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ADHESION HYSTERESIS IN MOLECULAR SYSTEMS: UNDERSTANDING THE DISSIPATION PROCESSES AT THE NANOSCALE WITH AFM AND THEORETICAL SIMULATIONS

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The Scanning Tunneling (STM) and the Atomic Force (AFM) microscopes, due to their high spatial resolution and manipulation capabilities, have greatly contributed to the emergence of Nanoscience and Nanotechnology. The advance has been particularly spectacular in Dynamic AFM, where the development of the frequency modulation operation mode (FM-AFM)[1] has paved the way for atomic-scale imaging [2], manipulation [3] and characterization of the tip-sample forces on all kinds of surfaces, including the chemical identification of individual atoms [4].

In this talk, we discuss how we can combine AFM experiments with the theoretical simulations performed in our group to study the nature of the dissipation processes at the nanoscale. Firstly, we'll introduce the main ideas reviewing our work on semiconductor surfaces with the AFM operated in the frequency modulation mode (FM-AFM), where we have determined the mechanisms for atomic-scale manipulation and identified a common dissipation channel due to single-atom contact adhesion [5,6]. Secondly, we explore, in two technologically relevant organic-based systems, the role of adhesion hysteresis as a dominant dissipation process and the atomistic mechanisms involved. In the case of a monolayer of sexithiophene molecules studied with Amplitude Modulation (AM) AFM, our approach [7-9] includes not only ground-state calculations of the tip-sample interaction, but an extensive set of molecular dynamics simulations at room temperature to include the folding deformation modes that are necessary to describe properly the mechanical response on the molecular layer. Finally, we investigate the origin of the intramolecular contrast in energy dissipation FM-AFM images of PTCDA molecules adsorbed on metal surfaces. Here we illustrate how different deformation mechanisms can contribute to dissipation at different tip-sample distances [10].

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