ADSORPTION OF C60 ON A Si(111) 7X7 SURFACE: A THEORETICAL STUDY

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Fullerenes and carbon-based nanostructures are continuously attracting a widespread interest in the scientific community, especially for what concerns their use as electronic materials [1]. Ordered nanostructure growth and manipulation on well-oriented crystalline surfaces must rely on a detailed knowledge of the microscopic interaction between the constituting building blocks and the local conformation of the surface. The deposition of fullerenes on silicon surfaces is the obvious step to approach the fabrication of a system which could be ideally suited as an interface capable of efficiently bridging biological systems to nanoelectronics devices.

In this paper we study the adsorption of C_{60} molecules on Si(111) 7x7 surface as an efficient model template of the interaction of fullerenes on silicon surfaces. We present a theoretical study based in density-functional theory, expanding the one-electron wave function as a series of numerical atomic orbitals [2,3].

The roughness and the complexity of the reconstruction of this surface offer the opportunity to study the C_{60} molecule in different local chemical environments. We have identified up to seven non-equivalent adsorption sites, fully relaxing the positions of the atoms of the fullerene and of a few surface bi-layers.

We have rationalized the different adsorption mechanisms in terms of the projected density of states to put in evidence the role of each molecular orbitals and estimate the extent of the charge transfer.

Simulations of the scanning tunneling microscopy images will be also presented [4].

References:

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Figures:

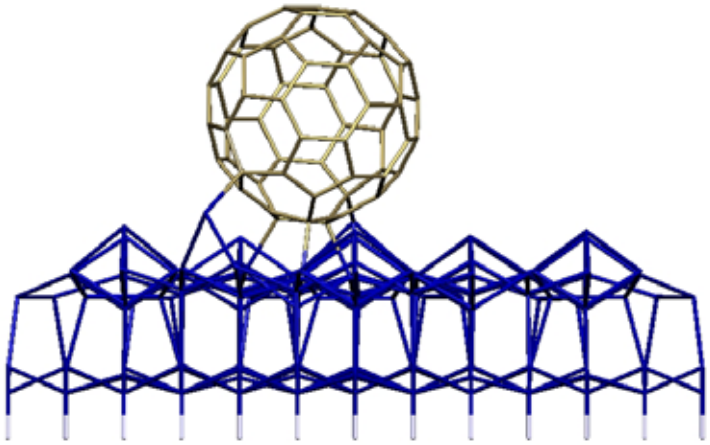

Figure 1 C60 adsorption at the unfaulted side

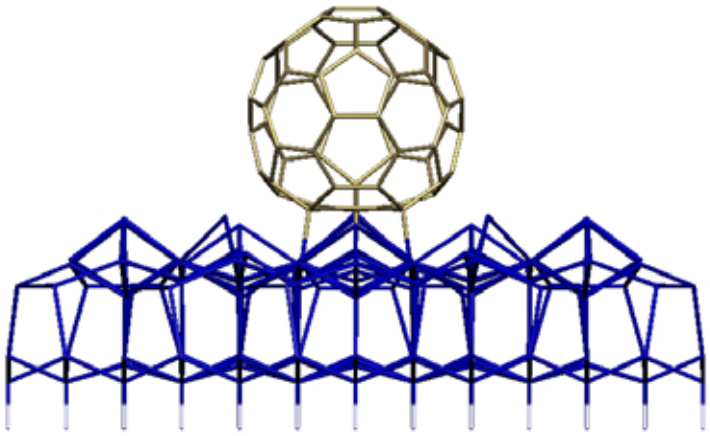

Figure 2 C60 adsorption at the faulted side