Journal of Surface Engineered Materials and Advanced Technology, 2015, 5, 169-176
Published Online October 2015 in SciRes. http://www.scirp.org/journal/jsemat
http://dx.doi.org/10.4236/jsemat.2015.54019

Adsorption of CO, CO_2, NO and NO_2 on Carbon Boron Nitride Hetero Junction: DFT Study

A. A. El-Barbary[1,2*], Kh. M. Eid[1,3], M. A. Kamel[1], H. O. Taha[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, Qassim, KSA
Email: *ahla_eg@yahoo.co.uk

Received 26 May 2015; accepted 13 July 2015; published 16 July 2015

Abstract

The adsorption of CO, CO_2, NO and CO_2 gas molecules on different diameters and chiralities of carbon nanotube-boron nitride nanotube (CNT-BNNT) heterojunctions 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 CNT-BNNT heterojunctions for adsorbing the CO, NO, CO_2 and NO_2 gas molecules is (5,0) CNT-BNNT heterojunction through forming C-N bonds with adsorption energy of −0.26, −0.41 eV, −0.33 and −0.63 eV, respectively. Also, the adsorption of CO, NO, CO_2 and NO_2 gas molecules on (5,5) and (6,6) CNT-BNNT heterojunctions does not affect the electronic character of the CNT-BNNT heterojunctions, however the adsorption of NO and NO_2 gas molecules on (5,0) and (9,0)CNT-BNNT heterojunctions in case of forming C-B bonds increases the band gaps to 1.21 eV and 1.52 eV, respectively. In addition, it is reported that the values of dipole moment for armchair (5,5) and (6,6) CNT-BNNT heterojunctions are not affected by gas adsorption. Also, for the zig-zag (5,0) and (9,0) CNT-BNNT heterojunctions, the values of dipole moment increase through forming C-N bonds and decrease through forming C-B bonds. In addition, it is reported that the highest dipole moment is obtained for (9,0) CNT-BNNT heterojunctions. Therefore, the zig-zag CNT-BNNT heterojunctions can be selected as good candidate for gas sensors.

Keywords

CNT-BNNT Heterojunctions, DFT, Gas Sensors

*Corresponding author.

How to cite this paper: El-Barbary, A.A., Eid, Kh.M., Kamel, M.A., Taha, H.O. and Ismail, G.H. (2015) Adsorption of CO, CO_2, NO and NO_2 on Carbon Boron Nitride Hetero Junction: DFT Study. *Journal of Surface Engineered Materials and Advanced Technology*, **5**, 169-176. http://dx.doi.org/10.4236/jsemat.2015.54019

1. Introduction

Heterojunction gas sensors have been widely fabricated due to their low cost and simple processing, such as high the triethylamine-sensing of NiO/SnO_2 hollowsphere P-N heterojunction sensors [1], the CuO-ZnO heterojunction gas sensors [2] the polypyrrole (Ppy)/TiO_2 heterojunction operated LPG sensor [3] the In_2O_3-WO_3 heterojunction nanofibers [4] the SnO_2/WO_3 heterojunction gas sensor [5] [6] and heterojunctions of B-C-N nanotubes [7]-[9]. Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima [10], they have attracted much attention due to their remarkable electrical, mechanical and thermal properties [11]-[13]. The single-walled CNTs (SWCNTs) can be metallic or semiconducting, depending on their chirality and diameter. Compared with CNTs, BNNTs are semiconducting with an uniform wide energy gap [14], and their electronic properties are independent of the tube chirality and diameter [15]. Also, the boron nitride nanotubes (BNNTs) do not react with molten metals, and have higher oxidation resistance than CNTs [16] [17]. By joining two NTs with same diameter and different materials, the heterojunction can be obtained [11] [18]. The combined advantages of CNTs and BNNTs make their structures are ideal components for applications requiring high strength, chemical stability, high-temperature resistance or electrical insulation, such as nanocables [19] [20]. The CNT-BNNT heterojunctions have investigated due to their unique electronic properties which can be controlled by adjusting the atomic composition and joint configurations [21]-[23]. Using, *ab initio* and semi-empirical approaches, the electronic properties of the CNT-BNNT heterojunctions have been studied [24]-[26].

In this paper, the adsorption of CO, NO, CO_2 and NO_2 gas molecules on the surfaces of the heterojunctions with the same diameters and different chiralities for (5,0), (9,0), (5,5) and (6,6) CNT-BNNTs is studied, using the density functional theory and basis set 6 - 31 g (d,p). Also, the electronic properties and surface reactivity of CNT-BNNT heterojunctions have been discussed.

2. Computational Methods

The density functional theory as implemented within G03W package [27]-[33], using B3LYP exchange-functional and applying basis set 6 - 31 g (d,p) are performed. All CNT-BNNT heterojunctions of (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 adsorption energies of gas molecules on CNT-BNNT heterojunctions (E_{ads}) [34] are calculated from the following relations:

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

where $E_{(\text{heterojunction+gas molecule})}$ is the total energy of nanotube and gas molecules, $E_{\text{heterojunction}}$ is the energy of the CNT-BNNT heterojunction, 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 the vacant site (above a center of a hexagon ring) of CNT-BNNT heterojunctions with different charilities and diameters (5,0) CNT-BNNT, (9,0) CNT-BNNT, (5,5) CNT-BNNT and (6,6) CNT-BNNT as shown in **Figure 1** and **Table 1**. For zig-zag (5,0) CNT-BNNT and (9,0) CNT-BNNT heterojunctions have two ways of joining, first through forming C-B bonds and second through forming C-N bonds, see **Figure 1**. However, the (5,5) CNT-BNNT and (6,6) CNT-BNNT are joined through one way.

Table 1. The configuration structures of the studied CNT-BNNT heterojunctions.

System	Configuration Structures
(5,0) CNT-BNNT	$C_{30}B_{15}N_{15}H_{10}$ $C_{30}N_{15}B_{15}H_{10}$
(9,0) CNT-BNNT	$C_{54}B_{27}N_{27}H_{18}$ $C_{54}N_{27}B_{27}H_{18}$
(5,5) CNT-BNNT	$C_{50}B_{25}N_{25}H_{20}$
(6,6) CNT-BNNT	$C_{60}B_{30}N_{30}H_{24}$

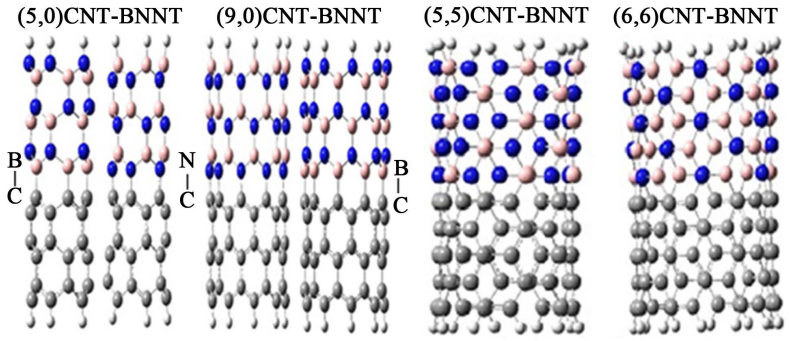

Figure 1. The fully optimized structures of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. Carbon atoms (gray), Nitrogen atoms (blue), Boron atom (pink) and hydrogen atoms (white).

3.1. Adsorption of CO, CO_2, NO and NO_2 Gas Molecules on CNT-BNNT Heterojunctions

We have adsorbed CO, NO, CO_2 and NO_2 gas molecules vertically on the vacant site (above a center of a hexagon ring) of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. The calculated adsorption energies of CO, NO, CO_2 and NO_2 are listed in **Table 2**. It is found that the best CNT-BNNT heterojunction for adsorbing the CO, NO, CO_2 and NO_2 gas molecules is (5,0) CNT-BNNT through forming C-N bonds with adsorption energy of −0.26 eV, −0.41 eV, −0.33 eV and −0.63 eV, respectively. Therefore, the (5,0) CNT-BNNT is considered to be the best heterojunction for adsorbing CO, NO, CO_2 and NO_2 gas molecules.

3.2. Energy Gaps of Adsorbed CO, CO_2, NO and NO_2 Gas Molecules on CNT-BNNT Heterojunctions

From **Table 3**, it is found that the adsorption of CO, NO, CO_2 and NO_2 gas molecules on (5,0), (5,5), (6,6) CNT-BNNT heterojunctions does not affect the electronic character of the CNT-BNNT heterojunctions, however the adsorption of NO and NO_2 gas molecules on (5,0) and (9,0) CNT-BNNT heterojunctions in case of forming C-B bonds is increased to 1.21 eV and 1.36 eV, respectively.

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

Our calculated band gaps show that the adsorption of CO, NO, CO_2 and NO_2 gas molecules on (5,0), (5,5), (6,6) CNT-BNNT heterojunctions does not affect the electronic character of the CNT-BNNT heterojunctions, however the adsorption of NO_2 gas molecules on (9,0) CNT-BNNT heterojunctions increases the band gap the of (9,0) CNT-BNNTs to ~1.52 eV. 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) CNT-BNNT heterojunctions are investigated, see **Figure 2** and **Figure 3**. The band gaps of the CNT-BNNT heterojunctions are calculated and are listed in **Table 3**. The HOMO and LUMO energy orbitals for (5,0) and (9,0) CNT-BNNT heterojunctions in case of forming C-N bonds are found to be (−4.08 eV, −2.99 eV), (−3.27 eV, −2.72 eV) and in case of forming C-B bonds are (−4.35 eV, −3.54 eV) and (−4.08 eV, −3.54 eV), respectively. The HOMO and LUMO energy orbitals for (5,5) and (6,6) CNT-BNNT heterojunctions are (−4.35 eV, −2.72 eV) and (−4.08 eV, −2.72 eV), respectively. Comparing the HOMO-LUMO energies of the CNT-BNNT heterojunctions 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 located at the carbon terminals except the (5,0) CNT-BNNT heterojunctions the electron density is distributed over all (5,0) heterojunctions, see **Figure 2**. Comparing the HOMO-LUMO energies of the (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions with ones after the NO and NO_2 gas molecules are adsorbed, it is clear that the values of energy gap are similar, except for (5,0) and (9,0) CNT-BNNT heterojunctions in case of forming C-B bonds the energy gap increases to 1.21 eV and 1.52 eV, respectively. Also, it is noticed that there are representations from the NO and NO_2 gas moleculeson the LUMO of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions and the electron density is localized on carbon terminals, see **Figure 3**.

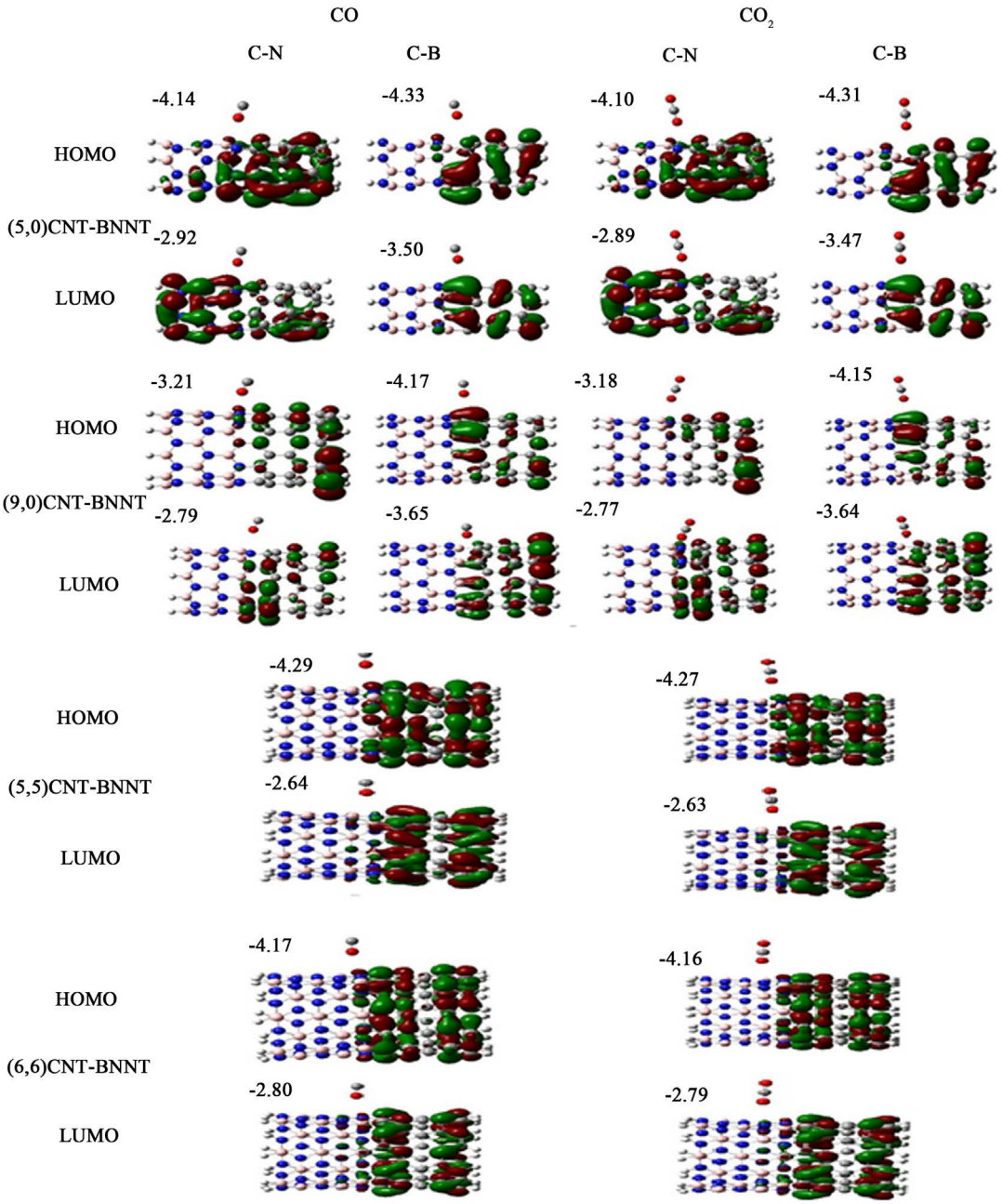

Figure 2. HOMO and LUMO molecular orbitals of adsorbing CO and CO_2 gas molecules on the (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. Energies of HOMO and LUMO are listed above the molecular orbitals and are given by eV.

Table 2. The calculated adsorption energies (E_{ads}) of CO, NO, CO_2 and NO_2 above a vacant site of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. All energies are given by eV.

	CO		NO		CO_2		NO_2	
Heterojunctions	C-N	C-B	C-N	C-B	C-N	C-B	C-N	C-B
(5,0) CNT-BNNT	−0.26	−0.20	−0.41	−0.33	−0.33	−0.22	−0.63	−0.60
(9,0) CNT-BNNT	−0.15	−0.05	−0.24	−0.12	−0.22	−0.25	−1.58	−0.40
(5,5) CNT-BNNT	−0.15		−0.18		−0.20		−0.24	
(6,6) CNT-BNNT	−0.17		−0.13		−0.15		−0.25	

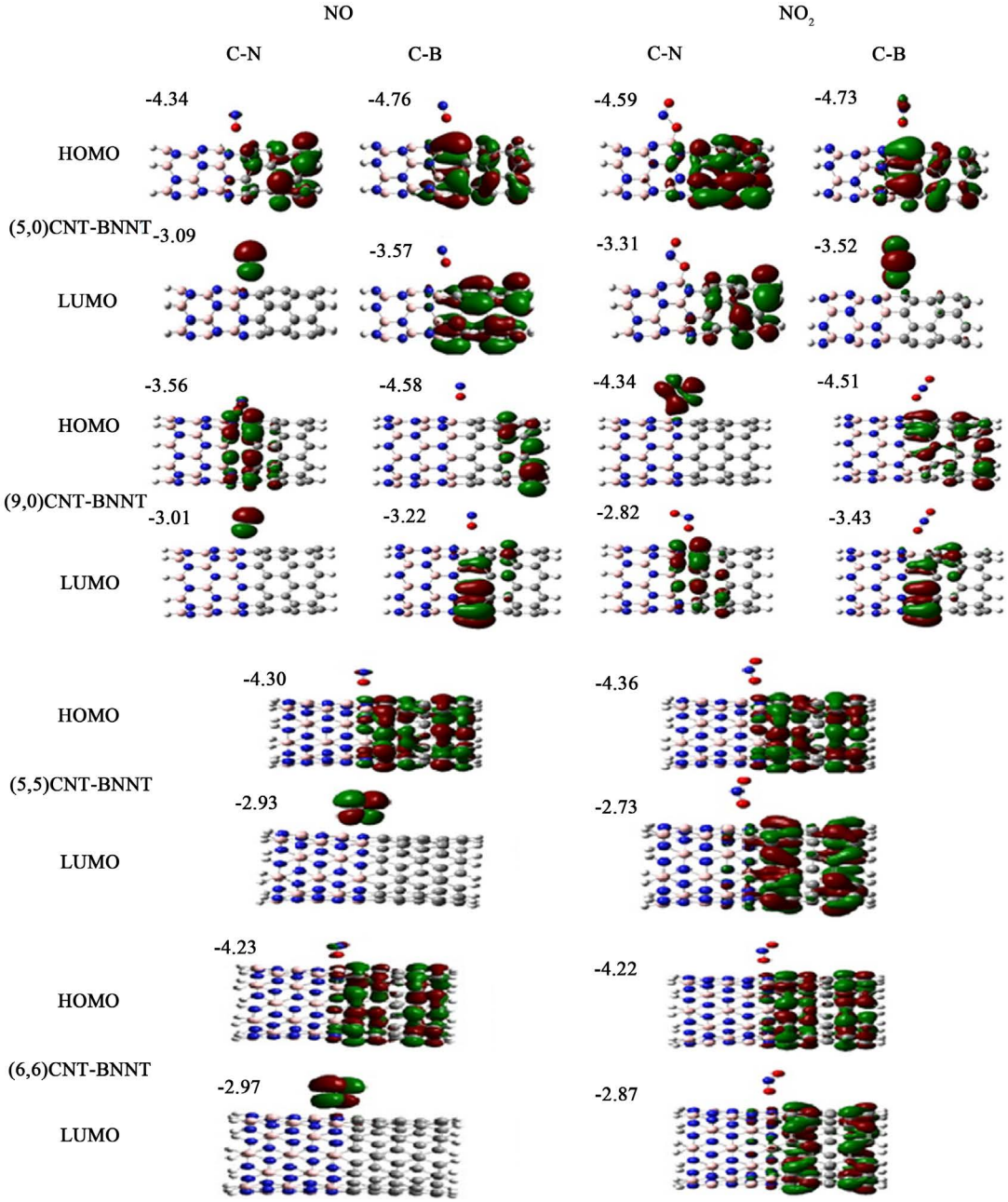

Figure 3. HOMO and LUMO molecular orbitals of adsorbing NO and NO_2 gas molecules on the (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. Energies of HOMO and LUMO are listed above the molecular orbitals and are given by eV.

3.4. The Reactivity of CNT-BNNT Heterojunction 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 CNT-BNNT heterojunctions does not change the band gaps of the CNT-BNNT heterojunctions but the adsorption of NO and NO_2 gas molecules strongly alters the band gaps and the molecular orbitals of (5,0) and (9,0) CNT-BNNT heterojunctions through forming C-B bonds. To clear that the reactivity of CNT-BNNT heterojunction surfaces before and after adsorbing CO, CO_2, NO and NO_2 gas molecules on (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions is studied, see **Table 4**. The surface reactivity of the CNT-BNNT heterojunctions is

Table 3. The calculated energy gaps (E_g) of adsorbing CO, NO, CO_2 and NO_2 above a vacant site of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. All energies are given by eV.

	CNT-BNNT		CO		NO		CO_2		NO_2	
Heterojunctions	C-N	C-B	C-N	C-B	C-N	C-B	C-N	C-B	C-N	C-B
(5,0) CNT-BNNT	1.21	0.8	1.22	0.82	1.25	1.19	1.21	0.84	1.28	1.21
(9,0) CNT-BNNT	0.44	0.52	0.42	0.52	0.55	1.36	0.41	0.51	0.52	1.52
(5,5) CNT-BNNT	1.63		1.64		1.64		1.64		1.63	
(6,6) CNT-BNNT	1.35		1.37		1.37		1.37		1.35	

Table 4. The calculated dipole moments of CNT-BNNT heterojunctions and after adsorbing CO, NO, CO_2 and NO_2 above a vacant site of (5,0), (9,0), (5,5) and (6,6) CNT-BNNT heterojunctions. All dipole moments are given by Debye.

	CNT-BNNT		CO		NO		CO_2		NO_2	
Heterojunctions	C-N	C-B	C-N	C-B	C-N	C-B	C-N	C-B	C-N	C-B
(5,0) CNT-BNNT	0.67	2.00	1.53	1.66	2.45	0.71	2.28	1.69	5.35	1.84
(9,0) CNT-BNNT	12.47	0.52	12.06	0.67	11.1	0.78	12.61	0.95	11.83	7.52
(5,5) CNT-BNNT	1.92		1.97		1.83		2.16		2.03	
(6,6) CNT-BNNT	2.59		2.61		2.21		2.86		3.05	

calculated and is listed in **Table 4**. The dipole moments of (5,5) and (6,6) CNT-BNNT heterojunctions are found to be 1.92 Debye and 2.59 Debye, respectively. The dipole moments of (5,0) and (9,0) CNT-BNNT heterojunctions through forming C-N bonds are found to be 0.67 Debye and 12.47 Debye and through forming C-B bonds are 2.0 Debye and 0.52 Debye, respectively.

Comparing the dipole moments of the CNT-BNNT heterojunctions with ones that the CO, CO_2, NO and NO_2 gas molecules are adsorbed, it is clear that the values of dipole moment do not change for armchair (5,5) and (6,6) CNT-BNNT heterojunctions. Also, for the zig-zag (5,0) and (9,0) CNT-BNNT heterojunctions, the values of dipole moment increase through forming C-N bonds and decrease through forming C-B bonds, see **Table 4**. Finally, one can report that the highest dipole moment is for (9,0) CNT-BNNT heterojunctions through forming C-N bonds.

4. Conclusion

The gas sensing behavior of CNT-BNNT heterojunctions, considering a range of different diameters and chiralities 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) CNT-BNNTs are studied using B3LYP/6-31 g(d, p). It is found that the best CNT-BNNT heterojunction for adsorbing the CO, NO, CO_2 and NO_2 gas molecules is (5,0) CNT-BNNT heterojunctions with adsorption energy of −0.26, −0.41 eV, −0.33 eV and −0.63 eV, respectively. It is reported that the adsorption of CO, NO, CO_2 and NO_2 gas molecules on (5,5) and (6,6) CNT-BNNT heterojunctions does not affect the electronic character of the CNT-BNNT heterojunctions, however the adsorption of NO and NO_2 gas molecules on (5,0) and (9,0) CNT-BNNT heterojunctions in case of forming C-B bonds increases the band gaps to 1.21 eV and 1.52 eV, respectively. Also, it is noticed that the highest dipole moment is for (9,0) CNT-BNNT heterojunctions through forming C-N bonds.

References

[1] Ju, D., Xu, H., Xu, Q., Gong, H., Qiu, Z., Guo, J., Zhang, J. and Cao, B. (2015) High Triethylamine-Sensing Properties of NiO/SnO_2 Hollow Sphere P-N Heterojunction Sensors. *Sensors and Actuators B*: *Chemical*, **215**, 39-44. http://dx.doi.org/10.1016/j.snb.2015.03.015

[2] Hu, Y., Zhou, X., Han, Q., Cao, Q. and Huan, Y. (2003) Sensing Properties of CuO-ZnO Heterojunction Gas Sensors. *Materials Science and Engineering*: *B*, **99**, 41-43. http://dx.doi.org/10.1016/S0921-5107(02)00446-4

[3] Bulakhe, R.N., Patil, S.V., Deshmukh, P.R., Shinde, N.M. and Lokhande, C.D. (2013) Fabrication and Performance of Polypyrrole (Ppy)/TiO_2 Heterojunction for Room Temperature Operated LPG Sensor. *Sensors and Actuators B*: *Chem-*

ical, **181**, 417-423. http://dx.doi.org/10.1016/j.snb.2013.01.056

[4] Feng, C., Li, X., Ma, J., Sun, Y., Wang, C., Sun, P., Zheng, J. and Lu, G. (2015) Facile Synthesis and Gas Sensing Properties of In_2O_3-WO_3 Heterojunction Nanofibers. *Sensors and Actuators B*: *Chemical*, **209**, 622-629. http://dx.doi.org/10.1016/j.snb.2014.12.019

[5] Ling, Z. and Leach, C. (2004) The Effect of Relative Humidity on the NO_2 Sensitivity of a SnO_2/WO_3 Heterojunction Gas Sensor. *Sensors and Actuators B*: *Chemical*, **102**, 102-106. http://dx.doi.org/10.1016/j.snb.2004.02.017

[6] Gui, Y., Dong, F., Zhang, Y., Zhang, Y. and Tia, J. (2013) Preparation and Gas Sensitivity of WO_3 Hollow Microspheres and SnO_2 Doped Heterojunction Sensors. *Materials Science in Semiconductor Processing*, **16**, 1531-1537. http://dx.doi.org/10.1016/j.mssp.2013.05.012

[7] Zhang, Y., Gu, H., Suenaga, K. and Iijima, S. (1997) Heterogeneous Growth of B-C-N Nanotubes by Laser Ablation. *Chemical Physics Letters*, **279**, 264. http://dx.doi.org/10.1016/S0009-2614(97)01048-8

[8] Suenaga, K., Colliex, C., Demoncy, N., Loiseau, A., Pascard, H. and Willaime, F. (1997) Synthesis of nanoparticles and nanotubes with well-separated layers of boron nitride and carbon. *Science*, **278**, 653. http://dx.doi.org/10.1126/science.278.5338.653

[9] Liu, H.X., Zhang, H.M., Song, J.X. and Yong, Z.Z. (2010) Electronic transport properties of an (8, 0) carbon/boron nitride nanotube heterojunction. *Chiniese Physics B*, **19**, 037104. http://dx.doi.org/10.1088/1674-1056/19/3/037104

[10] Iijima, S. (1991) Helical Microtubules of Graphitic Carbon. *Nature*, **354**, 56. http://dx.doi.org/10.1038/354056a0

[11] Saito, R., Dresselhaus, G. and Dresselhaus, M.S. (1998) Physical Properties of Carbon Nanotubes. Imperial College Press, London.

[12] Zhao, P., Wang, P.J., Zhang, Z., Fang, C.F., Wang, Y.M., Zhai, Y.X. and Liu, D.S. (2009) Electronic Transport Properties of DTE-Based Molecular Switch with SWCNT Electrodes: Effect of Chirality. *Solid State Communications*, **149**, 928-931. http://dx.doi.org/10.1016/j.ssc.2009.03.027

[13] Zhao, P., Wang, P.J., Zhang, Z. and Liu, D.S. (2010) Negative Differential Resistance in a Carbon Nanotube-Based Molecular Junction. *Physics Letters A*, **374**, 1167-1171. http://dx.doi.org/10.1016/j.physleta.2009.12.047

[14] Blase, X., Rubio, A., Louie, S.G. and Cohen, M.L. (1994) Stability and Band Gap Constancy of Boron Nitride Nanotubes. *Europhysics Letters* (*EPL*), **28**, 335-340. http://dx.doi.org/10.1209/0295-5075/28/5/007

[15] Rubio, A., Corkill, J.L. and Cohen, M.L. (1994) Theory of Graphitic Boron Nitride Nanotube. *Physical Review B*, **49**, 5081-5084. http://dx.doi.org/10.1103/PhysRevB.49.5081

[16] Chernozatonskii, L.A., Galpern, E.G., Stankevich, I.V. and Shimkus, Y.K. (1999) Nanotube C-BN Heterostructures: Electronic Properties. *Carbon*, **37**, 117-121. http://dx.doi.org/10.1016/S0008-6223(98)00194-8

[17] Golberg, D., Bando, Y., Mitome, M., Kurashima, K., Grobert, N., Reyes-Reyes, M., Terrones, H. and Terrones, M. (2002) Nanocomposites: Synthesis and Elemental Mapping of Aligned B-C-N Nanotubes. *Chemical Physics Letters*, **360**, 1-7. http://dx.doi.org/10.1016/S0009-2614(02)00783-2

[18] Lambin, Ph., Fonseca, A., Vigneron, J.P., Nagy, J.B. and Lucas, A.A. (1995) Structural and Electronic Properties of Bent Carbon Nanotubes. *Chemical Physics Letters*, **245**, 85-89. http://dx.doi.org/10.1016/0009-2614(95)00961-3

[19] Zhang, Z.H., Guo, W.L. and Tai, G. (2007) Coaxial Nanotubes: Carbon Nanotubes Sheathed with Boron Nitride Nanotubes. *Applied Physics Letters*, **90**, Article ID: 133103. http://dx.doi.org/10.1063/1.2714997

[20] Enyashin, A.N. and Ivanovskii, A.L. (2005) Mechanical and Electronic Properties of a C/BN Nanocable under Tensile Deformation. *Nanotechnology*, **16**, 1304-1310. http://dx.doi.org/10.1088/0957-4484/16/8/054

[21] Kawaguchi, M. (1997) B/C/N Materials Based on the Graphite Network. *Advanced Materials*, **9**, 615-625. http://dx.doi.org/10.1002/adma.19970090805

[22] Azevedo, S., de Paiva, R. and Kaschny, J.R. (2006) Stability and Electronic Structure of $B_xN_yC_z$ Nanotubes. *Journal of Physics*: *Condensed Matter*, **18**, 10871-10879. http://dx.doi.org/10.1088/0953-8984/18/48/014

[23] Kim, S.Y., Park, J., Choi, H.C., Ahn, J.P., Hou, J.Q. and Kang, H.S. (2007) X-Ray Photoelectron Spectroscopy and First Principles Calculation of BCN Nanotubes. *Journal of the American Chemical Society*, **129**, 1705-1716. http://dx.doi.org/10.1021/ja067592r

[24] Blase, X., Charlier, J.-C., De Vita, A. and Car, R. (1997) Theory of Composite $B_xC_yN_z$ Nanotube Heterojunctions. *Applied Physics Letters*, **70**, 197. http://dx.doi.org/10.1063/1.118354

[25] Liu, H.X., Zhang, H.M., Song, J.X. and Yong, Z.Z. (2010) Electronic Transport Properties of an (8, 0) Carbon/Boron Nitride Nanotube Heterojunction. *Chinese Physics B*, **19**, Article ID: 037104. http://dx.doi.org/10.1088/1674-1056/19/3/037104

[26] Zhao, P., Liu, D.S., Zhang, Y., Su, Y., Liu, H.Y., Li, S.J. and Chen, G. (2012) Electronic Transport Properties of Zigzag Carbon- and Boron-Nitride-Nanotube Heterostructures. *Solid State Communications*, **152**, 1061-1066.

http://dx.doi.org/10.1016/j.ssc.2012.03.018

[27] Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Zakrzewski, V.G., Montgomery, J.A., Stratmann, R.E., Burant, J.C., Dapprich, S., Millam, J.M., Daniels, A.D., Kudin, K.N., Strain, M.C., Farkas, O., Tomasi, J., Barone, V., Cossi, M., Cammi, R., Mennucci, B., Pomelli, C., Adamo, C., Clifford, S., Ochterski, J., Petersson, G.A., Ayala, P.Y., Cui, Q., Morokuma, K., Malick, D.K., Rabuck, A.D., Raghavachari, K., Foresman, J.B., Cioslowski, J., Ortiz, J.V., Stefanov, B.B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Gomperts, R., Martin, R.L., Fox, D.J., Keith, T., Al-Lamham, M.A., Peng, C.Y., Nanayakkara, A., Gonzalez, C., Challacombe, M., Gill, P.M.W., Johnson, B.G., Chen, W., Wong, M.W., Andres, J.L., Head-Gordon, M., Replogle, E.S. and Pople, J.A., Gaussian 2004 (Inc., Wallingford CT).

[28] EL-Barbary, A.A., Lebda, H.I. and Kamel, M.A. (2009) The High Conductivity of Defect Fullerene C_{40} Cage. *Computational Materials Science*, **46**, 128-132. http://dx.doi.org/10.1016/j.commatsci.2009.02.034

[29] El-Barbary, A.A., Eid, Kh.M., Kamel, M.A. and Hassan, M.M. (2013) Band Gap Engineering in Short Heteronanotube Segments via Monovacancy Defects. *Computational Materials Science*, **69**, 87-94. http://dx.doi.org/10.1016/j.commatsci.2012.10.035

[30] EL-Barbary, A.A., Ismail, G.H. and Babeer, A.M. (2013) Effect of Monovacancy Defects on Adsorbing of CO, CO_2, NO and NO_2 on Carbon Nanotubes: First Principle Calculations. *Journal of Surface Engineered Materials and Advanced Technology*, **3**, 287-294. http://dx.doi.org/10.4236/jsemat.2013.34039

[31] Hindi, A. and EL-Barbary, A.A. (2015) Hydrogen Binding Energy of Halogenated C_{40} Cage: An Intermediate between Physisorption and Chemisorption. *Journal of Molecular Structure*, **1080**, 169-175. http://dx.doi.org/10.1016/j.molstruc.2014.09.034

[32] EL-Barbary, A.A. (2015) ^{1}H and ^{13}C NMR Chemical Shift Investigations of Hydrogenated Small Fullerene Cages C_n, C_nH, C_nH_n and C_nH_{n+1}: n = 20, 40, 58, 60. *Journal of Molecular Structure*, **1097**, 76-86. http://dx.doi.org/10.1016/j.molstruc.2015.05.015

[33] E EL-Barbary, A.A., Eid, Kh.M., Kamel, M.A., Osman, H.M. and Ismail, G.H. (2014) Effect of Tubular Chiralities and Diameters of Single Carbon Nanotubes on Gas Sensing Behavior: A DFT Analysis. *Journal of Surface Engineered Materials and Advanced Technology*, **4**, 66-74. http://dx.doi.org/10.4236/jsemat.2014.42010

[34] Chang, H., Lee, J.D., Lee, S.M. and Lee, Y.H. (2001) Adsorption of NH_3 and NO_2 Molecules on Carbon Nanotubes. *Applied Physics Letters*, **79**, 3863. http://dx.doi.org/10.1063/1.1424069