

AFM imaging and C₆₀ diffusion on the Si(001) surface

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We present here both an *ab-initio* study of the energetics and image properties of the Si(001) surface and the adsorption and manipulation of C₆₀ molecules on Si(001). The adsorption of C₆₀ on surfaces is of particular interest as it has been proposed that a device constructed from endohedrally doped fullerenes could be used as a spin based, solid state quantum computer [1]. The *ab-initio* codes SIESTA and VASP have been used to perform electronic structure calculations of C₆₀ on the Si(001) surface in order to determine the most energetically favourable configurations. These codes utilise general gradient approximations, periodic boundary conditions and the method of pseudopotentials. Preliminary results from our calculations have been published [2] and contrasted with a previous LDA study of the system [3].

Here we complete our study and present results for all the possible adsorption configurations of C₆₀ on the Si(001) surface. We have furthermore simulated the diffusion of a C₆₀ molecule which rolls along the surface between equivalent bonding sites. This is directly related to current experimental work being performed at Nottingham University on the STM manipulation and imaging of C₆₀ on the Si(001) surface

Furthermore we have investigated the energetics of the Si(001) surface separately, which is in itself an interesting system. Being highly reactive due to Si atoms in the upper layer each having one dangling bond, the ground state arrangement is still open to debate due to several configurations lying close by in energy [4].

Contour plots of the Si(001) surface have been created by simulating the interaction of an AFM tip with the surface dimers in the non-contact regime. The close approach and retraction of the AFM tip created a permanent deformation of the surface dimers, these results are in agreement with a previous tight binding study [5]. The energy barriers needed for the surface dimers to flip between the different configurations have also been investigated. We find that it is possible for the surface to return to its initial geometry after the tip is retracted.

[1] http://www.thphys.may.ie/EC/ROSES/roses_project.htm

[2] C. Hobbs, L. Kantorovich, *Nanotechnology* **15** (2004) S1

[3] P.D. Godwin, S.D. Kenny, R. Smith, *Surf. Science* **529** (2003) 237-246

[4] Ramstad A, Brocks G and Kelly P J 1995 *Phys. Rev. B* **51** 20

[5] K. Tagami, M. Tsukada, *Surf. Science* **493** (2001) 56-62