Numerical Tools For Local Probe Based Methods: From Imaging To Single Molecule Manipulation

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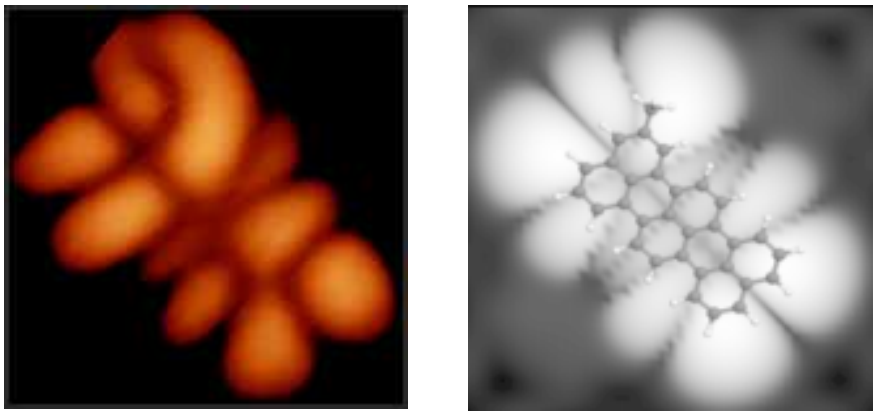
Since the invention of local probes based methods, like STM and AFM, an important theoretical effort of images interpretation has been performed. Actually, due to many physical effects inherent in these techniques, simulations were necessary to explain the experimental results. In this context, different theoretical models were proposed giving rise to different numerical codes, each of them having specific functionalities or at least having a particular range of validity. Even at the present time, a complete and integrated proposition is not yet available.
We will describe one of these codes and will present simulation results obtained with it. This code, called ESQC (Elastic Scattering Quantum Chemistry) is based on an extended Hückel approach and allows the determination of the tunnel current inside the STM junction for a broad variety of physical systems. Generally, molecular mechanics or molecular dynamics are coupled to the tunnel current calculations to fit experimental results with a better confidence, especially when adspecies (mostly large organic molecules) are purposely manipulated with the tip.
In a second part, we will show some results obtained recently with a virtual AFM. This code allows to simulate a dynamic atomic force microscope with a important versatility. In fact, one can tune many parameters, as physical parameters of the cantilever, oscillation amplitudes of the cantilever, the different gains of the feedback loops, the origin and the amount of noises as well... Such a numerical tool can match as close as possible an experimental setup and could be an interesting means to obtain information about local dissipation.



Experimental (left) and calculated (right) images of the HOMO of a methylterrylene molecule adsorbed on a 2ML NaCl(100) film deposited on a Cu(111) surface (C. Villagomez Ojeda, GNS-Cemes).