COMBINING *AB INITIO* AND SEMI – EMPIRICAL APPROACHES FOR SCANNING TUNNELING MICROSCOPY SIMULATIONS.

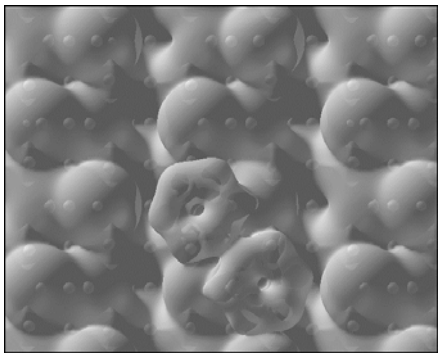
M. Dubois[1], C. Delerue[2] and A. Rubio[3]

1. DRFMC / SPSMS, CEA Grenoble, 17 rue des Martyrs, 38000 Grenoble (France)
2. IEMN / ISEN / Physique, Avenue Poincaré, Cité Scientifique, 59650 Villeneuve d'Ascq (France)
3. Dpto. Fisica de Materiales, Facultad de Quimicas, Universidad del Pais Vasco, 20018 San Sebastian. (Spain)

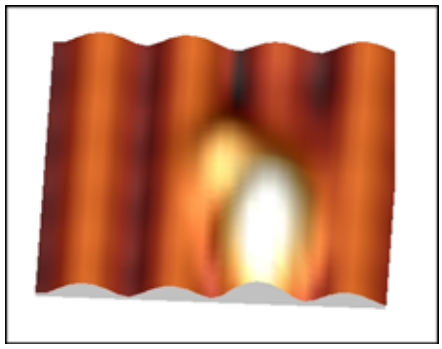
The Scanning Tunneling Microscope (STM) is a remarkable tool to probe object and materials at the atomic scale and is thus widely used to characterize the adsorption of molecules on surfaces. Measurements of the conductance through the molecules (STM spectroscopy) and bias dependent STM images provide indirect information on the molecular electronic structure and on the bonding of the molecule with the surface. In this context, many studies have dealt with molecules on metallic surfaces. Some works have concerned molecules deposited on semiconductor surfaces but the experiments are more difficult due to the lower conductivity of the sample. The interpretation of the results is also more difficult due to the complex electronic structure of the surface itself.

From a theoretical point of view, the development of an efficient tool for STM simulations is a challenging work and an important need for experimentalists. A strictly *ab initio* approach for those calculations is delicate due to the size and complexity of generally studied systems. On the other hand, semi – empirical methods are limited for the determination of the electronic structure and atomic relaxations.

In this work, we present how those two approaches are combined to allow efficient STM simulations. The tunneling current calculation is made within the tight binding approximation using a scattering formalism. Although this tight binding approach is quiet efficient in some cases, some limitations appear when we don't know how the molecule is adsorbed on the surface or how are positioned the electronic levels of the molecule with respect to the Fermi level of the surface. We will thus discuss how *ab initio* calculations can be helpful to solve some of those issues. We will illustrate this talk with two examples: the adsorption of a biphenyl molecule on Si(100), then the adsorption of a polymer (poly(3-alkylthipohene)) on HOPG.



a) charge density contour plot of a biphenyl molecule adsorbed on a reconstructed silicon surface. *(ab initio)*



b) simulated STM image of a biphenyl molecule adsorbed on a reconstructed silicon surface. (tight binding)