Instituto Universitario de Investigación en Nanociencia de Aragón
Universidad Zaragoza

Cátedra SAMCA de Nanotecnología
Universidad Zaragoza

SEMINARIOS INA

Calculating Tip-Sample Currents and Forces: From UHV to Liquids

Dr. Rubén Pérez

Scanning Probe Microscopy Theory & Nanomechanics Group
Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid

Miércoles 17 de junio, 12:00 h
Sala de conferencias
Edificio de I+D, Campus Río Ebro

Instituto Universitario de Investigación en Nanociencia de Aragón
Universidad Zaragoza

Cátedra SAMCA de Nanotecnología
Universidad Zaragoza

ABSTRACT:

Scanning Tunneling (STM) and Atomic Force (AFM) Microscopes, some of the basic tools in Nanotechnology, exploit currents and forces to visualize and manipulate matter at the nanoscale. In this talk, I'll review the theoretical developments necessary to describe tip-sample transport and interactions in technologically relevant materials like carbon nanostructures and reducible oxides, and the extra challenges involved in the imaging of surfaces and large biomolecules in their native liquid environment.

Understanding the interaction of graphene with metal surfaces is a necessary step for the development of a new graphene-based technology. We have combined high-resolution STM experiments by different groups and our DFT and STM calculations to explore the interplay between defects (point defects like vacancies and extended edges) and the metal interaction in the modification of the structure and electronic properties [1,2], and to characterize the moire patterns formed on both weakly (Pt, Cu) and strongly interacting (Rh)[3] cases. In G/Cu [4], we have exploited this tunable transparency to provide a comprehensive picture of the G-metal coupling with atomic precision and high energy resolution, with important implications for the improvement of our description of the van der Waals interaction.

TiO2 Anatase is a pivotal material in devices for energy-harvesting applications and catalysis. Methods for the accurate characterization of this reducible oxide at the atomic scale are critical in the exploration of its outstanding properties for technological developments. We'll discuss how combined STM/AFM measurements and first-principles simulations provide an unambiguous identification of atomic species at the (101) anatase surface. Based on key distinguishing features extracted from calculations and experiments, we identify candidates for the most common surface defects [5].

Finally, we'll face the challenges involved in simulating interactions in liquids. They will be illustrated with the study of the adsorption of Immunoglobulin G (IgG) antibodies (~13.000 atoms) on hydrophobic surfaces like graphene [6]. Our MD results and the AFM images demonstrate that the IgG antibodies are strongly adsorbed, do not unfold, and retain their secondary and tertiary structure upon deposition. Statistical analysis of the AFM images shows that many of the antibodies adopt vertical orientations, even at very small coverages, exposing both Fab binding sites for recognition events, making graphene a strong candidate for the future development of immunosensors.

[1] M. M. Ugeda, et al. Phys Rev Lett. 107, 116803 (2011).
[2] P. Merino et al., ACS Nano 8, 3590–3596 (2014).
[3] A. Martín-Recio et al. Nanoscale 10.1039/c5nr00825 (2015).
[4] H. González-Herrero et al., submitted to Nature Communications (2015).
[5] O. Stetsovych et al., accepted in Nature Communications (2015).
[6] J.G. Vilhena et al., submitted to JACS (2015).