Modelling and Patterning of Si(100) surface with $c(4 \times 2)$ reconstruction

by

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Declaration

I, Mauro Mantega, hereby declare that this dissertation has not been submitted as an exercise for a degree at this or any other University.

It comprises work performed entirely by myself during the course of my Ph.D. studies at Trinity College Dublin. I was involved in a number of collaborations, and where it is appropriate my collaborators are acknowledged for their contributions.

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Abstract

Despite the increasing interest in novel materials for the next generation of micro-electronic devices, such as graphene and topological insulators, Si(100) surface is still the most important substrate for nano-device applications. Its high stability and the possibility of manipulating and functionalizing the surface properties at an atomic level are opening up new perspectives for a wide range of applications ranging from transistor downscaling, dictated by Moore's law, to quantum computing.

The adsorption of single atoms and small inorganic molecules plays a fundamental role in controlling the passivation, oxidation and epitaxial growth of the surface. Hydrogen passivated Si(100) surfaces, for example, can be patterned by desorbing H atoms through the tip of a scanning tunneling microscope (STM) and a variety of arrangements of coupled dangling bonds (quantum dots) can be created. Furthermore, the morphology and electronic properties of the reconstructed Si(100) surface provide a template for exploring systems with low dimensionality and quantum confinement effects on a real system. The quasi one dimensional dispersion of the Si(100) surface states can be exploited to study the fundamental physics related to real quantum wells.

The dimer rows of the $p(2 \times 2)$ and $c(4 \times 2)$ reconstructed Si(100) surfaces exhibit interesting surface electronic properties originating from the dangling bonds: the empty dangling bond state (π^*) is situated within the silicon bulk band gap and reveals energy dispersion only along the dimer row. The standing wave pattern in the local density of states, affected by surface adspecies, is very sensitive to the precise nature and configuration of the adspecie and it inspired us to develope a non intrusive, non local approach to characterize them. The adsorption of the simplest adspecie, a single H atom, which has a fundamental rôle related to the passivation of the surface and nano-patterning procedures will be presented. The adsorbed H atom, on the otherwise bare Si(100) surface with $c(4 \times 2)$ reconstruction, passivates one of the Si dangling bonds, breaking the Si-Si π-bond and leaving an isolated dangling bond (named the single dangling bond, SDB) on the other site of the dimer. An exhaustive description of the bonding configuration of the single H atom on the surface is presented as a function of the doping of the sample. Two approaches have been adopted.

The first one, called local approach, consists of analyzing local data such as the topography and the LDOS in the proximity of the reacted site to extract information about the bonding configuration of the adspecie.

The second approach, called non-local approach, makes use of nonlocal information, such as the standing wave pattern in the nonlocal density of states far away from the reacted site, to determine the adsorption configuration of the H. The properties of the single dangling bond are also evaluated.

Data are obtained by performing *ab initio* computer simulations and compared with scanning tunneling microscopy and spectroscopy (STM/STS) experiments.

With these tools, we were able to characterize the geometry and the charging state of the SDB for different doping conditions. For n-doped systems, the H-produced SDB is doubly occupied with the H_B configuration being the lowest in energy. This

configuration coincides with the majority specie found in low temperature STM experiments. The H_T configuration is the lowest in energy for p-doped samples, with the SDB state being empty. Finally, according to our calculations, the H_B configuration is predicted to be the lowest in energy for the neutral intrinsic case, and the SDB state is partially occupied and spin-polarized.

The nonlocal approach enabled us to map the phase-shift $\Theta(k)$ and it proved to be a very precise fingerprint for discriminating different H adsorption configurations. It has the potential to become a very general tool to determine the configuration of molecules and adspecies deposited on surfaces where the topographic signatures of different configurations are indistinguishable.

We also found that the configuration and charging state of the SDB are responsible for a gating between the reacted row and a bare adjacent one. The charge present at the reacted site originates a depletion of charge in the adjacent row, due to the Coulomb interaction, which results in a gating effect. The magnitude of the gating is proportional to the charging of the SDB and to the directionality of the SDB orbital.

All the results presented in this thesis can provide an interesting perspective for exploring fundamental properties of coupled systems (e.g. quantum wells) as well as applicative aspects aimed at the fabrication of nano-devices. The gating effect, together with the ability to create quantum wells by nanopatterning the Si(100) with an STM tip, may offer the opportunity to study coupled real quantum wells.

The interplay between charging and geometry can be taken as the basic mechanism for fabricating an atomic-scale switch device. In fact, by tuning the surface doping from p-type to n-type, one may switch between the two H configurations. These have distinct scattering and transport properties, so that the switch can be detected electrically or by mapping the phase-shift using the nonlocal approach method.

At the end of my PhD I was involved in another project with the aim of modelling a heterostructure based on graphene and topological insulators, by means of

first-principles calculations. In the last part of this thesis, the preliminary results concerning the electronic properites of a graphene-Bi_2Se_3 heterostructure are presented. The main idea is to model a material which combines the roboustness of the topological protected surface states of a topological insulator (TI) with the promising transport properties of pristine graphene. For different graphene-TI separations, the evolution of the band gap and the of the band structure is studied. At a close distance between the two subsystems, a conical band in the proximity of the Fermi level originates at the graphene-Bi_2Se_3 interface region. Our preliminary results predict this band to be topologically protected even though further investigations are required. A topological protected state in graphene, once supported by experimental verification, would candidate this versatile material as a very promising replacement for silicon aimed at nanoelectronics applications.

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