SPAGS-STM, a true high performance tool for in-silico imaging

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The production of numerical STM images of large-scale molecular systems is often limited to the use of low-level theory such as the Tersoff-Hamann (TH) approach [1]. A significant amount of STM features are revealed by such a representation of surface states that are obtained from electronic structure calculations, except that the influence of the tip is totally excluded. Electron scattering approach such as the Laudauer-Buttiker formula (LBF) [2] considers the influence of the tip, but can also considers electron-electron, electron-phonon, and several other inelastic scattering events [3]. Due to all these features, the LBF approach represents one of the most accurate models for generating STM images.

Despite the high accuracy of such scattering approach, the associated computational complexity and effort needed to obtain STM images still constitute the major drawbacks of the LBF technique. Nevertheless, our recent development in parallel computing [4] and space discretization [5] in STM simulations open a route toward a next generation of real-time STM imaging. In addition, we are presently developing new software features where chemical and physical intrusions within the model framework can be performed. Following this chemical intrusion scheme, the composition of the molecular specie studied by STM can be modified, and the resulting STM image be rapidly computed and visualized. For example, it costs nearly 16 sec to evaluate a STM image of a (5,5) nanotube model containing 250 carbon atoms within TH limits, while around 1 sec is needed to evaluate a new STM image in which a carbon atom has been replaced by a nitrogen atom (see Figure 1) in the original model [6]. This improvement in rate of producing STM images was possible through a judicious use of matrix refreshment and iterative techniques for matrix diagonalization. This intrusive mode opens an efficient route for exploring the role of functional groups or heteroatoms on the origin of STM contrasts of adsorbed molecules.

In this presentation, a brief overview of our most recent contributions in the rapid production of accurate STM images will be given. In addition, several convincing examples related to electron confinement nearby nanostructures, to surface reshaping induced by adsorbates, and to more subtle molecular interactions such as π–π interactions will be discussed. Finally, I will show that quantitative analysis of STM contrasts can be used to understand, and in some cases to discriminate between possible surface mechanisms.

References:

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Figures:

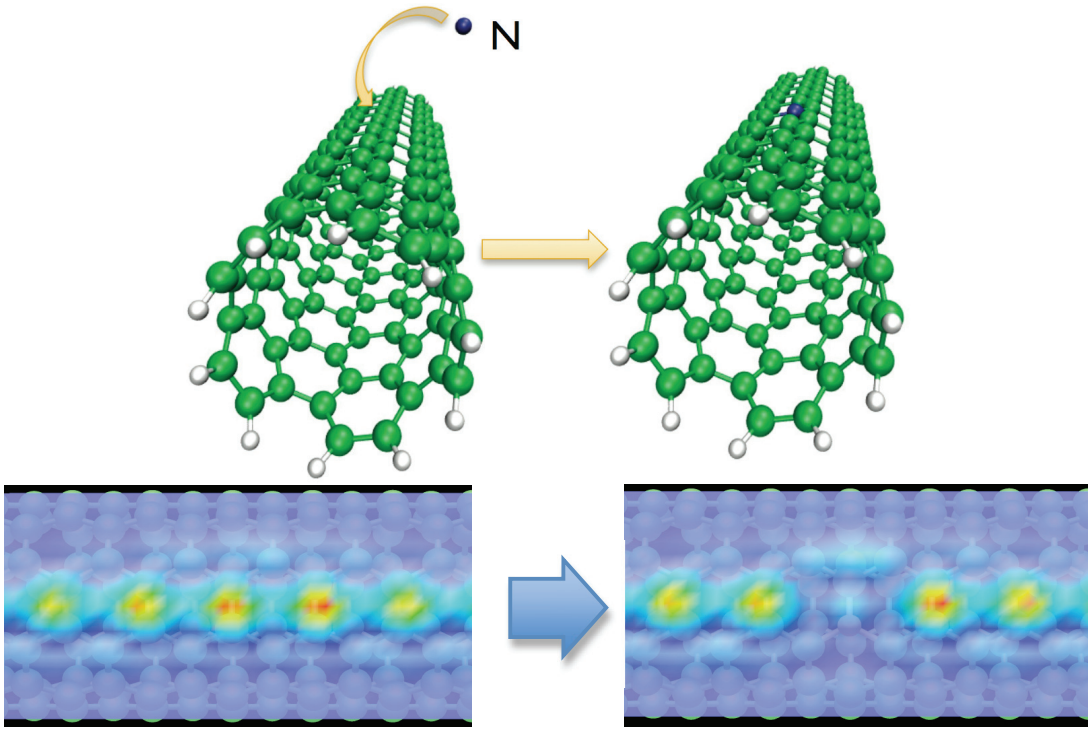

Figure 1. Representation of the chemical intrusion (top) in the evaluation of STM images (bottom) of a (5,5) carbon nanotube (left side) in which a carbon atom is replaced by a nitrogen atom (right side).