

# Adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> on Boron Nitride Nanotubes: DFT Study

A. A. El-Barbary<sup>1,2\*</sup>, Kh. M. Eid<sup>1,3</sup>, M. A. Kamel<sup>1</sup>, H. O. Taha<sup>1</sup>, G. H. Ismail<sup>1,2</sup>

<sup>1</sup>Physics Department, Faculty of Education, Ain Shams University, Cairo, Egypt

<sup>2</sup>Physics Department, Faculty of Science, Jazan University, Jazan, KSA

<sup>3</sup>Bukairiyah for Science, Qassim University, Qassim, KSA

Email: [\\*ahla\\_eg@yahoo.co.uk](mailto:ahla_eg@yahoo.co.uk)

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## Abstract

The adsorption of CO, CO<sub>2</sub>, NO and CO<sub>2</sub> gas molecules on different chiralities of single boron nitride nanotubes (BNNTs) is investigated, applying the density functional theory and using basis set 6 - 31 g (d,p). The energetic, electronic properties and surface reactivity have been discussed. We found that the best BNNT for adsorbing the CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules is (5,0) BNNT with adsorption energy of -0.27, -0.37 eV, -0.23 and -0.92 eV, respectively. Also, the electronic character of (5,0), (9,0), (5,5) and (6,6) BNNTs is found to be not affected by the adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules. It is found that the dipole moments of zig-zag (5,0) and (9,0) BNNTs are always higher than the arm-chair (5,5) and (6,6) BNNTs. Also, it is noticed that the highest dipole moment is for (9,0) BNNT.

## Keywords

BN Nanotubes, DFT, Gas Sensors

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## 1. Introduction

The BN nanotubes are interesting materials for technological applications because they can be used as hydrogen storage [1]-[3], catalysis [4] [5], molecular sensing [6]-[8], field emission displayers [9]-[11] and switching behaviors [12]. The emission of carbon and nitrogen oxides (CO, CO<sub>2</sub>, NO and NO<sub>2</sub>) results from the combustion of fossil fuels, contributing to both smog and acid precipitation, and affect both terrestrial and aquatic ecosystems [13]. Chemical gases CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules are strongly toxic to human beings and animals as they inhibit the consumption of oxygen by body tissues. Because they are colorless, odorless and tasteless the

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\*Corresponding author.

gas sensors with high sensitivity to their presence are very interesting.

Although many efforts have been made to use catalysts to reduce the amount of carbon or nitrogen oxides in the air [14]-[20], an efficient method of sensing and removing carbon and nitrogen oxides is still required. In the present study, our aim is to study the adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules on boron nitride nanotubes with different diameters and different chiralities. The structural characteristics of adsorbed CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules on BNNTs are investigated and the corresponding adsorption energies are computed. In order to find the preferred adsorption site, different positions are investigated. The energy gap and HOMO-LUMO energies are reported.

## 2. Computational Methods

All calculations were performed with the density functional theory as implemented within G03W package [21]-[27], using B3LYP exchange-functional and applying basis set 6 - 31 g (d,p). All Pristine BN nanotubes (5,0) and (9,0), (5,5) and (6,6) are fully optimized with spin average as well as the adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules. The adsorption energies of gas molecules on BNNTs ( $E_{\text{ads}}$ ) [28] are calculated from the following relations:

$$E_{\text{ads}} = E_{(\text{nanotube}+\text{gas molecules})} - E_{\text{nanotube}} - E_{\text{gas molecules}}$$

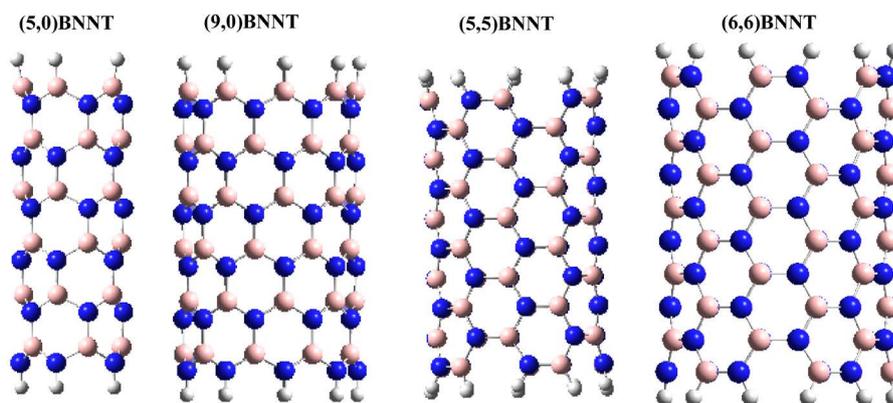
where  $E_{(\text{nanotube}+\text{gas molecules})}$  is the total energy of nanotube and gas molecules,  $E_{\text{nanotube}}$  is the energy of the BN nanotube, and  $E_{\text{gas molecules}}$  is the energy of gas molecules.

## 3. Results and Discussion

We will investigate the adsorption of gas molecules, CO, CO<sub>2</sub>, NO and NO<sub>2</sub> on four BN nanotubes with different chiralities and diameters (5,0) BNNT, (9,0) BNNT, (5,5) BNNT and (6,6) BNNT as shown in **Figure 1** and **Table 1**.

### 3.1. Adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> Gas Molecules on BNNTs

The CO and CO<sub>2</sub> gas molecules are vertically adsorbed on different three positions of (5,0), (9,0), (5,5) and (6,6)



**Figure 1.** The fully optimized structures of (5,0), (9,0), (5,5) and (6,6) BNNTs. Nitrogen atoms (blue), Boron atom (pink) and hydrogen atoms (white).

**Table 1.** The configuration structures of the studied BNNTs.

System	Configuration Structures
(5,0) BNNT	B <sub>30</sub> N <sub>30</sub> H <sub>10</sub>
(9,0) BNNT	B <sub>54</sub> N <sub>54</sub> H <sub>18</sub>
(5,5) BNNT	B <sub>50</sub> N <sub>50</sub> H <sub>20</sub>
(6,6) BNNT	B <sub>60</sub> N <sub>60</sub> H <sub>24</sub>

BNNTs: above a boron or nitrogen atom (atom site), above a bond between boron and nitrogen atoms (bond site) and above a center of a hexagon ring (vacant site). The calculated adsorption energies of CO and CO<sub>2</sub> gas molecules are listed in **Table 2**. It is found that the best BNNT for adsorbing the CO and CO<sub>2</sub> gas molecules is (5,0) BNNT with adsorption energy of  $-0.27$  and  $-0.37$  eV, respectively. All sites (atom, bond and vacant) have equivalent tendency for adsorbing the CO and CO<sub>2</sub> gas molecules on the (5,0) BNNT. Therefore, one can conclude that the best BNNT as gas sensors for CO and CO<sub>2</sub> gas molecules is (5,0) BNNT.

Also, the NO and NO<sub>2</sub> gas molecules are vertically adsorbed on different three positions of (5,0), (9,0), (5,5) and (6,6) BNNTs: above an atom site, above a bond site and above a vacant site. The calculated adsorption energies of NO and NO<sub>2</sub> gas molecules are listed in **Table 3**. It is found that the best adsorption energies of NO and NO<sub>2</sub> gas molecule are on the (5,0) BNNT. All sites (atom, bond and vacant) have equivalent tendency for adsorbing the NO gas molecule on the (5,0) BNNT with energy of  $\sim -0.2$  eV, however the best adsorption site for NO<sub>2</sub> gas molecule found to be above the bond site with adsorption energies  $-0.92$  eV. Therefore, one can conclude that the best BNNT as gas sensors for NO and NO<sub>2</sub> gas molecules is (5,0) BNNT.

From **Table 2** and **Table 3**, one can conclude that the adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules is independent on the diameters of BNNTs and the best adsorbed tubes are the (5,0) BNNTs.

### 3.2. Energy Gaps of Adsorbed CO, CO<sub>2</sub>, NO and NO<sub>2</sub> Gas Molecules on BNNTs

From **Table 4** and **Table 5**, it is found that the adsorption of CO and CO<sub>2</sub> gas molecules on BNNTs does not affect the electronic character of the BNNTs, however the adsorption of NO and NO<sub>2</sub> gas molecules on BNNTs is reduced the band gap the BNNTs to  $\sim 3$  eV.

**Table 2.** The calculated adsorption energies ( $E_{\text{ads}}$ ) of CO and CO<sub>2</sub> on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. All energies are given by eV.

System	CO			CO <sub>2</sub>		
	Atomsite	Bondsitesite	Vacantsite	Atomsite	Bondsitesite	Vacantsite
50	-0.23	-0.27	-0.26	-0.37	-0.36	-0.27
90	-0.22	-0.16	-0.23	-0.18	-0.12	-0.20
55	-0.12	-0.08	-0.13	-0.09	-0.14	-0.28
66	-0.14	-0.22	-0.14	-0.05	-0.20	-0.17

**Table 3.** The calculated adsorption energies ( $E_{\text{ads}}$ ) of NO and NO<sub>2</sub> on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. All energies are given by eV.

System	NO			NO <sub>2</sub>		
	Atomsite	Bondsitesite	Vacantsite	Atomsite	Bondsitesite	Vacantsite
50	-0.20	-0.21	-0.23	0.12	-0.92	-0.35
90	-0.14	-0.16	-0.26	-0.23	-0.21	-0.22
55	-0.13	-0.16	-0.11	-0.15	-0.37	-0.17
66	-0.17	-0.17	-0.19	-0.14	-0.38	-0.16

**Table 4.** The calculated energy gaps ( $E_g$ ) of CO and CO<sub>2</sub> on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. All energies are given by eV.

System	Pristine BNNTs	CO			CO <sub>2</sub>		
		Atomsite	Bondsitesite	Vacantsite	Atomsite	Bondsitesite	Vacantsite
50	3.37	3.39	3.39	3.39	3.40	3.41	3.39
90	5.72	5.63	5.42	5.45	5.72	5.72	5.72
55	6.08	5.48	5.63	5.45	6.07	6.06	6.06
66	6.11	5.50	5.51	5.50	6.10	6.10	6.10

**Table 5.** The calculated energy gaps ( $E_g$ ) of NO and NO<sub>2</sub> on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. All energies are given by eV.

System	NO			NO <sub>2</sub>		
	Carbonsite	Bondsite	Vacantsite	Carbonsite	Bondsite	Vacant site
50	2.92	2.50	2.63	2.65	2.89	2.72
90	2.97	2.97	3.00	3.36	3.54	3.23
55	2.98	2.98	2.98	3.14	3.30	3.14
66	2.96	2.97	2.97	3.36	3.30	3.15

### 3.3. HOMO-LUMO Orbitals of Adsorbing CO, CO<sub>2</sub>, NO and NO<sub>2</sub> Gas Molecules on BNNTs

Our calculated band gaps show that the adsorption of CO and CO<sub>2</sub> gas molecules on BNNTs does not affect the band gaps of the pristine BNNTs, however the adsorption of NO and NO<sub>2</sub> gas molecules reduces all the values of band gaps to ~3 eV. To explain that the molecular orbitals of adsorbing CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules on (5,0), (9,0), (5,5) and (6,6) BNNTs are investigated, see **Figure 2** and **Figure 3**. The band gaps of the pristine BNNTs are calculated and are listed in **Table 4**. The HOMO and LUMO energy orbitals for pristine (5,0), (9,0), (5,5) and (6,6) BNNTs are found to be (-6.12 eV, -2.75 eV), (-6.37 eV, -0.65 eV), (-6.35 eV, -0.27 eV) and (-6.36 eV, -0.25 eV), respectively. Comparing the HOMO-LUMO energies of the pristine BNNTs with ones after the adsorption of CO and CO<sub>2</sub> gas molecules, it is clear that the energy values are so close. Also, it is noticed that there is not any contribution from the gas molecules at the molecular orbitals except for (5,5), (6,6) BNNTs and the electron density of HOMO and LUMO is distributed either overall atoms of BNNTs as on (5,5), (6,6) BNNTs or is located at the terminals of the tube as on (5,0), (9,0) BNNTs, see **Figure 2**. Comparing the HOMO-LUMO energies of the pristine BNNTs with ones after the adsorption of NO and NO<sub>2</sub> gas molecules, it is clear that the energy gaps are reduced especially for (9,0), (5,5) and (6,6) BNNTs. The LUMO energy levels in case of (5,0) and (9,0) BNNTs after adsorbing NO and NO<sub>2</sub> gas molecular are getting deep (lower) in energy, results in reducing the band gap from ~6 eV to ~3 eV. Also, it is noticed that there is a representation from the NO and NO<sub>2</sub> gas molecules at HOMO and LUMO of (5,0), (9,0), (5,5) and (6,6) BNNTs, see **Figure 3**.

### 3.4. The Reactivity of BNNT Surfaces before and after Adsorbing Gas Molecules

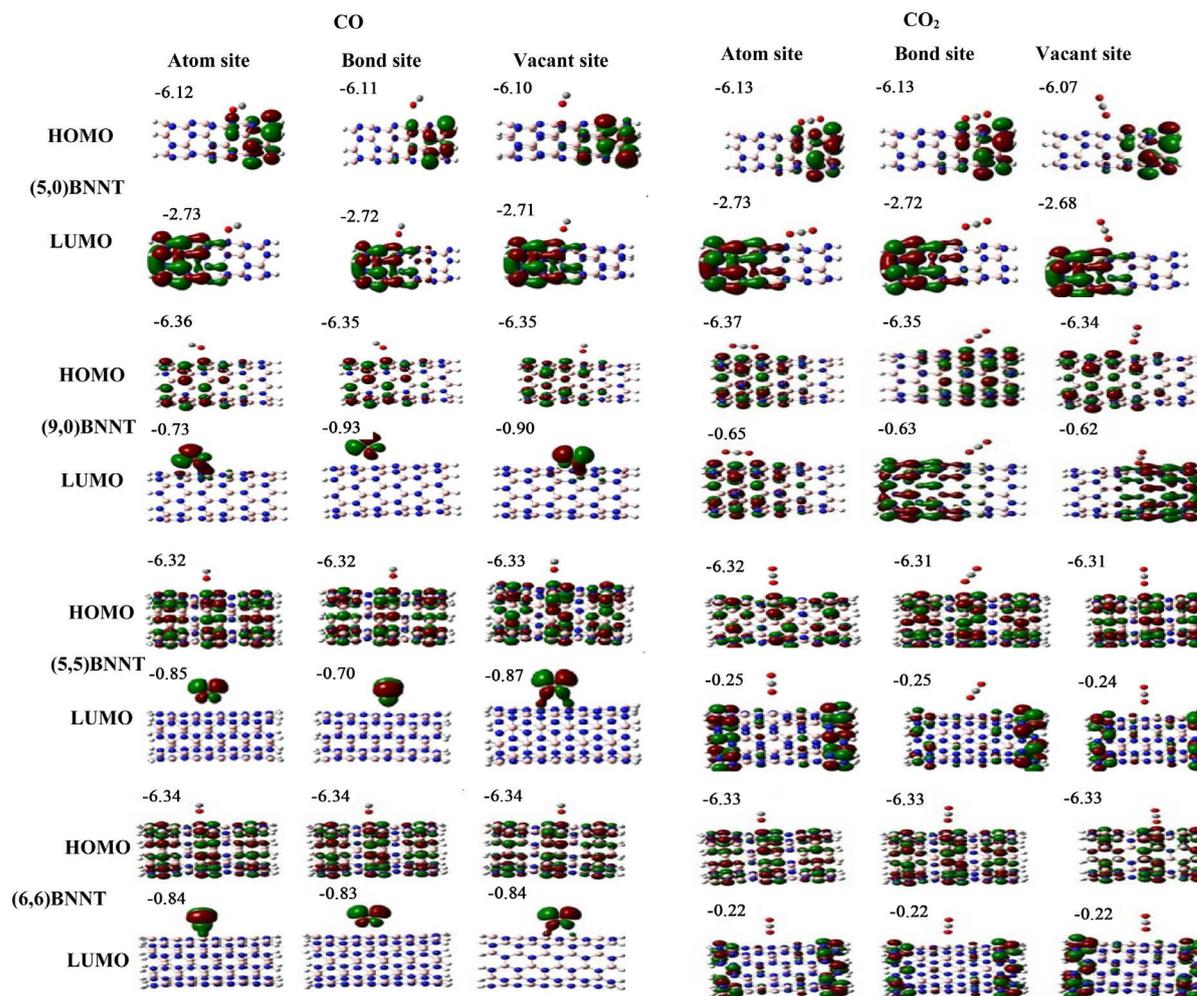
Our calculated band gaps and molecular orbitals show that the adsorption of CO and CO<sub>2</sub> gas molecules on BNNTs does not change the band gaps of the pristine BNNTs but the adsorption of NO and NO<sub>2</sub> gas molecules alters both of the band gaps and the molecular orbitals of (5,0), (9,0), (5,5) and (6,6) BNNTs. To clear that the reactivity of BNNT surfaces before and after adsorbing CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules on (5,0), (9,0), (5,5) and (6,6) BNNTs are studied, see **Table 6** and **Table 7**. The surface reactivity of the pristine BNNTs is calculated and is listed in **Table 6**. The dipole moments of pristine (5,0), (9,0), (5,5) and (6,6) BNNTs are found to be 4.67 Debye, 14.94 Debye 0.00 Debye and 0.00 Debye, respectively.

Comparing the dipole moments of the pristine BNNTs with ones after the CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules are adsorbed, it is clear that the values of dipole moments do not change for zig-zag (5,0) and (9,0) BNNTs but they increase in case of armchair (5,5), (6,6) BNNTs, see **Table 6**. Also, it is noticed that the highest dipole moment is for (9,0) BNNT. Comparing the dipole moments of the pristine BNNTs with ones after the NO and NO<sub>2</sub> gas molecules are adsorbed, it is found that the values of dipole moments do not change for zig-zag (5,0) and (9,0) BNNTs but they increase in case of armchair (5,5), (6,6) BNNTs, see **Table 7**. Also, it is noticed that the highest dipole moment is for (9,0) BNNT.

From **Table 6** and **Table 7**, it is clear that the dipole moments of zig-zag (5,0) and (9,0) BNNTs are always higher than the arm-chair (5,5) and (6,6) BNNTs. In addition, the highest e dipole moment is for (9,0) BNNT.

## 4. Conclusion

The gas sensing behavior of BNNTs, considering a range of different nanotube diameters and chiralities, as well as different adsorption sites are reported. The adsorption of CO, CO<sub>2</sub>, NO, and NO<sub>2</sub> gas molecules on the (5,0), (9,0), (5,5) and (6,6) BNNTs are studied using B3LYP/6-31 g(d, p). Three different adsorption sites (above an



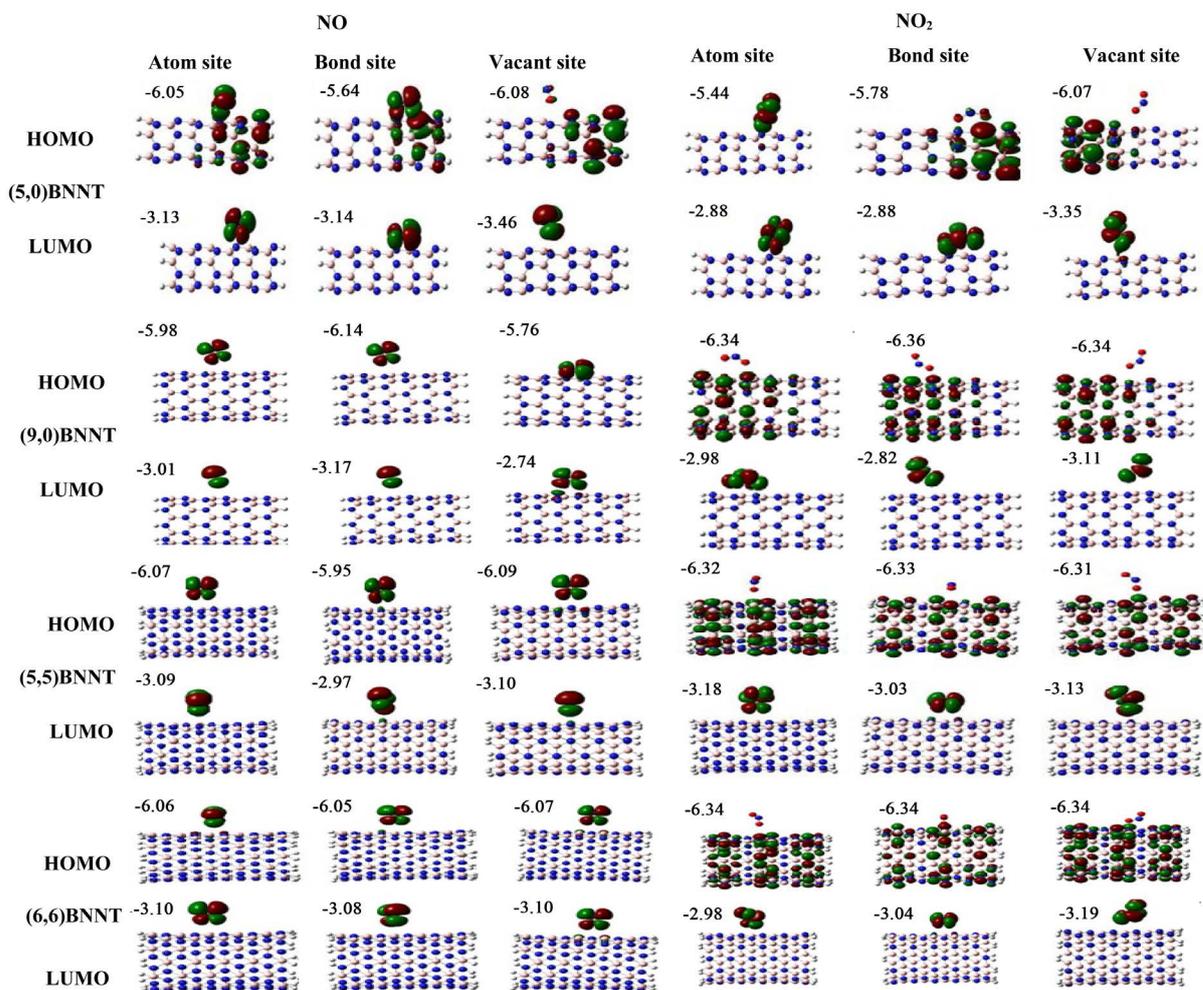
**Figure 2.** HOMO and LUMO molecular orbitals of adsorbing CO and CO<sub>2</sub> gas molecules on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. Energies of HOMO and LUMO are listed above the molecular orbitals and are given by eV.

**Table 6.** The calculated dipole moments of pristine and after adsorbing CO and CO<sub>2</sub> gas molecules on the (5,0), (9,0), (5,5) and (6,6) BNNTs. All dipole moments are given by Debye.

system	Pristine BNNTs	CO			CO <sub>2</sub>		
		Atomsite	Bondsite	Vacantsite	Atomsite	Bondsite	Vacantsite
(5,0) BNNT	4.67	4.79	4.83	4.72	4.77	4.85	4.86
(9,0) BNNT	14.94	14.92	14.93	14.94	14.96	14.96	14.95
(5,5) BNNT	0.00	0.51	0.51	0.44	0.47	0.79	0.80
(6,6) BNNT	0.00	0.45	0.48	0.41	0.77	0.79	0.74

**Table 7.** The calculated dipole moments of pristine and after adsorbing NO and NO<sub>2</sub> gas molecules on the (5,0), (9,0), (5,5) and (6,6) CNTs. All dipole moments are given by Debye.

system	NO			NO <sub>2</sub>		
	Atomsite	Bondsite	Vacantsite	Atomsite	Bondsite	Vacantsite
(5,0) BNNT	4.89	5.13	4.76	4.75	2.33	4.70
(9,0) BNNT	15.00	14.98	15.17	15.01	15.13	14.78
(5,5) BNNT	0.59	0.36	0.52	0.54	0.71	0.63
(6,6) BNNT	0.60	0.61	0.60	0.63	0.74	0.69



**Figure 3.** HOMO and LUMO molecular orbitals of adsorbing NO and NO<sub>2</sub> gas molecules on the pristine (5,0), (9,0), (5,5) and (6,6) BNNTs. Energies of HOMO and LUMO are listed above the molecular orbitals and are given by eV.

atom site, a bond site and a vacant site) are applied on BNNTs. It is found that the best BNNT for adsorbing the CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules is (5,0) BNNT with adsorption energy of  $-0.27$  eV,  $-0.37$  eV,  $-0.23$  and  $-0.92$  eV, respectively. Also, the electronic character of (5,0), (9,0), (5,5) and (6,6) BNNTs is found to be not affected by the adsorption of CO, CO<sub>2</sub>, NO and NO<sub>2</sub> gas molecules. It is found that the dipole moments of zig-zag (5,0) and (9,0) BNNTs are always higher than the arm-chair (5,5) and (6,6) BNNTs. Also, it is noticed that the highest dipole moment is for (9,0) BNNT.

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