Bulletin of Environment, Pharmacology and Life Sciences
Bull. Env.Pharmacol. Life Sci., Vol 4 [Spl issue 1] 2015: 390-395

Online ISSN 2277-1808
Journal's URL:http://www.bepls.com
CODEN: BEPLAD
Global Impact Factor 0.533
Universal Impact Factor 0.9804

FULL LENGTH ARTICLE **OPEN ACCESS**

Analysis the Optical Behavior and Stability Graphene Structures using DFT Method

Tahmineh Jalali[1], Tayebeh Davani [1,2], Hosein Mokhtari [2]
[1]Physics Department, Persian Gulf University, Bushehr 75169, Iran.
[2] Physics Department, Yazd University, Yazd , Iran.
Email: jalali@pgu.ac.ir

ABSTRACT
Employing DFT method, Graphene molecule whose zigzag edges are filled with hydrogen, is simulated and computed orthogonally based on B3LYP/6-311G in 4 structures with different numbers of carbon and hydrogen. Different quantities such as stability, density of states and band gap are investigated in each case. By Structure Development, the stability is increased and the computed band gap and hardness are decreased. However, the polarizability increases and Fermi level becomes higher.
Key words: Graphene, band gap, density of state, Fermi level, DFT

INTRODUCTION

Carbon is a fundamental material in Nano-engineering whose allotropes including Graphite, Nanotubes, Fullerenes and recently, Graphene, plays special and important role in this arena [1]. Graphene, two dimensional allotrope of Carbon, is separated from Graphite in 2004 [2]. Although it was very difficult to observe this material, Mermine and Winger had proved that two-dimensional material cannot have long-range order [3]. But Graphene is the first two-dimensional stable solid state material and because of its unique transition features is the most important Carbon structure now. Due to this feature, Graphene became an ideal material for the fields of nano-electronics, Optoelectronics, Superconductivity, Josephson junctions and also studying ballistic transport and modeling massless Dirac fermions [1]. A variety of methods has been used to study this material which DFT is one of their best [4].
In this paper employing DFT method, different structures of Graphene, which have hydrogenated zigzag edges, are simulated with B3LYP/6-311G hybrid basis in Gaussian03 software and various quantities such as stability, density of states and band gap are investigated for each case. Graphs are plotted utilizing Gauss Sum and Matlab software.

Graphene:

Graphene is a one-atom thick layer of Graphite which has interesting mechanical, optical and electrical features. Owing to high mobility of carriers in Graphene, this matter has become a new option for electronic materials, and is expected to replace silicon in the near future [5]. Graphene has no band gap around the Fermi level, something that determines the characteristics of semiconductor materials and is necessary to control the conductivity by use of electrical materials [6]. Since Graphene is a semi-metal with zero band gap and its band structure is linear at low energies, and also due to the observed anomalous Hall Effect in it and the cyclotron mass, the particles in Graphene shows relativistic behavior [5]. In terms of mechanical properties, this material is very resistant to pressure. . This material due to its integrated structure is one of the most rigid materials and also its thermal conductivity is as high as diamond and carbon nanotubes [7]. It has been shown that by adding chemical impurities to pure Graphene, electrical conductivity varies considerably [8]. Optical transition of Graphene has also been studied in the infrared spectrum and it is said that a single particle model can accurately describe the rate of transition with substantial agreement with

experiments [9]. Despite the extraordinary properties, unfortunately due to the lack of band gap, Graphene has a limited role in electronic equipment. In order to use in electronics industry, we need to open energy band gap in Graphene. The desired band gap can also be obtained through saturating the free electrons of the Graphene surface [10] which will be performed through bonding free electrons and an outer atom. Hydrogen can be one of these atoms. Hydrogenation causes that, hybrid varies from sp^2 to sp^3 and helps that the material be more stable. The hydrogenation of Graphene causes that a gap opens in it.

Today, Graphene is famous as a versatile material. This reputation is just because of its quirky features. Graphene as the lightest and strongest material, with extraordinary abilities in the electrical and thermal conductivity compared to the other materials, creates vast applications and it is expected that Graphene compounds create wider and more amazing applications in future. In addition to high electrical conductivity, small size and high strength are the features which have empowered Graphene to make huge advances in biology and medical devices. It is important to measure and normalize blood glucose and hemoglobin level, as well as modifying DNA. Moreover the light throughput of Graphene is more than 90%, this feature has made a significant impact on the field of Optoelectronics, especially, Graphene's role to construct LCDs, LEDs, tablets and computers is the result of this effectiveness.

Methodology

Studying many-particle systems has been one of the physicists' goals. A solid is a collection of light and heavy positively charged particles (nucleus) and negatively charged particles (electrons). For N nuclei, we have the problem of N+NZ particles interacting. This is an N body problem and since particles are very light, quantum mechanics should be employed to solve the problem. Density Functional Theory Density (DFT) is one of the most common and successfull methods of statistical mechanics of solids which nowadays is used to compute the chemical molecules bond energy and band structure of solids in Physics. The merit of this method over than the other ones, is that, density of the particles, which is the physical quantity and visible in the lab, has been considered as the main variable [11]. Therefore this method is used to compute the features of a Graphene which is limited by hydrogen [6].

Discussion

Since the hydrogenation of Graphene provides more stable material and hydrogenation modifies the band gap in Graphene, the Graphene molecule with orthogonal configuration such that the edges of these structures have zigzag shape, are simulated and investigated in different structures of $C_{16}H_{10}$, $C_{30}H_{14}$, $C_{48}H_{18}$, $C_{70}H_{22}$.

First, the structure of $C_{16}H_{10}$ is computed with the mentioned basis and method. This structure has been shown in the Figure 1. For this structure the obtained structure formation energy is equal to -615.755 Hartree. Furthermore, HOMO level and LUMO level were obtained -0.206 and –0.063 electronvolts respectively.

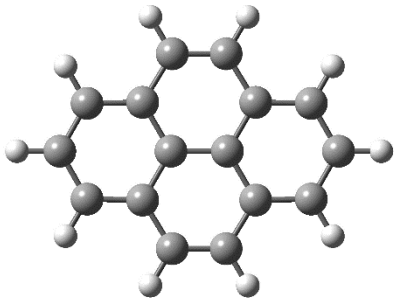

Fig. 1) $C_{16}H_{10}$ structure.

Then the $C_{30}H_{14}$ structure is investigated using the aforementioned method and basis. Structure formation energy is -1151.706 which is more negative than the preceding structure. HOMO level and LUMO level were computed -0.178 and –0.097 electronvolts respectively both of which have lower level in comparison with the first structure. Figure 2 shows this structure.

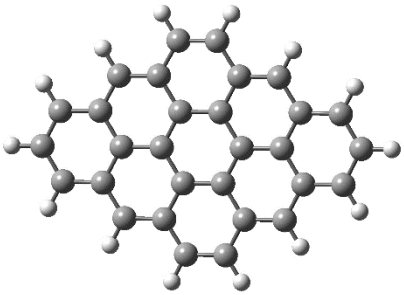

Fig. 2) $C_{30}H_{14}$ structure.

A larger structure i.e. $C_{48}H_{18}$ (Figures 3) is studied. Its structure formation energy is -1840.106 Hartree, as expected we observed that this is more negative than the preceding structures. -0.162 and –0.117 electronvolts were resulted for HOMO level and LUMO level respectively, both of which have lower level in comparison with the preceding structures.

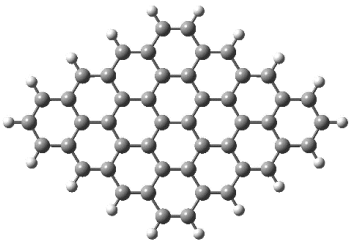

Fig. 3) $C_{48}H_{18}$ structure.

The largest structure which is simulated and computed is $C_{70}H_{22}$ structure (figure 4). Its structure formation energy is -2680.963 Hartree, which is the most negative value in comparison with the preceding structures. It, therefore, is the most stable state. For HOMO level and LUMO level, the values -0.153 and –0.129 electronvolts were also computed respectively, which are the lowest value in the computed structures.

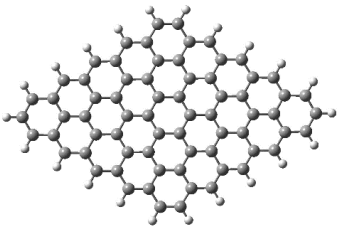

Fig. 4) $C_{70}H_{22}$structure.

By computing LUMO and HOMO level, the band gap can be obtained from difference between these two levels and also hardness, which assigns half of band gap to itself, is computed for each of four structures, as it was expected by structure expansion, both quantities decrease gradually (table 1).

Table 1

hardness) Electronvolts (	The size of the band gap (Electronvolts)	Structure formation energy) Hartree (	Graphene structure
0.715	0.143	615.755–	$C_{16}H_{10}$
0.405	0.081	-1151.706	$C_{30}H_{14}$
0.022	0.045	-1840.106	$C_{48}H_{18}$
0.012	0.024	2680. 963–	$C_{70}H_{22}$

Another quantity which is evaluated is polarizability of the three primary structures. By structure expansion, we observe more polarizability and this is obvious because the distance between atoms

increases by enlarging the structure and as a result dipole moment boosts and the polarizability which is proportional to dipole moment would be increased. This can be observed in Figure 5.

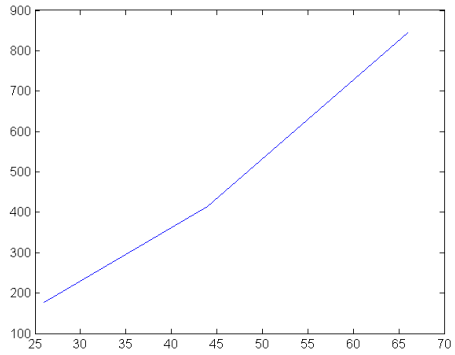

Fig. 5) Polarization diagram versus number of atoms constructing the structure

Figure 5 is plotted for $C_{16}H_{10}$ structure with 26 atoms and polarizability equal to 176.451, $C_{30}H_{14}$ structure with 44 atoms and polarizability equal to 414.105, and $C_{48}H_{18}$ structure with 66 atoms and polarizability equal to 843.709. Where the horizontal axis indicates the number of atoms and the vertical axis determines the amount of polarizability.

To study the optical behavior of materials, their electron behavior should be considered. Figures 6-9 indicate density of state (DOS) for these 4 structures in which Fermi level is increasing and this is in agreement with former reports [12].

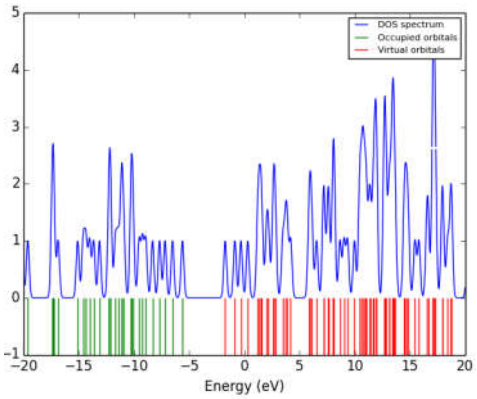

Fig. 6) Density of state diagram for $C_{16}H_{10}$ structure

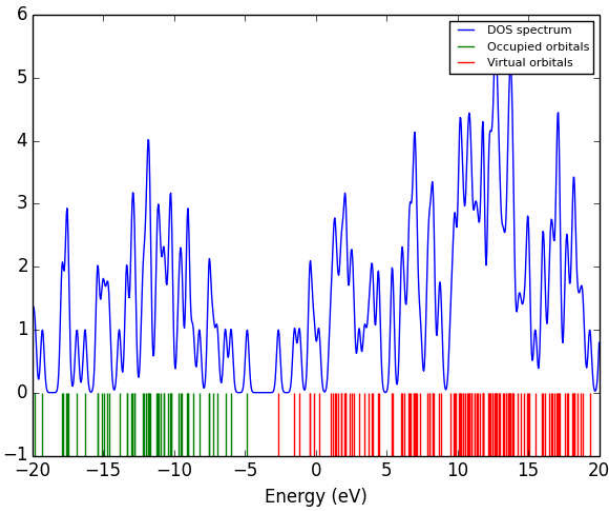

Fig. 7) Density of state diagram for $C_{30}H_{14}$ structure

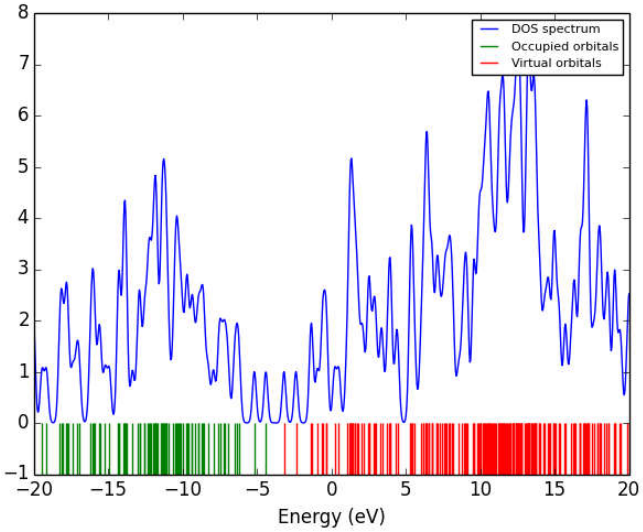

Fig. 8) Density of state diagram for $C_{48}H_{18}$ structure

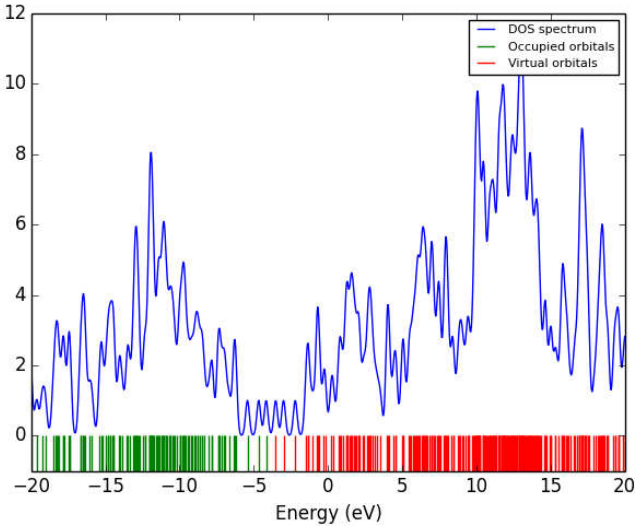

Fig. 9) Density of state diagram for $C_{70}H_{22}$ structure

RESULTS

The unique effect of Graphene in electronic and optoelectronic has encouraged the researchers of different fields, to employ various methods and experiments, to utilize Graphene and its compounds as a widely used subject in their plans and researches. In this paper employing DFT method, four orthogonal zigzag edge structures of Graphene, i.e. $C_{16}H_{10}$, $C_{30}H_{14}$, $C_{48}H_{18}$, $C_{70}H_{22}$, which have filled existing free bonds in the edges, are simulated and computed with hybrid basis B3LYP/6-311G; and it is observed that for the larger structures, more stability is achieved. Moreover, by expanding the structure, shorter band gap can be resulted. Therefore, the obtained hardness will be decreased while more polarizability is established. Besides, electronic density of states investigation suggests that Fermi level increment which is resulted due to structure enlargement, have an acceptable optical behavior in these four structures.

REFERENCES

1. Novoselov, K. S. A., Geim, A. K., Morozov, S., Jiang, D., Grigorieva, M. K. I., Dubonos, S. V., & Firsov, A. A, 2005, *Two-dimensional gas of massless Dirac fermions in graphene,* nature ,438(7065), 197-200.
2. Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang D., Zhang, Y., Dbonos, S. V., Grigorieva, I. V. and Firsov, A. A, 2004, *Electric field effect in atomically thin carbon films*, Science. vol. 306, no. 5696, pp. 666–669.
3. Mermin, N. D, *Crystalline Order in Two Dimensions*, Phys. Rev., vol. 176, pp. 250–254, 1968.
4. Dharma-Wandra, M.W., Zgierski, M.Z. 2008, *Magnetism and structure at vacant lattice sites in grapheme*, Physica E 41, 80-3.
5. Castro Neto, A. H.,Guinea, F., Peres, N. M. R., Novoselov, K. S. and Geim, A. K, 2009, The *electronic properties of grapheme.* Rev.Mod. Phys. 81,109.

6. Chang,Y. and Wang,Z, 2008, *Research on 3D Visualization of Crystal Molecular Structure Based on Augmented Reality*, Proc.International Conference on Computer Science and SoftwareEngineering. pp. 1146-1149.
7. Balandin, A. A., Ghosh, S., Bao, W., Calizo, I., Teweldebrhan, D., Miao, F. and Lau, C. N, 2008, *Superior thermal conductivity of single-layer grapheme*, Nano Lett. vol. 8, no. 3, pp.902–907.
8. Lu, X. K., Yu, M. F., Huang, H. & Ruoff, R. S., 2007,*Tailoring graphite with the goal of achieving singlesheets,* Nanotechnology,10(3), 269-2721999.
9. Sadowski, M. L., Martinez, G., Potemski, M., Berger, C., & De Heer, W. A, 2006, *Landau level spectroscopy of ultrathin graphite layers*, Physical review letters. 97(26), 266405.
10. Sofo, J. O., Chaudhari, A. S. and Barber, G. D, 2007, *Graphane: A two dimensional hydrocarbon*. Phys. Rev. B, Condense. Matter. vol. 75, no. 15, p. 153 401.
11. Sahni, V., 2004, *Quantal density functional Theory*, Springer.ISBN 3540408843.
12. Karki, D. B., & Adhikari, N. P., 2014, *First-principles DFT study for the structural stability of Hydrogen passivated graphene (H-graphene) and atomic adsorption of oxygen on H-graphene with different schemes.* arXiv preprint arXiv:1404.6446.