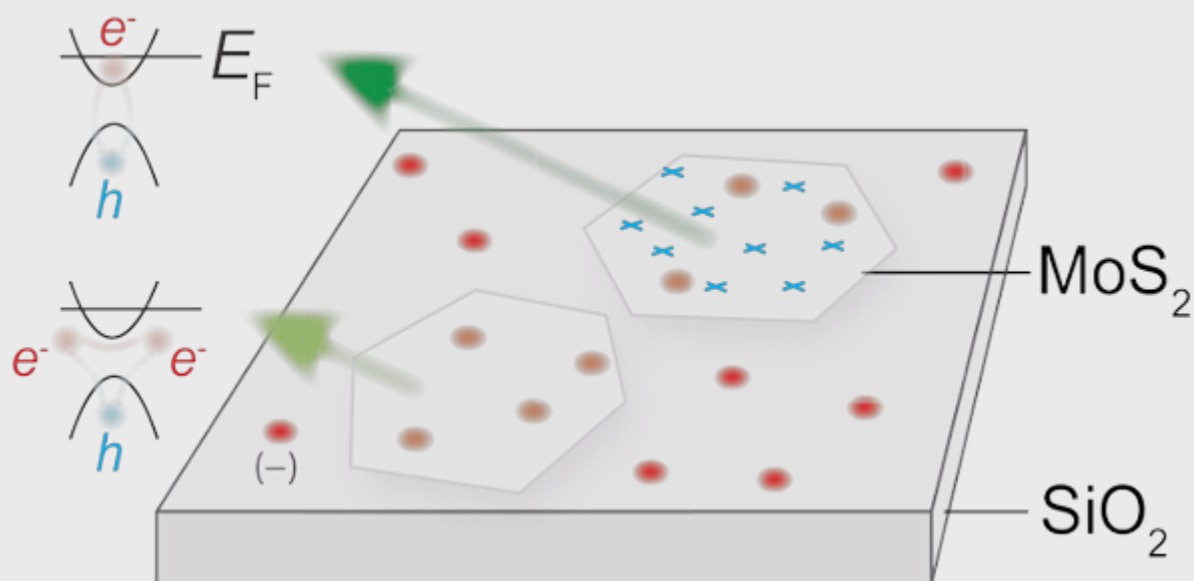


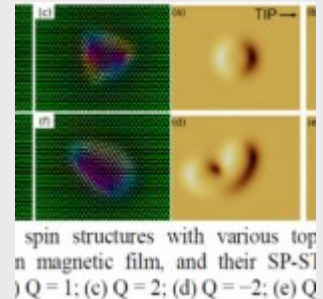
## Weakly Trapped, Charged, and Free Excitons in Single-Layer MoS<sub>2</sub> in the Presence of Defects, Strain, and Charged Impurities



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](#)]

## Principles



Title: Complex Magnetic Structures at Surfaces and Their Imaging with STM from First Principles.

When: Monday, June 12, (2017), 12:00.

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

Speaker: Krisztián Palotás, Department of Complex Physical Systems, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia.

**R**ecent advances in spin-polarized scanning tunneling microscopy (STM)

experiments allow the determination of complex (non-collinear) surface magnetic structures (like spin-spirals, skyrmions) in real space. Motivated by these advancements, there is a strong need for theoretical understanding of the observed magnetic structures. In the first part of the talk I present recent theoretical results on the formation of a diversity of complex magnetic structures in thin films obtained by a combination of ab initio and spin dynamics calculations [1].

Understanding STM image contrasts is of crucial importance in surface science and related technologies. In the second part of the talk I present various STM theories and highlight different tip effects on the STM contrast based on first principles calculations, going beyond the Tersoff-Hamann model, e.g., within 3D-WKB tunneling theory [2]. Examples include a prototype frustrated hexagonal antiferromagnet, Cr monolayer on Ag(111) [3], metastable skyrmionic structures with various topologies [4] and highly oriented pyrolytic graphite. By comparing STM topographic data between experiment and large scale simulations, we can determine particular tip orientations that are most/least likely present in the STM experiment [5]. Furthermore, I present an extension of Chen's derivative rule for STM simulations including tip-orbital interference effects, and demonstrate the importance of such effects on the STM contrast for two surface structures: N-doped graphene and a magnetic Mn<sub>2</sub>H complex on the Ag(111) surface [6]. Finally, the first steps towards the theoretical modeling of high resolution spin transfer torque imaging are presented [7].

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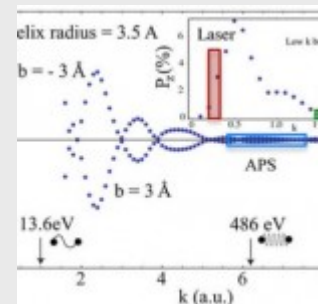
G. Mándi, K. Palotás, *Phys. Rev. B* 91, 165406 (2015).

K. Palotás et al., *Phys. Rev. B* 94, 064434 (2016).

[More information on IFIMAC Website](#)

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## 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.

# E

lectron 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.

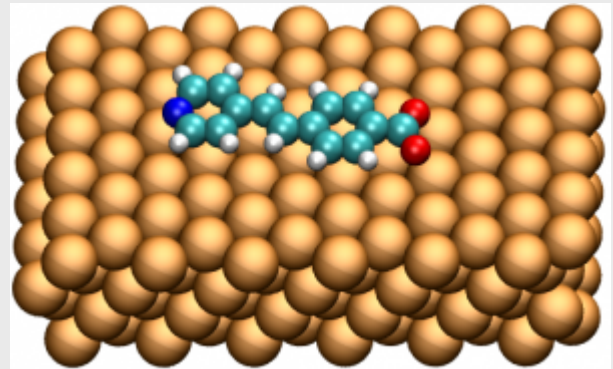
In this talk, a general theoretical framework for CISS will be presented and some recent experiments in molecular junctions using local probes like STM, where CISS manifests itself in asymmetries in the molecular conductance, will be discussed.

[More information on IFIMAC Website](#)

## DFT analysis of combined 3D NC-AFM and STM imaging of the Cu(100)-O oxide surface

Wednesday, 21th March 2012. 12:00-13:00

Milica Todorović



Departamento de Física Teórica de la Materia Condensada, UAM

### ABSTRACT:

Investigation of novel catalytically active surfaces requires a comprehensive experimental method for the identification and rapid characterization of prospective catalytically active sites. In a bid towards functional imaging, three-dimensional atomic force microscopy (3D-AFM) in non-contact mode [1] has been combined with scanning tunnelling microscopy (STM) to study the oxygen-terminated copper (100) surface. Complex 3D data sets, obtained by simultaneously recording the tunnelling current and the AFM frequency shift, allow for site-specific quantification of forces and tunneling currents. The wealth of information obtained is remarkable, but the interpretation of the wide range of contrast modes requires a thorough characterisation of the sources of contrast in AFM and STM imaging.

We combined DFT total-energy calculations with Non-Equilibrium Green's Function (NEGF) methods for electronic transport to determine the tip-surface interaction and tunnelling current [2, 3, 4] for a large set of tip models in order to clarify the different contrast modes obtained in the experiments. We studied the features of a stable Cu(100)( $2\sqrt{2}\times\sqrt{2}$ )R45deg-O surface reconstruction and identified prospective reaction sites, before introducing model AFM tips to conduct a series of tip approach simulations. The effect of tip changes on imaging modes was explored by considering tips of different reactivity. Our simulations, in comparison with AFM experimental images, identified a contaminated tip with a Cu-terminated experimental configuration. Charge density and current calculations further helped us investigate the STM imaging modes for tips of different reactivity. Through this work, were able to explain a large variety of experimental STM contrasts obtained. Lastly, simulations of different surface defect models enabled us to understand detailed STM image features and led us to consider the mechanisms of domain formation on the Cu(100)-O surface.

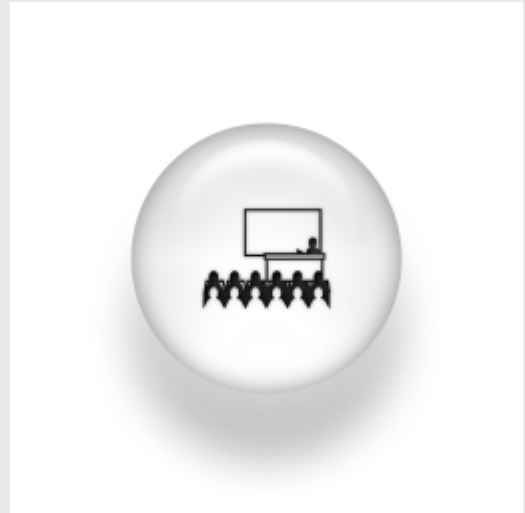
[1] B. J. Albers et al., Nature Nanotech. 4, 307 (2009)

[2] Y. Sugimoto et al., Nature 446, 64 (2007)

[3] P. Jelinek et al, Phys. Rev. Lett. 101, 176101 (2008)

## PFores and currents in carbon nanostructures

Wednesday, 30 March 2011, 12:00-13.00



*Prof. Pablo Pou*

Dpto. de Física Teórica de la Materia Condensada, UAM

### ABSTRACT:

STM [1] and FM-AFM [2] have been used for many years to study low-dimensional carbon materials. The simple honeycomb structure shared by these materials represents both a perfect testing ground and a fundamental challenge for scanning microscopy imaging. Graphite can be imaged with atomic resolution with Scanning Probe Microscopy even in ambient conditions but, after 25 years of research, still there is no consensus whether the maxima in the atomic scale images correspond to atoms or to the hollow sites. We have carried out a study that combines DFT total-energy calculations with NEGF methods for electronic transport in order to determine the interaction and the tunneling current between a large set of SPM tips with nanotubes, graphite and graphene [3]. Our results explain the rich variety of image patterns observed in both AFM and STM experiments in terms of two factors: (i) the tip-sample distance and (ii) the chemical reactivity of the tip. Furthermore, we demonstrate, contradicting the usual interpretation, that short-range chemical forces and not van der Waals interactions are the responsible for the atomic-scale contrast on the FM-AFM images.

Finally, we have extended our study to defects in these materials, which, instead of a problem, result on novel and promising electronic properties. For example, vacancies in a graphene layer support localized magnetic moments [4]. We present a study of the forces and currents on a graphene layer on Pt considering explicitly the presence of vacancies [5].

[1] Park et al, APL 48,112 (1986)

- [2] Holscher et al, PRB 62, 6967 (2000); Hembacher et al, PRL. 94 056101 (2005); Albers et al, Nat Nano 4, 307 (2009); Gross et al, Science 325, 1110 (2009)
- [3] Ondracek et al, PRL (2011).
- [4] Ugeda et al, PRL 104, 096804 (2010).
- [5] Ugeda et al, submitted to PRL (2011).
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