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Investigation of Molecular Selenium Adsorption to the Outer Surface of Single Wall Carbon Nanotubes

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Abstract

In this study the adsorption of selenium molecule (Se_2) on the outer surface of zigzag (5,0), (8,0) and (10,0) carbon nanotubes has been investigated. We examined number adsorbed orientations as well as different adsorption sites on nanotubes. The adsorption energies, equilibrium distances, energy differences between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and interaction angles between nanotubes and selenium molecule have been studied in details. The results showed that the best angle of the selenium molecule with the nanotubes is zero degree. Selenium adsorption on the external surface of zigzag nanotubes increased their electrical conductivity. It is found that an increase in nanotubes diameter leads to an increase in their stability. The adsorption energy values of selenium molecule on the surface of zigzag (5,0) and (8,0) nanotubes was low and negative; therefore this was a physical adsorption and exothermic. Independent to the orientation, the adsorption process of Se_2 on (10,0) nanotube showed chemisorption with large charge transfer from nanotube to adsorbed molecule.

Keywords: *Zigzag carbon nanotubes, Adsorption, Selenium, Density functional theory.*

1. INRODUCTION

Carbon nanotubes are of great research interest because they are used in physical, chemical, and nanotechnological applications since the discovery of single wall carbon nanotubes (SWCNTs) [1, 2]. Due to specific chemical and physical properties of carbon nanotubes, their practical applications have been extended in design of sensors, energy storage, electrochemical and electronic devices [3] and advanced technological innovation [4]. The electrical characteristic of SWCNTs depends on their chirality (n, m) and tube diameter [4]. The length and the sidewall curvature have influence on electronic structure and energetics of a nanotube [5-9]. Due to large current carrying capacity and thermal stability of metallic carbon nanotubes, they have been identified as potential candidates for interconnect applications [10] and emission devices [11]. The chemical reactivity of carbon nanotubes arises from the formation of the electron cloud on the wall of the tube. The physical properties and electronic structures of organic p-aromatic materials such as SWCNTs can be altered by molecular interactions. During the last decades, the research efforts have been carried out to investigate properties changes of SWCNTs due to adsorption of foreign molecules or atoms on external surface of carbon nanotubes [12-14]. The adsorption of different molecules such as oxygen, hydrogen, and methane on SWCNTs has been studied [15]. Using density functional theory (DFT), Rafati et al. [16] have investigated the adsorption of oxygen molecules and atoms. In their studies, adsorption of oxygen molecules on the inner and the outer walls of the SWCNTs has been found to be physical and chemical, respectively. Javid et al. have studied chemical adsorption of benzene on the inside and outside of the SWCNTs using the density functional theory [17]. Hydrogen storage has been investigated inside armchair SWCNTs using molecular dynamics simulation by Davoodi and co-workers. Their results showed hydrogen storage within SWCNTs for radius larger than (5,5) SWCNTs radius [18].

The synthesis of SWCNTs produces a mixture of metallic and semiconducting nanotubes and so their applications are limited in the presence of semiconducting [19, 20] because of their low density of states (DOS) around the Fermi level [13, 21]. To overcome this limitation, it is possible to change the semiconductor nanotubes to metallic ones or separate them. However, the challenge is separation of metallic nanotubes from the as-synthesized mixture [22]. One can functionalize SWCNTs with transition metals (TM) [23-28] and halogens [29] to change their electrical properties from semiconductor to metallic.

Selenium exhibits rich chemistry and semiconductor properties, and has several applications in electronics [30]. Nanostructured selenium has significant potential for applications in solar cells, sensors, photonic devices, rectifiers, xerography and photographic exposure meters [31-33].

Although, selenium is not metal and does not belong to halogen family, but Krishnan and co-workers's studies [34] showed that adsorption of atomic selenium on the outer surface of SWCNTs can convert the semiconductor nanotubes to metallic and increases the conductance of the metallic and semimetallic ones. First-principles calculations have been employed to determine and rationalize the structural and electronic properties of Se monomers, dimmers, trimmers and wires interacting with the semiconductor (8, 0) SWNT. These results revealed the formation of Se clusters on SWCNTs because Se−Se bonds show much favorite than Se−C ones [35]. For this reason, and in order to study the effect of molecular orientation on the adsorption, we investigated molecular selenium adsorption on the outer surface of SWCNT. It is the first *ab initio* theoretical study on the structural and electronic properties of the nano tube- selenium molecule system. This is the first time to gain a conclusive insight into the interaction of Se molecule (Se_2) with the zigzag SWCNTs. In this study, we investigate the orientation of adsorbed Se_2 on the outside surface of zigzag (5,0), (8,0) and (10,0) carbon nanotubes. We have determined the adsorption energies, equilibrium distances, the energy gaps between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and interaction angles between nanotubes and Se_2. This helps to make an understanding of the relationship between nanotubes electrical conductivity and their stability with the adsorption of Se_2.

2. COMPUTATIONAL METHOD

The Tube Gen [36] was used for drawing of all SWCNTs geometries. During the adsorption of Se_2 on SWCNTs, the structural and electronic properties of the tube-molecule systems have been investigated using the DFT. DFT calculations were performed using Becke's three-parameter exchange functional with the Lee-Yang-Parr correlation functional (B3LYP) [37, 38]. The Los Alamos effective core potential with second double-zeta (LANL2DZ) [39] was used as the basis set. Calculations were carried out using Gaussian 03 software [40]. The selection of this level of theory was based on the success of the applied methods in theoretical studies of the chemistry of

SWCNTs [41-45] and their substitutionally doped analogs by several research groups [46, 47] and limitation of computational costs arising from the size of the studied system and the inclusion of selenium dimmer. Abadir et al. in their study about the effect of the basis set choice on the results of carbon nanotubes DFT calculations, recommended a double-zeta polarized basis set for predicting the population analysis and electronic structure of a nanotube and a physisorbed biomolecule [48].

The calculated vibrational frequencies for all the structures indicate no imaginary frequency, but show that these conformers all correspond to the true minima on the potential energy surface.

In the present work, we have used a carbon nanotube of zigzag type. For SWCNTs, calculations were performed to obtain the adsorption energy curves as well as the equilibrium tube-molecule distance for each system. The natural bond orbital (NBO) has been used to obtain the total charge transfers (Q_{ct}) from the nanotubes to the Se_2.

To study the interactions of Se_2 with the zigzag (5,0), (8,0) and (10,0) SWCNTs, different adsorption sites on top of the carbon atoms of the nanotube were considered. Average distance between C-C atoms was 1.42 Å and diameter of the (5,0), (8,0) and (10,0) nanotubes were 3.96 , 6.3 and 7.86 Å, respectively. The number of carbon atoms in the (5,0), (8,0) and (10,0) nanotubes were 62, 82, and 102, respectively. Different possible orientations of the Se_2 for adsorption on the outside of the carbon nanotubes were investigated (in angles 0, 45, 90 and 135˚). We calculated the total energy of the tube-molecule system ($E_{tube-Se}$) as well as the distinct tube (E_{tube}) and Se_2 (E_{Se}). The adsorption energy (E_{ad}) can be calculated with the basis sets corrections by

$$E_{ad}=E_{(tube-Se)}-(E_{tube}+E_{Se})+BSSE \qquad (1)$$

where BSSE is basis set superposition error and is eliminated by the standard counterpoise correction method of Boys and Bernardi [49].

2. RESULTS AND DISCUSSION

In order to investigate the adsorption of Se_2 and find the most stable adsorption configurations, Se_2 are initially placed at different orientations and positions above the surface of tubes. Figure 1 demonstrates different locations on the nanotube where Se_2 can be placed. In site A, the selenium molecule is placed on carbon atom which is at the end of the tube. In position C, this molecule is placed on the middle carbon. In sites B and E the selenium molecule is placed on the bond between the two carbons and in location D it is placed at the center of the ring.

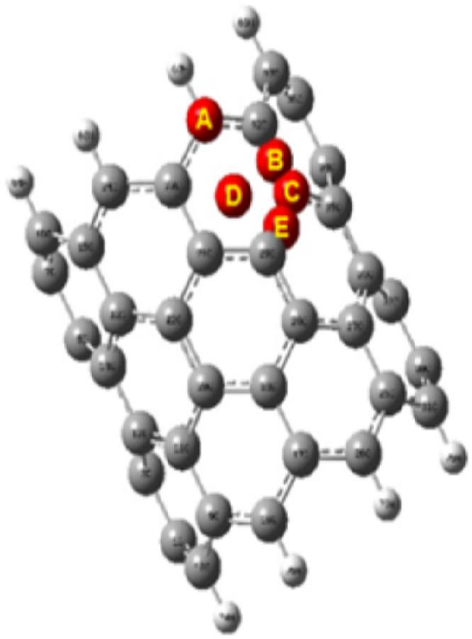

Figure 1. *Different orientations of selenium molecule on the nanotube.*

Figure 2 shows the energy of the (10,0) nanotube structure with selenium molecule in positions A, B, C, D and E based on the distance between selenium molecule and the nanotube. As Figure 2 demonstrates, the adsorption energy in location A is less negative than other positions which represents the weaker adsorption of selenium molecule with the nanotube. The most stable position for Se_2 on the nanotube is where the adsorption energy is the least. Therefore, site A is not suitable for selenium molecule.

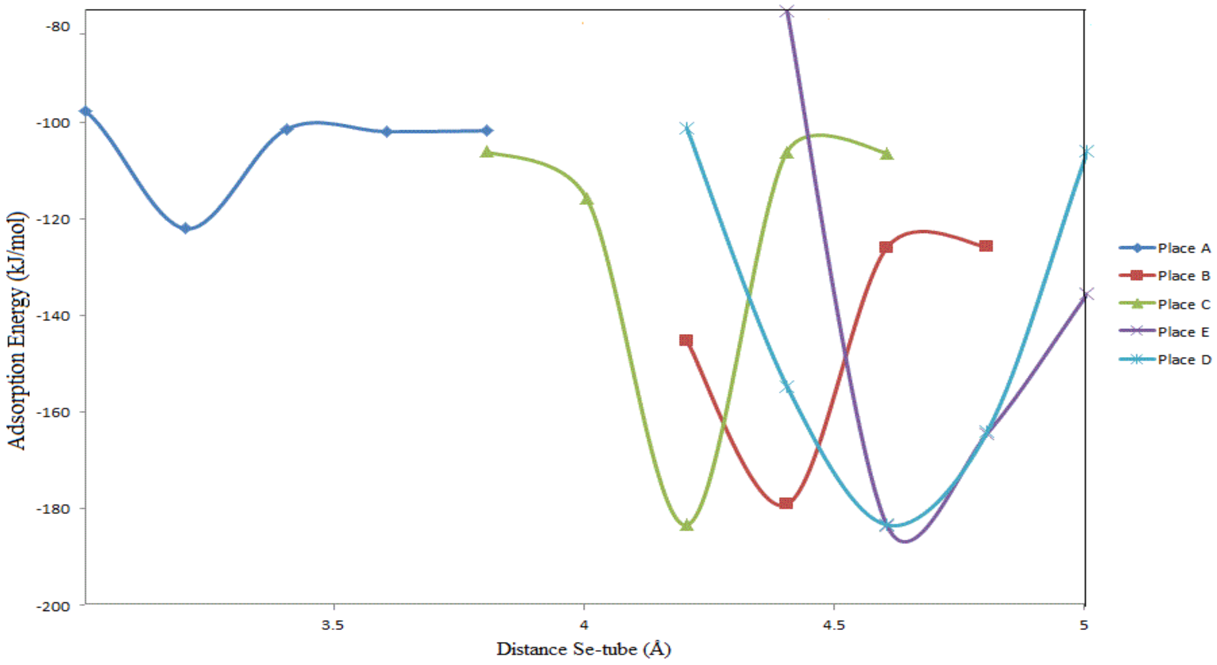

Figure 2. *Energy of the (10,0) nanotube structure with selenium molecule.*

The adsorption energy values of selenium molecule with nanotube in sites B, C, D and E are almost equal and they are more negative than location A. Thus, each of these positions is a suitable site for placement of Se_2, but the most negative adsorption energy belongs to location C and in this study, the Se_2 is placed in site C. Similar findings have also been obtained for the adsorption of Se_2 on (5,0) and (8,0) nanotubes.

By varying the direction of the placement of Se_2 with respect to carbon nanotube axis with angles 0˚, 45˚, 90˚, and 135˚, the best orientation of selenium can be achieved. This study was done at the above-mentioned angles.

Figure 3 demonstrates the placement of Se_2 at different angles with respect to the external surface of the (8,0) nanotube.

Table 1 shows the adsorption energy, HOMO, LUMO and energy gap and equilibrium distance between selenium molecule and the external surface of the (5,0), (8,0), and (10,0) nanotubes at angles 0˚,45˚,90˚, and 135˚ in site C.

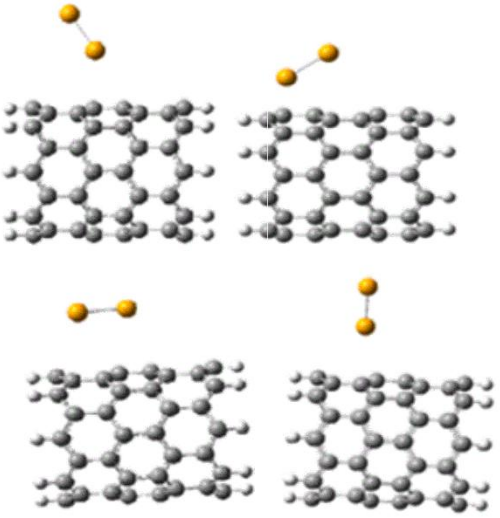

Figure 3. *Placement of Se_2 at different angles with respect to the external surface of the (8,0) nanotube.*

As Table 1 demonstrates, the best orientation of selenium with respect to carbon nanotube is angle 0˚. This can be attributed to selenium molecule being

Table 1. *The absorption energy, HOMO, LUMO energies, gap energy and equilibrium distance of Se_2 adsorbed on the external surface of the nanotubes at different angles.*

SWCNT (n,m)	θ (deg)	R_e(Å)	E_{ad} (kcal/mol)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{gap} (eV)
(5,0)	0	4.60	-10.56	-5.39	-4.85	0.54
(5,0)	45	3.00	-9.68	-4.49	-3.85	0.64
(5,0)	90	3.80	-6.92	-5.35	-4.59	0.75
(5,0)	135	4.00	-6.04	-5.19	-4.38	0.81
(8,0)	0	4.20	-14.00	-4.34	-4.04	0.30
(8,0)	45	4.80	-11.32	-4.32	-3.94	0.37
(8,0)	90	4.65	-9.25	-4.32	-3.91	0.41
(8,0)	135	4.20	-10.31	-4.34	-3.99	0.35
(10,0)	0	4.20	-25.37	-4.24	-3.89	0.35
(10,0)	45	4.20	-21.45	-4.31	-3.94	0.37
(10,0)	90	3.80	-23.29	-4.32	-3.96	0.36
(10,0)	135	3.30	-22.37	-4.30	-3.96	0.37

exactly in line with the axis of the zigzag nanotube. Selenium molecule prefers to have the smallest angle with the tube axis; this angle is in line with angle of the zigzag nanotube (Figure 4).

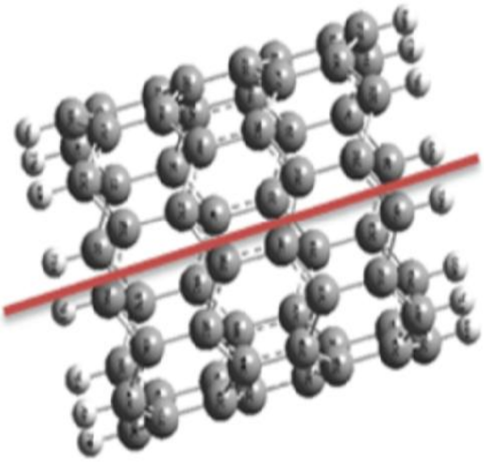

Figure 4. *The axis of the zigzas nanotube.*

As can be seen from table 1, the interaction distances are 4.20, 4.20, 3.80, 3.30 Å and adsorption energy values of the Se_2 on the external wall of the (10,0) carbon nanotube are -25.37, -21.45, -23.29 and -22.37 kcal/mol at angles 0˚, 45˚, 90˚, and 135˚, respectively, suggesting chemisorption. For the rest of the configurations, the adsorption energies are less negative than –15 kcal/mol, indicating that the adsorption process is physisorsption in nature and the Se_2 is stabilized on the surfaces of the (5,0) and (8,0) nanotubes without any type of chemical bonding between them as the adsorption values are negative and the phenomenon is exothermic. As table 1 shows, adsorption energies at 0˚ for (5,0), (8,0), and (10,0) nanotubes are -10.56, -14.00, and -25.37 kcal/mol, respectively. These results show that at the best orientation (0˚), adsorption energy decreases with the increase of the diameter of tube. Adsorption energy for (10,0) nanotube is more negative than that of (5,0) and (8,0) nanotubes. This is probably due to the large diameter of (10,0) nanotube as well as the larger number of carbons of this nanotube. As the diameter of (8,0) nanotube is larger than that of nanotube (5,0), its energy is lower too. In other words, as the nanotube diameter increases, the stability of the nanotube-selenium system increases.

The energy gap (E_{gap}) which is energy difference between the HOMO and LUMO for all nanotubes used in the present work before adsorption of selenium are collected in table 2. It is seen that the calculated band gaps of (8,0) and (10,0) tubes are almost the same, while the gap is much larger for (5,0) tube. This is due to the smaller diameter of this nanotube comparing to the other nanotubes, but, as the (8,0) and (10,0) nanotubes are not very different regarding their diameters, the difference in their energy gap is not noticeable.

Calculated E_{gap} for adsorption of selenium molecule on (5,0) nanotube range from 0.54 to 0.81 eV, while it is 0.93 eV for bare (5,0) nanotube. Therefore, adsorption of Se_2 has significant effect on the electronic structure of (5,0) nanotube. On the contrary, for adsorption of Se_2 on the (8,0) and (10,0) nanotubes, HOMO and LUMO levels change slightly and consequently

***Table 2.** HOMO energies (E_{HOMO}), LUMO energies (E_{LUMO}) and HOMO-LUMO energy gap (E_{gap}) and Fermi energies (E_F) of the nanotubes (eV).*

SWCNT (n,m)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_{gap} (eV)	E_F (eV)
(5,0)	**-4.21**	**-3.28**	**0.93**	**-3.75**
(8,0)	**-4.07**	**-3.65**	**0.42**	**-3.86**
(10,0)	**-4.10**	**-3.69**	**0.41**	**-3.90**

their E_{gap} values are almost unchanged. E_{gap} values for the configurations of (8,0) and (10,0) nanotubes vary in the range between 0.30-0.41 eV and 0.35-0.37 eV, respectively, compared to 0.42 eV for bare (8,0) nanotube and o.41 eV for bare (10,0) nanotube. E_{gap} has the least value at 0˚ for all nanotubes. Table 1 shows that variations in the orientation of selenium molecule at angles 45˚, 90˚, and 135˚ doesn't have an equal effect on the energy gap of (5,0), (8,0), and (10,0) nanotubes. Regarding (10,0) nanotube E_{gap} at 45˚, 90˚, and 135˚ does not have noticeable differences. The effect of selenium's approaching (8,0) nanotube at the mentioned angles is similar to that of (10,0) nanotube; but, in (5,0) nanotube, as the angle increases, the E_{gap} value increases. Compared with (8,0) and (10,0) nanotubes, the (5,0) nanotube has a smaller diameter, and the orientation variation of the adsorbed molecule on its energy gap is distinct. By the increase in the angle and selenium's receding from the nanotube axis, the amount of E_{gap} increases and electric conduction decreases.

As HOMO energy is usually used as a criterion for determining the electrophilicity ability of a molecule, an increase in the amount of HOMO energy with the appropriate orientation of the adsorbed molecule to give the electrons of this orbital to a suitable recipient, can lead to the increase in reaction, and finally leads to better adsorption. Table 1 indicates that the placement of selenium molecule at angle 0˚ relative to the axis of the nanotube leads to decrease in energy gap. Therefore, electric conduction of the nanotube increases by the adsorption of Se_2.

To verify the effect of the Se_2 adsorption on the electronic properties of nanotubes, the DOSs of some Se_2- nanotubes systems were calculated and indicated in Figure 5. Consistent with adsorption energies, the DOS analysis shows that interactions between Se_2 and (5,0) and (8,0) nanotubes are weaker than (10,0) nanotube. Inspection of the Figure 5 indicates that in Se_2-(10,0) nanotube system the strong interaction causes dramatic changes in the DOS on both sides near the Fermi level.

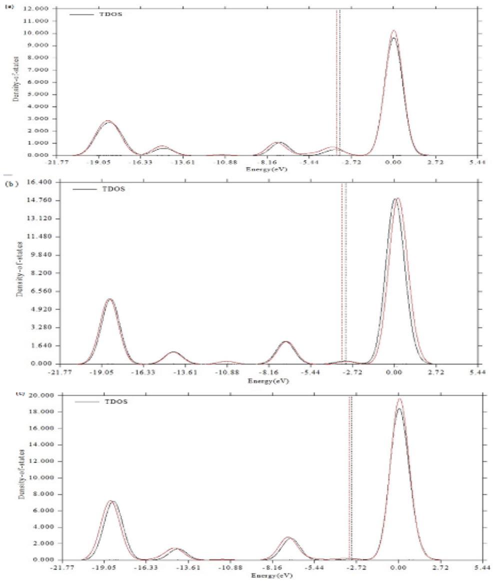

***Figure 5.** DOSs for the bar nanotubes (black curves) and Se_2-nanotubes systems (red curves) calculated for the configurations at 0^o shown in table 1. The dashed lines shows the Fermi energies. (a) (5,0) nanotube, (b) (8,0) nanotube, (c) (10,0) nanotube.*

To investigate the molecular properties, the total charge transfer (Q_{ct}), defined as the charge variation in considered nanotubes caused by the adsorption of Se_2 molecule, is calculated based on natural bond orbital (NBO) population schemes [50]. The NBO population analysis indicates charge transfers from nanotubes to the Se_2. High charge transfer from nanotubes to Se_2 is an indicator of acceptor character of selenium molecule. In the most stable configurations, the Se_2 adsorbed aligns along the carbon nanotube axis, the transferred charges from the (5,0), (8,0) and (10,0) nanotubes to Se_2 are -0.321 e, -0.451 e, and -0.297 e, respectively. These charge transfers can be predicted by the location of the HOMO and LUMO energy levels of Se_2 with respect to the Fermi levels of nanotubes. The HOMO and LUMO energies of Se_2 calculated at B3LYP level are -5.35 and -6.08 eV. The Fermi levels of (5,0), (8,0) and (10,0) nanotubes are -3.75, -3.86 and -3.90 eV, respectively (table 2). Previous investigations [51, 52] have shown that adsorbates with the LUMO lying below the graphene Fermi level, act as acceptor and graphene exhibits p-type semiconducting. Since graphenes have many properties similar to SWCNTs, so the results of present work for nanotubes are in agreement with previous studies for grapheme [51, 52]. Consequently, all studied nanotubes exhibit p-type semiconducting due to Se_2 adsorption.

3. CONCLUSION

Studying the energy curves of selenium molecule's approaching the nanotubes shows that the placement of selenium at the edges is not appropriate. The best angle at which selenium molecule can be placed with respect to the nanotubes is 0˚, which has the least adsorption energy and the least energy gap comparing to angles 45˚, 90˚, and 135˚. Since the energy gap decreases with adsorption of selenium on the external surface of the zigzag nanotubes which are semiconductors, so it leads to the increase in their electric conduction. This is more suitable regarding the nanotubes with bigger diameters. As the nanotube diameter increases, the stability of the nanotube-selenium system increases. This can be attributed to the more negative adsorption energy of the nanotube with the large diameter comparing to small diameters. Regarding the low amount of energy, adsorption of selenium on the external surface of the (5,0) and (8,0) zigzag nanotubes is physical adsorption, and as the value of the adsorption is negative, the phenomenon is exothermic. Adsorption energies of Se_2 on the (10,0) nanotube show strong interaction between Se_2 and the (10,0) nanotube.

REFERENCES

1. Iijima, S. (1991). “Helical Microtubes of Graphitetic Carbon”, *Nature*, 354: 56–58.
2. Moradi, O., Yari, M., Zare, K., Mirza, B., Najafi, F. (2012). “Carbon Nanotubes: A Review of Chemistry Principles and Reactions”, *Fullerenes, Nanotubes and Carbon Nanostructures*, 20: 138–151.
3. Charlier, J. C., Blase, X., Roche, S. (2007). “Electronic and Transport Properties of Nanotubes”, *Rev. Mod. Phys.*, 79: 677-711.
4. Baughman, R. H., Zakhidov, A. A., de Heer. W. A. (2002). “Carbon Nanotubes - The Route toward Applications”, *Science*, 297: 787-792.
5. Hamada, N., Sawada, S. I., Oshiyama, A. (1992). “New One-Dimensional Conductors: Graphitic Microtubules”, *Phys. Rev. Lett.*, 68: 1579-1581.
6. Saito, R., Fujita, M., Dresselhaus, G., Dresselhaus, M. S. (1992). “Electronic Structure of Chiral Graphene Tubules”, *Appl. Phys. Lett.*, 60: 2204-2206.
7. Odom, T. W., Huang, J. L., Kim, P., Lieber, C. M. (1998) "Atomic Structure and Electronic Properties of Single-walled Carbon Nanotubes”, *Nature*, 391: 62-64.
8. Jishi, R. A., Bragin, J., Lou, L. (1999) “Electronic Structure of Short and Long Carbon Nanotubes from First Principles”, *Phys. Rev. B*, 59: 9862-9865.
9. Gulseren, O., Yildirim, T., Ciraci, S. (2002) “Systematic ab initio Study of Curvature Effects in Carbon Nanotubes”, *Phys. Rev. Lett.*, 65: 153405(1-4).
10. Dresselhaus, M. S., Dresselhaus G**.,** Jorio, A. (2004) “Unusual Properties and Structure of Cnanotubes”, *Annu**.** Rev**.** Matter**.** Res.*, 34: 247–278.
11. Dresselhaus, M. S., Dresselhaus, G., Charlier, J. C., Hernandez, E. (2004) “Electronic, Thermal and Mechanical Properties of Carbon Nanotubes, in Nanotechnology of Carbon and Related Materials”, *Philos. Trans. R. Soc. London, Ser. A*, 362: 2065-2209.
12. Collins, P. G., Bradley, K., Ishigami, M., Zettl, A. (2000) “Extreme Oxygen Sensitivity of Electronic Properties of Carbon Nanotubes”, *Science*, 287: 1801-1804.
13. Kong, J., Franklin, N. R., Zhou, C., Chapline, M. G., Peng, S.; Cho, K., Dai, H. (2000) “Nanotube Molecular Wires as Chemical Sensors”, *Science*, 287: 622-625.

14. Dag, S., Gulseren, O., Ciraci, S. (2003) “A Comparative Study of O_2 Adsorbed Carbon Nanotubes”, *Chem. Phys. Lett.,* 380: 1-5.
15. Lithoxoos, G. P., Labropoulos, A., Peristeras, L. D., Kanellopoulos, N., Samios, J., Economou I. G. (2010) “A Combined Experimental and Monte Carlo Molecular Simulation Study”, *J. Supercrit. Fluid,* 55: 510–523.
16. Rafati, A. A., Hashemianzadeh, S. M., Nojini, Z. B. (2009) “Effect of the Adsorption of Oxygen on Electronic Structures and Geometrical Parameters of Armchair Single-Wall Carbon Nanotubes: A Density Functional Study”, *J. Colloid and Interface Sci.,* 336: 1–12.
17. Javid, A. H., Gorannevis, M., Moattar, F., Mashinchian Moradi, A., Saeeidi P. (2013) “Modeling of Benzene Adsorption in the Gas Phase on Single-Walled Carbon Nanotubes for Reducing Air Pollution”, *Int. J. Nanosci. Nanotechnol.,* 9: 227-234.
18. Davoodi, J., Alizade, H., (2011) “Radius Dependence of Hydrogen Storage Inside Single Walled Carbon Nanotubes in an Array”, *Int. J. Nanosci. Nanotechnol.,* 7: 143-146.
19. Hohenberg, P., Kohn, W. (1964), “Inhomogeneous Electron Gas”, *Phys. Rev. B,* 136: 864-871.
20. Kohn, W., Sham, L. J. (1965), “Self-Consistent Equations Including Exchange and Correlation Effects”, *Phys. Rev. A,* 140: 1133-1138.
21. Collins, P. G., Bradley, K., Ishigami, M., Zettl, A. (2000), “Extreme Oxygen Sensitivity of Electronic Properties of Carbon Nanotubes”, *Science,* 287: 1801-1804.
22. Zhou, Y., Sreekala, S., Ajayan, P. M., Nayak, S. K. (2008), “Resistance of Copper Nanowires and Comparison with Carbon nanotube Bundles for Interconnect Applications using First Principles Calculations”, *J. Phys.: Condens. Matter,* 20: 095209(1-5).
23. Fagan, S. B., Fazzio, A., Mota, R. (2006), “Titanium Monomers and Wires Adsorbed on Carbon Nanotubes: A First Principle Study”, *Nanotechnology,* 17: 1154-1159.
24. Yang, C. K., Zhao, J., Lu J. P. (2002) “Binding Energies and Electronic Structures of Adsorbed Titanium Chains on Carbon Nanotubes”, *Phys. Rev. B,* 66: 041403(1-4).
25. Yang, C. K., Zhao, J., Lu, J. P. (2004) “Complete Spin Polarization for A Carbon Nanotube with an Adsorbed Atomic Transition-Metal Chain”, *Nano Lett.,* 4: 561-563.
26. Voggu, R., Pal, S., Pati, S. K., Rao, C. N. R. (2008) “Semiconductor to Metal Transition in SWNT Caused by Interaction with Gold and Platinum Nano Particles”, *J. Phys.: Condens. Matter,* 20: 215211(1-16).
27. Kim, Y. L., Li, B., An, X., Hahm, M. G., Chen, L., Washington, M., Ajayan, P. M., Nayak, S. K., Busnaina, A., Kar, S., Jung, Y. J. (2009) “Highly Aligned Scalable Platinum-Decorated Single-Wall Carbon Nanotube Arrays for Nanoscale Electrical Interconnects”, *ACS Nano,* 3: 2818-2826.
28. Dag, S., Durgun, E., Ciraci, S. (2004) “Nanotechnology-An Introduction for the Standards Community”, *Phys. Rev. B,* 69: 121407(1-4).
29. Han, S. S., Hyuck, M. L. (2004) “Adsorption Properties of Hydrogen on (10,0) Single-Walled Carbon Nanotube through Density Functional Theory”, *Carbon,* 42: 2169-2177.
30. Gates, B., Mayers, B., Cattle, B., Xia, Y. N. (2002), “Synthesis and Characterization of Uniform Nanowires of Trigonal Selenium”, *Adv. Funct. Mater.* 12: 219–227.
31. Li, X., Li, Y., Li, S., Zhou, W., Chu, H., Chen, W., Li, I. L., Tang, Z. (2005) “Single Crystalline Trigonal Selenium Nanotubes and Nanowires Synthesized by Sonochemical Process”, *Cryst. Growth Des.* 5: 911-916.
32. Zhang, X. Y., Xu, L. H., Dai, J. Y., Cai, Y., Wang, N. (2006) “Photoconductivity of Single-Crystalline Selenium Nanotubes”, *Mater. Res. Bull.* 41: 1729-1734.
33. Liu, P., Ma, Y., Cai, W., Wang, Z., Wang, J., Qi, L., Chen, D. (2007) “Photoconductivity of Single-Crystalline Selenium Nanotubes”, *Nanotechnology,* 18: 205704-205716.
34. Krishnan, S., Yilmaz, H., Vadapoo, R., Marin, C. (2010) “Selenium Adsorbed Single Wall Carbon Nanotubes as a Potential Candidate for Nanoscale Interconnects”, *Appl. Phys. Lett.* 97: 163107(1-3).
35. Bergoli, R., Mota, R, Zanella, I. ,da Silva, L. B. ,Fagan, S. B. (2011) “Selenium Nanostructures Adsorbed on Carbon Nanotubes: A DFT Investigation”, *J. Comput. Theor. Nanosci.* 8: 1710-1715.
36. Frey, J. T.; Doren, D. J. (2011) Tube Gen 3.4; University of Delaware, Newark, DE.
37. Beche A. D. (1993) “Density-Functional Thermochemistry. III. The Role of Exact Exchange”, *J. Chem. Phys.* 98: 5648-5652.
38. Lee, C. T., Yang, W. T., Parr, R. G. (1988) “Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density”, *Phys. Rev. B,* 37: 785-789.
39. Hay, P. J., Wadt, W. R. (1985) “Ab initio Effective Core Potentials for Molecular Calculations. Potentials for Transition Metal Atoms Sc to Hg” *J. Chem. Phys.* 82: 270-283.
40. Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Montgomery, J. A., Jr., Vreven, T., Kudin, K. N., Burant, J. C., Millam, J. M., Iyengar, S. S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G. A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K. Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J. E., Hratchian, H. P., Cross, J. B., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J., Ayala, W., Morokuma, P. Y., Voth, K.,

Salvador, G. A., Dannenberg, P., Zakrzewski, J. J., Dapprich, V. G., Daniels, S., Strain, A. D., Farkas, M. C., Malick, O., Rabuck, D. K., Raghavachari, A. D., Foresman, K., Ortiz, J. B., Cui, J. V., Baboul, Q., Clifford, A. G., Cioslowski, S., Stefanov, J., Liu, B., Liashenko, B., Piskorz, G. A., Komaromi, P., Martin, I., Fox, R. L., Keith, D. J. T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C., Pople, J. A. (2003) Gaussian 03, Revision B. 05, Gaussian, Inc., Pittsburg, PA.

41. Mpourmpakis, G., Tylianakis, E., Froudakis, G. E. (2007) “Carbon Nanoscrolls: A Promising Material for Hydrogen Storage”, *Nano Lett.,* 7: 1893-1897.
42. Mpourmpakis, G., Froudakis, G. E. (2007) “Why Boron Nitride Nanotubes Are Preferable to Carbon Nanotubes for Hydrogen Storage? An ab initio Theoretical Study”, *Catal. Today,* 120: 341-345.
43. Baei, M. T., Soltani, A. R., Moradi, A. V., Lemeski, E. T. (2011) “Adsorption Properties of NO on (6, 0), (7, 0), and (8, 0) Zigzag Single-Walled Boron Nitride Nanotubes: A Computational Study”, *Comput. Theor. Chem.,* 970: 30-35.
44. Chen, Z., Nagase, S., Hirsch, A. C., Haddon, R., Thiel, W., Schleyer P. von R. (2004) “Side-Wall Opening of Single-Walled Carbon Nanotubes (SWCNTs) by Chemical Modification: A Critical Theoretical Study”, *Angew. Chem.,* 116: 1578-1580.
45. Bai, J., Zeng, X. C., Tanaka, H., Zeng, J. Y. (2004) “Metallic Single-Walled Silicon Nanotubes”, *Proc. Natl. Ac. Sci.,* 101: 2664-2668.
46. Yeung, C. S., Chen, Y. K., Wang, Y. A. (2010) “Theoretical Studies of Substitutionally Doped Single-Walled Nanotubes”, *J. Nanotechnol*. 2010: 801789(1–42).
47. Chen, Y. K., Liu, L. V., Tian, W. Q., Wang, Y. A. (2011) “ Theoretical Studies of Transition–Metal–Doped Single–Walled Carbon Nanotubes”, *J. Phys. Chem. C*, 115: 9306–9311.
48. Abadir, G. B., Walus, K., Pulfrey, D. L. (2008) “Basis-Set Choice for DFT/NEGF Simulations of Carbon Nanotubes”, *J. Comput. Electron.* 8: 35-42.
49. Boys S. F., Bernardi, F. (1970) “The Calculation of Small Molecular Interactions by the Differences of Separate Total Energies. Some Procedures with Reduced Errors”, *Mol. Phys.* 19: 553-566.
50. Reed, A. E., Curtiss L. A., Weinhold, F. A. (1988) “"Intermolecular Interactions from a Natural Bond Orbital, Donor-Acceptor Viewpoint", *Chem. Rev.,* 88: 899–926.
51. Pinto, H., Markevich, A. (2014) “Electronic and Electrochemical Doping of Graphene by Surface Adsorbates”, *Beilstein J. Nanotechnol.,* 5: 1842–1848.
52. Omidvar, A., Mohajeri A. (2015) “Promotional Effect of the Electron Donating Functional Groups on the Gas Sensing Properties of Graphene Nanofakes”, *RAS Adv.* 5: 54535-54543.