

**Conferencia:**  
**Exciting Molecules Once at a  
Time: A Physicist of Molecular  
Science**

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# **EXCITING MOLECULES ONCE AT A TIME: A PHYSICIST VIEW OF MOLECULAR SCIENCE**

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Scanning tunneling microscopy is an unique method to visualize surfaces, and individual atoms and molecules. It allows also manipulation of one molecule at a time. Tunneling electrons injected from a sharp tip are the fundamental element in scanning tunneling microscopy. By tuning their energy they allow us to additionally perform high resolution spectroscopy resolved at the nanometer scale. In this seminar, I will review several works in the field of nanoscale molecular physics at surfaces, studied with tunneling microscopy and spectroscopy.

In our group, one of the main interests is detection and manipulation of the magnetism of molecular species. One of the most curious findings is the charge transfer compound TTF-TCNQ, which on the surface of a metal transfers one full electron, converting TCNQ in a paramagnetic anion [1]. The magnetic properties can be inherited by transition metal atoms embedded in the molecular species. Spectroscopy measurements reveal the spin state of the atom in the molecule and also information about their local environment [2]. Finally, I will also describe current studies about molecular reaction induced on the surface of the metal: the so-called “on-surface synthesis”. In this field, we explored several reactions, ranging from intra-molecular transformations [3] to the formation of graphene nanoribbons.

[1] I. Fernandez-Torrente, K. J. Franke, and J. I. Pascual, Physical Review Letters 101, 217203 (2008).

[2] B.W. Heinrich, L. Braun, J.I. Pascual, K.F. Franke, Nano Letters 15, 4024 (2015)

[3] B. W. Heinrich, G. Ahmadi, V. L. Müller, L. Braun, J. I. Pascual, K. J. Franke, Nano Letters 13, 4840 (2013).

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- Birth place/date: Madrid, Spain/ April 6<sup>th</sup>, 1968
- ResearchID: F-3489-2011

*Background on experimental physics, with major experience in low temperature scanning tunneling microscopy and spectroscopy.*

**Summary:**

Nacho Pascual holds a PhD in Physical Sciences obtained in 1998 from the Universidad Autónoma de Madrid, Department of Condensed Matter Physics. His various research topics expanded in the field of electronic transport through atoms and molecules. In 1999, he moved to Berlin, to the Fritz-Haber Institute der Max-Planck Gesellschaft, hosting there a Marie Curie Fellowship and contributing to developing the field of single-molecule vibrational spectroscopy with STM. After a short stay in Barcelona, at the Institut de Ciencia de Materiales (ICMAB-CSIC), hosting a Ramon y Cajal Fellowship, he moved back to Berlin, to the Free University, first (2004) as a Junior Professor and posteriorly (2008) tenured as full Professor. There, he expanded his research in the field of Molecular Physics at Surfaces, dealing with various molecular-scale phenomena ranging from molecular switches and charge transfer processes, to magnetism and superconductivity. In 2012, he joined CIC nanoGUNE at San Sebastian (Basque Country), where he currently leads a basic research group aiming at resolving quantum-phenomena in new materials.

**Academic Degrees:**

- [1991] M.Sc. ( Licenciatura) in Physical Sciences, Universidad Autónoma de Madrid.
- [1998] Doctor in Physical Sciences, Department Física de la Materia Condensada, Universidad Autónoma de Madrid. Director: Dr. Julio Gómez Herrero.  
Title of the dissertation: "Propiedades Electrónicas de Sistemas Nanométricos", (*Electronic properties of nanometer-sized systems*).

**Merits, contributions and status:**

- [1999] Dissertation awarded with the “Extraordinary Prize of physical sciences”.
- [2000] Awarded with a “Marie Curie” research contract by the European Union.
- [2002] Awarded with a “Ramon y Cajal” research contract by the Spanish Ministry of Science and Technology
- Referee of international journals (*Nature, Appl. Phys. A, Surf. Sci., Phys. Rev. Lett., PNAS, J. Am. Chem. Soc., J. Phys. Chem. B, Phys. Rev. B, Science, Ang. Chemie,...*).
- Referee of research projects and grants for the Spanish science ministry, the Chilean science funding agency, Argentinian Research Agency, the Catalan Science Office, Dutch Technology Foundation STW, German Research Association (DFG), and Swiss National Science Foundation.

- 88 publications in indexed international refereed journals (3000 citations, h28), including publications in Nature Journals (4), Science (3), Physical Review Letters (16), Nanoletters (2),...
- More than 100 invited talks in international meetings and research centers.

## Post-doctoral Activities:

- April 1998: Assistant Researcher at UAM.
- June 1999: “Marie Curie” research grant from the European Union, at Fritz-Haber Institut der Max-Planck Gesellschaft (FHI-MPG).
- January 2002: “Ramon y Cajal” research contract from the Spanish Ministry of Science and Technology, Institut de Ciències de Materials de Barcelona, CSIC.
- January 2004: Juniorprofessor (W1), Dept. of Physics, Freie Universität Berlin (FUB).
- January 2009: Professor (W2), Dept. of Physics, FUB
- January 2010: Guest Professor at the Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragon, Zaragoza (Spain).
- September 2012: Ikerbasque Research Professor in CIC nanoGUNE, San Sebastian

## Teaching and Academic Activities:

- [2004-2012] Freie Universität Berlin: Continuous lecturer of undergraduate and Master courses
- Tutor of 12 undergraduate students completing the German *Diploma or Master*.
- Tutor of 9 Ph. D. Students (six of them successfully concluded).

## Major Research Areas:

- Electronic structure of surfaces: band structure and electron dynamics resolved with STM.
- Electronic transport through single molecules: vibronic effects and heat dissipation.
- Single-molecule vibrational (inelastic) spectroscopy and electron induced manipulation.
- Intramolecular conformational dynamics of molecular switches at surfaces.
- Molecular magnetism on metal, semimetal and superconducting surfaces

## Six representing publications:

### Electron transport:

1. *Quantum contact in gold nanostructures by scanning tunneling microscopy*. J.I. Pascual, J. Méndez, J. Gómez-Herrero, A.M. Baró, N. García, and Vu Thien Binh. **Physical Review Letters** **71**, 1852 (1993).
2. *Resonant electron heating and molecular phonon cooling in single C<sub>60</sub> junctions*. G. Schulze, K. J. Franke, A. Gagliardi, G. Romano, C. S. Lin, A. Da Rosa, T. A. Niehaus, Th. Frauenheim, A. Di Carlo, A. Pecchia, and J. I. Pascual, **Physical Review Letters** **100**, 136801 (2008)

### Single molecule vibrations

3. *Selectivity in vibrationally mediated single-molecule chemistry*. J.I. Pascual, N. Lorente, Z. Song, H. Conrad, and H.-P. Rust. **Nature** **423**, 525 (2003).
4. *Driving a macroscopic oscillator by the stochastic motion of a hydrogen molecule*, Ch. Lotze, M. Corso, K.J. Franke, F. von Oppen, J.I. Pascual, **Science** **338**, 779 (2012).

### Molecular magnetism

5. *Competition between Kondo screening and superconducting phenomena* K. J. Franke, G. Schulze, J. I. Pascual, **Science** **332**, 94 (2011).
6. *Protection of excited spin states by a superconducting energy gap*, B. W. Heinrich, L. Braun, J.I. Pascual, K.J. Franke, **Nature Physics** **9**, 765 (2013).