Diversity of the nanotubes, which are possible?

J. D. Santos[1], E. Moraes[1], C.A. Taft[2], E. Longo[3] and J. B. L. Martins[4]
[1]*UEG, Universidade Estadual de Goiás, GO, Brazil*
[2]*CBPF, Centro Brasileiro de Pesquisas Físicas, RJ, Brazil*
[3]*UNESP, Universidade Paulista, Araraquara, SP, Brazil*
[4]*UnB, Universidade de Brasília, DF, Brazil*

The literature describes presently diverse nanotubes such as C, Si, Ge as well as other oxides (ZnO, SnO_2, TiO_2) and nitrates (BN). However which elements and combination of chemical elements can form a structure characterized by nanotubes.? Making combinations with the elements Al, B, Ge, Si e P, we made simulations of the nanotubes with these elements as well as their combinations in the armchair [n,n] and zigzag [n,0] models. Using the semi-empirical method AM1, we optimized these structures analyzing their stabilities, electronic properties and their characteristics having a nanotube structure. The combinations AlB, AlGe, AlP, AlSi, GeB, BP, SiP, GeP and SiB indicated nanotube characteristics after optimization by AM1 method, whereas the Gap (|Homo-Lumo|) remained at about 4 a 5 eV, indicating semiconductor characteristics (Figura 1). Notwithstanding, some systems could not be characterized as nanotubes after optimization, some of which involved Zn, such that ZnB, ZnGe, ZnP and ZnAl did not tend to crystals or nanotubes.

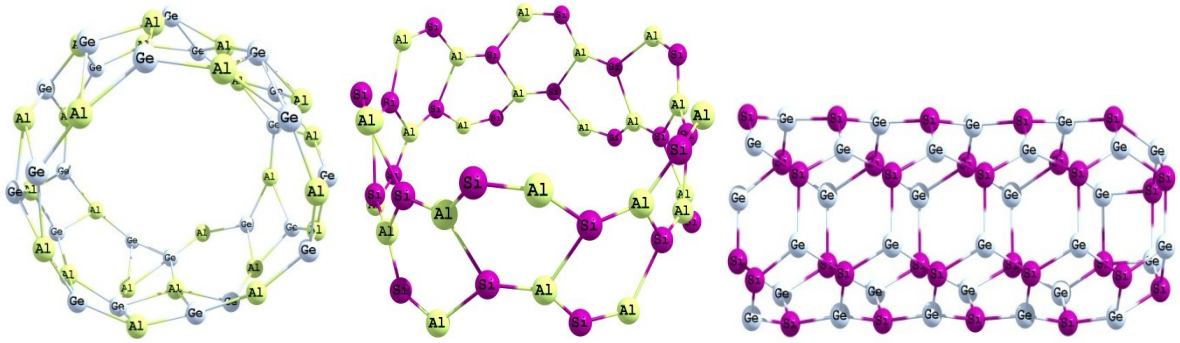

Figure 1 – Nanotubes of AlGe, AlSi and SiGe, respectively, otimized by the semi-empirical AM1method.

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e-mail:eduquimica2003@yahoo.com.br Cep 75120-220 Anápolis-GO - Brazil