Poster

DENSITY FUNCTIONAL STUDY OF MOLECULAR HYDROGEN COVERAGE ON HEXAGONAL AND PENTAHEPTITE CARBON NANOTUBES

I. Cabria, M. J. López and J. A. Alonso
Departamento de Física Teórica, Universidad de Valladolid, 47005 Valladolid, Spain
E-mail: cabria@fta.uva.es
http://lab2.fam.cie.uva.es

Hydrogen storage is a materials science challenge and relevant for onboard automotive applications. One of the storage methods is the physisorption of hydrogen on materials with high specific surface area, as carbon nanotubes. Density functional calculations of the adsorption of molecular hydrogen on the external surface of usual hexagonal nanotubes and pentaheptite (generated by rolling up a two-dimensional three-fold coordinated carbon network composed of pentagons and heptagons) carbon nanotubes and have been carried out. Binding energies of single molecules have been studied as a function of orientation of the molecules and type of nanotube. We have found weak adsorption, with binding energies near 100 meV/molecule in the most stable configurations on both types of nanotubes. The binding energies of a single molecule on hexagonal and pentaheptite nanotubes are similar. Also the binding energies on metallic and semiconducting hexagonal nanotubes are similar. When the nanotube surface is fully covered with one molecule per polygon (pentagon, hexagon or heptagon), the binding energy per molecule decreases for some nanotubes due to repulsive interactions between neighbor molecules. For the same reason, direct adsorption of a single hydrogen layer with a coverage of more than one molecule per polygon is not possible, even at low temperatures. However, adsorption of two layers (14.3 wt % hydrogen adsorbed when all the surface is covered) leads to binding energies between 40 and 80 meV/molecule, although the molecules of the outer layer are more weakly bound compared to those of the inner one. All the small binding energies calculated indicate that substantial adsorption is only possible at very low temperatures.

Acknowledgements: Work supported by MCyT (Grant MAT2002-04499-C02-01) and Junta de Castilla y León (Grant CO01/102).

Figures:

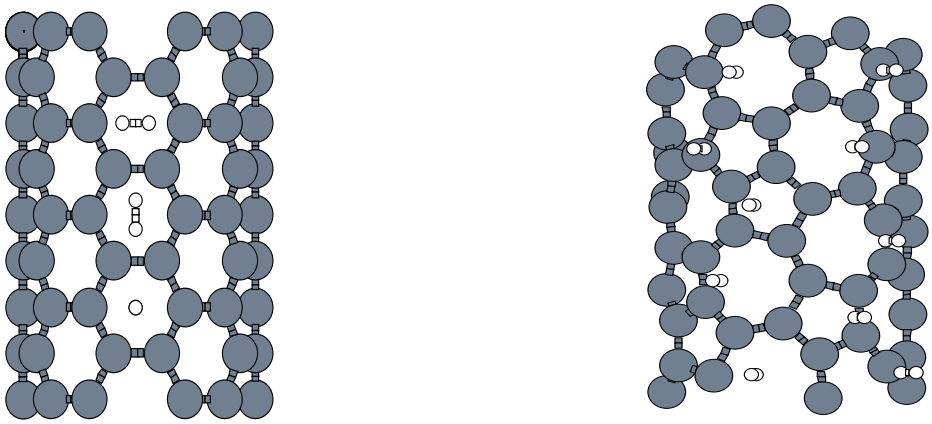

Figure 1. Left panel: Different adsorption configurations for a hydrogen molecule on the external surface of a carbon nanotube. Right panel: Adsorption of molecular hydrogen on the external surface of a pentaheptite carbon nanotube, formed by pentagons and heptagons.