

A Density Functional Theory Study of Boron Nitride Nano-Ribbons

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ABSTRACT

The electronic and structural properties of pristine and carbon doped (C-doped) boron nitride nano-ribbons (BNNRs) have been studied employing density functional theory (DFT) calculations. Total energies, gap energies, dipole moments, and quadrupole coupling constants (qcc) have been calculated in the optimized structures of the investigated BNNRs. The results indicated that the stability and gap energy of the BNNR were decreased whereas the polarizability was increased because in the C-doped structure. The calculated qcc values indicated that the electronic properties of the nitrogen atoms were influenced because of the C-doping more than the boron atoms.

Keywords: Boron nitride; Nano-ribbon; Carbon doping; Density functional theory

INTRODUCTION

Fullerene discovery has raised intensive studies on the various kinds of the carbon based nano-materials including nanotubes, nanocones, etc., because of their potential applications in nano-scale devices [1-4]. By recent progresses in the experimental techniques, graphene, as the latest member, has been added to this family [5]. The graphene layer consists of a planar honeycomb arrangement of the carbon atoms and the layer is terminated by two different zigzag and armchair ends. The electronic and structural properties of carbon nano-ribbon (CNR), boron nitride nano-ribbon (BNNR) (Fig. 1), and aluminum nitride nano-ribbon (AlNNR) have been studied by earlier works [6-11]. In present study, the electronic and structural properties of pristine and carbon doped (C-doped) BNNRs (Fig. 1) have been investigated employing density functional theory (DFT) calculations. To this aim, the geometries of the investigated structures have been allowed to relax during the optimization processes and then the structural parameters including total energy, gap energy, dipole moment, and quadrupole coupling constant (qcc) have been calculated (Table 1). The BNNRs are important to

be studied because of their applications in forming other nanostructures such as nanotubes [12] and also their stabilities in the high temperature environments [8].

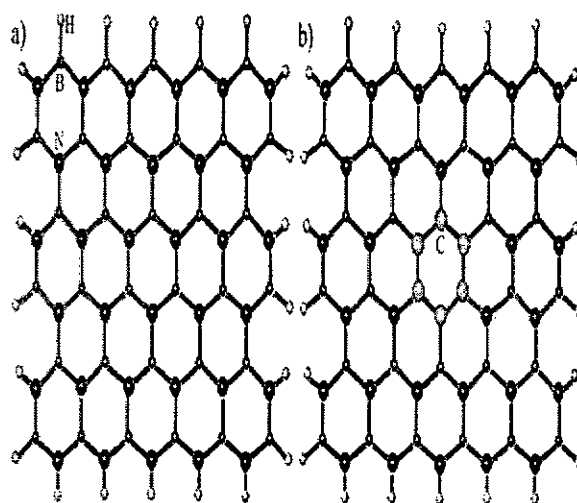


Fig. 1. The 2D views of the pristine (a) and the C-doped (b) BNNRs.

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METHOD

The DFT calculations have been performed using the Gaussian 98 [13] program at the levels of the BLYP and the B3LYP exchange-correlation functionals and the 6-31G* standard basis set [14,15]. The pristine BNNR (Fig. 1a) consists of 33 boron atoms and 33 nitrogen atoms. The C-doped BNNR (Fig. 1b) consists of 30 boron atoms, 30 nitrogen atoms, and 6 carbon atoms. The ends of both structures have been saturated by the hydrogen atoms. The geometries of the investigated structures have been allowed to relax by performing all-atomic optimizations. The structural parameters including total energy, gap energy, dipole moment, quadrupole coupling constant (qcc) have been calculated for the optimized structures (Table 1). The qcc value means the interaction energy between electric field gradient (EFG) tensors and nuclear electric quadrupole moment (eQ) at the sites of quadrupole nuclei. Eq. (1) has been used to evaluate the qcc values from the calculated EFG tensors in which the standard Q values reported by Pyykkö [16] have been employed in Eq. (1); $Q(\text{B-11}) = 40.59 \text{ mb}$ and $Q(\text{N-14}) = 20.44 \text{ mb}$. In recent studies, we have shown that the qcc values could reveal insightful trends about the electronic structural properties of the boron nitride nanotubes [17].

$$\text{qcc (MHz)} = e^2 Q q_{zz} h^{-1} \quad (1)$$

Table 1. The structural parameters*

	Pristine	C-Doped
Total energy	-71917 [-71946]	-71628 [-71657]
Gap energy	4.11 [5.91]	3.49 [4.92]
Dipole moment	4.21 [3.96]	4.35 [4.06]
qcc (B-11)	2.80 [2.97]	2.83 [2.99]
qcc (N-14)	0.84 [0.90]	1.13 [1.11]

*The units of energies, dipole moment and qcc are eV, Debye and MHz, respectively. The brackets include the results obtained by the B3LYP functional whereas the other results are obtained by the BLYP functional.

RESULTS AND DISCUSSION

Two exchange-correlation functionals including BLYP and B3LYP have been employed in the current calculations. Due to different implemented theories [18-20], different values of parameters are obtained by two functionals. However, the orders of values for the pristine and the C-doped models are not changed by the two functionals. Therefore, the aim of this study could be followed by both functionals. Within the text, the values obtained by the BLYP functional are discussed. It is noted that similar results are observed by the B3LYP functional.

Total energies

Fig. 1. shows the investigated structures of the pristine and the C-doped BNNRs. The two structures have the same numbers of atoms; however, in the C-doped BNNR, 3 B atoms and 3 N atoms have been doped by 6 C atoms. The doped C atoms make a ring in the center of the BNNR (Fig. 1b). The calculated total energies (Table 1) reveal that the structure of the pristine BNNR is 289 eV more stable than the C-doped BNNR. There are only B-N bonds in the pristine BNNR by the calculated average value of 1.45 Å but there are also B-C and C-N bonds, in addition to the B-N bonds, in the C-doped BNNR. Although the calculated average value of B-N bonds is remained unchanged in the C-doped BNNR, different B-C and C-N bonds by the calculated values of 1.52 and 1.44 Å, respectively, are arisen because of the C-doped region. Therefore, the stability of the pristine BNNR is influenced by this structural perturbation and different total energy is yielded for the C-doped BNNR.

Gap energies

Previous works proposed that the BN nanomaterials are wide band gap semiconductors but the C nanomaterials are either semiconductors or metals depending on the structural factors. This trend made the BN nanomaterials as proper candidates instead of the C ones for the more specific purposes. The calculated gap energies of this study for the pristine and the C-doped BNNRs are in the category of the semiconductors (Table 1). However, the calculated value for the pristine BNNR is 0.62 eV larger than the C-doped model.

Indeed, it is due to the influence of C-doping on the electronic properties of the BNNR which could be well detected by the calculated gap energies.

Dipole moments

The C-doped ring plays as an impurity in the structure and as a perturbation to the properties of the pristine BNNR. Therefore, the value of dipole moment is changed from 4.21 Debye in the pristine model to 4.35 Debye in the C-doped model. This trend could mean that the polarizability of the BNNR is increased because of C-doping. This result is in agreement with the calculated total energies of the pristine and the C-doped BNNRs in which the C-doped structure is less stable than the pristine one.

Quadrupole coupling constants

The calculated average values of the qcc for the B-11 and the N-14 nuclei in the optimized structures of the pristine and the C-doped BNNRs are listed in Table 1. The EFG tensors are very sensitive to the electronic distributions at the sites of the quadruple nuclei and detect any perturbations to these environments [17]. The comparison of the values of the qcc for the B-11 nuclei in the pristine and the C-doped BNNRs indicates that the electronic properties of the B atoms are not changed significantly. However,

this comparison for the N-14 nuclei indicates that the electronic properties of the N atoms are significantly influenced because of C-doping. Since the B atom has lack of electron in the valence shell whereas the N atom has a lone pair of electrons in the valence shell, the significant change of the electronic properties of the N atoms is reasonable.

CONCLUSIONS

The DFT calculations have been performed to study the electronic and structural properties of the pristine and the C-doped BNNRs. The calculated total energies indicated that the C-doped structure was less stable than the pristine one. The calculated gap energies indicated that the value was smaller for the C-doped structure. The calculated dipole moments indicated that the polarizability of the C-doped model was more than the pristine one. The calculated qcc values indicated that the electronic properties of the N atoms were influenced more than the B atoms because of C-doping.

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