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# Investigating the Effects of Molecular Oxygen Impurity on the Quadrupole Coupling Constants of Boron Nitride Nanotubes: Computational Studies

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## ABSTRACT

Density functional theory (DFT) calculations have been performed to investigating the effects of the molecular oxygen impurity on the quadrupole coupling constant (*Qcc*) parameters of armchair and zigzag boron nitride nanotubes (BNNTs). Optimization processes have been performed to relax the original and impure structures of the investigated BNNTs. Afterwards, the *Qcc* parameters have been evaluated for the boron and nitrogen atoms of the optimized BNNTs. The results have indicated that the *Qcc* parameters of boron and nitrogen atoms could detect the effects of oxygen impurity in the structure of BNNTs, in which the changes of those nitrogen atoms close to the impure region are more obvious. The B3LYP and B3PW91 exchange-correlation functional methods and the 6-31G* standard basis set as implemented in the Gaussian 98 package have been employed for performing the calculations.

**Keywords**: Density functional theory; Molecular oxygen impurity; Boron nitride nanotube; Nuclear quadrupole resonance

## INTRODUCTION

The discovery of carbon nanotube (CNT) by Iijima has increased numerous research on characterizing the properties and applications of this novel material [1-5]. Further studies indicated that the electronic properties of CNTs are mainly dependent on their structural topologies, in which the CNTs are categorized as metal or semiconductors [6]. Due to this task, the syntheses of CNTs for desired purposes are difficult because distinguishing the armchair and zigzag models of nanotube during the syntheses of CNT is not easy [7]. Therefore, considerable efforts have been done to identifying other structures of nanotubes with properties independent of the restricting factor of structural topologies. Among which, the tubular form of counterparts of boron and nitrogen atoms has been proposed as a suitable non-carbon nanotube [8]. The new boron nitride nanotube (BNNT) has been observed to be always semiconductor independent of the structural topologies [9]. Furthermore, since the electronegativities of boron and nitrogen atoms are different, the BNNT is observed to be a polar material in contrast with the CNT, which is a non-polar material. Having hetero atoms at the edges of nanotube is another obvious difference between the BNNTs and the CNTs, in which the studies indicated that the properties of two edges of the zigzag BNNTs are significantly different [10]. The BNNTs were firstly introduced through calculations but soon after their syntheses were also reported [11,12]. To this time, the properties of BNNTs have been studied using different computational and experimental techniques [13-15]. The studies also indicated that the presence of impurities such as carbon or oxygen atoms in the tubular structures could yield new properties for the impure BNNTs [16-19]. Earlier studies

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indicated that nuclear quadruple resonance (NQR) spectroscopy could reveal insightful trends for the properties of original and impure BNNTs [16,20].

Among the techniques of characterizing the properties of matters, NQR spectroscopy is considered as an insightful technique [21]. The properties of nuclei with nuclear spin angular momentum ($I$) greater than one-half, so called quadrupole nuclei, could be detected by the NQR measurements. These nuclei have nuclear electric quadruple moment ($eQ$), which interacts with electric field gradient (EFG) tensors at the electronic sites of atoms. The EFG tensors ($|q_{zz}|>|q_{xx}|>|q_{yy}|$) are very sensitive elements to the electronic sites of atoms and they could detect any perturbations to these sites. The interaction energy between the $eQ$ and the $q_{zz}$ component of EFG tensors is measured as quadrupole coupling constant ($Qcc$) which could be reproduced by either computations or experiments. Therefore, the magnitude of $Qcc$ is proportional to the electronic density of the atoms. It is important to note that performing experimental NQR measurements on the nanotubes is almost a formidable task due to the complex electronic environments of the nanotubes. Therefore, reproducing the NQR parameters by computations is an advantage of computational studies for the complex electronic structures of nanotubes [22].

Within this work, we have chosen the representative models of armchair and zigzag BNNTs to computationally investigating the effects of presence of molecular oxygen impurity on the $Qcc$ parameters of BNNTs. As mentioned above, since the $Qcc$ parameters are mainly dependent on the electronic sites of atoms, tracking their changes between the original and impure BNNTs could reveal insightful trends about their electronic properties. To achieve the purpose of study, we have firstly performed optimization processes on the original and impure models of (4,4) armchair and (6,0) zigzag BNNTs (Figs. 1 and 2). Subsequently, we have computed the $Qcc$ parameters for the boron ($^{11}$B) and nitrogen ($^{14}$N) atoms of the optimized models of the investigated BNNTs. It is noted that the geometrical difference between the original and impure models is that one boron atom and one nitrogen atom of the original models are substituted by two oxygen atoms to make the impure models. The computed $Qcc$ parameters for the $^{11}$B and $^{14}$N atoms of the original and impure BNNTs are tabulated in Tab. 1–4.

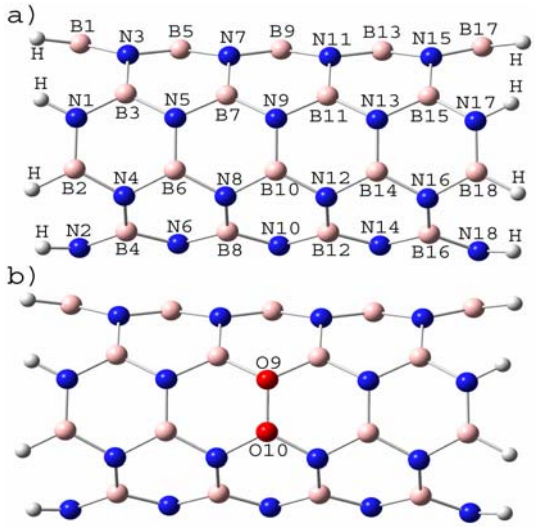


**Fig. 1.** To ease, 2D views of the models are shown. The original armchair model is shown in panel (a) and the impure armchair model is shown in panel (b).

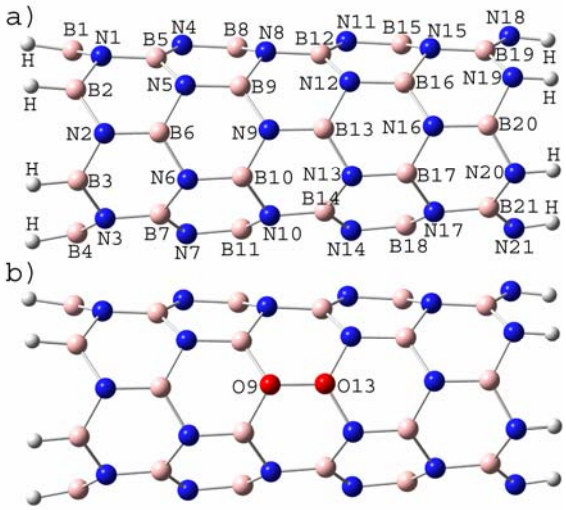


**Fig. 2.** To ease, 2D views of the models are shown. The original armchair model is shown in panel (a) and the impure armchair model is shown in panel (b).

## METHOD

Quantum chemical calculations based on density functional theory (DFT) as implemented in the Gaussian 98 package [23] have been employed within this work. The original (4,4) armchair model of BNNT consists of thirty-six boron and thirty-six nitrogen atoms in which the tubular

edges are saturated by sixteen hydrogen atoms to avoid the dangling effects (Fig. 1a). To make the molecular oxygen impure model, one boron atom and one nitrogen atom are replaced by two oxygen atoms (Fig. 1b). The original (6,0) zigzag model consists of thirty-six boron and thirty-six nitrogen atoms, in which the tubular edges of this nanotube are also saturated by twelve hydrogen atoms to avoid the dangling effects (Fig. 2a). To make the molecular oxygen impure model, one boron atom and one nitrogen atom are substituted by two oxygen atoms (Fig. 2b). Firstly, each of the four structures have been individually relaxed during the all-atomic optimization process using the B3LYP exchange-correlation functional method and the 6-31G* standard Pople type basis set [23]. Subsequently, the electric field gradient (EFG) tensors have been calculated at the sites of boron ($^{11}$B) and nitrogen ($^{14}$N) atoms of the optimized structures. Since the quantum calculations yield the EFG tensors in the principal axes system (PAS) ($|q_{zz}|>|q_{xx}|>|q_{yy}|$), Eq. (1) is used to convert them to the quadrupole coupling constants (*Qcc*) [21]. It is remembered that the *Qcc* is a measure of interaction energy between the nuclear electric quadrupole moment (*eQ*) and the $q_{zz}$ compnete of the EFG tensors. The standard values of quadrupole moments (*Q*) reported by Pyykkö [24] are used in Eq. (1): $Q(^{11}B)$ = 40.59 and $Q(^{14}N)$ = 20.44 mb. To calculate the EFG tensors, the B3LYP and B3PW91 exchange-correlation functional methods and the 6-31G* standard Pople type basis set have been used [23]. The evaluated values of *Qcc* parameters for $^{11}$B and $^{14}$N atoms are tabulated in Tables 1 – 4 for the original and molecular oxygen impure models of the investigated BNNTs (Figs. 1 and 2).

$$Qcc\ (\mathrm{MHz}) = e^2Qq_{zz}/h^{-1} \quad (1)$$

**Table 1.** Quadrupole coupling constants of B-11 atoms for the armchair BNNTs*

| Atoms | Original Model | | Impure Model | |
|---|---|---|---|---|
| | B3LYP/6-31G* | B3PW91/6-31G* | B3LYP/6-31G* | B3PW91/6-31G* |
| B1 | 3.32 | 3.26 | 3.30 | 3.24 |
| B2 | 3.32 | 3.26 | 3.30 | 3.24 |
| B3 | 2.90 | 2.83 | 2.97 | 2.90 |
| B4 | 2.90 | 2.83 | 2.84 | 2.77 |
| B5 | 2.90 | 2.83 | 2.90 | 2.82 |
| B6 | 2.90 | 2.83 | 2.69 | 2.62 |
| B7 | 2.90 | 2.83 | 2.87 | 2.80 |
| B8 | 2.90 | 2.83 | 2.69 | 2.61 |
| B9 | 2.91 | 2.84 | 2.84 | 2.77 |
| B10 | 2.91 | 2.84 | — | — |
| B11 | 2.90 | 2.83 | 2.87 | 2.80 |
| B12 | 2.90 | 2.83 | 2.69 | 2.61 |
| B13 | 2.90 | 2.83 | 2.93 | 2.82 |
| B14 | 2.90 | 2.83 | 2.70 | 2.62 |
| B15 | 2.90 | 2.83 | 2.97 | 2.90 |
| B16 | 2.90 | 2.83 | 2.84 | 2.77 |
| B17 | 3.32 | 3.26 | 3.30 | 3.24 |
| B18 | 3.32 | 3.26 | 3.30 | 3.24 |

* See Fig. 1 for the atomic numbers.

**Table 2.** Quadrupole coupling constants of N-14 atoms for the armchair BNNTs*

| Atoms | Original Model | | Impure Model | |
|---|---|---|---|---|
| | B3LYP/6-31G* | B3PW91/6-31G* | B3LYP/6-31G* | B3PW91/6-31G* |
| N1 | 1.85 | 1.79 | 1.92 | 1.86 |
| N2 | 1.85 | 1.79 | 1.82 | 1.77 |
| N3 | 0.94 | 0.99 | 0.80 | 0.86 |
| N4 | 0.94 | 0.99 | 1.14 | 1.18 |
| N5 | 0.82 | 0.86 | 1.19 | 1.24 |
| N6 | 0.82 | 0.86 | 0.73 | 0.79 |
| N7 | 0.87 | 0.92 | 0.80 | 0.85 |
| N8 | 0.87 | 0.92 | 4.49 | 4.41 |
| N9 | 0.81 | 0.86 | — | — |
| N10 | 0.81 | 0.86 | 0.80 | 0.85 |
| N11 | 0.87 | 0.92 | 0.80 | 0.85 |
| N12 | 0.87 | 0.92 | 4.49 | 4.41 |
| N13 | 0.82 | 0.86 | 1.19 | 1.24 |
| N14 | 0.82 | 0.86 | 0.73 | 0.73 |
| N15 | 0.94 | 0.99 | 0.80 | 0.86 |
| N16 | 0.94 | 0.99 | 1.14 | 1.18 |
| N17 | 1.85 | 1.79 | 1.92 | 1.86 |
| N18 | 1.85 | 1.79 | 1.82 | 1.77 |

* See Fig. 1 for the atomic numbers.

# RESULTS AND DISCUSSIONS

The major purpose of this study is to investigating the effects of presence of molecular oxygen impurity in the tubular structure on the *Qcc* parameters of the (4,4) armchair and (6,0) zigzag BNNTs. To achieve the purpose, we have performed DFT calculations to evaluate the *Qcc* parameters for the $^{11}B$ and $^{14}N$ atoms in the optimized structures of the original and impure models of the investigated BNNT. The evaluated values of *Qcc* parameters obtained by two levels of calculations are tabulated in Tables 1 – 4. Comparison of the values of the obtained parameters of the two levels, B3LYP/6-31G* and B3PW91/6-31G*, indicates that there are no significant differences between the values of the two computational levels and the values are supported by the both levels. Therefore, through the following text, the values obtained at the level of B3LYP/6-31G* calculations are only referred to.

**Armchair models**

The original model of the (4,4) armchair BNNT consists of thirty-six boron atoms and thirty-six nitrogen atoms, in which the tubular edges are saturated by sixteen hydrogen atoms (Fig. 1a). As could be seen in Fig. 1b, in the impure model of the investigated (4,4) armchair BNNT, the boron atom number 10 and the nitrogen atom number 9 are substituted by two oxygen atoms. The 2D views of the investigated models are shown in Fig. 1 and also the values of *Qcc* parameters for one side of nanotubes are tabulated in the Tables 1 and 2 which well represent the properties of the original and impure models of the (4,4) armchair BNNT.

The obtained values of *Qcc* parameters for the $^{11}B$ atoms of the original and impure armchair models are tabulated in Table 1. The results of the original model indicate that, with the exception of B1, B2, B17 and B18 atoms, which are located at the edges of nanotube, other boron atoms detect similar electronic environments, which are observed by their values of *Qcc* parameters. This trend reveals that the boron atoms of the edges of the original model of the armchair BNNT play different roles in comparison with the other boron atoms of the structure. In the impure model (Fig. 1b), in which B10 atom is substituted by O10 atom, the boron atoms of the edges of the nanotube do not show significant differences in comparison with the boron atoms at the edges of the original model. This trend reveals that, since the boron atoms of the edges of nanotubes do not show significant differences, the considered length of

nanotube for investigating the properties of the impure model could well represent the armchair nanotubes. In the impure model of armchair nanotube, B7 and B11 atoms are directly bonded to O9 atom, in which their *Qcc* parameters do not detect significant changes with respect to the original model. This trend reveals that since the electronegativities of nitrogen and oxygen atoms are close to each other, the nature of B-O bond is not significantly different from the original B-N bond. Therefore, the values of *Qcc* parameters for B7 and B11 atoms of the impure model are not different from the original model. The most changes of the electronic sites of the boron atoms due to the presence of the oxygen molecule in the structure are observed for B6, B8, B12 and B14 atoms which are located in the oxygen-membered rings. These boron atoms are bonded to N8 and N12 atoms, in which the two nitrogen atoms are directly bonded to the oxygen atom. Therefore, it could be concluded that the significant changes of the electronic properties of the mentioned boron atoms could be considered due to the significant changes of the electronic properties of N8 and N12 atoms. In other cases, the changes of *Qcc* parameters for the boron atoms of the impure model could be neglected with respect to the values of *Qcc* parameters for the boron atoms of the original model of the investigated armchair BNNT.

It is important to note that the electronic sites of boron and nitrogen atoms are different because, in the bonding situations, the former one has a lack of electrons but the latter one has an excess of electrons in their valance shells. Therefore, different behaviors for these atoms in the structure of the investigated BNNT could be expected. In the original model of the investigated armchair BNNT (Fig. 1a), comparing the evaluated values of *Qcc* parameters for the nitrogen atoms indicates that N1, N2, N17 and N18, which are located at the edges of nanotubes have the largest values of *Qcc* parameters among other nitrogen atoms. For other nitrogen atoms, the values of *Qcc* parameters indicate that the electronic environments of the nitrogen atoms detect slight changes through the structure of the original model of the armchair BNNT. In comparison with the boron atoms of the original model, the electronic environments of the nitrogen atoms detect more changes in the structure of the original armchair BNNT. In the impure model of the investigated armchair BNNT (Fig. 1b), in which N9 atom is substituted by O9 atom, the values of *Qcc* parameters for N1, N2, N17 and N18 atoms do not detect any significant changes with respect to the original model. This trend is in agreement with the earlier trend about the values of *Qcc* parameters for the boron atoms of the edges of nanotube which both confirm that our considered lengths of nanotubes are proper for achieving our purpose of this study. In comparison with the original model, the surprising values of *Qcc* parameters for N8 and N12 atoms of impure model, which are directly bonded to O10 atom, indicate that the natures of B-N and O-N bonds are completely different. The values of *Qcc* for other nitrogen atoms also detect notable changes due to the existence of molecular oxygen impurity in the structure of armchair BNNT.

**Zigzag models**

The original and impure models of the investigated (6,0) zigzag BNNT are shown in panels a and b of Fig. 2. The original model consists of thirty-six boron atoms and thirty-six nitrogen atoms, in which the tubular edges are saturated by twelve hydrogen atoms. In the impure model, N9 and B13 atoms are substituted by O9 and O13 atoms to consider the presence of molecular oxygen impurity in the structure of the investigated zigzag BNNT. It is important to note that in contrast with the armchair BNNTs, which have two similar edges, the zigzag BNNTs have different tubular edges of B-edge and N-edge. As shown in Fig. 2, B1, B2, B3 and B4 atoms make the B-edge and N18, N19, N20 and N21 make the N-edge of the investigated (6,0) zigzag BNNT. The evaluated *Qcc* values for the $^{11}B$ and $^{14}N$ atoms of the original and impure zigzag models are tabulated in Tables 3 and 4.

**Table 3.** Quadrupole coupling constants of B-11 atoms for the zigzag BNNTs*

| Atoms | Original Model | | Impure Model | |
|---|---|---|---|---|
| | B3LYP/6-31G* | B3PW91/6-31G* | B3LYP/6-31G* | B3PW91/6-31G* |
| B1 | 3.71 | 3.65 | 3.73 | 3.67 |
| B2 | 3.71 | 3.65 | 3.71 | 3.65 |
| B3 | 3.71 | 3.65 | 3.71 | 3.65 |
| B4 | 3.71 | 3.65 | 3.73 | 3.67 |
| B5 | 2.97 | 2.90 | 2.98 | 2.91 |
| B6 | 2.97 | 2.90 | 2.96 | 2.89 |
| B7 | 2.97 | 2.90 | 2.98 | 2.91 |
| B8 | 2.95 | 2.86 | 2.92 | 2.85 |
| B9 | 2.95 | 2.86 | 2.93 | 2.87 |
| B10 | 2.95 | 2.86 | 2.93 | 2.85 |
| B11 | 2.95 | 2.86 | 2.92 | 2.87 |
| B12 | 2.94 | 2.87 | 2.76 | 2.69 |
| B13 | 2.94 | 2.87 | — | — |
| B14 | 2.94 | 2.87 | 2.76 | 2.69 |
| B15 | 2.93 | 2.85 | 2.84 | 2.77 |
| B16 | 2.93 | 2.85 | 2.80 | 2.73 |
| B17 | 2.93 | 2.85 | 2.80 | 2.73 |
| B18 | 2.93 | 2.85 | 2.84 | 2.77 |
| B19 | 2.77 | 2.70 | 2.75 | 2.68 |
| B20 | 2.77 | 2.70 | 2.78 | 2.71 |
| B21 | 2.77 | 2.70 | 2.75 | 2.68 |

* See Fig. 2 for the atomic numbers.

**Table 4.** Quadrupole coupling constants of N-14 atoms for the zigzag BNNTs*

| Atoms | Original Model | | Impure Model | |
|---|---|---|---|---|
| | B3LYP/6-31G* | B3PW91/6-31G* | B3LYP/6-31G* | B3PW91/6-31G* |
| N1 | 0.96 | 0.99 | 0.96 | 0.99 |
| N2 | 0.96 | 0.99 | 0.98 | 1.01 |
| N3 | 0.96 | 0.99 | 0.96 | 0.99 |
| N4 | 1.07 | 1.10 | 0.94 | 0.99 |
| N5 | 1.07 | 1.10 | 1.11 | 1.14 |
| N6 | 1.07 | 1.10 | 1.11 | 1.14 |
| N7 | 1.07 | 1.10 | 0.94 | 0.99 |
| N8 | 1.11 | 1.15 | 0.91 | 0.98 |
| N9 | 1.11 | 1.15 | — | — |
| N10 | 1.11 | 1.15 | 0.91 | 0.98 |
| N11 | 1.12 | 1.16 | 1.18 | 1.22 |
| N12 | 1.12 | 1.16 | 4.29 | 4.26 |
| N13 | 1.12 | 1.16 | 4.29 | 4.26 |
| N14 | 1.12 | 1.16 | 1.18 | 1.22 |
| N15 | 1.17 | 1.21 | 1.14 | 1.18 |
| N16 | 1.17 | 1.21 | 1.28 | 1.31 |
| N17 | 1.17 | 1.21 | 1.14 | 1.18 |
| N18 | 2.54 | 2.52 | 2.52 | 2.50 |
| N19 | 2.54 | 2.52 | 2.57 | 2.55 |
| N20 | 2.54 | 2.52 | 2.57 | 2.55 |
| N21 | 2.54 | 2.52 | 2.52 | 2.50 |

* See Fig. 2 for the atomic numbers.

Tab. 3 presents the values of *Qcc* parameters for the $^{11}$B atoms of the original and impure models of the (6,0) zigzag BNNTs. In the original model (Fig. 2a), the results indicate that the values of *Qcc* for those boron atoms which are located at the B-edge of nanotube are the largest ones among the values of *Qcc* parameters for boron atoms. B19, B20 and B21 atoms are located close to the N-edge of nanotube, in which their *Qcc* values are the smallest ones among the boron atoms of the investigated zigzag BNNT. From the B-edge to the N-edge, the values of *Qcc* parameters for the $^{11}$B atoms are decreased, in which the changes of the values of *Qcc* parameters for the boron atoms of the inner shells, from B5 to B18, are occurred slightly. In the impure model (Fig. 2b), in which B13 atom is substituted by O13 atom, the values of *Qcc* parameters for the boron atoms of the B-edge of BNNT do not detect notable changes with respect to the original model. This trend reveals that the considered length of the investigated zigzag BNNT is proper for achieving our purpose of this study. Among the boron atoms, B9 and B10 atoms are directly bonded to O9 atom, in which their values of *Qcc* values in the impure model do not detect significant changes in comparison with the original model. However, the values of *Qcc* parameters for B12 and B14 atoms, which are in the O-membered ring, detect the most significant changes among other boron atoms. The main reason is that the properties of N12 and N13 atoms which are directly bonded to B12 and B14 atoms are significantly changed in the impure model with respect to the original model of the investigated zigzag BNNT. The effects on the properties of B16 and B17, which are also in direct bonding with the N12 and N13 atoms, are also notable. However, the changes of the properties of other boron atoms, which are detected based on the changes of the values of *Qcc* parameters in the original and impure models, due to the presence of the molecular oxygen impurity in the structure of the (6,0) zigzag BNNT are almost negligible.

The evaluated values of *Qcc* parameters for the $^{14}$N atoms of the original and impure models of the investigated (6,0) zigzag BNNT (Fig. 2) are tabulated in Table 4. In the original model (Fig. 2a), N18, N19, N20 and N21 atoms make the N-edge of the zigzag nanotube, in which their values of *Qcc* parameters are the largest ones among other nitrogen atoms. The values of *Qcc* parameters for the $^{14}$N atoms are decreased from the N-edge to the B-edge of nanotube, from N21 atom to N1 atom. N1, N2, and N3 atoms are located close to the B-edge of nanotube, in which their values of *Qcc* parameters are the smallest ones among other nitrogen atoms. In parallel with the results of *Qcc* parameters for the $^{11}$B atoms at the B-edge of nanotube, the results of *Qcc* parameters for the $^{14}$N atoms also confirm that the atoms of the edges of nanotubes play different roles with respect to other atoms in the structures of the investigated zigzag BNNT. In the impure model (Fig. 2b), N9 atom is substituted by O9 atom, which brings some changes to the natures of chemical bondings with respect to the original model. Due to the presence of molecular oxygen impurity, the values of *Qcc* parameters for the $^{14}$N atoms at the N-edge of the nanotube do not detect any significant changes with respect to the original model. This trend, in agreement with the trend about the values of *Qcc* parameters for the $^{11}$B atoms of the B-edge of impure model, confirms that the length of model is proper for achieving our purpose of this study. The most changes of the values of *Qcc* parameters for the $^{14}$N atoms of the impure model with respect to the original model are observed for N12 and N13 atoms which are directly bonded to O13 atom. Since the natures of B-N atoms are completely different from the O-N atoms, significant effects of the molecular oxygen impurity are observed for the properties of N12 and N13 atoms. The values of *Qcc* parameters for other nitrogen atoms indicate that, with the exceptions of the nitrogen atoms at the N-edge and close to the B-edge, they detect the notable effects of the molecular oxygen impurity in structure of zigzag BNNT. However, the magnitudes of changes are very smaller than the changes of N12 and N13 atoms.

## CONCLUSIONS

We have performed DFT calculations to investigate the effects of molecular oxygen doping on the *Qcc* parameters of the representative (4,4) armchair and (6,0) zigzag BNNTs. The results indicated that the properties of boron and nitrogen atoms detect the effects of the oxygen impurity, in which the changes of the

values of *Qcc* parameters between the original and impure models could be considered as a measure of the effects. The values of those boron and nitrogen atoms located close to the impurity region detect the most significant changes of the values of *Qcc* parameters. For other atoms, smaller effects are observed. Comparing the changes of the properties of boron and nitrogen atoms of the impure models also indicated that the changes of the properties of nitrogen atoms are better observed.

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## REFERENCES

[1] S. Iijima, Nature 354 (1991) 56.
[2] H. Aghaie, M.R. Gholami, M. Monajjemi, M.D. Ganji, Physica E 40 (2008) 2965.
[3] M.D. Ganji, I. Rungger, J. Iran. Chem. Soc. 5 (2008) 566.
[4] G. Guisbiers, M. Wautelet, L. Buchaillot, Phys. Rev. B 79 (2009) 155426.
[5] G. Guisbiers, D. Liu, Q. Jiang, L. Buchaillot, Phys. Chem. Chem. Phys. 12 (2010) 7203.
[6] I. Vurgaftman, J.R. Meyer, J. Appl. Phys. 94 (2003) 3575.
[7] P.J.F. Harris, Carbon Nanotubes and Related Structures, Cambridge University Press, Cambridge, 1999.
[8] A. Loiseau, F. Willaime, N. Demoncy, N. Schramcheko, G. Hug, C. Colliex, H. Pascard, Carbon 36 (1998) 743.
[9] X. Balasé , A. Rubio, S.G. Louie, M.L. Cohen, Europhys. Lett. 28 (1994) 335.
[10] S. Hou, Z. Shen, J. Zhang, X. Zhao, Z. Xue, Chem. Phys. Lett. 393 (2004) 179.
[11] A. Rubio, J. L. Corkill, M. L. Cohen, Phys. Rev. B 49 (1994) 5081.
[12] N. G. Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, S. G. Louie, A. Zettl, Science 269 (1995) 966.
[13] L.A. Thesing, P. Piquini, T. Kar, Nanotechnology 17 (2006) 1637.
[14] H. S. Kang, J. Phys. Chem. B 110 (2006) 4621.
[15] H.–S. Wu, X.–H. Xu, F.–Q. Zhang, H. Jiao, J. Phys. Chem. A 107 (2003) 6609.
[16] M. Mirzaei, N.L. Hadipour, M.R. Abolhassani, Z. Naturforsch. A 62 (2007) 56.
[17] G. Gou, B. Pan, L. Shi, J. Am. Chem. Soc. 131 (2009) 4839.
[18] L.A. Silva, S.C. Guerini, V. Lemos, J.M. Filho, IEEE Trans. Nanotechnology 5 (2006) 517.
[19] R. Moradian, S. Azadi, Europhys. Lett. 83 (2008) 17007.
[20] M. Mirzaei, N.L. Hadipour, Physica E 40 (2008) 800.
[21] T.P. Das and E.L. Han, Nuclear Quadrupole Resonance Spectroscopy, Academic Press, New York, 1958.
[22] E. Zurek, J. Autschbach, J. Am. Chem. Soc. 126 (2004) 13079.
[23] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery, Jr., R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, A.G. Baboul, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, C. Gonzalez, M. Head-Gordon, E.S. Replogle, J.A. Pople, GAUSSIAN 98, Gaussian, Inc., Pittsburgh, PA, 1998.
[24] P. Pyykkö, Mol. Phys. 99 (2001) 1617.