Carbide and Nitride nanotubes

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Abstract

In recent years, investigation of nanotube materials have resulted in new research areas, and received significant attention due to their technological applications, eg., photoluminescence semiconductor devices, solar cells, and catalysis. Studies were reported MgF_2 nanotubes using Hartree-Fock and B3LYP methods with Huzinaga basis set [1].Nano-sized tubular structures have stimulated intensive research interests, because these materials have enabled studies on fundamental physical properties. Nanotubular structures have only only been grown for few materials, which have bulk lamellar structures, such as graphite-like structures (BN, BCN, WS_2, MoS_2[1], GaN, Ba_2O, BeB_2 nanotubes have been reported in the literatures. GaN is technologically the most interesting compound and has attracted attention because of the importance in science and technology for optoelectronic applications[2,3]. The optimized structures of carbides and nitride nanotubes of the Hartree-Fock and DFT methods using 3-21G and 6-31G as well as Huzinaga basis set. The figure 1 presents various BN nanotubes and Fig 2 the SiC nanotubes.
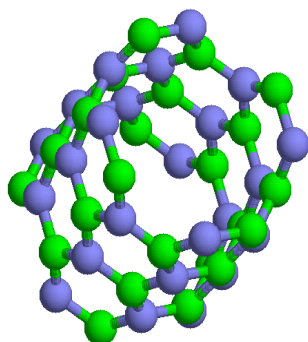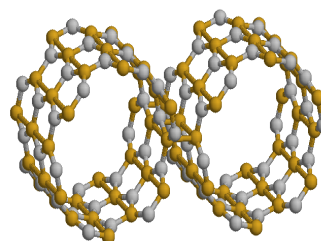
Figure 2: Nanotubes of SiC.

Figure1: Nanotubes of BN.

References:

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