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Effect of Tubular Chiralities and Diameters of Single Carbon Nanotubes on Gas Sensing Behavior: A DFT Analysis

A. A. EL-Barbary[1,2*], Kh. M. Eid[1,3], M. A. Kamel[1], H. M. Osman[1], G. H. Ismail[1,2]

[1]Physics Department, Faculty of Education, Ain Shams University, Cairo, Egypt
[2]Physics Department, Faculty of Science, Jazan University, Jazan, KSA
[3]Bukairiayh for Science, Qassim University, Buraydah, KSA
Email: *ahla_eg@yahoo.co.uk

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Abstract

Using density functional theory, the adsorption of CO, CO_2, NO and CO_2 gas molecules on different chiralities and diameters of single carbon nanotubes is investigated in terms of energetic, electronic properties and surface reactivity. We found that the adsorption of CO and CO_2 gas molecules is dependent on the chiralities and diameters of CNTs and it is vice versa for NO and NO_2 gas molecules. Also, the electronic character of CNTs is not affected by the adsorption of CO and CO_2 gas molecules while it is strongly affected by NO and NO_2 gas molecules. In addition, it is found that the dipole moments of zig-zag CNTs are always higher than the arm-chair CNTs. Therefore, we conclude that the zig-zag carbon nanotubes are more preferred as gas sensors than the arm-chair carbon nanotubes, especially for detecting NO and NO_2 gas molecules.

Keywords

Carbon Nanotubes, DFT, Gas Sensors

1. Introduction

Monitoring of combustible gas alarms, gas leak detection, and environmental pollution is of great concern in public security. Advances in nanotechnology give great promise for achieving new sensing materials. Since the discovery of carbon nanotubes in 1991, the single-walled carbon nanotubes (SWCNTs) have been intensively investigated as nanoscale gas sensors because of their great surface areas to bulk ratio and their abilities to mod-

*Corresponding author.

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ulate electrical properties upon adsorption of various kinds of gas molecules [1]-[17]. The emission of carbon and nitrogen oxides (CO, CO_2, NO and NO_2) results from the combustion of fossil fuels, contributing to both smog and acid precipitation, and affecting both terrestrial and aquatic ecosystems [18]. Although many efforts have been made to use catalysts to reduce the amount of carbon or nitrogen oxides in the air [19]-[25], an efficient method of sensing and removing carbon and nitrogen oxides is still required.

Because carbon and nitrogen oxides are the most dangerous air pollutants, toxic and global warming gases, our work is concentrated on investigating the effect of tubular chiralities and diameters of single carbon nanotubes on gas sensing behavior for CO, CO_2, NO and NO_2 gas molecules, applying the first principle calculations.

2. Computational Methods

All calculations were performed with the density functional theory as implemented within G03W package [26]-[29], using B3LYP exchange-functional and applying basis set 6 - 31g (d,p). Pure carbon 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_2, NO and NO_2 gas molecules.

The obtained diameters [30] and the adsorption energies of gas molecules on CNTs (E_{ads}) [31] are calculated from the following relations:

$$D = 0.73\left(n^2 + nm + m^2\right)^{1/2}$$

where *n* and m are integral numbers, the composition of chiral vector.

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

where $E_{(\text{nanotube+gas molecules})}$ is the total energy of nanotube and gas molecules, E_{nanotube} is the energy of the carbon 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_2, NO and NO_2 on four carbon nanotubes with different charilities and diameters $(5,0)$ CNT, $(9,0)$ CNT, $(5,5)$ CNT and $(6,6)$ CNT as shown in **Figure 1** and **Table 1**.

3.1. Adsorption of CO, CO_2, NO and NO_2 Gas Molecules on CNTs

We have adsorbed CO and CO_2 gas molecules vertically on different three positions of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs: above a carbon atom (carbon site), above a bond between two carbon atoms (bond site) and above a center of a hexagon ring (vacant site). The calculated adsorption energies of CO and CO_2 gas molecules

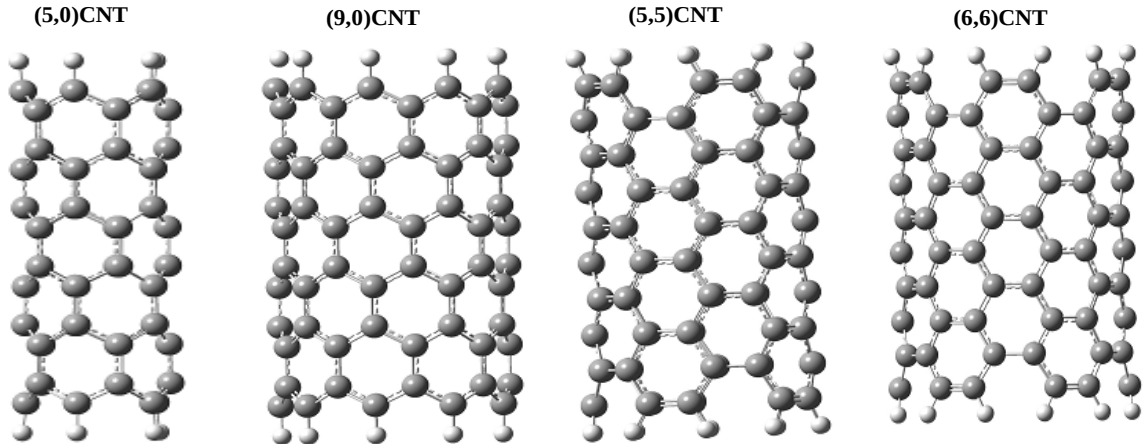

Figure 1. The fully optimized structures of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. Carbon atoms (gray) and hydrogen atoms (white).

are listed in **Table 2**. It is found that the best position and adsorption energy for CO gas molecule is above the bond site on $(9,0)$ CNT with adsorption energy of −0.43 eV, however for CO_2 gas molecule is above the vacant site on $(9,0)$ CNT with adsorption energy of −0.26 eV. Therefore, one can conclude that the best CNT gas sensor for CO and CO_2 gas molecules is the $(9,0)$ CNT.

Also, we have adsorbed NO and NO_2 gas molecules vertically on different three positions of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs: above a carbon site, above a bond site and above a vacant site. The calculated adsorption energies of NO and NO_2 gas molecules are listed in **Table 3**. It is found that the best adsorption energies of NO gas molecule are on the $(9,0)$ CNT above a bond site, then above a carbon site and after that above a vacant site with adsorption energies of −1.65 eV, −1.55 eV and −1.34 eV, respectively. However, for NO_2 gas molecule is found to be above the bond site on $(9,0)$ CNT with adsorption energy of −1.75 eV. Also, it is noticed that the vacant site is always preferred for NO_2 gas adsorption on all the studied CNTs except for $(9,0)$ CNT. Therefore, one can conclude that all CNTs can be used as gas sensors for NO and NO_2 gas molecules.

From **Table 2**, **Table 3**, one can investigate the effect of the chiralities and the diameters on the CNT gas sensors behavior. It is clear that the adsorption of CO and CO_2 gas molecules is dependent on the chiralities and the diameters of CNTs. The adsorption of CO and CO_2 gas molecules is enhanced with increasing the diameter of the zig-zag CNTs. However, the adsorption of NO and NO_2 gas molecules is independent on the chiralities and the diameters of CNTs.

3.2. Energy Gaps of Adsorbed CO, CO_2, NO and NO_2 Gas Molecules on CNTs

From **Table 4**, it is clear that the adsorption of CO and CO_2 gas molecules on CNTs does not affect the elec-

Table 1. The configuration structures and diameters of the studied CNTs.

System	Configuration Structures	Diameters/Å
$(5,0)$ CNT	$C_{60}H_{10}$	3.65
$(9,0)$ CNT	$C_{108}H_{18}$	6.57
$(5,5)$ CNT	$C_{100}H_{20}$	6.32
$(6,6)$ CNT	$C_{120}H_{24}$	7.59

Table 2. The calculated adsorption energies (E_{ads}) of CO and CO_2 above a carbon site, a bond site and a vacant site of pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All energies are given by eV.

	CO			CO_2		
System	Carbon site	Bond site	Vacant site	Carbon site	Bond Site	Vacant Site
$(5,0)$ CNT	0.04	−0.00	−0.04	−0.00	0.00	0.00
$(9,0)$ CNT	0.03	−0.43	−0.24	−0.23	−0.00	−0.26
$(5,5)$ CNT	0.04	0.04	0.04	0.13	0.003	2.19
$(6,6)$ CNT	−0.01	−0.01	−0.03	−0.00	−0.00	−0.16

Table 3. The calculated adsorption energies (E_{ads}) of NO and NO_2 above a carbon site, a bond site and a vacant site of pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All energies are given by eV.

	NO			NO_2		
System	Carbon site	Bond site	Vacant site	Carbon Site	Bond site	Vacant site
$(5,0)$ CNT	−0.35	−0.34	0.29	0.07	−0.36	−1.04
$(9,0)$ CNT	−1.55	−1.65	−1.34	−1.19	−1.75	−1.40
$(5,5)$ CNT	0.06	0.22	0.07	2.26	0.92	−1.32
$(6,6)$ CNT	−0.01	0.25	0.07	0.06	0.35	−1.34

tronic character of the CNTs. Also, the band gaps of pristine CNTs and the adsorbed CO and CO_2 gas molecules on CNTs are so close.

From **Table 5**, the adsorption of NO and NO_2 gas molecules on CNTs is strongly affected the electronic character of the $(9,0)$ and $(5,0)$CNTs. However, there is not any change of the electronic character for $(5,5)$ and $(6,6)$ CNTs. The band gap of pristine $(5,0)$ CNT is increased from 0.70 eV to 1.61 eV and to 1.37 eV when NO and NO_2 gas molecules are adsorbed on it, respectively. Also, The band gap of pristine $(9,0)$ CNT is increased from 0.25 eV to 1.34 eV and to 1.25 eV when NO and NO_2 gas molecules are adsorbed on it, respectively. One can conclude that the electronic character of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs is not affected by the adsorption of CO and CO_2 gas molecules. The adsorption of NO and NO_2 gas molecules on CNTs is only strongly affected the electronic character of the $(9,0)$ and $(5,0)$CNTs, however the $(5,5)$ and $(6,6)$ CNTs are not affected at all.

3.3. HOMO-LUMO Orbitals of Adsorbing CO, CO_2, NO and NO_2 Gas Molecules on CNTs

Our calculated band gaps show that the adsorption of CO and CO_2 gas molecules on CNTs is not affected the band gaps of the pristine CNTs, however the adsorption of NO and NO_2 gas molecules is strongly affected the band gaps. To explain that the molecular orbitals of adsorbing CO, CO_2, NO and NO_2 gas molecules on $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs are investigated, see **Figure 2**, **Figure 3**. The band gaps of the pristine CNTs are calculated and are listed in **Table 4**. The HOMO and LUMO energy orbitals for pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs are found to be (−4.13 eV, −3.42 eV), (−3.93 eV, −3.68 eV), (−4.62 eV, −2.82 eV) and (−4.70 eV, −2.82 eV), respectively. Comparing the HOMO-LUMO energies of the pristine CNTs with ones after the adsorption of CO and CO_2 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 and the electron density of HOMO and LUMO is distributed over all the carbon atoms of CNTs except for $(9,0)$ CNT is located at the terminals of the tube, see **Figure 2**. Comparing the HOMO-LUMO energies of the pristine CNTs with ones after the adsorption of NO and NO_2 gas molecules, it is clear that the energy values are so close in case of $(5,5)$ and $(6,6)$ CNTs and are quite far in case of $(5,0)$ and $(9,0)$ CNTs. The HOMO energy levels in case of $(5,0)$ and $(9,0)$ CNTs after adsorbing NO and NO_2 gas molecular are getting deep (lower) in energy however the LUMO energy levels are getting higher in energy. Results in increasing the band gap from 0.70 eV to 1.81 eV in

Table 4. The calculated energy gaps (E_g) of CO and CO_2 above a carbon site, a bond site and a vacant site of pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All energies are given by eV.

		CO			CO_2		
System	Pristine CNTs	Carbon site	Bond site	Vacant site	Carbon Site	Bond site	Vacant Site
$(5,0)$ CNT	0.70	0.61	0.70	0.70	0.61	0.61	0.60
$(9,0)$ CNT	0.25	0.25	0.25	0.25	0.25	0.24	0.25
$(5,5)$ CNT	1.79	1.80	1.79	1.80	1.80	1.79	1.75
$(6,6)$ CNT	1.90	1.92	1.92	1.92	1.92	1.92	1.92

Table 5. The calculated energy gaps (E_g) of NO and NO_2 above a carbon site, a bond site and a vacant site of pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All energies are given by eV.

	NO			NO_2		
system	Carbon site	Bond Site	Vacant Site	Carbon site	Bond Site	Vacant site
$(5,0)$ CNT	1.61	0.99	0.94	0.61	0.99	1.37
$(9,0)$ CNT	1.34	1.24	1.14	1.25	1.25	1.14
$(5,5)$ CNT	1.79	1.81	1.79	1.72	1.76	1.79
$(6,6)$ CNT	1.92	1.90	1.92	1.94	1.88	1.91

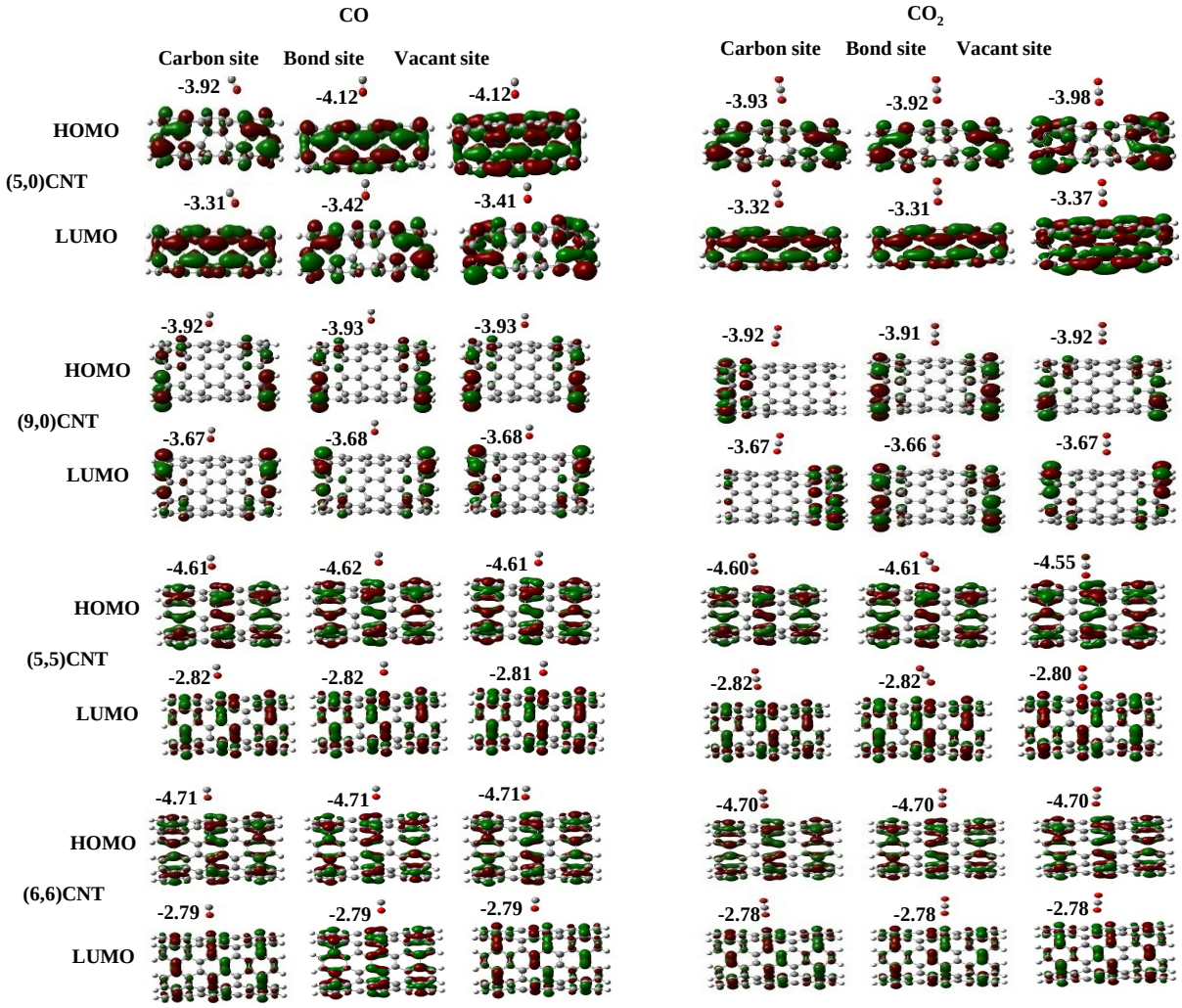

Figure 2. HOMO and LUMO molecular orbitals of adsorbing CO and CO_2 gas molecules on the pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. Energies of HOMO and LUMO are listed above the molecular orbitals and are given by eV.

case of $(5,0)$ CNT and from 0.25 eV to 1.34 eV in case of $(9,0)$ CNT. Also, it is noticed that there is representation from the NO gas molecule at LUMO of $(9,0)$ and $(6,6)$ CNTs, see **Figure 3**.

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

Our calculated band gaps and molecular orbitals show that the adsorption of CO and CO_2 gas molecules on CNTs is not affected neither the band gaps nor the molecular orbitals of the pristine CNTs but the adsorption of NO and NO_2 gas molecules is strongly affected both of the band gaps and the molecular orbitals of $(5,0)$ and $(9,0)$ CNTs. To clear that the reactivity of CNT surfaces before and after adsorbing CO, CO_2, NO and NO_2 gas molecules on $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs are studied, see **Table 6**, **Table 7**. The surface reactivity of the pristine CNTs is calculated and is listed in Table 6. The dipole moments of pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs are found to be 0.54 Debye, 0.20 Debye 0.00 Debye and 0.00 Debye, respectively.

Comparing the dipole moments of the pristine CNTs with ones that are adsorbed the CO and CO_2 gas molecules, it is clear that the dipole moment values are so close in case of the adsorption of the CO gas molecule but they are higher in case of the adsorption of the CO_2 gas molecule, see **Table 6**. Also, it is noticed that the highest dipole moments after the adsorption of the CO_2 gas molecule are 0.74 Debye (when CO_2 is adsorbed above the bond site of $(9,0)$ CNT) and 0.77 Debye (when CO_2 is adsorbed above the vacant site of $(5,5)$ CNT), re-

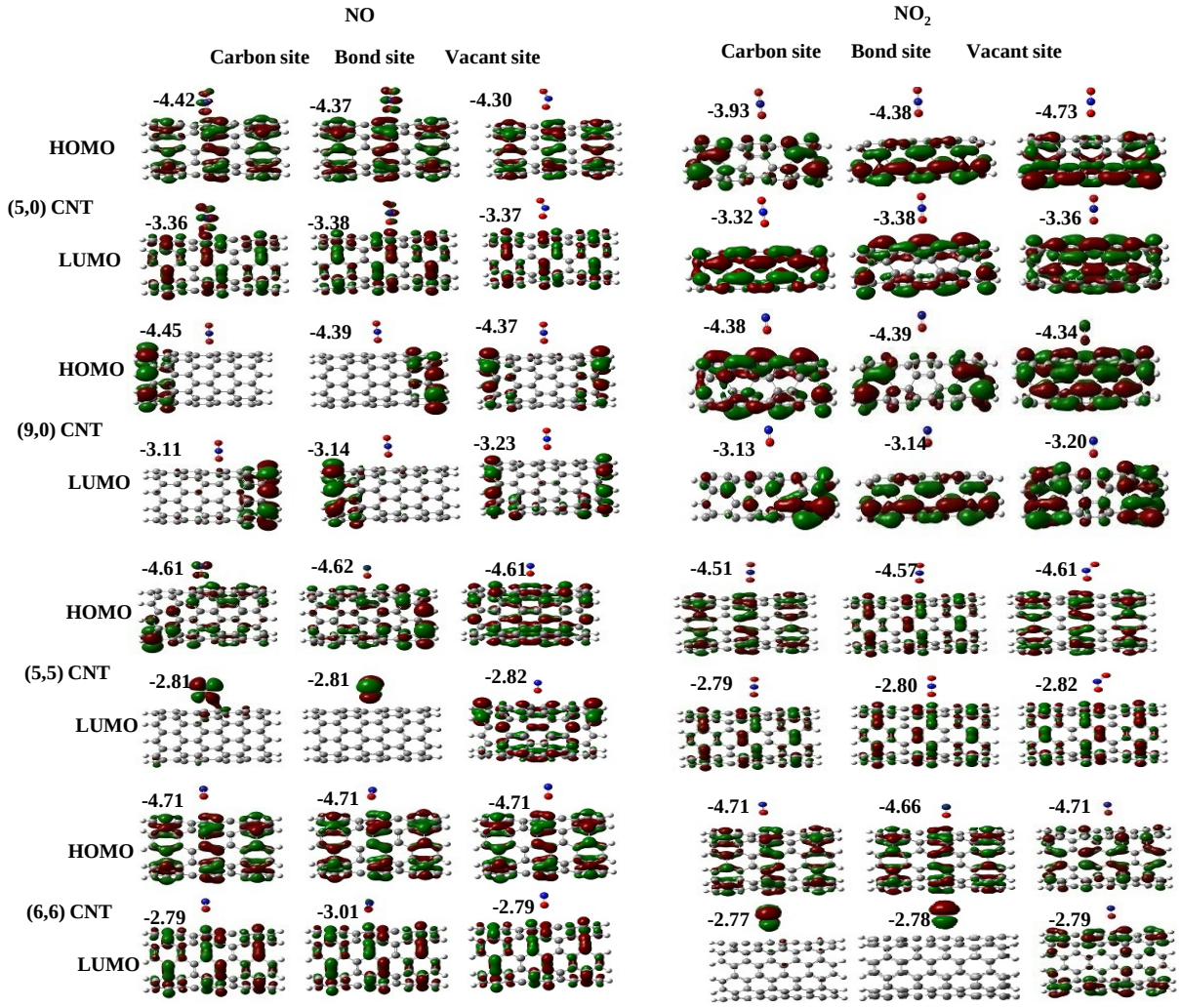

Figure 3. HOMO and LUMO molecular orbitals of adsorbing NO and NO_2 gas molecules on the pristine $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. Energies of HOMO and LUMO are listed above their molecular orbitals and are given by eV.

Table 6. The calculated dipole moments of pristine and after adsorbing CO and CO_2 gas molecules above a carbon site, a bond site and a vacant site of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All dipole moments are given by Debye.

		CO			CO_2		
system	Pristine CNTs	Carbon site	Bond site	Vacant Site	Carbon Site	Bond Site	Vacant Site
$(5,0)$ CNT	0.54	0.54	0.56	0.49	0.46	0.47	0.62
$(9,0)$ CNT	0.20	0.40	0.21	0.10	0.23	0.74	0.30
$(5,5)$ CNT	0.00	0.04	0.12	0.06	0.21	0.25	0.77
$(6,6)$ CNT	0.00	0.06	0.05	0.06	0.23	0.23	0.26

spectively. Comparing the dipole moments of the pristine CNTs with ones that are adsorbed the NO and NO_2 gas molecules, it is found that the dipole moments are getting higher. When the NO and NO_2 gas molecules are adsorbed on the vacant sites of CNTs, their dipole moments are either quite close to or are lower than the dipole moments of pristine CNTs, except in case of adsorbing NO_2 on $(5,0)$ CNT, the dipole moment is increased. Also, all the calculated dipole moments of adsorbing NO and NO_2 gas molecules on the carbon sites of CNTs

Table 7. The calculated dipole moments of pristine and after adsorbing NO and NO_2 gas molecules above a carbon site, a bond site and a vacant site of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs. All dipole moments are given by Debye.

	NO			NO_2		
system	Carbon site	Bond Site	Vacant Site	Carbon Site	Bond Site	Vacant site
$(5,0)$ CNT	5.58	1.12	0.36	0.28	0.97	1.47
$(9,0)$ CNT	0.46	0.48	0.11	0.69	0.11	0.07
$(5,5)$ CNT	0.14	0.11	0.11	1.48	0.58	0.13
$(6,6)$ CNT	0.15	0.31	0.17	0.20	0.53	0.17

are increased, except in case of adsorbing NO_2 on $(5,0)$ CNT, the dipole moment is decreased. In case of adsorbing NO and NO_2 gas molecules on the bond sites of CNTs the dipole moments are also increased, except in case of adsorbing NO_2 on $(9,0)$ CNT is decreased, see **Table 7**.

From **Table 6**, **Table 7**, it is clear that the dipole moments of zig-zag $(5,0)$ and $(9,0)$ CNTs are always higher than the arm-chair $(5,5)$ and $(6,6)$ CNTs. Also, it is noticed that the dipole moment of adsorbing NO gas molecule on the bond site of $(5,0)$ CNT is increased by ten times comparing with the dipole moment of pristine $(5,0)$CNT.

4. Conclusion

The gas sensing behavior of CNTs, considering a range of different nanotube diameters and chiralities, as well as different adsorption sites is reported. The adsorption of CO, CO_2, NO, and NO_2 gas molecules on the $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$ CNTs are studied using B3LYP/6-31 g(d, p). Three different adsorption sites (above a carbon site, a bond site and a vacant site) are applied on CNTs. It is found that the adsorption of CO and CO_2 gas molecules is dependent on the chiralities and the diameters of CNTs and it is enhanced with increasing the diameter of the zig-zag CNTs. However, the adsorption of NO and NO_2 gas molecules is independent on the chiralities and the diameters of CNTs. Also, the electronic character of $(5,0)$, $(9,0)$, $(5,5)$ and $(6,6)$CNTs is not affected by the adsorption of CO and CO_2 gas molecules. While, the adsorption of NO and NO_2 gas molecules on CNTs is only strongly affected by the electronic character of the $(9,0)$ and $(5,0)$CNTs but the $(5,5)$ and $(6,6)$ CNTs are not affected at all. It is found that the dipole moments of zig-zag $(5,0)$ and $(9,0)$ CNTs are always higher than the arm-chair $(5,5)$ and $(6,6)$ CNTs. Also, it is noticed that the dipole moment of adsorbing NO gas molecule on the bond site of $(5,0)$ CNT is increased by ten times compared with the dipole moment of pristine $(5,0)$CNT. Therefore, these findings prove that the zig-zag carbon nanotubes are better than the arm-chair carbon nanotubes as gas sensors, especially for NO and NO_2 gas molecules.

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