IMAGING, MANIPULATION AND CHEMICAL IDENTIFICATION OF INDIVIDUAL ATOMS WITH DYNAMIC FORCE MICROSCOPY: A THEORETICAL PERSPECTIVE.

Rubén Pérez

Nanomechanics & SPM Theory Group
Departamento de Física Teórica de la Materia Condensada
Universidad Autónoma de Madrid, E-28049 Madrid, Spain

ruben.perez@uam.es

Dynamic Force Microscopy is a powerful tool for the characterization and manipulation of matter at the nanometer scale [1]. The most-extended operation mode (amplitude modulation, AM-AFM, also known as "tapping") allows the imaging with nanometer resolution of heterogeneous materials in their natural environment and state. Measuring the phase lag of the vibrating probe with respect to the external excitation, AM-AFM can map simultaneously the shape and the compositional variations of the surface and provide access to the dissipated energy [2].

In this talk, we focus on the frequency modulation mode (FM-AFM) that has fulfilled the long standing goal of achieving atomic resolution in all kind of surfaces. We'll show how the combination of force spectroscopy measurements with our large-scale first principles calculations, can be used to understand and extend the FM-AFM capabilities in key areas including single-atom manipulation [3,4] and chemical identification [5]. Tip-sample interactions are also relevant to the STM operation in the near-to-contact regime, where they can induce a substantial decrease of the current when approaching semiconductor surfaces under low bias conditions [6].

Finally, we extend this collaboration between theory and experiment in the analysis of force curves measured in a technologically relevant oxide surface: the rutile TiO2(110) surface. We have characterized the interaction between clean and contaminated Si-based tips in order to understand the rich variety of atomic contrasts observed on this surface. Our calculations show that the relative contribution of the weak short-range electrostatic interaction and the onset of chemical bonding between the closest tip and surface atoms is very sensitive to the tip-sample distance, defining di erent interaction regimes along the tip-sample distance. In particular, we show the short-range electrostatic interaction in weak interaction regime can provide a complex atomic contrast such as the experimentally reported neutral and all-inclusive [7] contrast modes.

References:

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