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Oxi-reduction of nanotube structures of the form [(XY)n]m, with ARMCHAIR and ZIGZAG configurations, +1, 0, -1 charges, using both semiempírical, Ab-initio HF, and DFT methods with 3-21G, 6-31G and Huzinaga basis sets, whereas X, Y: B, Al, C, Si, Ge, N, P, O, S; n, m = 4, ..., 10

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The discovery of various forms of carbon BUCKBALLS and carbon nanotubes are making possible new frontier research lines for possible structures that have conformations not foreseen in the traditional studies in interatomic interactions, in Chemistry as well as other related areas whereas theory could not predict the exotic conformations/configurations detected experimentally and are actually being synthesized and investigated by various researchers, [1-4]. With possible applications in strategic technological areas, such as new sensor materials, semiconductors, catalysts, varistors and new conformations that were not foreseen from a theoretical-experimental point of view,[5].

Progress in this area yields new perspectives for studies in various fields of Chemistry, Physics, Engineering, Biology and many others research lines. In this work we use quantum-mechanical semi-empirical Am1 as well as Ab-intio Hartree-Fock and Density Functional methods with 3-21G, 6-31G and Huzinaga basis sets to investigate the oxidation and reduction of various species of nanotubes of the forms:

$$\left[\left(XY\right)_n\right]_m^{1+} \xrightarrow{1e^-} \left[\left(XY\right)_n\right]_m^{0} \xrightarrow{1e^-} \left[\left(XY\right)_n\right]_m^{1-}$$

X, Y: B, Al, C, Si, Ge, N, P, O, S; n, m = 4, ..., 10

Our results permits important, conclusion leading- comparisons of the variations of energies of these systems, due to the injections of electrons, as well as their stabilities, | Homo – Lumo |, charge distributions, dipoles, of the many possibilities that are obtained varying the nature of X, Y, n, m, the charges and the ARMACHAIR and ZIGZAG geometries.

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