

Title: Fabrication of Gold Nano-Crystal Arrays for Molecular Electronics: High Frequency Molecular Rectifiers and π - π 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].

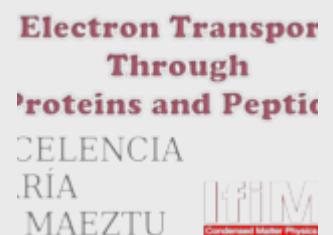
In a first study, we demonstrate molecular diodes operating up to 17.8 GHz. Direct current and radio frequency (RF) properties were simultaneously measured with the tip of an interferometric scanning microwave microscope and S11 parameters show a diode rectification ratio of 12 dB. In a second investigation, we explore the π - π 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.

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



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](mailto:linda.zotti@uam.es) (linda.zotti(at)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.

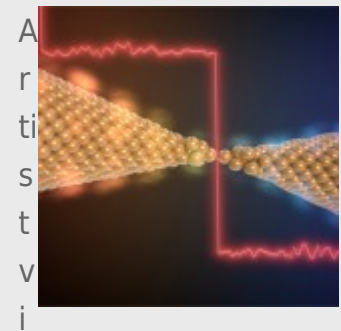
Fortran and bash-script programming skills, experience in UNIX-based operating systems.

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](#).

Quantized Thermal Transport in Single-Atom Junctions



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ew 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.

What 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,

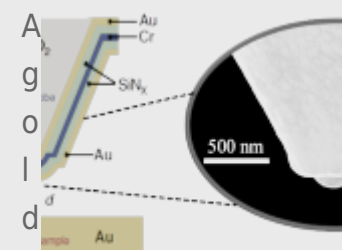
even at room temperature. However, the experimental study of thermal conduction in these atomic-scale systems continues to be a formidable challenge and it has remained elusive to date in spite of its fundamental interest.

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

Radiative Heat Transfer in Ångström and Nanometer-sized Gaps



coated scanning thermal microscopy probe is brought into close proximity of a heated gold

substrate.

Article: published in [Nature Communications](#) by Víctor Fernández-Hurtado, [Johannes Feist](#), [Francisco J. García-Vidal](#) and [Juan Carlos Cuevas](#), Department of Theoretical Condensed Matter Physics and [IFIMAC](#) researchers.

Radiative heat transfer between closely placed objects is attracting a lot of attention for several reasons. First, recent experiments have finally verified the long-standing prediction that radiative heat transfer can be greatly enhanced over the classical far-field limit set by the Stefan-Boltzmann law for blackbodies if the gap between two objects is smaller than the thermal wavelength, which is of the order of 10 μm at room temperature. This is possible due to the contribution of the near field in the form of evanescent waves (or photon tunneling). Second, this confirmation has triggered the hope that near-field radiative heat transfer could have an impact in different technologies that make use of thermal radiation such as thermophotovoltaics, thermal management, lithography, data storage, and thermal microscopy.

In spite of the progress made in recent years in the understanding of thermal radiation at the nanoscale, several recent experiments exploring the radiative thermal transport in nanometric gaps have seriously questioned this understanding. In particular, measurements on two gold-coated surfaces with gap sizes in the range of 0.2-10 nm have suggested an extraordinarily large near-field enhancement more than 3 orders of magnitude larger than the predictions of fluctuational electrodynamics, which is presently the standard theory used for the description of near-field thermal radiation.

A possible solution to this puzzle has now been proposed in a work published in [Nature Communications](#) by a collaboration between the groups of Pramod Reddy and Edgar Meyhofer (University of Michigan) and [IFIMAC](#) researchers Víctor Fernández-Hurtado, Johannes Feist, Francisco J. García-Vidal and Juan Carlos Cuevas. In this work, the authors explore the radiative heat transfer in Ångström- and nanometer-sized gaps between an Au-coated scanning thermal microscopy probe and a planar Au substrate in an ultrahigh vacuum environment. Using the apparent tunneling barrier height as a measure of cleanliness, it was found that upon systematically cleaning via plasma-cleaning or locally pushing the tip into the substrate by a few nanometers, the observed radiative conductances decreased from unexpectedly large values to extremely small ones—below the detection limit of the probe—as expected from computational results obtained within the framework of fluctuational electrodynamics. These results suggest that the huge signal reported in recent experiments might be an artifact due to the presence of contaminants bridging the gap between the tip and the substrate, thus providing an additional path for heat transfer via conduction. Moreover, this work shows that it is possible to avoid the confounding effects of surface contamination and systematically study thermal radiation in Ångström- and nanometer-

sized gaps. [\[Full article\]](#)

References

Study of Radiative Heat Transfer in Ångström and Nanometre Sized Gaps, L. Cui, W. Jeong, V. Fernández-Hurtado, J. Feist, F.J. García-Vidal, J.C. Cuevas, E. Meyhofer, and P. Reddy, Nature Communications 8, 14479, (2017). [\[URL\]](#)

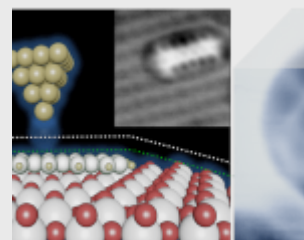
Submolecular AFM Imaging and Spectroscopy on Single Molecules Using KolibriSensor™ and Cantilevers

Title: Submolecular AFM Imaging and Spectroscopy on Single Molecules Using KolibriSensor™ and Cantilevers.

When: Monday, October 17, (2016), 12:00.

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

Speaker: Tomoko K. Shimizu, Research Center for Advanced Measurement and Characterization National Institute for Materials Science (NIMS), Tsukuba, Japan.



Submolecular imaging using frequency-modulation (FM) atomic force microscopy (AFM) has recently been established as a stunning technique to reveal the chemical structure of unknown molecules, to characterize intra-molecular charge distributions, and to observe chemical transformations. So far, most of these feats were achieved on planar molecules using the so-called qPlus sensor, a specially designed quartz AFM sensor. The KolibriSensor, another type of quartz AFM sensor, is also expected to be capable of high-resolution imaging, but only very few experimental results have been reported to date.

Here, we present submolecular resolution images and spectroscopic data on single molecules of a porphycene derivative [1] using small oscillation amplitudes with KolibriSensors. Force volume measurements with CO-functionalized probes [2] revealed features that may be related to the isomers of porphycene molecules. We also report a novel imaging method to achieve submolecular resolution on three-dimensional molecules and structures using a silicon (Si) cantilever-based AFM operated with large oscillation amplitudes. At variance with previous implementations, this method allowed us to simultaneously image both intra-molecular structures and the atomic arrangement of the substrate [3]. Force volume measurements over C60 molecules clarified the validity of our method to achieve submolecular resolution [3].

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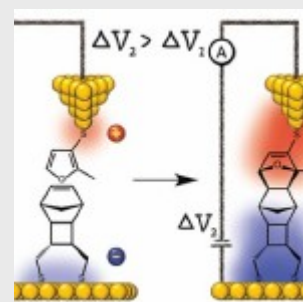
Probing Concepts in Single-Molecule Wires: Diodes, Electromechanics, FETs, Spinterface, Photo-switches and... Single-molecule Chemistry?

Title: Probing Concepts in Single-Molecule Wires: Diodes, Electromechanics, FETs, Spinterface, Photo-switches and... Single-molecule Chemistry?

When: Friday, 10 June (2016), 12:00h.

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

Speaker: Ismael Díez Pérez, Institute for Bioengineering of Catalonia (IBEC), University of Barcelona, Spain.



Inspired by the vision that single molecules could ever be functional elements in future nano-optoelectronic devices, there has been considerable interest in understanding charge transport in individual molecular backbones [1]. The birth of the Single-molecule Electronics field occurred with the first experimental realization of single-molecule wires [2]. Today, this field is powered by the combined efforts from very different disciplines; engineering, physics, chemistry and, lately, molecular biology. Our contributions to this field come from the Chemistry branch, with a vision based on developing new molecular moieties to provide new electrical capabilities into the single-molecule device. Along this adventure, it is also our goal to deepen into the understanding of chemistry-related charge transport in order to ultimately transfer all this knowledge into the biological electron transport, undoubtedly one of the key fundamental processes in life. As the title suggests, this seminar will show you a list of recent examples reporting newly designed molecules with a very specific electronic target when placed as a single-molecule wire [3-7]. We hope to convince you of the pivotal paper of molecular design in this field and of the vision that the Single-molecule Electronics field can directly profit from well-described chemistry supra-molecular chemistry processes. In this vein, the last example will show you our first attempt of using Single-molecule Electronics tools to analyze the catalytic aspects of a textbook chemical reaction [8].

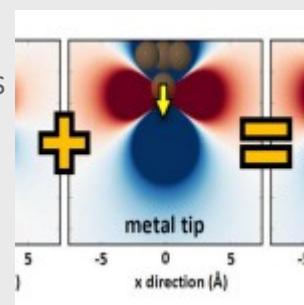
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[More information on IFIMAC Website](#)

The Electric Field of CO Tips and Its Relevance for Atomic Force Microscopy

Article: published in [Nano Letters](#) by Michael Ellner, [Pablo Pou](#) and [Rubén Pérez](#), Department of Theoretical Condensed Matter Physics and IFIMAC researchers.



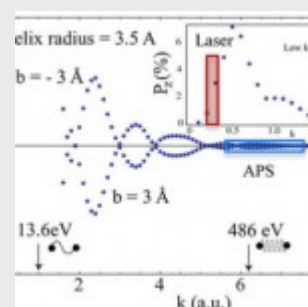
Frequency modulation atomic force microscopy (FM-AFM) has been recognized for a long time as one of the best tools for materials characterization at the atomic scale. The use of metal tips decorated with CO molecules represented a significant step forward in this technique that paved the way for the visualization of the internal structures of molecules with unprecedented resolution. This high resolution has been explained in terms of the strong Pauli repulsion between the closed-shell molecule acting as the probe and the electronic charge of the molecule probed. In addition, the associated tilting of the CO molecule amplifies the spatial variations of the charge density on the sample.

Notwithstanding, experiments on polar and metallic systems show that electrostatic interactions are necessary to understand the complex contrast observed and its distance evolution. Attempts to describe those interactions in terms of a single electrostatic dipole replacing the tip have led to contradictory statements about its nature and strength.

Here, we solve this puzzle with a comprehensive experimental and theoretical characterization of the AFM contrast on Cl vacancies. Our model, based on density functional theory (DFT) calculations, reproduces the complex evolution of the contrast

between both the Na cation and Cl anion sites, and the positively charged vacancy as a function of tip height, and highlights the key contribution of electrostatic interactions for tip-sample distances larger than 500 pm. For smaller separations, Pauli repulsion and the associated CO tilting start to dominate the contrast. The electrostatic field of the CO-metal tip can be represented by the superposition of the fields from the metal tip and the CO molecule. The long-range behavior is defined by the metal tip that contributes the field of a dipole with its positive pole at the apex. At short-range, the CO exhibits an opposite field that prevails. The interplay of these fields, with opposite sign in the near-field and rather different spatial extensions, explains the contrast evolution observed in our experiments and reconciles the apparently contradictory claims in the literature. [\[Full article\]](#)

Spin Polarization and Molecular Chirality In STM Junctions



Title: Spin Polarization and Molecular Chirality In STM Junctions

When: Wednesday, 24 February (2016), 12:00h

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

Speaker: Vladimiro Mujica, Arizona State University, USA.

Electron spin polarization is usually associated to the presence of external fields or magnetic interfaces. However, Chiral-Induced Spin Selectivity (CISS) refers to a symmetry-breaking effect whereby chiral molecules are capable of filtering an electronic spin component. This effect has been verified in electron photo-emission experiments but it also has important consequences in other instances of electron transport and transfer, e.g., STM and chemical reactions.

In this talk, a general theoretical framework for CISS will be presented and some recent experiments in molecular junctions using local probes like STM, where CISS manifests itself in asymmetries in the molecular conductance, will be discussed.

[More information on IFIMAC Website](#)

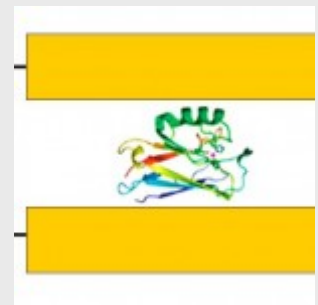
Protein-based Electronics

Title: Protein-based Electronics

Funding Agency: Spanish Ministry of Science and Innovation (MAT2014-58982-JIN).

Principal Investigator: [Linda Angela Zotti](#).

Duration: October 2015 – October 2018.



Description:

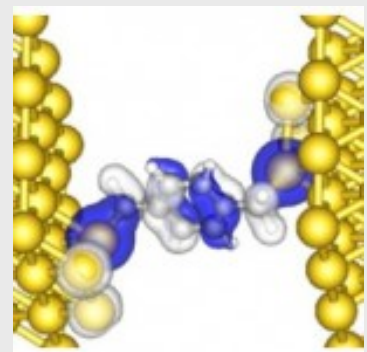
The project will explore the electronic transport through single-protein junctions. It will be focused on how the conductance changes depending on either chemical or geometrical differences in the protein. A combination of Density functional theory, Non-equilibrium Green's Function techniques and molecular dynamics will be used.

Calculating the Conductance of Single Molecule Junctions from First Principles

When: Friday, 11 September (2015), 12:00h

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

Speaker: Héctor Vázquez, Center Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic.



Abstract:

In this talk I will present the group's recent work on single molecule transport. Our work uses DFT-NEGF methods to investigate the conducting properties of molecules placed between two metallic electrodes. I will first discuss the importance of linker chemistry and molecular chemical properties on elastic transmission. I will then briefly describe our recent efforts in mapping the different contributions to the inelastic vibrational signal.

[More information on IFIMAC Website](#)
