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Effect of adsorption sensitivity of armchair single-walled BN nanotube toward thiocyanate anion: A systematic evaluation of length and diameter effects



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ABSTRACT

The first-principles calculations to investigate the adsorption behavior of thiocyanate anion (SCN⁻) on the external surface of H-capped (6, 0), (3, 3), and Al and Ga doped (3, 3) single-walled boron nitride nanotubes (SWBNNTs) has been performed. Binding energy and the equilibrium distance corresponding to the most stable state of SCN⁻/(3, 3) BNNT is found to be -1.747 eV and 1.546 A, respectively, which can represent mainly a polar covalent bond. The calculation results have shown that both doped aluminum and gallium can enhance the adsorption energy of SCN⁻ into the (3, 3) BNNTs. For the SCN⁻ /BNNT complexes, the energy gaps, NBO, dipole moments, natural atomic orbital occupancies and global indices have been computed using DFT theoretical method at B3LYP level and $6-31G^{**}$ basis set. Finally, a novel type of the adsorbent that can be used to remove of SCN⁻ anion has been reported.

1. Introduction

After the discovery of carbon nanotubes (CNT) by Ijima [1], scientists investigated new properties of this fascinating novel material by numerous theoretical and experimental research projects [2,3]. Furthermore, the investigations have detected the tubular structure of BNNT which has initially stabilized by the calculations [4] and subsequently synthesized [5]. Stable structures of non-carbon based nanotubes in which boron nitride nanotubes (BNNT) are among the most important ones have very interesting characteristics [6]. After that, a rapidly growing number of experimental and theoretical investigations have been performed to study the structural and electronic properties of the BNNT [7-10]. In contrary to CNTs, which have metal or semiconductor characteristics based on the tubular diameter and chirality, the BNNT has always the behavior of semiconductors, which is independent of the structural factors [11]. Previous studies have demonstrated the influence of doped atoms on the electronic and structural properties of BNNT [12,13]. The functionalized or doped BNNTs, which exhibit dramatic changes in electronic properties to their pristine counterparts, further enlarge the application in the nanomolecular range. It was found that either single boron or single nitrogen atom substituted in the C-doped BNNTs has induced spontaneous magnetization [14]. An insulator-to-semiconductor transition has been observed on the successfully synthesized F-doped BNNTs [15], also the effect of doped fluorine on the structural and electronic properties of the (5, 5) BNNTs has been theoretically investigated [16]. Recently, Zhang et al. [17] have studied the adsorption of the H₂ on the Rh-, Ni-, and Pd-doped SWBNNTs. Moreover, Zhang et al. [18] have investigated the adsorption of O_2 on the pure and C-doped (5, 5) armchair BNNTs via first-principles theory based on DFT calculations. They reported that the interaction of C-doped on BNNTs can improve the O2 storage capacity. Electronic conductance changes in BNNTs upon exposure to gas molecules [19]. A lot of studies have been indicated the influence of doping and impurities on the adsorption behavior of BNNTs [20,21]. Based on this feather, they can be served as nanotube molecular sensors [22,23]. Furthermore, the adsorption behavior of dimethyl and trimethyl amine molecules on borophene nanotube has been studied using DFT method [24]. Recently, the electronic properties of bismuthene nanotube (Bi-NT) (7, 0) for detection of V-series vapors have been also studied using SIESTA theoretical package [25]. Moreover, the

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Fig. 1. Schematic structure of (6, 0) and (3, 3) BNNTs, Al-, and Ga-doped (3, 3) BNNTs with their density of state plots.

adsorption behavior of hazardous phosgene gas and amine vapors on antimonene nanotube [26] and black phosphorene nanotubes [27] have investigated using first-principles method. On the other hand, the reaction between \mbox{CS}_2 and \mbox{NH}_2^{-} species and also reaction between CH₃SCN and e- generate thiocyanate anion (SCN⁻) [28], and it can be found in interstellar ice and dust clouds [29]. SCN^- is one of the pseudohalogens arise from several sources such as industrial processes, e.g. hydrometallurgy, electroplating, fabric dyeing, and photofinishing, tabacoo smoke, diet and even car exhaust, poses potential threat to environment and human body because of its cumulative effect [30]. Also, a fade away or reducing SCN⁻ in the human body [31] is of high prominence regarding the human host defense system [32–36]. It may happen via biosynthesis of hypothiocyanite by a lactoperoxidase [37-40]. Since SCN⁻ has attracted the interests of environmental scientists, the information about how different nano surfaces interact with SCN⁻ seems to be important. In this research, the adsorption behaviors of the SCN⁻ on the pristine zigzag (6, 0), armchair (3, 3), Al-doped and Ga-doped (3, 3) BNNTs have been studied in which the ends of the BN nanotubes are saturated by hydrogen atoms. We hope that our results provide experiments with useful information on designing sensors employing the BN nano-materials

2. Computational methods

All the geometry optimizations and energy calculations are performed using the Gaussian 03 program package [41] using density functional theory (DFT) method at B3LYP quantum chemical level and 6-31G** basis orbital set [42-44]. The hydrogenated (6, 0), (3, 3), Sidoped (3,3) Al-doped (3,3) and Ga-doped (3,3) zigzag BNNTs have 72 $(B_{30}N_{30}H_{12})$, 66 $(B_{27}N_{27}H_{12})$, 66 $(B_{26}N_{27}H_{12}Si)$, 66 $(B_{26}N_{27}H_{12}Al)$, and (B26N27H12Ga) atoms, respectively. To calculate total energies, selfconsistent field (SCF) and electron density calculations are performed with a convergence criterion of 1.0×10^{-6} Hartree. In geometry optimizations, the cut-off values for force and displacement are 0.00045 Hartree/Bohr and 0.0018 Bohr, respectively. The binding energy (Ebin) of an SCN⁻ to the BNNT has determined using the following equations:

$$\Delta E_{bin} = E_{BNNT-SCN^{-}} - \left(E_{BNNT} + E_{SCN^{-}}\right) \tag{1}$$

$$\Delta E_{\text{bin}} = E_{Al-BNNT-SCN^{-}} - \left(E_{Al-BNNT} + E_{SCN^{-}}\right)$$
⁽²⁾

$$\Delta E_{\text{bin}} = E_{Ga-BNNT-SCN^{-}} - \left(E_{Ga-BNNT} + E_{SCN^{-}}\right)$$
(3)

Where E(BNNT- SCN) is the total energy of the BNNTs interacting with the SCN $\bar{}$. E_{BNNT} is the total energy of the pure BNNT and E_{SCN} is the total energy of an isolated SCN⁻. E_{Al-BNNT} and E_{Ga-BNNT} are the total energies of the Al- and Ga-doped BNNTs, respectively. EAI-BNNT-SCN and E_{Ga-BNNT-SCN}⁻ are is the total energies of the Al- and Ga-doped BNNTs interacting with the SCN⁻. Natural charge analysis with full NBO calculations was performed using the DFT theoretical method at B3LYP level and 6-31G** basis set to optimize the structures. The electrophilicity concept was stated for the first time in 1999 by Parr et al. [45]. μ is defined according to the following equation [46]:

$$\mu = (E_{HOMO} + E_{LUMO})/2 \tag{4}$$

where E_{HOMO} is the energy of the Fermi level (E_F) and E_{LUMO} is the first eigenvalue of the valance band. Electronegativity (χ) is defined as the negative of chemical potential (μ), as follows: $\chi = -\mu$. Furthermore, chemical hardness (η) can be approximated using the Koopmans' theorem [47,48] as $\eta = (E_{LUMO} - E_{HOMO})/2$. Softness (S) and electrophilicity index (ω) are defined as the following equations, respectively. 5)

$$S = 1/2\eta \tag{5}$$



Fig. 2. MEP maps for both zigzag and armchair BNNTs.

Table 1

Calculated bond length (Å), adsorbate-surface distance D/Å, binding energy E_{bin}/eV , HOMO energies (E_{HOMO}/eV), LUMO energies (E_{LUMO}/eV), dipole moment ($D_M/Debye$), and HOMO–LUMO energy gap (E_g/eV) for the pure BNNTs.

Property	(3,3) BNNT	(4,4) BNNT	(6,0) BNNT	(8,0) BNNT	Ι	п	III	IV
R _{Al-N1} ∕ Å	1.448	1.451	1.460	1.449	1.563	1.555	1.550	1.540
R _{Ga−N1} / Å	1.460	1.455	1.455	1.454	1.547	1.538	1.576	1.537
R _{N1-Al-N2} /°	-	-	-	-	1.554	1.558	1.546	1.566
R _{N1-Ga-N2} /°	-	-	-	-	1.624	1.624	1.623	1.610
R _{SCN-BNNT} /Å	-	-	-	-	1.178	1.178	1.178	1.182
R _{C -S} / Å	5.012	5.407	4.195	6.412	5.490	6.661	4.289	5.119
D _M /Debye	0.008	0.009	7.936	11.867	11.69	35.43	32.09	31.98
E _{HOMO} /eV	-6.48	-6.43	-6.45	-6.47	-3.21	-3.23	-3.11	-2.79
E_{LUMO} /eV	-0.11	-0.14	-2.03	-1.08	2.00	0.93	2.32	0.65
E_g /eV	6.37	6.29	4.42	5.39	5.21	4.16	5.43	3.44
$\Delta E_g / \%$	-	-	-	-	17.17	22.82	14.75	22.17
I/eV	6.48	6.43	6.45	6.47	3.21	3.23	3.11	2.79
A /eV	0.11	0.14	2.03	1.08	-2.00	-0.93	-2.32	-0.65
η /eV	3.18	3.15	2.21	2.70	2.61	2.08	2.72	1.72
μ /eV	-3.30	-3.29	-4.21	- 3.78	-0.61	-1.15	-0.40	-1.07
S / eV^{-1}	0.16	0.16	0.23	0.18	0.19	0.32	0.18	0.29
ω/eV	1.71	1.72	4.01	2.64	0.23	0.32	0.03	0.33



Fig. 3. The optimized structure for the most stable configuration (N-side) of (a) SCN⁻/(6, 0) BNNTs and (b) SCN⁻/(3, 3) BNNTs complexes.



Fig. 4. The optimized structure for the most stable configuration (N-side) of (a) SCN⁻/Al-doped (3, 3) BNNTs and (b) SCN⁻/Ga-doped (3, 3) BNNTs complexes.

 $\omega = \mu^2/2\eta$

(6) **3. Results and discussion**

3.1. Adsorption of SCN^{-} on the pristine (6, 0) and (3, 3) BNNTs

Firstly, the structure of SCN⁻, pristine BNNTs including *zigzag* (6, 0) and *armchair* (3, 3) BNNT have been optimized for the anion adsorption. Several adsorption configurations of SCN⁻ binding from its N

Table 2

Calculated bond length (Å), adsorbate-surface distance D/Å, binding energy E_{bin}/eV , HOMO energies (E_{HOMO}/eV), LUMO energies (E_{LUMO}/eV), dipole moment ($D_M/Debye$), and HOMO–LUMO energy gap (E_g/eV) for the SCN⁻ interacting with the pristine Al- and Ga-doped (3, 3) BNNTs.

Property	SCN ⁻	Al (3,3)BNNT	Ga(3,3)BNNT	Х	Z
R _{Al-N1} ∕ Å	-	1.802	-	1.881	_
R _{Ga−N1} / Å	-	-	1.853	-	1.923
R _{N1-Al-N2} /°	-	114.37	-	103.28	-
R _{N1-Ga-N2} /°	-	-	113.86	-	102.94
R _{SCN-BNNT} /Å	-	-	-	1.875	1.906
R _{C -S} / Å	1.676	-	-	1.612	1.615
$R_{C \equiv N} / Å$	1.181	-	-	1.187	1.186
Diameter/Å	-	4.12	4.24	4.246	4.253
D _M /Debye	7.480	1.469	1.309	29.73	29.79
E _{HOMO} /eV	-0.41	-6.44	-6.45	-3.55	-3.60
E_{LUMO} /eV	7.41	-1.65	-2.13	2.42	2.40
E_g / eV	7.82	4.79	4.32	5.97	6.00
$\Delta E_g /\%$	-	-	-	24.63	38.89
I/eV	0.41	6.44	6.45	3.55	3.60
A /eV	-7.41	1.65	2.13	-2.42	-2.40
η /eV	3.91	2.40	2.16	2.99	3.00
μ /eV	3.50	-4.04	-4.29	-0.56	-0.6
S / eV^{-1}	0.13	0.21	0.23	0.17	0.17
ω /eV	1.57	3.40	4.26	0.05	0.06

head to the B atom of *zigzag* and *armchair* BN nanotubes on its surface have been considered, as shown in Fig. 1. To explore the interaction mechanism between SCN⁻ and the BNNTs, we investigated molecular electrostatic potential (MEP) maps for these processes, where the positive and negative charges over the boron and nitrogen atoms are represented by the blue and red colors (see Fig. 2). In previous reports, it has been shown that the adsorption of SCN⁻ from its N head is much more stable than the adsorption from its S head on the different surfaces of nanotubes and nano-cages [29,30,32].

The optimized geometries of (6, 0) and (8, 0) *zigzag* and (3, 3) and (4, 4) *armchair* of pristine BNNTs for B1–N1 bond length were found to be about 1.460 Å, 1.449 Å, 1.448 Å, and 1.451 Å, and the diameter of the nanotubes about 4.195 Å, 6.412 Å, 5.012 Å, and 5.407 Å, respectively. The equilibrium distance in each case is summarized in Table 1.

The results of calculations for the potential energy surfaces for the band length of SCN⁻ from BN nanotube with different lengths and diameters are reported in Table 1. The effects of the tube diameter and length on the stability of BN nanotubes interacting with SCN⁻ molecule are interesting, as with increases of tube diameter and length decreases in the stability of these systems are observed. In general, SCN⁻ molecules are strongly bound to the surface of BN nanotubes and the nanotube-molecules interactions can be recognized as a polar covalent bond. The most stable configuration of SCN⁻ from its nitrogen head on the (3, 3) *armchair* BNNT is the B site, i.e., the perpendicular approach of SCN⁻ with the nitrogen Lewis base on BNNT wall, which is defined as the π -hole bonds [49,50]. Studies on the bonding



Fig. 5. Charge distribution of HOMO and LUMO orbitals on the (3, 3) BNNTs, Al-, and Ga-doped (3, 3) BNNTs loaded with one SCN⁻.



Fig. 6. TDOS plots for both zigzag and armchair BNNTs.

comportments indicate that the adsorption energy for SCN⁻ on the extern surface of pristine (6, 0) and (8, 0) *zigzag* and (3, 3) and (4, 4) *armchair* BNNTs for the most stable configuration (N-side) are about -1.661 eV, -1.440 eV, -1.747 eV, and -1.508 eV, and the equilibrium distance between the closet atoms of these species are 1.566 Å, 1.588 Å, 1.546 Å, and 1.554 Å, respectively (Fig. 3).

Addition of extra diffuse function leads to a nominal impact on the E_{bin} values in the interaction between the SCN⁻ and the BN nanotube. The values of E_{bin} for the pristine (6, 0) zigzag and (3, 3) armchair BNNTs with the SCN⁻ are -1.470 and -1.498 eV obtained, respectively, at B3LYP/6-31 + G^{**} level of theory. To see the effect of dispersion contribution in the interaction between the SCN⁻ and the BN nanotube, the E_{bin} values were also computed by the B3LYP-D functional for the most stable complexes. The interaction of pristine (6, 0)zigzag and (3, 3) armchair BNNTs with the SCN⁻have the values of -1.899 and -1.918 eV, respectively. The B3LYP-D functional represents a little difference in the prediction of absorption energy between the SCN⁻ and the BN nanotube. The slight difference of E_{bin} for the different BNNT configurations indicate that the binding energies of SCN^{-} on (3, 3) armchair BNNT is more stable than (6, 0) *zigzag* BNNT. It is obvious that after perfect optimization of the energetically favorable configuration, the binding energy is significantly changed comparing to the single point energy (SPE) calculations. Highlighting that SPE cannot accurately suggest the adsorption nature between two species [29,32]. Moreover, the results have shown that the interaction of SCN⁻ with (3, 3) armchair BNNT surface has the stronger binding energy comparing to the other BNNTs. Baei and Varasteh Moradi [51] reported that the binding energy for SCN^- is a weak physisorption on (6, 0), (7, 0), (8, 0), and Ga-doped (6, 0) BNNTs surfaces, however, the reaction between SCN^- and BNNTs is an exothermic process and possible. Natural charge analysis has shown that in these configuration 0.45 e and 0.46 e charges have transferred from SCN^- to the (6, 0), and (3, 3) BNNTs. These findings have suggested the attachment of the strong interaction (polar covalent bond) in these adsorption processes.

3.2. Adsorption of SCN^- on the Al- and Ga-doped (3,3) BNNTs

To examine the effect of metal doping on the adsorption behavior of the most stable configuration of (3, 3) BNNTs system, the nitrogen and boron atoms of (3, 3) BNNT were substituted by Al and Ga atoms. Afterwards, the interaction of perpendicularly approaching of SCNdirectly above Al and Ga atoms of Al- and Ga-doped (3, 3) BNNT were studied. The results of these interactions on Al- and Ga-doped (3, 3) BNNTs, were represented in Fig. 4.

A similar trend was considered for Al- and Ga- doped (3, 3) BNNT systems to find the approximate stable approach. Thus, the potential energy surface (PES) for both cases, including SCN- approaching to the Al- and Ga-doped (3, 3) BNNTs have been obtained. The average Ga-N and Al-N bond lengths are about 1.853 A and 1.802 A, respectively [52,53]. The N-Al-N and N-Ga-N bond angles in Al- and Ga-doped (3, 3) BNNTs have calculated 114.37° and 113.86°, respectively (see Table 2).

Considering PES results, it reveals that there exists the attractive



Fig. 7. TDOS plots of the SCN⁻interacting with BNNTs.

potential in all pathways with a well maximum about -3.694 and -3.528 eV for Al- and Ga-doped BNNT/SCN⁻ systems, respectively. While, the energy of SCN⁻ binding which have approached from its Sside to the Al- and Ga-doped (3, 3) BNNT systems were obtained -2.782 eV and -2.512 eV with an equilibrium distance (D) of 2.31 Å and 2.38 Å. It seems that because of Al- and Ga-doped atoms on (3, 3) BNNT, the binding energy significantly increase in comparison with pristine (6, 0) and (3, 3) BNNT systems which reflect the significant role of Al and Ga atoms in adsorption behavior of BNNTs. It should be note that the SCN⁻ binding from its N-side has provided higher adsorption energy than the SCN⁻ binding from its S-side. For the Al-doped BNNT system, the equilibrium Al-N distance and binding energy has calculated to be 1.873 Å and -3.694 eV, respectively. For the Ga-doped BNNT system, the corresponding values have calculated to be 1.867 Å and -3.528 eV. The computations have indicated that the interaction between SCN⁻ and Al-doped BNNT is stronger than the interaction between SCN⁻ and Ga-doped BNNT [27]. Charge analyses for both corresponding complexes have shown that the charge transferred from Al-doped and Ga-doped (3, 3) BNNTs to SCN⁻ were 0.706 e and 0.702 e, respectively.

3.3. Electronic energies and frontier molecular orbitals

The frontier molecular orbitals, namely, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) in the SCN⁻ and in pristine (6, 0), (3, 3) BNNTs, Ga-doped and

Al-doped (3, 3) BNNTs have had the most important description in determining chemical reactivity and spectral properties of these structures (Tables 1 and 2). Tables 1 and 2 present the results of DFT computations including the LUMO and HOMO energies for the most stable configuration of SCN⁻ adsorption on (3, 3) BNNT and Al-doped (3, 3) BNNT. The band gaps (Eg) of pristine (3, 3) BNNT and (6, 0) BNNT were 6.37 eV and 4.42 eV, and the bond gaps of Al-doped and Ga-doped (3, 3) armchair BNNTs were 4.79 eV and 4.32 eV, respectively. These findings have shown that when the SCN⁻ absorbed on (3, 3) BNNT and Al-doped (3, 3) BNNT, ELUMO and EHOMO for whole systems have reduced, therefore, both groups of occupied and unoccupied molecular orbital are lower and more stable than those of (3, 3) BNNT, and Al-doped (3, 3) BNNT, respectively (Fig. 5). It is found that the HOMO orbital for pristine (3,3) armchair BNNT was localized on N atom in end and the opposite end of the nanotube axes which corresponds to the lone pair of electron on the nitrogen atoms. While the LUMO orbital has more localized on B atoms and has more slightly distributed throughout the B-N orbitals. In SCN⁻, HOMO and LUMO orbitals have uniformly distributed throughout the S-C-N orbitals (Fig. 4). The distribution of frontier orbital in Al-doped (3, 3) BNNTs systems exhibit that HOMO was localized on the S-C-N orbitals and also slight aggregation on more electronegative nitrogen atoms at the center of the nanotube axis, which was corresponded to the lone pair of electron on the nitrogen atom. Also, the LUMO was more localized on boron and nitrogen atoms in the edge and end of the BNNTs (Fig. 5). The density of state (DOS) plot (with FWHM=0.3 eV) of all these configurations have been obtained using DFT theoretical method at B3LYP level and 6-31G** basis set (Figs. 6 and 7). The GaussSum program was used to calculate the DOS [54]. These spectra have clearly shown the value of energy gap and Fermi energy of all contributing materials and their complexes as well. The DOS demonstrates that the E_{bin} of SCN⁻on doping metals is a strong hybridization between the nitrogen atom of molecule and the aluminum, gallium atoms on BNNT sidewall. Therefore, the significant differences in the E_g of the pristine Al- and Gadoped (3, 3) BNNTs are about 4.79 and 4.32 eV, and for SCN⁻/Al-, Gadoped (3, 3) BNNT are 5.97 and 6.00 eV, respectively. These results clearly reveal a strong charge transfer of Al-, Ga-doped (3,3) BNNT to SCN⁻molecule. Our calculations reveal the stability of Al- and Gadoped on BNNT that may propose an acceptable sensor for detecting the SCN⁻molecule.

3.4. Quantum molecular descriptors

The quantum molecular descriptors for the SCN⁻, pristine (6, 0) BNNT, pristine (3,3) BNNT, Al-doped (3,3) BNNT, Ga-doped (3,3) BNNT, SCN⁻/Al-doped (3, 3) BNNT, and SCN⁻/Ga-doped (3, 3) BNNT models have been calculated and summarized in Tables 1 and 2. It seems that the energy gaps (E_{LUMO} - E_{HOMO}) for SCN⁻/Al-doped (3, 3) BNNT and SCN⁻/Ga-doped (3, 3) BNNT models, have decrease. This decrease of energy gaps when SCN⁻ adsorption has led to increase the reactivity of the complexes, and has shown the charge occurs between the SCN⁻ molecule and pristine (3,3) BNNT sidewalls. Decrease in global hardness, energy gap, and ionization potential and also, increase in electron affinity and electrophilicity of the complexes when SCNadsorption, have shown the charge transfer from SCN⁻ molecule (nucleophilic agent) to the nanotube models (electrophilic agent) [55-57].

4. Conclusions

In this research, SCN⁻ adsorption on the surface of zigzag and armchair configurations of (6, 0) BNNT, (3, 3) BNNT, Al-doped (3, 3) BNNT, and Ga-doped (3, 3) BNNT have been studied using first-principles computations. The interaction between SCN^- and (6, 0), (3, 3) BNNTs for the most stable configurations, are found to be -1.661 eVand -1.747 eV, which is an evidence of strong interaction between SCN⁻ and these two configurations. The obtained results have shown that the transfer of charge from SCN- to BNNTs is a significant factor in the change of the electrical conductance of the BN nanotubes. Also, Ga and Al doping on (3, 3) BNNT can noticeably increase the adsorption capability of these systems, indicating that Al- and Ga-doped (3, 3) BNNTs are the suitable systems to be applied as a detector of SCN⁻. The decrease of HOMO-LUMO energy gaps, ionization potential, and global hardness when the adsorption of SCN- on BNNTs surface due to the increase of chemical reactivity also lead to a decrease of stability in these systems.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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