

# Theoretical study on the functionalization of BC<sub>2</sub>N nanotube with amino groups

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**Abstract** Using density functional theory calculations, we investigated properties of a functionalized BC<sub>2</sub>N nanotube with NH<sub>3</sub> and five other NH<sub>2</sub>-X molecules in which one of the hydrogen atoms of NH<sub>3</sub> is substituted by X = -CH<sub>3</sub>, -CH<sub>2</sub>CH<sub>3</sub>, -COOH, -CH<sub>2</sub>COOH and -CH<sub>2</sub>CN functional groups. It was found that NH<sub>3</sub> can be preferentially adsorbed on top of the boron atom, with adsorption energy of -12.0 kcal mol<sup>-1</sup>. The trend of adsorption-energy change can be correlated with the trend of relative electron-withdrawing or -donating capability of the functional groups. The adsorption energies are calculated to be in the range of -1.8 to -14.2 kcal mol<sup>-1</sup>, and their relative magnitude order is found as follows: H<sub>2</sub>N(CH<sub>2</sub>CH<sub>3</sub>) > H<sub>2</sub>N(CH<sub>3</sub>) > NH<sub>3</sub> > H<sub>2</sub>N(CH<sub>2</sub>COOH) > H<sub>2</sub>N(CH<sub>2</sub>CN) > H<sub>2</sub>N(COOH). Overall, the functionalization of BC<sub>2</sub>N nanotube with the amino groups results in little change in its electronic properties. The preservation of electronic properties of BC<sub>2</sub>N coupled with the enhancement of solubility renders their chemical modification with either NH<sub>3</sub> or amino functional groups to be a way for the purification of BC<sub>2</sub>N nanotubes.

**Keywords** Amine · B3LYP · DFT · Functionalization · Nanostructures

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## Introduction

Carbon nanotubes (CNTs) have been widely studied in different applications of nanotechnology regarding their interesting physico-chemical properties [1–4]. Purification or controlled synthesis of CNTs with selected helicity has not been achieved so far which has made electronic device making with CNTs difficult. Therefore, it is interesting and important to further find or design other new low-dimensional tube-like nanostructured materials, being suitable for miniaturization of electronic devices. In addition to CNTs, extensively studied over the last decade, nanotubes may form in the B–C–N system. The structures of graphite and hexagonal boron nitride (BN) are nearly identical (unit cell, atomic distances), making the ternary B–C–N nanotubes a unique material due to the possibility of random and/or ordered substitution of B and N atoms for C atoms in the graphitic sheet [5–7]. Moreover, the ionicity properties of CNT and those of BN nanotubes are predicted to be opposite. CNTs are known to be non-ionic metals or semiconductors, while BN nanotubes are expected to be insulators with partially ionic nature. So preparation of ternary B–C–N NTs of various compositions may allow one to tune transport properties over a wide range. However, the formation of B–B and N–N bond pairs can be avoided if there is a C–C pair in B–C–N nanotubes. As a result, among different B–C–N nanotubes, the BC<sub>2</sub>N nanotube (BC<sub>2</sub>NNT) stoichiometry is the most stable stoichiometry [8–10].

Considerable experimental efforts have been devoted to the synthesis of C<sub>x</sub>(BN)<sub>y</sub> nanotubes, and they have been successfully obtained by electrical pyrolysis [11], laser ablation [12], hot-filament chemical vapor deposition [13], and the template route [14]. Unfortunately, the poor solubility and difficulties of purifying and processing have hampered the future application of BC<sub>2</sub>NNTs. Nonetheless, recent

advances in linking specific groups or molecules to the nanotubes clearly testify the strong potential of chemical functionalization not only for tuning the tubes' electronic properties, but also to enable their assembly into more-complex architectures required for integrated device operation [15–21]. The electronic structure properties of BC<sub>2</sub>NNTs have been theoretically studied by different groups [9, 10]. Recently, theoretical calculations on the pristine C<sub>x</sub>(BN)<sub>y</sub> compound nanotubes have shown that these nanostructures are promising for energy-storage applications [22]. However, neither experiments nor theoretical investigation have been reported on BC<sub>2</sub>NNT surfaces under both covalent and noncovalent functionalization, so further study of the electronic properties of BC<sub>2</sub>NNT under functionalization remains interesting.

In present work, we have investigated the functionalization of BC<sub>2</sub>NNTs by different amino groups using density functional theory (DFT). Five functional groups have been introduced as substituents in the molecule of NH<sub>2</sub>X, in which X denotes (i) –CH<sub>3</sub>, (ii) –CH<sub>2</sub>CH<sub>3</sub>, (iii) –CN, (iv) –COOH and (v) –CH<sub>2</sub>COOH. These groups can serve as starting sites for further nanotube functionalization.

### Computational methods

Geometry optimizations, and density of states (DOS) analysis were performed on a (8, 0) zigzag BC<sub>2</sub>NNT (constructed of 24 B, 24 N and 48 C atoms), and different functionalized BC<sub>2</sub>NNT complexes at B3LYP/6-31G(d) level of theory as implemented in GAMESS suite of program [23]. This level of theory is a popular approach which has been commonly used for nanotube structures [24–28]. It has also been demonstrated that the B3LYP provides an efficient and robust basis for calculations of several semiconductors by Tomic et al. [29], capable of reliably predicting both the ground state energies and the electronic structure. GaussSum program has been used to obtain the DOS results [30]. The length and the diameter of the optimized pure BC<sub>2</sub>NNT were computed to be about 11.42 Å and 6.22 Å, respectively. In order to reduce boundary effects, atoms at the open ends of the tube were saturated with hydrogen atoms. We define the chemical functionalization energy ( $E_{CF}$ ) of molecules as follows:

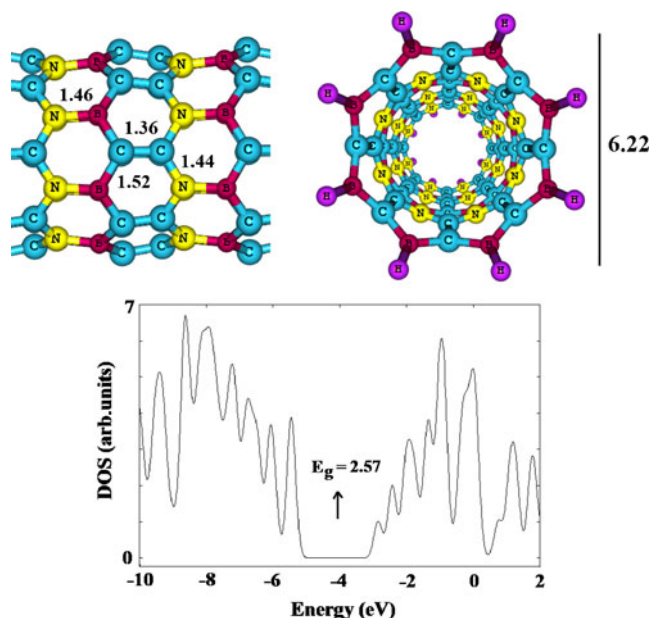
$$E_{CF} = E_{\text{molecule-tube}} - E_{\text{tube}} - E_{\text{molecule}}, \quad (1)$$

where  $E_{\text{molecule-tube}}$  is the total energy of mentioned molecule adsorbed on the BC<sub>2</sub>NNT surface, and  $E_{\text{tube}}$  and  $E_{\text{molecule}}$  are the total energies of the pristine BC<sub>2</sub>NNT and a molecule, respectively.  $E_{BSSE}$  is the basis set superposition error (BSSE) corrected for the all interaction energies. By the definition, a negative value of  $E_{CF}$  corresponds to exothermic functionalization. The canonical assumption for

Fermi level is that in a molecule (at  $T = 0$  K) it lies approximately in the middle of the HOMO-LUMO energy gap ( $E_g$ ). In fact, what lies in the middle of the  $E_g$  is the chemical potential, and since the chemical potential of a free gas of electrons is equal to its Fermi level as traditionally defined, herein, the Fermi level of the considered systems is at the center of the  $E_g$ .

### Results and discussion

At first, the accuracy of the method used in this work has been tested initially to describe the properties of NH<sub>3</sub> molecule in gas phase. The bond length of individual N-H and bond angle of free NH<sub>3</sub> from our approach are 1.01 Å and 108°, which are in good agreement with the experimental values of 1.01 Å and 107° [31], respectively. In Fig. 1, we have shown top and side views of the optimized structure of the BC<sub>2</sub>NNT, where four types of bonds namely B–N, B–C, N–C and C–C can be identified, with corresponding lengths of 1.46, 1.52, 1.44 and 1.36 Å, respectively. There are two types of carbon atoms in BC<sub>2</sub>NNT; C.I is a carbon atom that is bonded to two B atoms and one C atom, while C.II is a carbon atom that is bonded to two N atoms and one C atom. Buckling of B–N and C–C bonds was found in the structures. After optimization this buckling moves N atoms inward and B atoms outward of the nanotube surface in the B–N bonds. On the other hand, for C–C bonds, the C.I atoms are relaxed outward while the C.II atom inward of the nanotube surface. Calculated DOS (Fig. 1) plot shows that the tube is a semiconductor with the HOMO (the highest



**Fig. 1** Partial structure of optimized BC<sub>2</sub>NNT and its density of state (DOS). Bonds are in Å

occupied molecular orbital)-LUMO (the lowest unoccupied molecular orbital) energy gap ( $E_g$ ) of 2.57 eV.

#### Adsorption of $\text{NH}_3$ on the $\text{BC}_2\text{NNT}$

In order to find minimum adsorption configurations, the  $\text{NH}_3$  molecule was initially placed at different positions above a  $\text{BC}_2\text{NNT}$  including on top of a sidewall B, C.I, C.II or N atom from its H or N head. Full geometrical optimization was then performed with several different orientations of the  $\text{NH}_3$  molecule. Figure 2 displays a side view of stable (local minimum) configurations of the  $\text{NH}_3$  molecule on the tube. It was found that the  $\text{NH}_3$  molecule can be adsorbed with two orientations with respect to the sidewall surface: (A) a hydrogen atom of the molecule is nearest to an N atom of the surface, or (B) the nitrogen atom is nearest to a B atom of the surface. Other initial configurations have reoriented to one of these stable structures during relax optimization. More detailed information including values of  $E_{\text{CF}}$  and the charge transfer ( $Q_{\text{T}}$ ) are listed in Table 1.

In configuration A with  $E_{\text{CF}}$  of  $-2.7 \text{ kcal mol}^{-1}$ , only a weak hydrogen bond between an N atom of the tube and an H atom of  $\text{NH}_3$  is formed ( $\text{N} \cdots \text{H}$ , 2.99 Å), along with a charge transfer of 0.013  $e$ . Further indication of the negligible deformation degree in the geometry of  $\text{NH}_3$  upon the adsorption process, is given by the bond reorganization energy ( $E_{\text{br}}$ ), calculated as the energy difference between the full relaxed  $\text{NH}_3$  molecule and its adsorbed state.  $E_{\text{br}}$  of the  $\text{NH}_3$  in configuration A is about  $0.14 \text{ kcal mol}^{-1}$ ,

confirming the weak interaction. Calculated DOS plots (Fig. 2) show that the  $\text{NH}_3$  adsorption through this configuration has no sensible effects on the electronic properties of the tube so that the  $E_g$  of the tube has slightly increased from 2.57 to 2.60 eV.

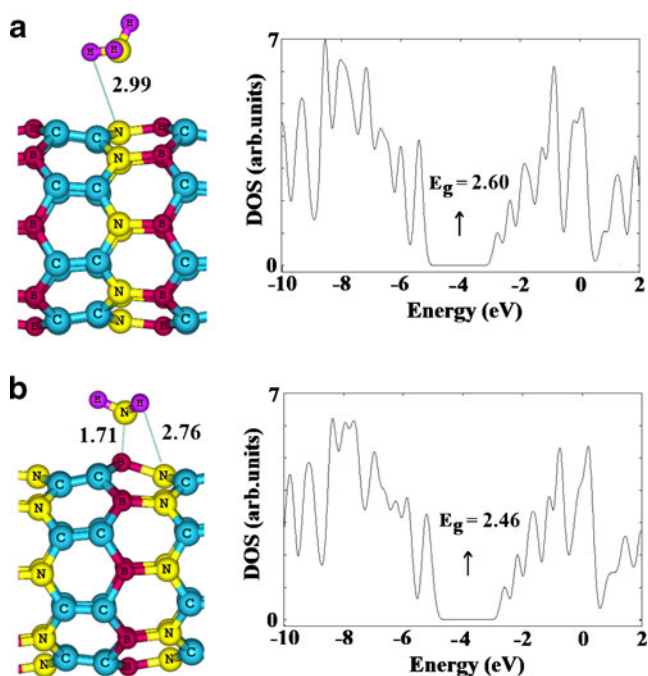
In the most stable configuration (Fig. 2b), a new B–N bond was formed between the nitrogen atom of  $\text{NH}_3$  and the boron atom on the sidewall of the  $\text{BC}_2\text{NNT}$  (with bond length 1.71 Å). This configuration has  $E_{\text{CF}}$  of  $-12.0 \text{ kcal mol}^{-1}$  and the boron atom is slightly pulled out of the surface. It has also been found that the  $\text{BC}_2\text{NNT}$  undergoes an obvious distortion upon  $\text{NH}_3$  adsorption via configuration A, so that the C–B and B–N bonds of tube in adsorption area were elongated to 1.57 and 1.53 Å, respectively. Calculated  $E_{\text{br}}$  of the  $\text{NH}_3$  molecule in configuration B is about  $0.09 \text{ kcal mol}^{-1}$ , which is smaller than that of configuration A. The adsorption of the  $\text{NH}_3$  on the B site in  $\text{BC}_2\text{NNT}$  can be rationalized by the fact that the LUMO is mainly located on the B atoms. As a result, the HOMO of  $\text{NH}_3$ , located on N atom, donates electrons preferentially to the LUMO centered on the B sites. The transferred charge (0.237  $e$ ) from  $\text{NH}_3$  to the tube in configuration B is remarkably more than that of configuration A. Change of  $E_g$  in configuration B (0.11 eV, Table 1) is also more than that of the A one (0.03 eV).

#### Influence of different organic groups on $\text{BC}_2\text{NNT}$ functionalization

In order to investigate the chemical functionalization of the  $\text{BC}_2\text{NNT}$  exterior surface, we have studied properties of a chemically modified tube with five amino functional groups, including  $\text{H}_2\text{N}(\text{CH}_3)$ ,  $\text{H}_2\text{N}(\text{CH}_2\text{CH}_3)$ ,  $\text{H}_2\text{N}(\text{COOH})$ ,  $\text{H}_2\text{N}(\text{CH}_2\text{COOH})$  and  $\text{H}_2\text{N}(\text{CH}_2\text{CN})$ . The most stable structures are shown in Fig. 3. We found that all the amino groups, except  $\text{NH}_2\text{COOH}$ , can be chemically adsorbed on the tube sidewall and covalently bonded with a boron atom, namely, forming a B–N bond. The B–N bond length ranges from 1.69 to 1.73 Å. The corresponding  $E_{\text{FC}}$  and charge transfer from the five adsorbates to  $\text{BC}_2\text{NNT}$  are listed in Table 2. The relative magnitude order of  $E_{\text{CF}}$  for different functional groups is as follows:

$$\text{H}_2\text{N}(\text{CH}_2\text{CH}_3) > \text{H}_2\text{N}(\text{CH}_3) > \text{NH}_3 > \text{H}_2\text{N}(\text{CH}_2\text{COOH}) \\ > \text{H}_2\text{N}(\text{CH}_2\text{CN}) > \text{H}_2\text{N}(\text{COOH}).$$

The largest  $E_{\text{CF}}$  belongs to the case of  $\text{H}_2\text{N}(\text{CH}_2\text{CH}_3)$  which is  $-14.2 \text{ kcal mol}^{-1}$ . This phenomenon may be explained by the fact that the  $-\text{CH}_2\text{CH}_3$  group is an electron donating functional and facilitated electron transfer to the tube surface. Furthermore, the charge transfer from the  $\text{H}_2\text{N}(\text{CH}_2\text{CH}_3)$  functional group to the  $\text{BC}_2\text{NNT}$  is about 0.249  $e$ ,



**Fig. 2** Models for two stable different functionalization of  $\text{BC}_2\text{NNT}$  by  $\text{NH}_3$  and related DOS

**Table 1** Chemical functionalization energy ( $E_{CF}$  in kcal mol<sup>-1</sup>), HOMO energies ( $E_{HOMO}$ ), LUMO energies ( $E_{LUMO}$ ), HOMO-LUMO energy gap ( $E_g$ ) and effective work function ( $\phi_{eff}$ ) of systems (Fig. 2) in eV

Configuration	$E_{CF}$	${}^aQ_T$ ( e )	$E_{HOMO}$	$E_{LUMO}$	$E_g$	$\phi_{eff}$	${}^b\Delta E_g$ (%)
BC <sub>2</sub> NNT	–	–	–5.41	–2.84	2.57	1.28	–
A	–2.8	0.013	–5.36	–2.76	2.60	1.30	1.1
B	–12.0	0.237	–5.06	–2.60	2.46	1.23	4.3

<sup>a</sup>  $Q_T$  is defined as the total Mulliken charge on the molecules

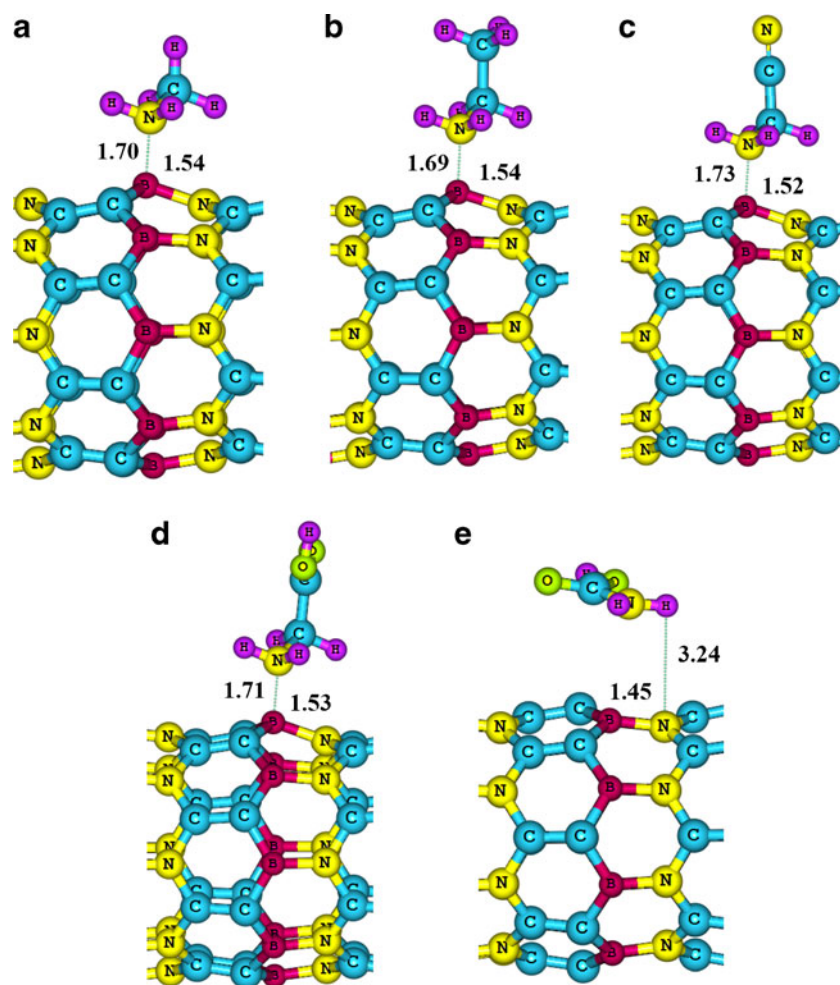
<sup>b</sup> Change of  $E_g$  of BC<sub>2</sub>NNT after functionalization

slightly larger than NH<sub>3</sub> group. This trend is also predicted in the case of –CH<sub>3</sub> so that in this case the  $E_{CF}$  is –12.9 kcal mol<sup>-1</sup> and a net charge of 0.240  $e$  is transferred from functional group to the BC<sub>2</sub>NNT. Unlike –CH<sub>3</sub> and –CH<sub>2</sub>CH<sub>3</sub>, the –CH<sub>2</sub>COOH and –CN are relatively strong electron-withdrawing functional groups. Thus, by replacing –H with the –CH<sub>2</sub>COOH and –CN groups, the charge transfer to the BC<sub>2</sub>NNT should be reduced, thereby weakening the interaction between the amino functional group and the BC<sub>2</sub>NNT. Calculated  $E_{CF}$  values for these cases are about –10.8 and –8.1 kcal mol<sup>-1</sup> and a net charge of 0.228 and 0.183  $e$  is transferred from H<sub>2</sub>N(CH<sub>2</sub>COOH) and H<sub>2</sub>N(CH<sub>2</sub>CN) to the

BC<sub>2</sub>NNT, respectively. For NH<sub>2</sub>COOH functional group, this molecule is only physically adsorbed on the tube with one N–H bond of NH<sub>2</sub>COOH directing toward a sidewall nitrogen atom, as shown in Fig. 3e. In this configuration, a net charge of about 0.136  $e$  transfers to the tube and its corresponding calculated  $E_{CF}$  value (Table 2) is about –1.8 kcal mol<sup>-1</sup>.

To verify the effects of the mentioned molecules adsorption on BC<sub>2</sub>NNT electronic properties, the DOSs of the functionalized–BC<sub>2</sub>NNT systems are calculated and Fig. 4 shows the DOS for representative systems. Table 2 summarizes the HOMO, LUMO, and  $E_g$  of different functionalized BC<sub>2</sub>NNT. After functionalization, the conduction and

**Fig. 3** Most stable configurations of chemically modified BC<sub>2</sub>NNT with the amino functional groups; (a) H<sub>2</sub>N(CH<sub>3</sub>), (b) H<sub>2</sub>N(CH<sub>2</sub>CH<sub>3</sub>), (c), H<sub>2</sub>N(CH<sub>2</sub>CN) (d) H<sub>2</sub>N(CH<sub>2</sub>COOH) and (e) H<sub>2</sub>N(COOH). Bonds are in Å



**Table 2** Chemical functionalization energy ( $E_{CF}$  in kcal mol<sup>-1</sup>), HOMO energies ( $E_{HOMO}$ ), LUMO energies ( $E_{LUMO}$ ), HOMO-LUMO energy gap ( $E_g$ ) and effective work function ( $\phi_{eff}$ ) of systems (Fig. 3) in eV

Functional component	$E_{CF}$	<sup>a</sup> $Q_T$ ( $ e $ )	$E_{HOMO}$	$E_{LUMO}$	$E_g$ (eV)	$\phi_{eff}$	<sup>b</sup> $\Delta E_g$ (%)
BC <sub>2</sub> NNT	–	–	–5.41	–2.84	2.57	1.28	–
H <sub>2</sub> N(COOH)	–1.8	0.136	–5.20	–2.77	2.43	1.21	–5.4
H <sub>2</sub> N(CH <sub>2</sub> CN)	–8.1	0.183	–5.22	–2.72	2.50	1.25	–2.7
H <sub>2</sub> N(CH <sub>2</sub> COOH)	–10.8	0.228	–5.06	–2.67	2.39	1.19	–7.0
H <sub>2</sub> N(CH <sub>3</sub> )	–12.9	0.240	–5.08	–2.59	2.49	1.24	–3.1
H <sub>2</sub> N(CH <sub>2</sub> CH <sub>3</sub> )	–14.2	0.249	–5.04	–2.59	2.45	1.22	–4.6

<sup>a</sup> $Q_T$  is defined as the total Mulliken charge on the adsorbed molecules

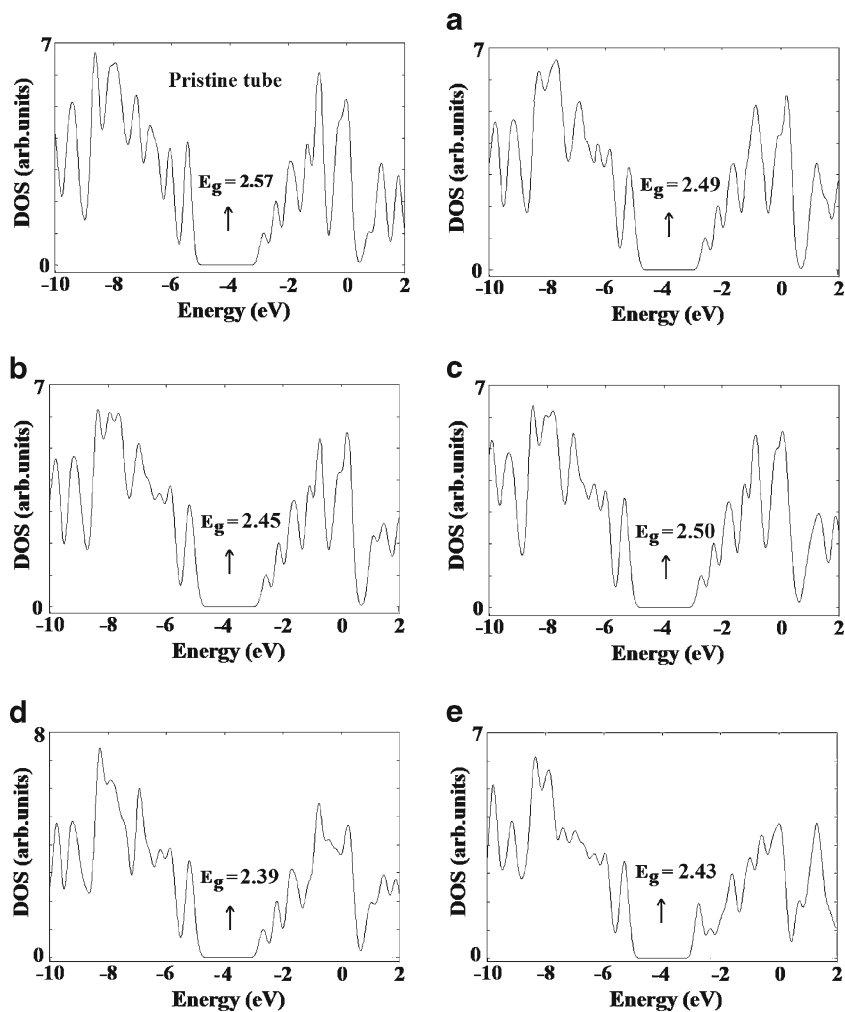
<sup>b</sup>Change of  $E_g$  of BC<sub>2</sub>NNT after functionalization

valence levels slightly shift to lower energies so that  $E_g$  changed very slightly between 0.07 and 0.18 eV and the contribution of functional groups is largely away from the Fermi level. It can be found that all functionalized-BC<sub>2</sub>NNTs are still semiconductors with a wide band gap close to that of the pristine BC<sub>2</sub>NNT.

Theoretical investigations have shown that introducing adsorbates on nanotube surface might effectively modify the

field emission properties [32], which is necessary to estimate the potential for the design of efficient field emission display. Thus, we analyze the modifications of the effective work function ( $\phi_{eff}$ ) due to amino functionalization on BC<sub>2</sub>NNT. Note that  $\phi_{eff}$  is defined as the energy difference between the Fermi level ( $E_F$ ) and the LUMO. Compared to the pristine BC<sub>2</sub>NNT ( $\phi_{eff}=1.28$  eV), we note that the amino adsorption can not alter significantly  $\phi_{eff}$  (ranged between

**Fig. 4** The DOS plots for pristine and amino functional group-modified BC<sub>2</sub>NNT. (a) H<sub>2</sub>N(CH<sub>3</sub>), (b) H<sub>2</sub>N(CH<sub>2</sub>CH<sub>3</sub>), (c) H<sub>2</sub>N(CH<sub>2</sub>CN) (d) H<sub>2</sub>N(CH<sub>2</sub>COOH) and (e) H<sub>2</sub>N(COOH)



1.19 and 1.25 eV). In short, chemical modification of BC<sub>2</sub>NNT with amino species can be supposed as some kind of “*harmless modification*”. On the other hand, the preservation of electronic properties of BC<sub>2</sub>NNTs coupled with the enhancement of solubility renders the chemical modification of BC<sub>2</sub>NNTs with either NH<sub>3</sub> or amino functional groups to be an effective way for the purification of BC<sub>2</sub>NNTs.

## Conclusions

We have studied chemical modification of a BC<sub>2</sub>NNT with NH<sub>3</sub> and amino groups of (H<sub>2</sub>N(CH<sub>3</sub>), H<sub>2</sub>N(CH<sub>2</sub>CH<sub>3</sub>), H<sub>2</sub>N(COOH), H<sub>2</sub>N(CH<sub>2</sub>COOH) and H<sub>2</sub>N(CH<sub>2</sub>CN)) using DFT calculations. It was found that NH<sub>3</sub> can be attached to boron atom of the BC<sub>2</sub>NNT with functionalization energy of  $-12.0 \text{ kcal mol}^{-1}$ . For chemically modified BC<sub>2</sub>NNT with various functional groups, the functionalization energies can be correlated with the trend of relative electron-withdrawing or -donating capability of the adsorbates. The functionalization energies are calculated to be in the range of  $-1.8$  to  $-14.2 \text{ kcal mol}^{-1}$ , and their relative magnitude order is found as follows: H<sub>2</sub>N(CH<sub>2</sub>CH<sub>3</sub>) > H<sub>2</sub>N(CH<sub>3</sub>) > NH<sub>3</sub> > H<sub>2</sub>N(CH<sub>2</sub>COOH) > H<sub>2</sub>N(CH<sub>2</sub>CN) > H<sub>2</sub>N(COOH). The calculated DOSs show that the functionalization of BC<sub>2</sub>NNT with these functional groups can be generally classified as a certain type of “*electronically harmless modification*”. In other words, the electronic properties of the BC<sub>2</sub>NNT are negligibly changed by the chemical functionalization and may be an effective way of BC<sub>2</sub>NNTs purification.

## References

- Iijima S (1991) Nature 354:56–58
- Sun SL, Hu YY, Xu HL, Su ZM, Hao LZ (2012) J Mol Model 18:3219–3225
- Politzer P, Murray JS, Lane P, Concha MC, Jin P, Peralta-Inga Z (2005) J Mol Model 11:258–264
- Chelmecka E, Pasterny K, Kupka T, Stobiński L (2012) J Mol Model 18:2241–2246
- Redlich P, Loeffler J, Ajayan PM, Bill J, Aldinger F, Rühle M (1996) Chem Phys Lett 260:465–470
- Zhang Y, Gu H, Suenaga K, Iijima S (1997) Chem Phys Lett 279:264–269
- Zhang Y, Suenaga K, Colliex C, Iijima S (1998) Science 281:973–975
- Rossato J, Baierle RJ (2007) Phys Rev B 75:235401–235407
- Pan H, Feng YP, Lin JY (2006) Phys Rev B 73:035420–035425
- Hernandez E, Goze C, Bernier P, Rubio A (1998) Phys Rev Lett 80:4502–4505
- Sen R, Satishkumar BC, Govindaraj A, Harikumar KR, Gargi R, Zhang JP, Cheetham AK, Rao CNR (1998) Chem Phys Lett 287:671–676
- Redlich P, Loeffler J, Ajayan PM, Bill J, Aldinger F, Rühle M (1996) Chem Phys Lett 26:465–470
- Bai XD, Guo JD, Yu J, Wang EG, Yuan J, Zhou WZ (2000) Appl Phys Lett 76:2624–2626
- Raidongia K, Jagadeesan D, Upadhyay-Kahaly M, Waghmare UV, Pati SK, Eswaramoorthy M, Rao CNR (2008) J Mater Chem 18:83–90
- Niyogi S, Hamon MA, Hu H, Zhao B, Bhowmik P, Sen R, Itkis ME, Haddon RC (2002) Accounts Chem Res 35:1105–1113
- Ahmadi Peyghan A, Omidvar A, Hadipour NL, Bagheri Z, Kamfiroozi M (2012) Physica E 44:1357–1360
- Beheshtian J, Peyghan AA, Bagheri Z (2012) Sens Actuators B: Chem 171–172:846–852
- Beheshtian J, Baei MT, Peyghan AA, Bagheri Z (2012) J Mol Model 18:4745–4750
- Beheshtian J, Bagheri Z, Kamfiroozi M, Ahmadi A (2012) Struct Chem 23:653–657
- Beheshtian J, Soleymanabadi H, Kamfiroozi M, Ahmadi A (2012) J Mol Model 18:2343–2348
- Beheshtian J, Peyghan AA, Bagheri Z (2012) Physica E 44:1963–1968
- Zhou Z, Zhao J, Gao X, Chen Z, Yan J, Schleyer PR, Morinaga M (2005) Chem Mater 17:992–1000
- Schmidt M et al (1993) J Comput Chem 14:1347–1363
- Moradi M, Peyghan A, Bagheri Z, Kamfiroozi M (2012) J Mol Model 18:3535–3540
- Beheshtian J, Peyghan A, Bagheri Z, Kamfiroozi M (2012) Struct Chem 5:1567–1572
- Beheshtian J, Peyghan AA, Bagheri Z (2012) Comput Theor Chem 992:164–167
- Wanbayor R, Ruangpornvisuti V (2012) Appl Surf Sci 258:3298–3301
- Beheshtian J, Peyghan AA, Bagheri Z (2012) Appl Surf Sci 258:8171–8176
- Tomić S, Montanari B, Harrison NM (2008) Physica E 40:2125–2127
- O’Boyle N, Tenderholt A, Langner K (2008) J Comput Chem 29:839–845
- Olmsted J, Williams GM (1997) Chemistry: the molecular science. WCB, Iowa
- Zhang J, Wang X, Yang W, Yu W, Feng T, Li Q, Liu X, Yang C (2006) Carbon 44:418–422