11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Zigzag and armchair nanotubes interacting in the forms { [$(XY)_n]_m$ .... [$(XY)_n]_m$ $\}_k$, using molecular mechanics, quantum mechanics semi-empirical as well as Ab-initio, HF and DFT methods, with k = 2,...,5; X e Y: B, Al, C, Si, Ge, N, P, O, S

E. Longo[4], J. D. Santos[2], J. B. L. Martins[3] and C. A. Taft[1]

1 - Department of Physics, Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, Brazil, e-mail:catff@terra.com.br
2 - Department of Chemistry, Universidade Estadual de Goiás - jdsantos@ueg.br
3 - Department of Chemistry, Universidade de Brasília, Distrito Federal, Brazil – Lopes@unb.br
4- LIEC - Araraquara, Universidade Estadual Paulista, São Paulo, Brazil – elson@iq.unesp.br

Structures in the form of nanotubes such as $[(CC)_{n1}]_{m2}$, $[(BN)_{n3}]_{m4}$, $[(ZnO)_{n5}]_{m6}$, with ZIGZAG, ARMCHAIR conformations have been synthetized in order to study new properties which have been measured and detected in these new materials [1, 2]. yielding new perspectives with potential technological applications such as new materials with different type of conductivities and catalytic properties as well as the fabrication of different types of gas sensors.due to the interaction with gases and molecules with these structures or even nanotubes with different stechiometric conformations with smaller or larger radii. The study of different distances of interaction, the conformations of the various types of nanotubes that are today synthetized [3] and studied giving more support to the knowledge of the forms of the structures that are formed from a macroscopic point of view.

Thus, a study is made of an entire series of nanotubes, ARMCHAR as well as ZIGZAG with varying number of nearest neighbors { [$(XY)_n]_m$ .... [$(XY)_n]_m$ $\}_k$, yielding distances of interactions, conformations among them, HOMO-LUMO of the system, distribution of the charge, dipole, variations of interactions energies as a function of the number k of nanotubes, Figure 1, which can still have as variables the types of atoms X,Y and the values of n, m that are associated to the dimeter and length of the nanotubes..

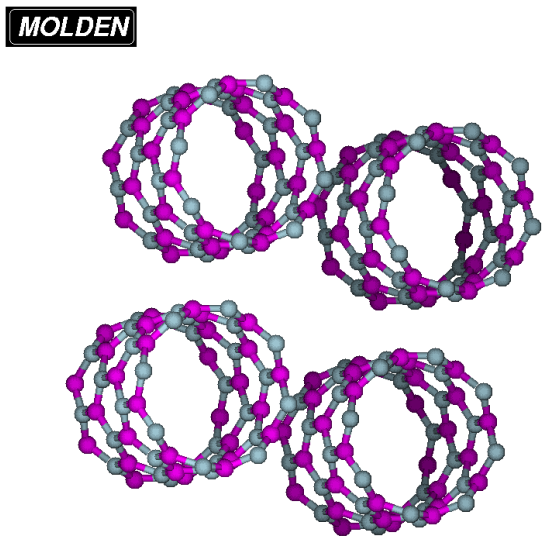

Figure 1. Interactions among zigzag nanotubes, { [$(BN)_8]_4$ .... [$(BN)_8]_4$ $\}_4$

[1] H.D. Yu, Z.P. Zhang, M.Y. Han, X.T. Hao, F.R. Zhu, J. Am. Chem. Soc. 2378, 127 (2005).
[2] B. WANG, et al. Nanotechnology **18**, 1 (2007).