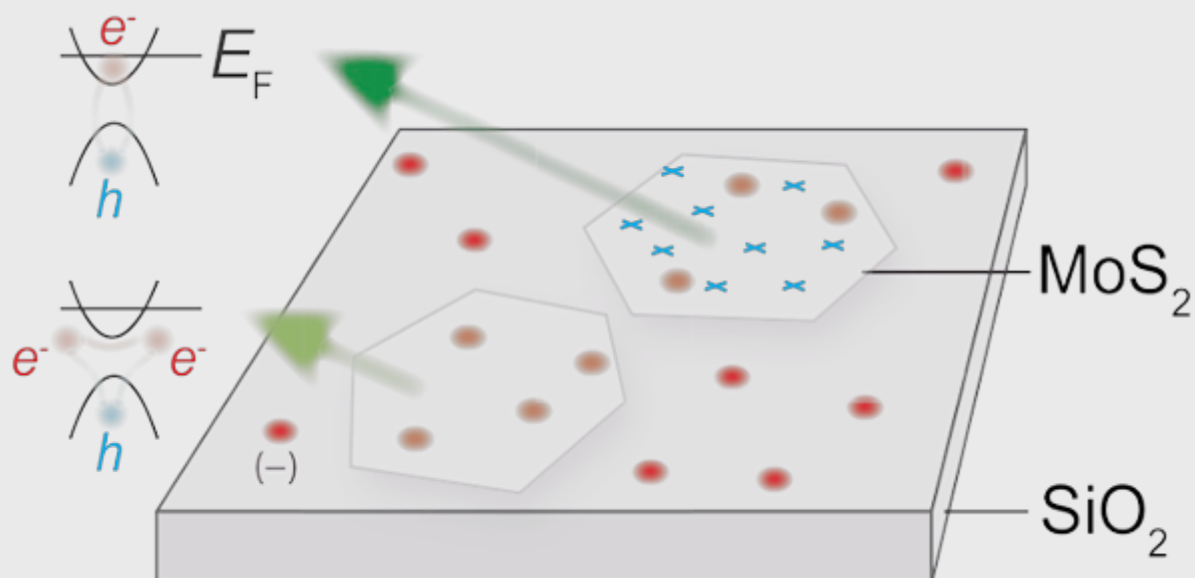
The advances reported in this work are expected to stimulate the exploration of atomic- and molecular-scale thermal transport and the quantification of the thermoelectric figure of merit in a variety of interesting molecules, nanostructures and materials. [[Full article](#)]

#### Reference

Peltier Cooling in Molecular Junctions, L. Cui, R. Miao, K. Wang, D. Thompson, L.A. Zotti, J.C. Cuevas, E. Meyhofer, P. Reddy, Nature Nanotechnology, doi:10.1038/s41565-01-0020-z, (2017). [[URL](#)]

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[Weakly Trapped, Charged, and Free Excitons in Single-Layer MoS<sub>2</sub> in the Presence of Defects, Strain, and Charged Impurities](#)



Article: published in [ACS Nano](#) by César González, [IFIMAC](#) researcher and member of the Department of Theoretical Condensed Matter Physics.

**F**ew- and single-layer MoS<sub>2</sub> host substantial densities of defects. They are thought to influence the doping level, the crystal structure, and the binding of electron–hole pairs. We disentangle the concomitant spectroscopic expression of all three effects and identify to what extent they are intrinsic to the material or extrinsic to it, i.e., related to its local environment. We do so by using different sources of MoS<sub>2</sub> -a natural one and one prepared at high pressure and high temperature- and different substrates bringing varying amounts of charged impurities and by separating the contributions of internal strain and doping in Raman spectra. Photoluminescence unveils various optically active excitonic complexes. We discover a defect-bound state having a low binding energy of 20 meV that does not appear sensitive to strain and doping, unlike charged excitons. Conversely, the defect does not significantly dope or strain MoS<sub>2</sub>. Scanning tunneling microscopy and density functional theory simulations point to substitutional atoms, presumably individual nitrogen atoms at the sulfur site. Our work shows the way to a systematic understanding of the effect of external and internal fields on the optical properties of two-dimensional materials. [[Full article](#)]

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[Fabrication of Gold Nano-Crystal Arrays for Molecular Electronics: High Frequency Molecular Rectifiers and  \$\pi\$ - \$\pi\$  Inter Molecular Interaction Energy](#)

# IfiMAC's SEMINAR

## ***Fabrication of Gold Nano-Crystal Arrays for Molecular Electronics: High Frequency Molecular Rectifiers and $\pi$ - $\pi$ Inter Molecular Interaction Energy***

**Jorge Trasobares**

National University of Singapore

Title: Fabrication of Gold Nano-Crystal Arrays for Molecular Electronics: High Frequency Molecular Rectifiers and  $\pi$ - $\pi$  Inter Molecular Interaction Energy.

When: Monday, September 18, (2017), 12:00.

Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).

Speaker: Dr. Jorge Trasobares, National University of Singapore, Singapore.

**E**-beam lithography was used for versatile fabrication of sub-15 nm single-crystal gold nanoarrays at wafer-scale by the so-called dot on the fly (DOTF) technique [1]. Here DOTF and other methods are compared evidencing the limiting factors for the writing speed. Wafer-scale fabrication of such arrays with 50 nm pitch allowed XPS analysis of a ferrocenylalkyl thiol self-assembled monolayer coated gold nanoarray. We exploit these arrays as a suitable test bed for Molecular Electronics (ME) [2] and propose two studies on high frequency molecular rectifiers [3] and inter molecular Interactions [4].

In a first study, we demonstrate molecular diodes operating up to 17.8 GHz. Direct current and radio frequency (RF) properties were simultaneously measured with the tip of an interferometric scanning microwave microscope and S11 parameters show a diode rectification ratio of 12 dB. In a second investigation, we explore the  $\pi$ - $\pi$  intermolecular interactions. This factor is one of the most important to optimize the transport and optical properties of organic transistors, light-emitting diodes or (bio-) molecular devices. Electrochemical measurements indicate two different phases localized on top and facets of the nanocrystals with clear intermolecular interactions and electrical current statistics on  $\sim$ 3000 molecular junctions confirm the theoretical prediction [5] of asymmetrical histograms due to cooperative effects.

References

J. Trasobares, F. Vaurette, M. François, H. Romijn, J-L. Codron, D. Vuillaume, D. Théron

and N. Clément. High speed e-beam lithography for gold nanoarray fabrication and use in nanotechnology. *Beilstein J. Nanotechnol.* 5, 1918-1925 (2014).

N. Clement, G. Patriarche, K. Smaali, F. Vaurette, K. Nishiguchi, D. Troadec, A. Fujiwara, D. Vuillaume. Large array of sub-10-nm single-grain Au nanodots for use in nanotechnology. *Small*, 7, 2607 (2011).

J. Trasobares, D. Vuillaume, D. Théron, N. Clement, A 17 GHz Molecular Rectifier, *Nat. Commun.* 7, 12850 (2016).

J. Trasobares, J. Rech, T. Jonckere, T. Martin, O. Aleveque, E. Levillain, V. Diez-Cabanes, Y. Olivier, J. Cornil, J.P. Nys, R. Sivakumarasamy, K. Smaali, Ph. Leclère, A. Fujiwara, D. Théron, D. Vuillaume, N. Clément. Estimation of  $\pi$ - $\pi$  Electronic Couplings from Current Measurements. *Nano Letters*, 17, 3215-3224 (2017).

M.G. Reuter, M.C. Hersam, T. Seideman, M.A. Ratner. Signatures of cooperative effects and transport mechanisms in conductance histograms. *Nano Letters*, 12, 2243-2248 (2012).

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XXIV International Summer School Nicolás Cabrera - 2017

# Quantum Transport in Topological Materials

XXIV International Summer School 'Nicolás Cabrera'

September 4-8, 2017

Miraflores de la Sierra

When: September 4-8, 2017

Where: Residencia La Cristalera, Miraflores de la Sierra, Madrid, Spain

Contacts:

Inés Ortiz – e-mail: [school@nicolascabrera.es](mailto:school@nicolascabrera.es)

Manuela Moreno – e-mail: [manuela.moreno@uam.es](mailto:manuela.moreno@uam.es)

Organizers:

Eduardo Lee, IFIMAC, UAM.

Elsa Prada, IFIMAC, UAM.

Alfredo Levy Yeyati, IFIMAC, UAM

## School Scopes and Goals

**T**opological materials constitute an exciting and very active research area in condensed matter physics. It studies new states of matter whose bulk properties are similar to those of 'ordinary' materials but that, at the same time, display edge or boundary states with very exotic properties. Since the discovery of topological insulators, roughly a decade ago, the field has rapidly expanded with the identification of other topological materials, such as topological superconductors and Weyl semimetals. This Summer School will gather leading international experts to provide an introduction to the basic concepts underlying topology in condensed matter systems, followed by a discussion of recent developments, with a focus on quantum transport and hybrid devices. The goal is to cover not only theoretical aspects, but to also address the experimental progress, including the detection and manipulation of states associated with these materials.

### School Topics

Hybrid devices (quantum dots, nanowires, heterostructures).

Topological insulators and superconductors.

Weyl semimetals.

Topological quantum computing.

### Invited Speakers

Ramón Aguado (ICMM-CSIC, Madrid)

Alberto Cortijo (ICMM-CSIC, Madrid)

Silvano De Franceschi (CEA, Grenoble)

Reinhold Egger (Heinrich Heine Univ., Düsseldorf)

Klaus Ensslin (ETH, Zürich)

Claudia Felser (Max Planck Inst. for Chemical Physics of Solids, Dresden)

Marcelo Goffman (CEA, Saclay)

Sophie Guéron (Univ. Paris Sud, Orsay)

Jelena Klinovaja (Univ. Basel)

Leo Kouwenhoven (QuTech, Delft Univ. of Technology)

Rosa López (Univ. Balears)

Fabrizio Nichele (Niels Bohr Institute, Copenhagen)

Yuval Oreg (Weizmann Inst. of Science)

Pablo San-Jose (ICMM-CSIC, Madrid)

Jörg Schäfer (Univ. Würzburg)

Patrik Recher (TU Braunschweig)

Shinsei Ryu (Univ. Chicago)

Felix von Oppen (Freie Univ. Berlin)

Organized with the collaboration of

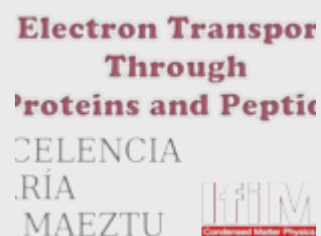
Further information:

Nicolás Cabrera Institute - [INC website](#)

XXIV International Summer School Nicolás Cabrera in the newspapers - [Atlasagencia](#)

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## Postdoctoral Position at UAM-IFIMAC in Electron Transport Through Proteins and Peptides - Closed



**A** postdoctoral position is available at UAM ([Universidad Autónoma de Madrid](#)) and funded by the [Condensed Matter Physics Center - IFIMAC](#). The candidate will work under the supervision of Prof. [Juan Carlos Cuevas](#) and Dr. [Linda A. Zotti](#) on the theory of electron transport through proteins and peptides. Funding is available for 18 months. The successful applicant will carry out theoretical simulations on the electron transport through proteins and peptides by means of Density Functional Theory (DFT) calculations, Non-Equilibrium Green's Function Techniques and tight-binding models. It will be based on a close cooperation with experimental partners. Applicants are invited to send a cover letter, a curriculum vitae and contact details of 2 referees who may be contacted to Dr. [Linda A. Zotti](#) ([linda.zotti@uam.es](mailto:linda.zotti@uam.es)) Applications will be accepted until the position is filled, but those received before the 20th of July 2017 will be guaranteed full consideration.

Requirements:

PhD in solid-state physics or computational chemistry.

Fortran and bash-script programming skills, experience in UNIX-based operating systems.

Strong background in solid state physics (basic knowledge of DFT and Green's function



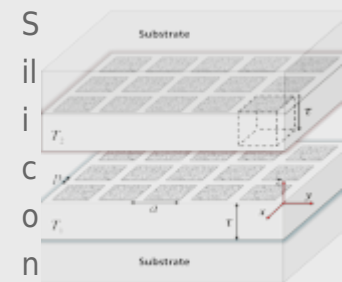
techniques would be beneficial but not necessary).

Good written and oral English language communication skills.

For further information please visit [IFIMAC's website](#).

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## Enhancing Radiative Heat Transfer With Silicon Metasurfaces



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etasurfaces made of  
2D periodic arrays of  
square holes.

Article: published in [Physical Review Letters](#) by Víctor Fernández Hurtado, [Francisco J. García Vidal](#) and [Juan Carlos Cuevas](#), IFIMAC researchers and members of the Department of Theoretical Condensed Matter Physics.

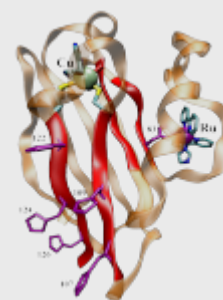
**T**hermal radiation is a universal physical phenomenon of great importance for different disciplines of science and engineering. In recent years, there has been a renewed interest in this topic due to the discovery that radiative heat transfer between two bodies can be drastically enhanced if they are brought sufficiently close to each other. This enhancement, which occurs when the separation is smaller than the thermal wavelength (10 microns at room temperature), is due to the contribution of evanescent waves that dominate the near-field regime. The fact that this near-field radiative heat transfer (NFRHT) between closely spaced bodies can overcome the far-field limit set by the Stefan-Boltzmann law for black bodies has now been verified in a variety of experiments exploring different materials, geometrical shapes, and gaps ranging from micrometers to a few nanometers.

In this context, the question on the fundamental limits of thermal emission is attracting a lot of attention. So far, the largest NFRHT enhancements have been reported for polar dielectrics (SiC, SiO<sub>2</sub>, SiN, etc), in which thermal radiation is dominated by surface phonon polaritons. Now, in a work published in [Physical Review Letters](#), the IFIMAC researchers Víctor Fernández Hurtado, [Francisco J. García Vidal](#) and [Juan Carlos Cuevas](#), together with Professor Shanhui Fan (Stanford University), have shown that

metasurfaces of doped silicon can be used to boost NFRHT. In particular, they demonstrate that one can design silicon metasurfaces that not only exhibit a room-temperature NFRHT much larger than that of bulk Si or other proposed periodic structures, but they also outperform the best unstructured polar dielectric. The underlying physical mechanisms responsible for this striking behavior are the existence of broadband spoof surface-plasmon polaritons (SPPs) in doped silicon and the ability to tune via nanostructuring the dispersion relation of these SPPs that dominate NFRHT in this structure. This work illustrates the great potential of metasurfaces for the field of radiative heat transfer. [\[Full article\]](#)

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## Molecular and Biomolecular Electron Transfer Processes: From the Single Molecule to the Cellular Length Scales



Title: Molecular and Biomolecular Electron Transfer Processes: From the Single Molecule to the Cellular Length Scales.

When: Tuesday, May 23, (2017), 12:00.

Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).

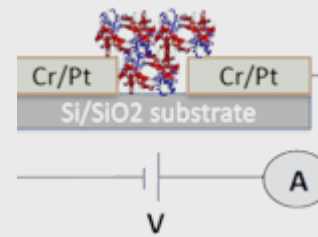
Speaker: Prof. Spiros S. Skourtis, Department of Physics, University of Cyprus, Nicosia Cyprus.

**M**olecular electron transfer processes are ubiquitous in biology and chemistry and are central to the molecular electronics and energy materials technologies. Biological electron transfer mechanisms are particularly rich, ranging from coherent tunneling to incoherent thermally-activated hopping. I will give a review of recent trends in the theory and simulation of biomolecular electron transfer rates, focusing on the roles of electronic coupling and energy level fluctuations. I will also discuss electron-transport pathway control over length scales that range from the small-molecule to the cellular levels.

[More information on IFIMAC Website](#)

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## Bottom-up Nanoelectronics: Contacting Single Molecules and Nanoparticles



Title: Bottom-up Nanoelectronics: Contacting Single Molecules and Nanoparticles.

When: Monday, May 22, (2017), 12:00.

Place: Departamento de Física de la Materia Condensada, Facultad Ciencias, Module 3, Seminar Room (5th Floor).

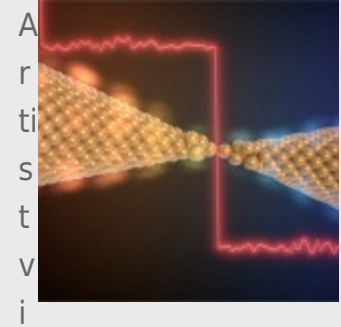
Speaker: Herre S.J. van der Zant, Delft University of Technology, Universidad Autonoma de Madrid and IMDEA Nanociencia Madrid.

**O**ur research focus is on bottom-up nanoelectronics and in particular the electronic characterization of single molecules and nanoparticles for device applications. For this purpose, we employ several methods to create electrodes, such as direct e-beam patterning, electromigration of Au wires, electroburning of multilayer graphene flakes, (gateable) mechanically-controllable break junctions (MCBJs) and a self-aligned fabrication technique for fabricating nano-spaced electrodes over large lengths. Typical experiments consist of measuring current-voltage characteristics as a function of various external stimuli such as electrode separation, gate voltage, temperature, and/or magnetic field. In this talk, I will discuss experiments on spincrossover nanoparticles and molecules, protein networks, biological nanowires and the use of superconducting electrodes as a new direction to study Shiba states in one-level quantum dot systems.

[More information on IFIMAC Website](#)

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## Quantized Thermal Transport in Single-Atom Junctions



View of quantized heat transport in a gold single-atom contact.

Article: published in [Science](#) by [Juan Carlos Cuevas](#), IFIMAC researcher and member of the Department of Theoretical Condensed Matter Physics.

**W**hat does determine the heat flow through a single atom? This is the ultimate question in the field of nanoscale energy transport and its answer is crucial to establish the fundamental laws that should describe the thermal transport in a variety of nanoelectronic devices. In the context of electrical circuits, the atomic scale was first reached with the advent of metallic atomic-size contacts and single-molecule junctions in the 1990s. These systems constitute the ultimate limit of miniaturization and have emerged as an ideal playground to investigate quantum effects related to charge and energy transport. Thus for instance, in recent years it has been shown that transport properties of metallic atomic-size contacts such as the electrical conductance, shot noise, thermopower, or Joule heating are completely dominated by quantum effects, even at room temperature. However, the experimental study of thermal conduction in these atomic-scale systems continues to be a formidable challenge and it has remained elusive to date in spite of its fundamental interest.

This basic open problem has now been resolved in a work published in [Science](#) by a collaboration between the groups of Pramod Reddy and Edgar Meyhofer (University of Michigan), Fabian Pauly and Peter Nielaba (University of Konstanz), and the [IFIMAC](#) researcher [Juan Carlos Cuevas](#). In this work, the authors made use of custom-designed picowatt-resolution calorimetric scanning probes to measure simultaneously the electrical and thermal conductance of gold and platinum atomic contacts all the way down to the single-atom level. This study reveals that the thermal conductance of gold single-atom junctions is quantized at room temperature in units of the universal thermal conductance quantum. It also shows that the Wiedemann-Franz law relating thermal and electrical conductance is satisfied even in single-atom contacts, irrespective of the metal. Furthermore, this work shows that all these observations can be quantitatively explained within the Landauer picture for quantum coherent thermal transport. In particular, this theory clarifies that the observations described above are due to the fact

that electrons dominate the thermal conductance in these metallic nanowires, and in the gold case electrons proceed ballistically through the contacts via fully open conduction channels.

The experimental techniques developed in this work will enable systematic studies of thermal transport in atomic chains and molecular junctions, which is key to investigating numerous fundamental issues that have remained inaccessible despite great theoretical interest. [\[Full article\]](#)

Quantized Thermal Transport in Single-Atom Junctions

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