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JASER

Electronic Properties of Graphene Ribbons and Their Adducts Using Density Function Theory

Article Info

Received: 10/10/2016
Accepted:5/11/ 2016
Published online: 1/12/2016

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ISSN 2231-8844

Abstract

In this research, we study the electronic properties of two pure graphene ribbon and their adducts by adding the Al / N compound. We showed that the electronic softness of the pure Graphene Ribbon was increased with increasing the thickness of the Ribbon, adding the Al / N atoms leads to decrease the electronic softness. The electrochemical hardness has inversely behavior to the softness. Increasing the thickness of the Graphene Ribbon leads to decrease the forbidden energy gap of the Ribbon, but the energy gap is increase due to the addition of the Al / N atoms in the Ribbon

Keywords: **DFT, Graphene Ribbon, Energy gap, Electronic softness and Electron affinity.**

1. Introduction

Graphene was first discovered in 2004 by Novoselov et al. Graphene is a single atomic layer with a thickness of only 0.34 nm of sp^2 hybridized carbon atoms covalently bonded to three other atoms arranged in a honeycomb lattice (Novoselov et al. 2004: Layek and Nandi, 2013: Singh et al. 2011). Graphene's unique structural and electronic properties and high carrier mobility makes it one of the most important topics in materials science today (Basua and Bhattacharyya, 2012: Chao et al., 2014). Graphene forms the basic structure of other carbon-based materials such as fullerene (wrapped-up graphene) (Craciun et al., 2011: Acik and Chabal 2011), carbon nanotubes (several graphene sheets rolled up along a vertical axis) (Chabal 2011), and graphite (stacked graphene) (Raza 2012; Choi W, Lee). Some of the carbon-based materials are illustrated in Figure 1. Graphene has unique properties with tremendous potential applications, such as chemical sensors (Chao et al., 2014, Craciun et al., 2011: Acik and Chabal 2011; Raza 2012; Choi W, Lee; Basu et al., 2012)[5-10], nanoelectronic devices, hydrogen storage systems (Chao et al., 2014), or polymer

nanocomposites (Pumera 2009. Graphene could be considered as a prototypical material to study the properties of other two-dimensional nanosystems. Several two-dimensional structures have been explored in the literature (Kuilla et al., 2010). Graphene-like two-dimensional silicon carbide, silicon (Bekaroglu et al., 2010, germanium (Voon et al., 2010), boron nitride (Cahangirov et al., 2009), and zinc oxide (Zhang et al., 2010 have been explored in the literature.

Graphene is a zero-gap semiconductor, because its conduction and valence bands meet at the Dirac points. The Dirac points are six locations in momentum space, on the edge of the Brillouin zone, divided into two non-equivalent sets of three points, where momentum is zero (Voon et al., 2010) .

2. Theoretical Methods and Computational Details

Density functional theory have been used to calculate the molecular properties for these molecules at [Becke three parameters with the Lee - Yang – Parr functional (B3LYP)] level with 6-31G** basis sets. All calculations were carried out using the Gaussian 2009 and Gaussian View -5(G09W, 2009).

3. Results and Discussion

Figure 1 illustrates the geometrical optimization of the suggested structures in this research, these structures are included four species; the first two are pure Graphene Ribbon 1 and 2, respectively, and the second two are constructed by adding Al / N compound in place of carbon atoms in phenylene rings, we denoted 1a and 2a, respectively.

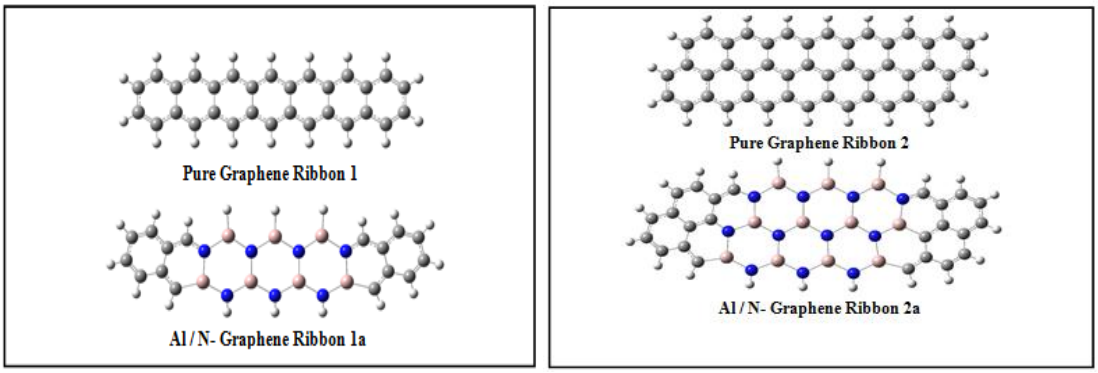

Figure 1: The geometry structure of the studied molecules

Table 1 shows the ground state calculations of the pure Graphene Ribbon 1 and it is adduct 1a relax at the minimum energy. These calculations are included the total energy in a. u, ionization potential and electron affinity in eV calculated due to Koopman's theorem, forbidden energy gap in eV, electronic softness in $(eV)^{-1}$, electrochemical hardness in eV , chemical potential in eV. Table 2 shows these calculations of the pure Graphene 2 and it is adduct 2a. From these tables, the total energy was decreased with increasing the thickness of the Ribbon and with increasing the number of Al / N atoms in the Ribbon, as we see in Figure

2, this result is a reflection of the binding energy of each structure. The carbon-carbon bond of the relaxed structures under study are in the ranges (C=C: 1.354-1382 ; C-C: 1.452-1.455 : C:::C: 1.394-1.408), this result is in a good agreement with those of aromatic rings[]. The electronic softness of the structure was increased with the increasing of the thickness of the Ribbon but it decreases with adding the Al / N compound in the structure. While the electrochemical hardness has inversely behavior of the electronic softness, the hardness is decrease with increasing the thickness of the Ribbon and increase with adding the Al / N compound in the structure. These results are indicate to that the pure Graphene Ribbon high reactivity than the doped Graphenen and became more reactive with increasing it is dimensions (n and m). The above results are correspond to the IP and EA of the structures, where the IP is decrease and EA is increase with increasing the thickness of the pure Graphene Ribbon. Adding the Al / N compound to the Ribbon leads to increasing the IP and decreasing the EA, that means the doped Graphene Ribbon has low ability to donating or accepting an electron to become cation or anion. Increasing the thickness of the pure Graphene Ribbon gave it high ability to donating or accepting electrons because the larger Graphene Ribbons and therefore the Graphene sheets have high conductivity and small forbidden energy gap. Adding the Al / N compound leads to increase the space between the conduction and the valence band in the structure due to the linear combination of atomic orbitals of all carbon atoms in the phenylene rings and the new atoms (Al and N). Figures 3-7 illustrate the above electronic properties.

Table (1) Electronic Properties of Graphene Ribbon 1 and it is Adduct.

Structure	E_T a. u	$S(ev)^{-1}$	η (ev)	M (ev)	EA (ev)	IE (ev)	E_g (ev)
Pure Graphene Ribbon 1	-1153.81	17.966	0.028	-0.13	0.102	0.158	0.056
Al / N- Graphene Ribbon 1a	-2701.04	8.841	0.057	-0.112	0.056	0.169	0.113

Table (2) Electronic Properties of Graphene Ribbon 2 and it is Adduct.

Structure	E_T a. u	$S(ev)^{-1}$	η (ev)	M (ev)	EA (ev)	IE (ev)	E_g (ev)
Pure Graphene Ribbon 2	-1764.71	25.934	0.019	-0.131	0.112	0.151	0.039
Al / N- Graphene Ribbon 2a	-4196.08	15.893	0.031	-0.112	0.081	0.144	0.063

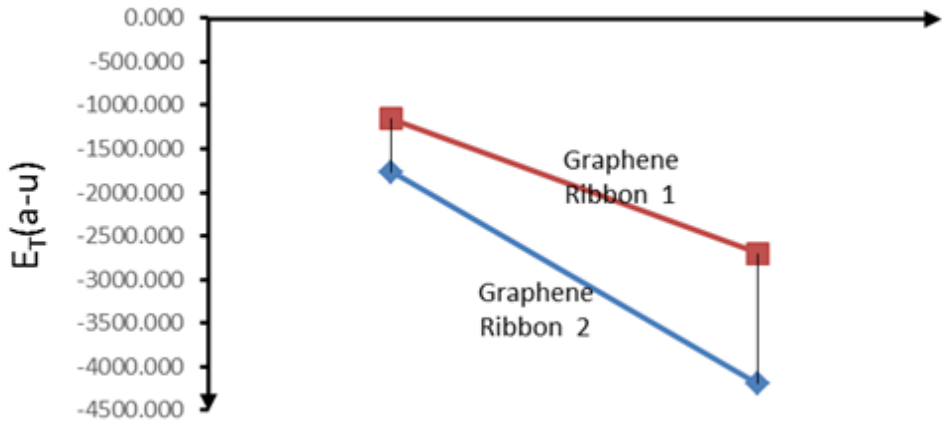

Figure 2:The total energy E_T in a.u of the Graphene Ribbons and their adducts

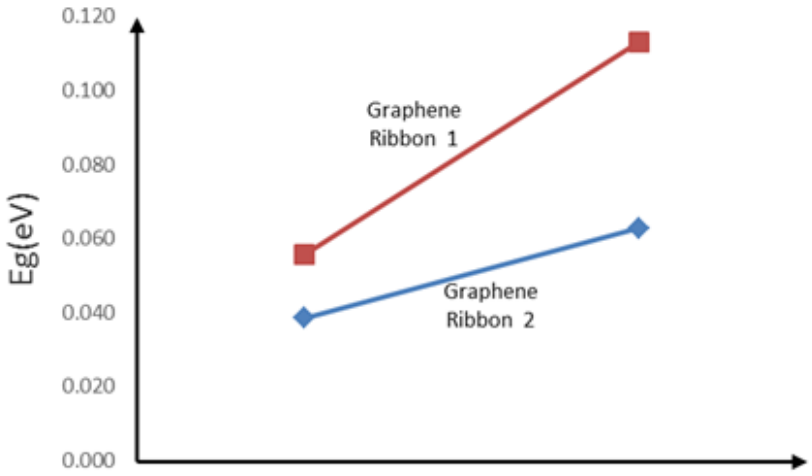

Figure 3: The E_g in eV of the Graphene Ribbons and their adducts .

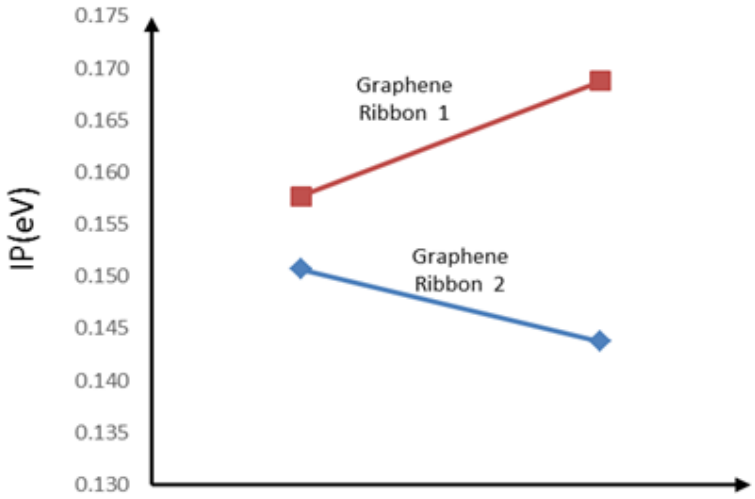

Figure 4: The IP in eV of the Graphene Ribbons and their adducts .

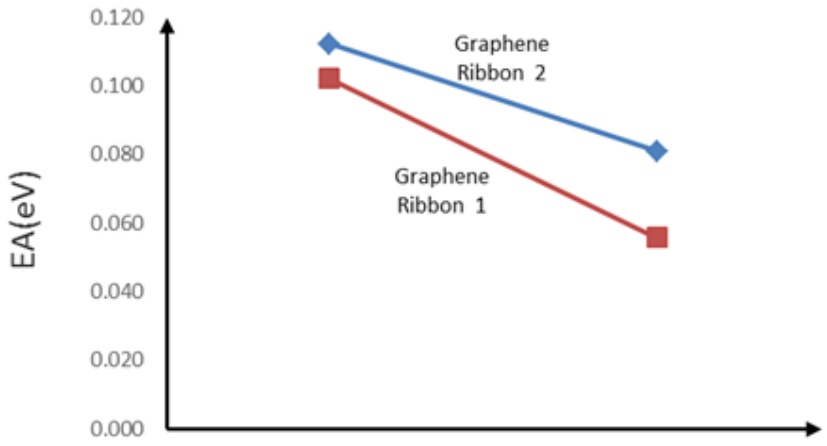

Figure 5: The EA in eV of the Graphene Ribbons and their adducts

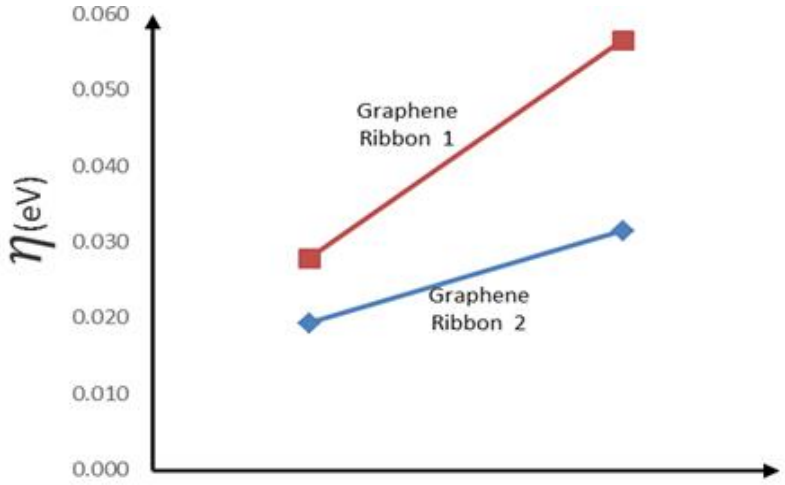

Figure 6: The molecular electrochemical hardness of the Graphene Ribbons and their adducts .

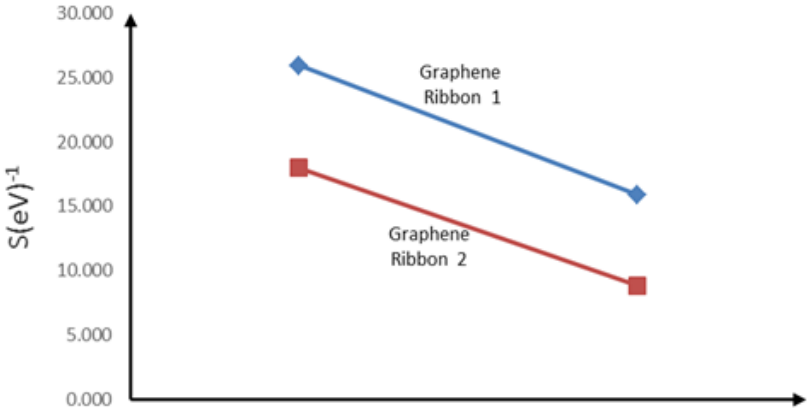

Figure 7: The electronic softness of the Graphene Ribbons and their adducts .

4. Conclusions

The electronic properties of two pure Graphene Ribbon and their adducts were calculated by employing the DFT using Gaussian 09 package of program. From the results, one can conclude the following:

1- The relax structures under study have geometrical parameters lie in the same range of the aromatic rings, that means the method we used in the relaxation is a suitable for these kinds of structures.

2- The total energy of the Graphene Ribbon is decrease with increasing both the thickness of the Ribbon and the number of Al / N atoms added in place of carbon atoms in the phenylene rings.

3- The electronic softness is increase with increasing the thickness of the Graphene Ribbon and decrease with adding the Al / N compound in the Ribbon, while the electrochemical hardness has inversely behavior to the electronic softness. These results come from the change of the calculated ionization potential and electron affinity of each structure due to the difference in the electronegativity of the carbon, aluminum and nitrogen atoms.

4- Increasing the thickness of the pure Graphene Ribbon decreased the forbidden energy gap, this is a sign to that the Graphene Sheet has high conductive than the Graphene Ribbon, the main factor of the electric conductance of the Graphene is the number of n and m that construct the structure.

References

Acik M, Chabal YJ: Nature of graphene edges: a review. Jpn J Appl Phys 2011, 50:070101.

Basu S, Bhattacharyya P: Recent developments on graphene and grapheneoxide based solid state gas sensors. Sens Actuators B 2012, 173:21.

Basua S, Bhattacharyya P: Recent developments on graphene and graphene oxide based solid state gas sensors. Sens Actuators B 2012, 173:1.

Bekaroglu E, Topsakal M, Cahangirov S, Ciraci S: First-principles study of defects and adatoms in silicon carbide honeycomb structures. Phys Rev B 2010, 81:075433.

Cahangirov S, Topsakal M, Akturk E, Sahin H, Ciraci S: Two-and one-dimensional honeycomb structures of silicon and germanium. Phys Rev Lett 2009, 102:236804.

Chao Z, Sihao C, Jianzhong L, Jihu W, Qiujie Y, Chuanrong L, Dapeng H and Tonghe Z : Graphene's cousin: the present and future of graphane. Nanoscale Research Letters 2014, 9:26

Choi W, Lee JW: Graphene: Synthesis and Applications. New York, USA: CRC Press (Taylor and Francis group); 2012.

Craciun MF, Russo S, Yamamoto M, Tarucha S: Tuneable electronic properties in graphene. Nano Today 2011, 6:42.

G09W programs. (2009) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al- Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, and E. S. Replogle Gaussian 09, Gaussian, Inc., Pittsburgh PA, 2009.

Kuilla T, Bhadra S, Yao D, Kim NH, Bose S, Lee JH: Recent advances in graphene based polymer composites. Prog Polym Sci 2010, 35:1350.

Layek RK, Nandi AK: A review on synthesis and properties of polymer functionalized graphene. Polymer 2013, 54:5087.

Novoselov KS, Geim AK, Morozov SV, Jiang D, Zhang Y, Dubonos SV,Grigorieva IV, Firsov AA: Electric field effect in atomically thin carbon films. Sci 2004, 306:666.

Pumera M: Electrochemistry of graphene: new horizons for sensing and energy storage. Chem Rec 2009, 9:211.

Raza H: (Ed): Graphene Nanoelectronics: Metrology, Synthesis Properties and Applications. Berlin, Germany: Springer; 2012.

Singh V, Joung D, Zhai L, Das S, Khondaker SI, Seal S: Graphene based materials: past, present and future. Prog Mater Sci 2011, 56:1178.

Voon LCLY, Sandberg E, Aga RS, Farajian AAA: Hydrogen compounds of group-IV nanosheets. Phys Lett 2010, 97:163114.

Zhang Y, Wu SQ, Wen YH, Zhu ZZA: Surface-passivation-induced metallic and magnetic properties of ZnO graphitic sheet. Phys Lett 2010, 96:223113.