11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Interactions of gases on the surface of carbon nanotubes of the armchair and zigzag type using AM1, MNDO, HF and DFT methods with 3-21G, 6-31G and Huzinaga basis sets

M. R. Vargas(1)*, J. D. Santos(1), J. B. L. Martins(2), E. Longo(3) and C. A. Taft(4)

(1) Department of Chemistry, Universidade Estadual de Goiás, e-mail: marcosrv@yahoo.com.br
(2) Department of Chemistry, Universidade de Brasília, Distrito Federal, Brazil
(3) LIEC, Universidade Estadual Paulista, São Paulo, Brazil
(4) Department of Physics, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brazil
* Corresponding author.

Abstract – We investigated the interaction of carbon nanotubes of Ge, Si, Al and B with gas CH_4, CO, CO_2, O_2 and N_2 on the internal as well as the external surface. In the manner it was observed that there occurs adsorption of these gases on the surface of the nanotubes with alteration of their electric properties showing in this manner the possibility of using these structures as sensors.

Gas sensors based on `functional` nanotubes are frequently related to direct changes of their electric properties as a response to the interaction with molecules. This has been one of the forms of exploring the potential of these structures that indicate electronic and mechanical properties different from gas sensors based on `functional` nanotubes which is frequently correlated to a direct change in their electric properties as a response to the interaction with molecules. This has been one of the ways of exploring the potential of these structures that indicate electronic and mechanical properties different from the `non functional` nanotubes. The changes of these types of nanotubes have been made both theoretically and experimentally via adsorption of atoms and molecules on nanotubes with substitutional doping. Single wall carbon nanotubes (SWNTs) with their unidimensional structure are structures that possess the components necessary to be used as sensors due to the delocalized electronic structure. A high sensibility of the electronic properties of the SWNTs in the presence of various gases was observed such as H_2, NO_2 and NH_3 [1, 2].

Via the optimized coordinates of the armchair and zigzag nanotubes doping was made with Ge, Si, Al, N e B in the middle of the structure as well as interactions with CH_4, CO, CO_2, O_2, N_2, NH_3, NO_2 and H_2 on the external surface and on the internal surface of the nanotube as shown in Figure 1.

For the interaction of methane with the carbon nanotube we analyzed the interaction distances between H and the surface of the structure as well as the C-H Bond distances. It was observed that there occurs a physical interaction with the C-H Bond at a distance of 1.11 Å.

For the other gas molecules we also observed a physical adsorption with the modification of the electronic structures of the molecules such as Gap (HOMO-LUMO). This study has indicated that these species can be used as sensors. The stabilization energy was calculated as the energy differences according to equation 1 for the methane molecule.

$$\text{Nanotube} \ldots CH_4 \rightarrow \text{Nanotube - } CH_4 \quad \Delta E = E_2(\text{Nanotube} \ldots CH_4) - E_1(\text{Nanotube - } CH_4) \qquad (1)$$

The left side of equation 1 represents the interaction of the methane molecule with the carbon nanotube at a distance of approximately 12 Å which yields an approximation term on the right hand side of the equation. The variation of energy was calculated via subtraction of energy of the interacting system from the non interacting system.

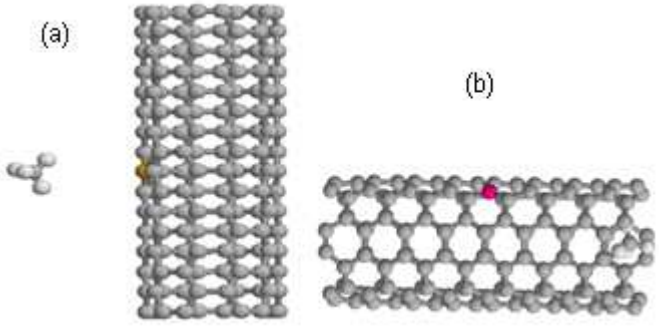

Fig. 1Model used for the interaction of gases with carbon nanotubes a)Ext. surface (b) Internal surrface

[1] A. G. Souza Filho and S. B. Fagan, Quim. Nova. 30 (2007).
[2] E. Bekyarova, M. Davis, T. Burch, M. E. Itkis, B. Zhao, S. Sunshine, and R. C. Haddon. J. Phys. Chem. B. 108 (2004).