METAL-SEMICONDUCTING BEHAVIOR OF CARBON NANOTUBES ADSORBED ON HYDROGENATED Si(001) SURFACES

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The direct integration of CNTs into the well-established silicon technology may be an efficient alternative to achieve nanoscale devices and circuits in the near future. Recently, Albrecht and Lyding have demonstrated the feasibility to characterize single-walled CNTs adsorbed on H-passivated silicon surfaces using ultra-high vacuum scanning-tunneling microscopy (UHV-STM) techniques [1]. Following this way, the study of atomistic processes occurring at the CNT–surface interface and the effect of the substrate in the electronic properties of the adsorbed CNT, are important questions for the future realization of silicon-based nanoelectronics.

In this work, the adsorption of a metallic single-walled carbon nanotube (CNT) on hydrogenated Si(001) surfaces are studied from first-principles calculations. Our results indicate that the electronic properties of the adsorbed CNT can be ruled by the H concentration along the CNT–H/Si(001) contact region. On the fully hydrogenated Si(001), the CNT is physisorbed, preserving almost unchanged its metallic character. Removing half the H atoms along the adsorption site, we find an enhancement on the metallicity of the adsorbed CNT. In contrast, removing all the H atoms along the adsorption site, the adsorbed CNT becomes semiconducting, exhibiting an energy gap. These results suggest that metallic CNTs adsorbed on H/Si(001) could be transformed into metal-semiconductor junctions by grading the H concentration along the CNT–surface interface.

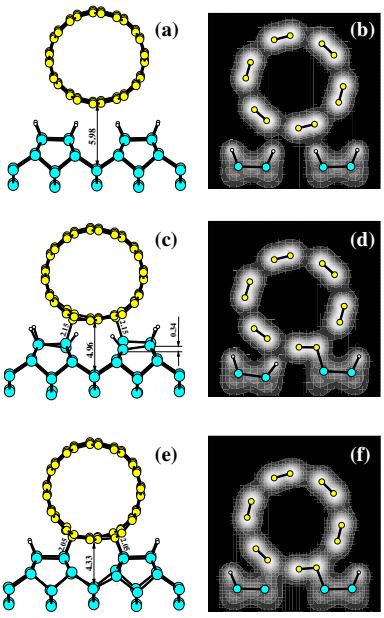

FIG. 1: Equilibrium geometries (left) and total charge densities contour plots (right), for the carbon nanotube adsorbed on the hydrogenated Si surfaces. The charge densities are depicted on a plane passes through the Si dimers. The numbers represent distances in Å.

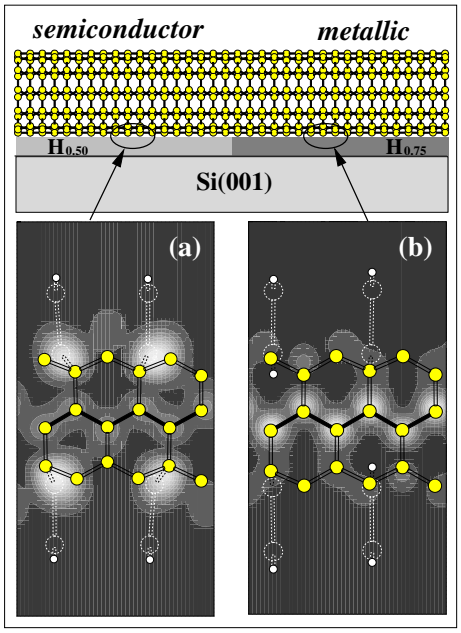

FIG. 2: (Top) Schematic representation of our proposed metal-semiconductor junction constructed with a single metallic CNT adsorbed on the surface trench of H/Si(001) with two different H concentrations. (Bottom) Charge density contour plots for the states just above the Fermi level

This work was supported by FAPESP, FAPEMIG and CNPq. We also would like to thank to CENAPAD-SP for computer time.

[1] P.M. Albrecht and J.W. Lyding, Appl. Phys. Lett. **83**, 5029 (2003).