Semiempirical strain energy for nanotubes

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The stability of nanotubes have been largely studied [1-2]. For the ZnO, ZnS, SiC, BN, AlP, C, Si, Ge e GeSi nanotubes we studied the strain energy,i.e the the variation of energy among the different forms of the crystalline plane and the form of the nanotube (Figure 1) We have optimized the structures with the semiempirical AM1 method, and also using the *ab initio* Hartree-Fock method with 3-21G basis. These structures were investigated searching for the structural properties of the compounds. In Table 1 we present the strain energy of the nanotubes investigated using the *ab initio* HF method. These results show that nanotubes are more stable than the crystalline planes. Nonetheless, the zigzag configuration (3,0) of some of the nanotubes have indicated to be unstable, although this result tends to change for structures with larger diameters.

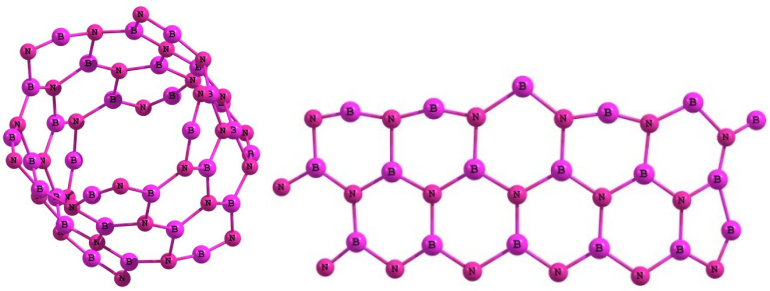

Figure 1 – BM nanotube and the crystalline plane, respectively

Tabela 1 – Strain energy of the nanotubes calculated by the ab-initio HF/3-21G method for various compounds

Configuration	Strain energy (eV)	Configuration	Strain energy (eV)
AlP[3,3]4	-6,0107	GeSi[3,0]4	2,4839
AlP[3,0]4	-13,3994	SiC[3,3]4	-7,6508
BN[3,3]4	-9,6821	SiC[3,0]4	0,0400
BN[3,0]4	-7,0888	Si[3,3]4	-8,9391
C[3,3]4	-1,5375	Si[3,0]4	13,7064
C[3,0]4	6,5043	ZnO[3,3]3	-20,9069
Ge[3,3]4	2,8614	ZnO[3,0]3	-12,9801
Ge[3,0]4	1,3708	ZnS[3,3]4	-23,0234
GeSi[3,3]4	-3,0341	ZnS[3,0]4	-3,4008

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[2] M ZHANG et al.Chemical Physics Letters. **379,** 81 (2003).