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Study of the new structures of nanotubes $[(XY)_n]_m$ with the armchair and CHIRAL forms, according to the folding of planes, using the quantum theoretical methods of AM1, MNDO, HF and DFT with the 3-21G, 6-31G and Huzinaga basis sets

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Abstract – The construction of carbon nanotubes can be made by folding sheets of graphite. From this knowledge, we constructed models of single and multiple wall nanotubes with the structures $[(XY)_n]_m$, where X = Al, Si, Ge, C, B e Zn and Y = P, Si, Ge, N, S and C. From the optimized structures we analyzed the stabilization energies, charge distribution, energy Gap (HOMO-LUMO) as well as the HOMO and LUMO surfaces.

Carbon nanotubes are identified by their chiral indexes (n, m) or equivalently by the diameter and the chiral angles. These structures are well recognized by their potential application in electronic devices, and can be classified according to the number of layers in two forms: multilayer and simple nanotubes. The form used depends on the application [1, 2].

The construction of a carbon nanotube can be made by considering a sheet of graphite rolled in the the cylindrical form as shown in Figure 1. Using this method it was possible to study the structures $[(XY)_n]_m$, where X = Al, Si, Ge, C, B e Zn and Y = P, Si, Ge, N, S and C. We calculated the stabilization energy when the sheet is folded to give origin to the nanotube as shown in equation 1.

$$\text{Sheet of atoms XY} \rightarrow \text{Nanotube } [(XY)_n]_m \quad \Delta E = E_{Nanotube} - E_{Sheet} \qquad (1)$$

From the energy variation we observed that some species are stabilized, such as the nanotubes $[(AlP)_n]_m$, $[(SiSi)_n]_m$, $[(CC)_n]_m$, $[(GeGe)_n]_m$, $[(SiSi)_n]_m$, $[(BN)_n]_m$ and $[(SiC)_n]_m$. From the optimized structures we analyzed the charge distribution, energy Gap (HOMO-LUMO) and the HOMO and LUMO surfaces. Using the same folding methodology we analyzed the formation of multiple wall nanotubes (Figure 2).

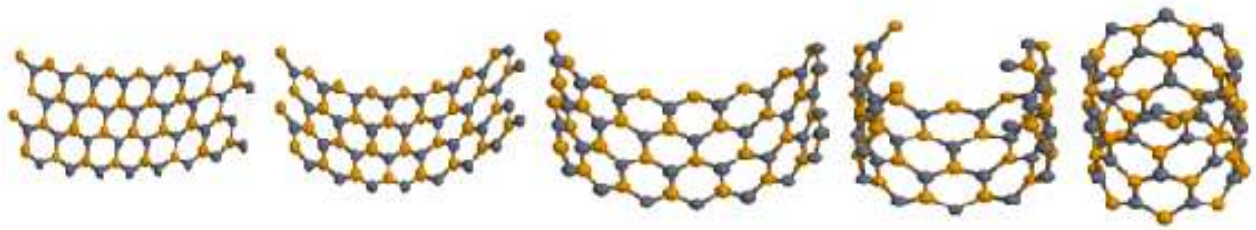

Figure 1. Model used for the construction of nanotubes $[(XY)_n]_m$.

Figure 2. Folding the sheets of XY atoms to form multiple layer nanotubes.

[1] A. G. Souza Filho, S. B. Fagan, Quim. Nova. 30 (2007).