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A QUANTUM CHEMICAL STUDY ON BORON NITRIDE AND CARBON NITRIDE NANOTUBES

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ABSTRACT. In order to use tubes for constructing electronic nanodevices we determined the energetic and electronic properties of the boron nitride and carbon nitride nanotubes.

Keywords: carbon-nitrogen and boron nitride nanotubes, semiempirical calculations, electronic properties, nanodevices.

INTRODUCTION

The discovery of carbon nanotubes [1] bring about unprecedented opportunities for obtaining materials with nanoscale structures. Recently, classes of tubes originating in compounds hexagonal tessellation: BN, CN_x have been synthesized [2-4]. Carbon and boron nitride nanotubes are promising systems for manufacturing of electronic devices, such as transistors, actuators and logic circuits [5-10]. These devices require precise control of the electronic properties. The fact that the electronic properties of the carbon nanotubes depend upon their chirality and diameter makes them unsuitable for some electronic devices.

The effect of chirality on energetic and electronic properties of zigzag boron nitride and carbon nitride nanotubes with 1:1 stoechiometry have been considered in this contribution.

METHOD OF CALCULATION

Carbon-nitrogen and boron nitride nanotubes with zigzag geometry have been considered theoretically by performing *PM3-RHF* [11] type semiempirical molecular orbital calculations by using Spartan '02 package [12].

The densities of states (*DOS*) have been calculated by the extended Hückel tight-binding method using BICON-CEDIT package [13].

RESULTS AND DISCUSSION

A) Thermodynamic stability

In the present work we have calculated the enthalpies of formation (ΔH) for (n,0)CN nanotubes with n=5, 6,….,12 depending on the chiral vector, n of the tube and compared them with the corresponding results for boron nitride nanotubes, **figure 1**.

Accordingly, the PM3 results show that both BN and CN nanotubes are thermodynamically stabilized with increasing of the chiral vector, n. All BN nanotubes are more stable than their carbon nitride analogues. This might explain the synthesis of carbon nitride nanotubes containing no more than 13% nitrogen [14].

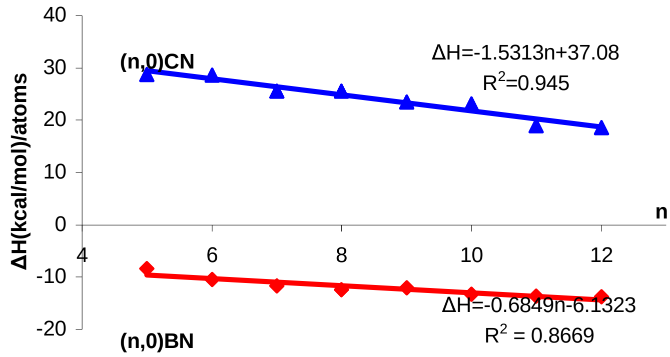

Figure 1. Enthalpies of formation (per atom) of the (n,0)CN/BN tubes as a function of chiral parameter (n).

B) Polarizability (α)

One of the current research topics in this area is the influence of different chiralities of the tubes on polarizabilities for possible applications on nanodevices. Polarizability measures the ability of an atom or molecule to deform the electric cloud in the presence of an electric field.

The calculated data have been plotted on graph in **figure 2**. This finding suggests that the polarizabilities of these tubes increases almost linearly with the chiral vector, n [15]. It is also important to notice that the polarizabilities of the CN nanotubes are higher than that of the BN analogues due to the higher polarizability of the carbon relative to boron.

C) Density of states (DOS)

The electronic properties of the nanotubes are examined using the information provided by density of states. The total DOS, IDOS (integrated DOS) and the N(2s, 2p), B(2s, 2p) contributions for (10,0)BN tube (with the 1:1 stoechiometry) are given in **figure 3**.

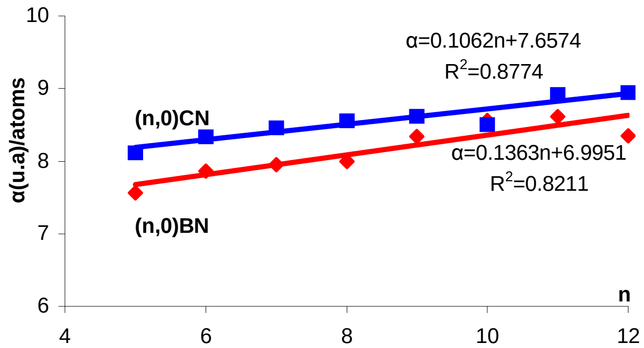

Figure 2. Polarizability (per atom) of the nanotubes as a function of chiral vector, n.

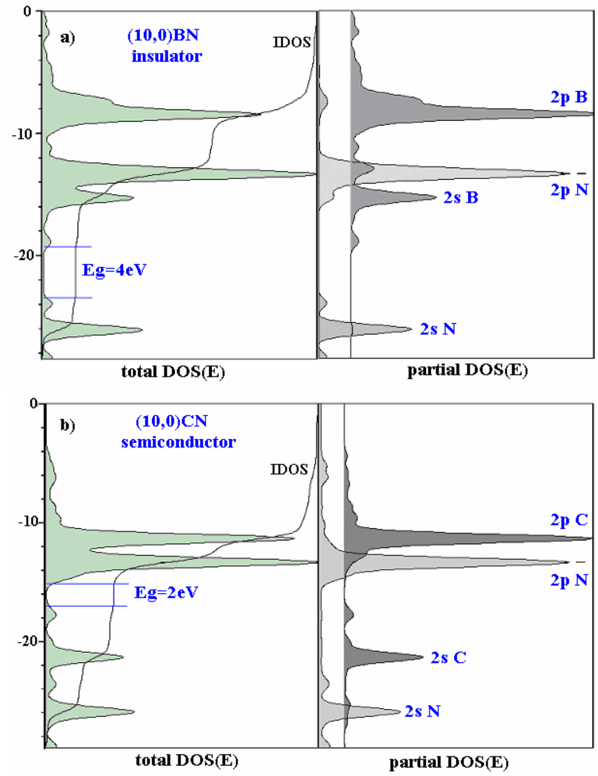

Figure 3. The total, partial *DOS* and *IDOS* diagrams for (10,0)BN and (10,0)CN tube.

The partial DOS(E) plot shows that the lowest band is derived from N(2s) orbitals and conduction bands are composed of 2s orbitals of the boron mixed with the 2p orbitals of the nitrogen and boron respectively. Since the gap between the valence and conduction bands (4eV) is greater than 3eV [16], indicates that the BN nanotube is an insulator. This finding is in agreement with the resultants published by Blasé [17] (tube is an insulator with a gap of 5,5eV).

From the DOS(E) plot indicates in **figure 3b** it is evident that the lowest bands (valence bands) are composed of N(2s), C(2s) derived states while the conduction bands are consisted of N(2p) and C(2p) derived states. Similar results indicates the DOS diagrams of the (n,0)BN and (n,0)CN with n=5, 6, 7, 8, 9, 11, 12. So that, all BN nanotubes are insulators while the CN nanotubes exhibit semiconductor properties, with constant gap independent of their chiral vector, n.

CONCLUSION

The carbon nitride nanotubes are thermodynamically stabilized with the increasing of the chiral vector, n. A higher polarizability and a semiconductor behaviour suggests that the carbon nitride nanotubes are good candidate for possible applications in nanodevices.

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