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Study Adsorption Ability Of Pure Single Walled Carbon Nano Tube To Detection Some Toxic Gases Using DFT Calculation

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Abstract. In this present study Density Function Theory (DFT) method was used to determine geometrical, electronic and adsorption proprieties. In this study assume that 0 eV is ideal adsorption energy because all interaction strength gave positive value. Result show that during interaction of gas molecule with surface of carbon nano tube sence methane (CH_4) gas physically grater than carbon dioxide (CO_2) and sulfide dihydride (H_2S) because interaction energy approximately to ideal zero. Result show that also, resulting from physical adsorption any effect on electronic and geometrical priorities was absence. Molecular orbital and energy gap doesn't effect during adsorption process. Charge transfer show that very small electrons transport between interaction systems.

Keywords: Adsorption energy. Molecular orbital, Charge transfer.

INTRODUCTION

In recent year, carbon nanotubes have been investigated by researchers due to special properties. It has special geometry and unique properties of carbon allotropes also, offer great potential application such as electronic devices, energy storage, chemical props and biosensors[1-4]. Because high surface to volume ratio and hollow structure of nano materials is ideal to for gas chemical and physical adsorption. Gas sensor based on one dimensional material such as nano-wire, carbon nanotubes and nano-fiber. Two-dimensional material such as graphene and it is derivative[5]. First discover of carbon nanotubes by Lijima in 1991[6]. In the last few years thermal, electronic, electron transport, mechanical and structural proprieties of carbon nanotubes widely has been investigated by researchers[7]. Carbon nanotubes divided to two types on single walled carbon nanotubes (SWCNT) and other was multi walled carbon nanotubes (MWCNT). The diameter of SWCNT was about 1 nm for MWCNT varies in ranges 5-100 nm[8]. The gas molecules that adsorbed with surface of carbon nanotubes change several properties such as structural and electronic[9, 10]. Carbon nanotubes have faster response, high sensitivity, smaller size and low operation temperature[11-12]. These characteristics make carbon nanotubes better application in environmental field, pharmaceuticals and biomedical[13-16]. Aim of present study determine strength of physical adsorption of gases molecule under research, also pointed ideal case of adsorption process that approximate to ideal interaction energy. Gases under study was Methane (CH_4), Carbon dioxide (CO_2) and Sulfide dihydride (H_2S).

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COMPUTATIONAL METHOD

Nano tube modular is used in this study to generate graphene nano-ribbon structure n=m=3 and tube length 1 nm. Export structure to Gaussian 5.0 version for display system. Then exporting the input data to Gaussian 09, this is to compute geometrical and electronical properties, also adsorption energy. DFT method was used to compute the ground state properties depending on electron density. Molecular orbital energy provides a Higher Occupied Molecular Orbital (HOMO) and Lower Unoccupied Molecular Orbitals (LUMO), Energy gap and Relaxation structure were computed by DFT method. UV-Visible properties are computed by the time depending-density function theory. Basis set used in present study was 6-31G and hybrid function B3LYP [14].

RESULT AND DISCUSSIONS

Geometrical Proprieties

Figure (1) represent geometrical structure for single walled carbon nano tube (SWCNT). Nano system conation several bond between atom that formed structure. Structure have four types of bond between atoms they are C-C, C=C, C-C (aromatic) and C-H. The bond length was (1.4481-1.4769), (1.3546), (1.4173-1.4421) and (1.0852) Å respectively. Bond length of C=C and C-H have one value because symmetry of atom that arranged on edge of structure. All bond length related to SWCNT was agreement with experimental and theoretical measurement [17].

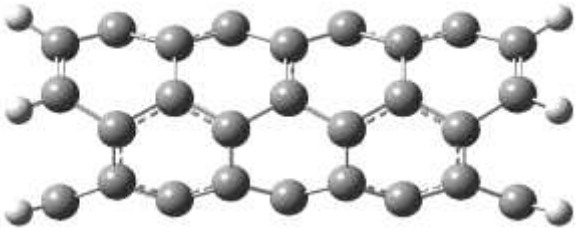

FIGURE 1. Represent geometrical structure for SWCNT before interaction.

Electronic Proprieties And Adsorption Energy

In this section used DFT calculation at basis set 3-21G with hybrid function B3LYP to computed electronic proprieties for SWCNT before and after interaction. Table 1 listed electronic proprieties for nano system in absence the gases molecule. Result show that nano system has semiconductor properties, also have same behavior of graphene nano-ribbon in same degree of charity [18]. Degree of charity mean n, m and length values, present calculation indicates that SWCNT have same electronic proprieties of graphene nano-ribbon. Table 2 listed electronic proprieties of SWCNT in presence gases molecule. Result show that total energy of interaction system was decreased that mean interaction process stable. Figure 2 represent molecular orbital distribution for adsorption system. Before interaction process all molecular orbital overlap C-C bonding and distribution was symmetry[16]. After molecule placed on surface of SWCNT molecular orbital remain distribution over C-C bonding. From this result indicate that because a weak physical adsorption molecular orbital doesn't effect. Also, probability of electron transport was low. Energy gap during adsorption system was approximately equal SWCNT band energy, because physical interaction between systems.

TABLE 1. Listed electronic proprieties for nano system in absence the gases molecule.

Property	Absence gases molecule
E_T (a.u.)	-2053.0914
HOMO (eV)	-4.7085
LUMO (eV)	-2.3292
E_g (eV)	2.379

TABLE 2. Listed electronic proprieties of SWCNT in presence gases molecule.

Gases	E_T (a.u.)	HOMO (eV)	LUMO (eV)	E_g (eV)
CH_4	-2093.3941	-4.7186	-2.3450	2.373
CO_2	-2240.6179	-4.7194	-2.3363	2.383
H_2S	-2450.5083	-4.7815	-2.4068	2.374

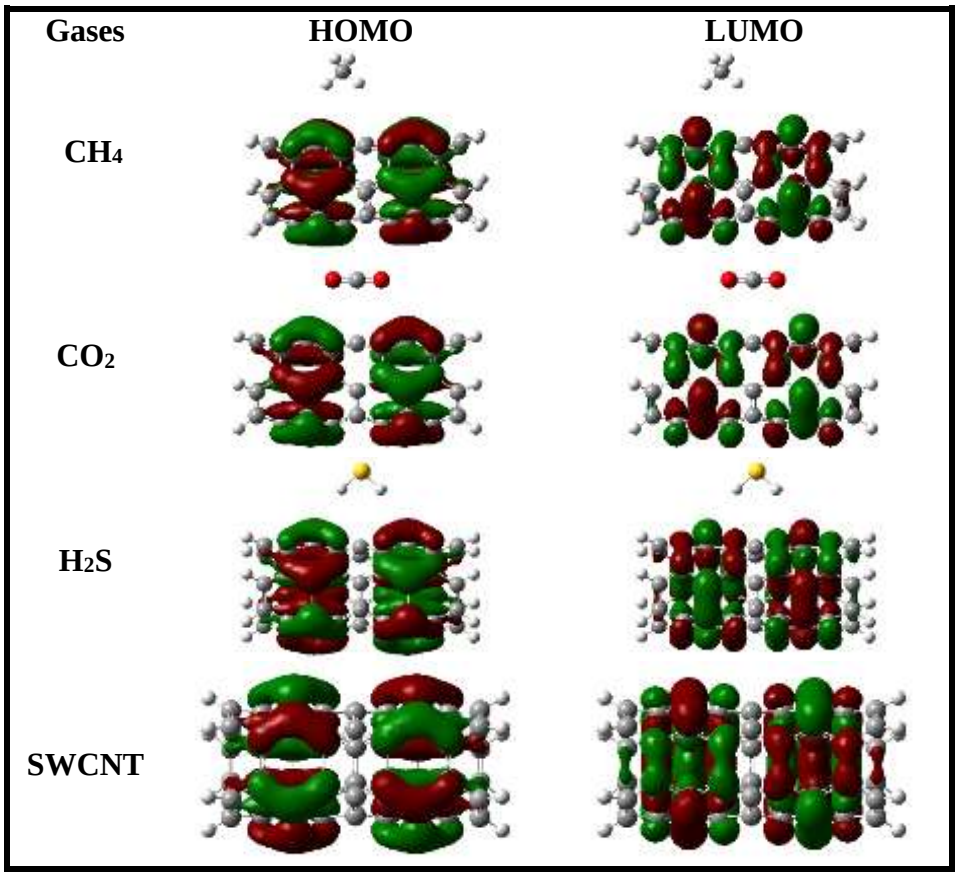

FIGURE 2. Represent molecular orbital distribution for systems under study.

Adsorption energy consider important factor that describe interaction process between gases molecule and surface on SWCNT. It pointed amount of energy raising during surface interaction phenomena. Table 3 listed adsorption energy measured in eV unit. In general case structure who have adsorption energy near 0eV is more stable mean system have good binding[19]. In this study all adsorption energy has positive value. So that we assume good sensitive system that have absorption energy near ideal 0 eV refer to stable state. Result show that methane gas has exactable interaction energy compared with other gases. Adsorption calculation proved that type of interaction was physical, because all proprieties of SWCNT remain constant in presence gases molecule. Result of adsorption energy of methane gas in study[18] was 0.082 eV. In present study show CH_4 gas molecule more exactable than graphene nano-ribbon. Figure 3 represent SWCNT interaction with gases molecule. Figure 4 represent adsorption energy diagram measured in eV unit.

TABLE 3. Represent adsorption energy for interaction gases molecule with SWCNT in eV unit.

Gases	Adsorption energy (eV)
CH_4	0.0303
CO_2	0.0784
H_2S	0.0833

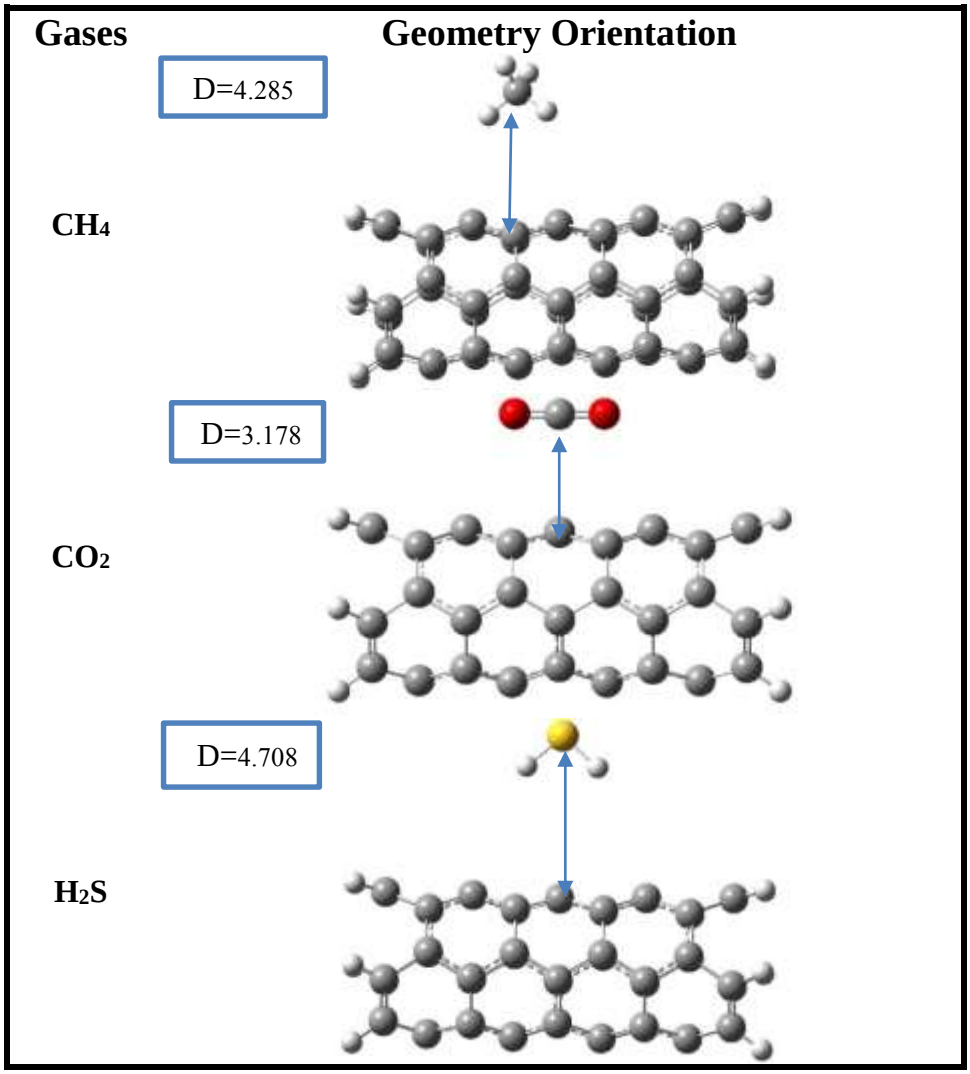

FIGURE 3. Represent geometry orientation of gases molecule over surface of SWCNT

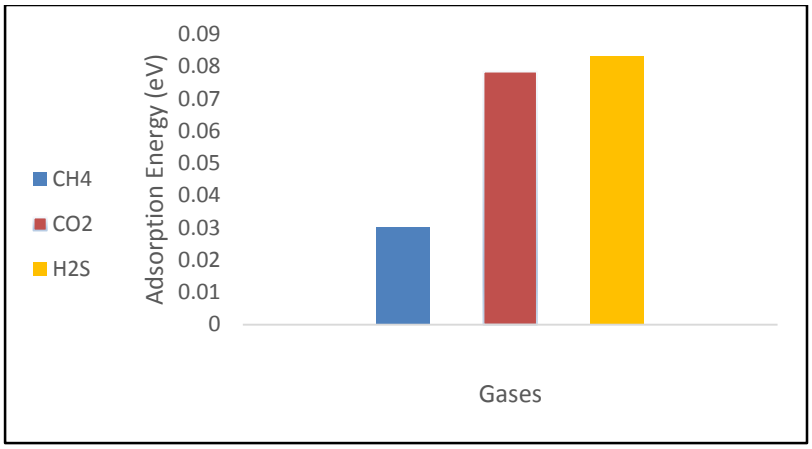

FIGURE 4. Represent adsorption energy diagram for interaction gases molecule.

Charge Transfer Analysis

Charge transfer (CT) calculation is important tool to determine amount of charge transfer between two reactors. By this calculation can be pointed track of charge direction. Track of charge direction depended on sign of charge transfer between two rectors. If CT have positive value this mean charge transfer from gas molecule to graphene nano-ribbon. CT have negative value this mean track of charge transport was from graphene nano-ribbon to gas molecule[20]. Table 4 represent charge transfer value for adsorbed gas molecule. Result show that charge transfer from SWCNT to adsorbed gas molecule. Also, because a physical adsorption and low interaction energy charge analysis show that small amount of electron transfer between two reactor system[20].

TABLE 4. Represent charge transfer value for adsorbed gas molecule.

Gases	Charge transfer
CH_4	-0.0062
CO_2	-0.0028
H_2S	-0.0012

CONCLUSIONS

In present research, study interaction between toxic gases and surface of SWCNT by DFT calculation. Geometrical and electronic proprieties of SWCNT not appear any change because physical adsorption. Present study proved SWCNT was modify phase from graphene nano-ribbon. molecular orbital doesn't effect during interaction process resulting from low physical adsorption energy raise Also, energy gap doesn't effect. Charge transfer calculation show that small amount of charge transfer from SWCNT to gases molecule. adsorption phenomena show that CH_4 gas molecule more favorite compared from H_2S and CO_2.

REFERENCES

1- M.S.Dresselhaus, G.Dressehaus, P.C.Eklund, Science of Fullenrenes and Carbon Nanotubes, (Academic Press, New York, 1996).
2- T.Ebbesen ed., Carbon Nanotube: Preparation and Properties, (CRC Press, Boca Raton, 1997).
3- [3] R.Saito, G.Dressehaus, M.S.Dresselhaus, Physics Properties of Carbon Nanotubes, (World Scientific, New York, 1998).
4- J.P.Lu, J.Han, Inter.J.High Electronics and System 9, 101(1998).

5- Reena Srivastavaa,c, , Harshika Sumanb , Sadhana Shrivastavaa , Anurag Srivastavac, " DFT analysis of pristine and functionalized zigzag CNT: A case of H2S sensing", Chemical Physics Letters, vol. 731, (2019.
6- S. Iijima, Nature 354, 56–58, (1991).
7- R.H. Baughman, A.A. Zakhidov, W.A. de Heer, Science 787–792, (2002).
8- N. Sinha, J. Ma, J.T. Yeow, J. Nanosci. Nanotechnol. 6, 573–590, (2006).
9- X.-X. Zhang, W.-T. Liu, J. Tang, P. Xiao, Study on PD detection in SF6 using multi- wall carbon nanotube films sensor, IEEE Trans. Dielectr. Electr. Insul. 17, 838–844, (2010).
10- J. Kong, N.R. Franklin, C. Zhou, M.G. Chapline, S. Peng, C. Kyeongjae, D. Hongjie, Nanotube molecular wires as chemical sensors, Science 287, 622–625, (2000).
11- X.-X. Zhang, Y. Bing, X.-J. Wang, C.-C. Luo, Effect of plasma treatment on multi- walled carbon nanotubes for the detection of H2S and SO2, Sensors 12, 9375–9385, (2012).
12- X.-X. Zhang, Y. Bing, Z.-Q. Dai, C.-C. Luo, The gas response of hydroxyl modified SWCNTs and carboxyl modified SWCNTs to H2S and SO2, PrzegladElektrotechniczny 88, 311–314, (2012).
13- T. Wei-Cheng, L. Hung-Ling, K. Chun-Yen, L. Chia-Jung, H. Chang-Jung, Sensors, IEEE 2011, pp. 1036–1039, (2011).
14- Y. Hizhnyi, S.G. Nedilko, V. Borysiuk, V.A. Gubanov, Int. J. Quan. Chem. 115, 1475–1482, (2015).
15- D.W.H. Fam, A.L. Palaniappan, A.I.Y. Tok, B. Liedberg, S.M. Moochhala, Sens. Actuators B Chem. 15, (2012).
16- M. Mittal, A. Kumar, Sens. Actuators B Chem. 203 (2014) 349, (2014). F. Mofidi and A. Reisi-Vanani, "Investigation of the electronic and structural properties of graphyne oxide toward CO, CO2 and NH3 adsorption: A DFT and MD study", Applied Surface Science. 507, 145134, (2020).
17- Mohammed A. Al-Seady and Hayder M. Abduljalil, "Study of Some Environmental Applications of Graphene and Boron-Nitride Nano-Ribbons Using Density Function Theory", Master Thesis, University of Babylon, Collage of Science, (2020).
18- S. Aghaei, M. Monshi, I. Torres, and I. Calizo, "Adsorption and Dissociation of Toxic Gas Molecules on Graphene-like BC3: A Search for Highly Sensitive Molecular Sensors and Catalysts", arXiv preprint arXiv:1706.00774, 2017.
19- R. Chandiramouli, A. Srivastava, and V. Nagarajan, "NO adsorption studies on silicene nanosheet: DFT investigation", Applied Surface Science, vol. 351, no. 2 pp. 662-672, 2015.
20- S. Sakina, Z. Johari, Z. Auzar, N. E. Alias, M. Abidin, and M. F. M. Yusoff, "Improving graphene nanoribbon gas sensing behavior through warping", Materials Research Express, vol. 4, no. 1, p. 015003, 2017.