Proyectos para Trabajos de Fin de Master

Curso 2017-18

1. Atomic-scale imaging of water networks with Atomic Force Microscopy
(tutor: Rubén Pérez, ruben.perez@uam.es, www.uam.es/spmth**)**

Understanding the growth mechanisms of ice on metal clusters and surfaces is relevant for many key practical issues, from catalysis to meteorology. The growth of thick ice layers is determined by the adsorption structure of the first water layer. In this layer, the competition between the interaction with the substrate and the hydrogen (H)-bonding among water molecules gives rise to 1D, 2D and 3D structures where the ice rules are frequently broken. Nowadays, we can use the Atomic Force Microscope (AFM), a basic tool in nanotechnology, to image these structures with atomic-scale resolution [1] using the quantum mechanical forces that appear when the tip of the AFM approaches the water molecules.

In this project, we'll explore how we can understand and simulate these AFM images using an accurate and efficient model that we have recently developed [2]. This model is based on quantum mechanical calculations and properly describes all the different contributions to the interaction, in particular, the Pauli repulsion associated with the overlap of the electronic clouds of the tip and the sample. The student will learn about the theory behind the calculation of forces with quantum mechanics, will get familiar with the tools that we have developed for the simulation of AFM, and will develop simple models to understand the experimental AFM results.

[1] A. Shiotari and Y. Sugimoto
Nature Communications 8:14313 (2017) | DOI: 10.1038/ncomms14313
[2] M. Ellner, N. Pavlicek, P. Pou, B. Schuler, N. Moll, G. Meyer, L. Gross, and R. Pérez
Nano Letters 16, 1974 (2016) | DOI: 10.1021/acs.nanolett.5b05251

2. Modeling the cysteine-gold interaction with quantum mechanical calculations and classical potentials.
(tutor: Rubén Pérez, ruben.perez@uam.es, www.uam.es/spmth**)**

Proteins with metal centers are emerging as interesting candidates for nanotechnology applications, including biomolecular electronics and nanosensing. Electronic transport through proteins can be now characterized in single-molecule experiments with electrochemical STM where a tip-protein-metal surface junction is formed. Achieving a good protein contact with the tip and sample electrodes, a key issue in molecular electronics, is particularly challenging in the case of biomolecules.

Cysteine aminoacids, with side chain thiols that can anchor it to an Au substrate by the formation of S–Au bonds, are good candidates to form stable electric contacts. In this project, the student will study the interaction of cysteine with a gold surface using quantum mechanical methods based on density functional theory. First, the adsorption of an isolated cysteine will be considered. Next, she/he will explore the adsorption of a pair of cysteines in a configuration that is commonly found in proteins. Finally, using these first-principles results as benchmarks, the student will assess the ability of classical interaction potentials to describe the cysteine-gold interaction.