# Electron Transport in Graphene-B/P compound Heterojunction Using LDA/SZ

Sabah N. Mazhir[1] , Hamid I. Abbood[2], Hawraa A. Abdulridha[3]

[1,3]Department of Physics/ college of science for women/ University of Baghdad, Baghdad-Iraq
[2] Physics department, Faculty of Science, Babylon University, Hilla-Iraq

***Abstract—*** *Present study deals with the effect of B/P compound as a point in the middle of grapheme sheet on the electron transport of pure graphene. The calculations are carried out using GOLLUM program. We showed that good relax of the studied graphene sheets was obtained using LDA/SZ DFT at SIESTA - trunk - 462 of program. Electrical and thermal conductivities of the graphene are in the order of pure graphene sheet > G-B/P (Point) sheet. The I-V characteristic was analyzed and the transmission value of the pure graphene sheet is higher than that of G-B/P (Point) sheet.*

***Keywords— Graphene sheet, Electrical conductivity, Thermal conductivity , I-V characteristic, and Transmission coefficient.***

## I. INTRODUCTION

Graphene is a 2-D atomic layer of carbon atoms, the building block of the 3-D structure graphite. While graphite has been a well-known and utilized material since antiquity, a single graphene layer was not isolated and studied until relatively recently [1,2,3]. Graphene was generated by several different chemical techniques in the 1960s and 1970s, but it was not until 2004 when K. S. Novoselov, A. K. Geim, and coworkers at the University of Manchester introduced a simple technique involving the mechanical exfoliation of graphite to isolate single graphene layers [1,4,5].

The availability of graphene flakes made the study of its properties possible and led to the enormous interest and intense activity in graphene research currently ongoing [5,6,7,8]. Graphene is a material with unique electronic transport properties such as a high Fermi level, outstanding carrier mobility, and a high carrier saturation velocity. These properties are complemented by excellent thermal conductivity, high mechanical strength, thinness, and flexibility. These characteristics make graphene an excellent candidate for advanced applications in future electronics [7,9,10,11].

In particular, the potential of graphene in high-speed analog electronics is currently being extensively explored [3,6,8]. In this paper, we discuss briefly the basic electronic structure and transport properties, I-V characteristic, conductance and transmission coefficient of pure and doped graphene sheets.

## II. THEORETICAL METHODS AND COMPUTATIONAL DETAILS

The calculated properties of molecules in Figure 1 are carried out using Density functional theory LDA/SZ basis sets method. The structures of the studied sheets are designed at Gaussian View 5.0.8 program[12,13], and all the calculations are carried out using the SIESTA – trunk - 462 program [14], GOLLUM program " version 1.0 " [15].

## III. RESULTS AND DISCUSSION

Figure 1 illustrates the geometrical optimization of the suggested structures in this research, these structures are included two species; the first is a pure graphene sheet and the second is the G-B/P (Point) sheet. Local density approximation LDA/SZ was shown to be highly successful for calculation the electronic properties such as electrical conductivity in (μs), thermal conductivity in (W / m. K), I-V characteristics and transmission coefficient.

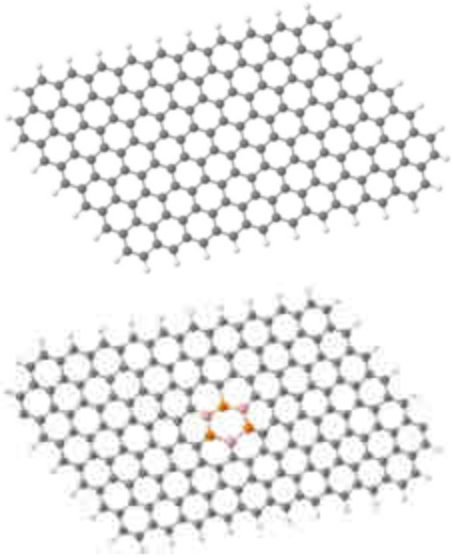

*Fig.1: The optimized structures of pure grapheme sheet and grapheme-B/P(point) sheet. (Hydrogen(H)≡ white: Carbon (C)≡ gray: Boron (B)≡ violet: Phosphorus (P) ≡ orange).*

The relaxed structures in figure 1 are designed at Gauss View 5.0.8. and relax by employing the B3LYP/DFT at SIESTA – trunk - 462 of program. We showed the addition of B and P atoms in pure graphene sheet to construct the doped graphene sheet has not effect on the structural properties of the structure, the C-C and C==C and C-H bonds remain in the same ranges of carbon rings structures[16,17].

Figure 2 shows that the electrical conductivity of the graphene sheets studied in this study is in the order of pure graphene sheet > G-B/P (Point) sheet, The electrical conductivity of pure graphene sheet is the highest value 6.14 μs, this due to the multi channels that the pure graphene has without any scattering region, the G-B/P (Point) sheet has electrical conductivity equal to 4.83 μs. The reason is due to the value of the forbidden energy gap, where the higher the value of the energy gap decreased electrical conductivity[18,19].

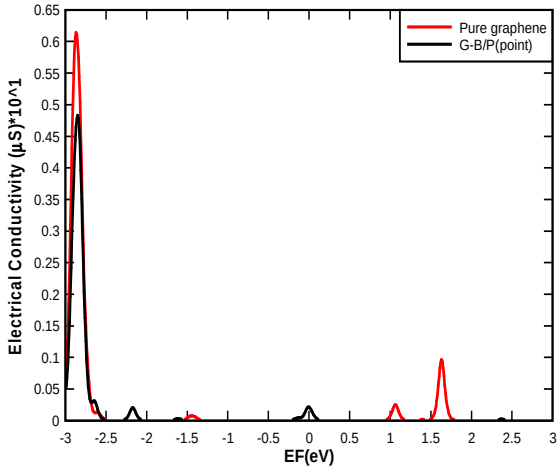


*Figure 2: Electric conductivity in (μs) of the pure graphene sheet and G-B/P (Point) sheet.*

Figure 3 shows the behavior of the thermal conductivity of the two pure and doped grapheme sheets, it can be seen that the thermal conductivity of the pure graphene sheet is $1.76*10^{-10}$ W / m. K, it decreased to $1.321*10^{-10}$ W / m. K for G-B/P (Point) sheet. Means, the presence of B/P compound as a point in the middle of the sheet decreases the number of channels that the electrons can pass and therefore reduced the electrical and thermal conductivities of the graphene sheet[18,19].

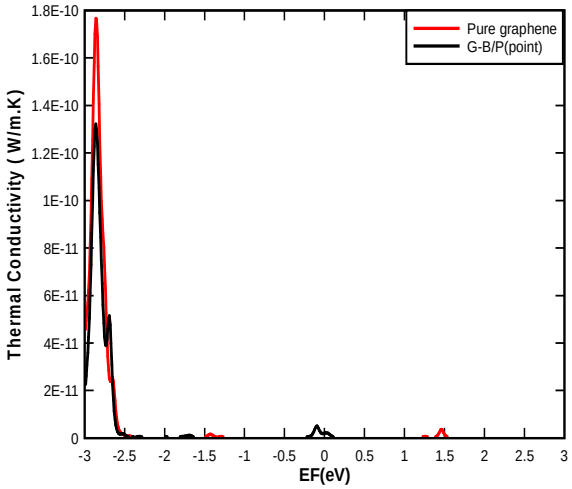


*Fig.3: Thermal conductivity in of the pure graphene sheet and G-B/P (Point) sheet.*

Figure 4 illustrates the analyze of the current-voltage characteristics of the pure and doped graphene sheets. Initially, each sheet is inserted in between two gold contacts electrodes with a suitable anchor atom between the electrode and the sheet. Then a bias voltage 3 Volt is applied in the direction of the axis connecting both the anchor atoms. From the calculations we can suggest that the symmetric interaction with the electrodes have rather limited influence on the sensing behavior of the pure graphene sheet and its adduct[18,20]. It is clear that pure graphene sheet shows the required bias voltage and reverse voltage for sensing are (1.6 and -1.6) Volts the doping ring (point) in the middle of the sheet) gave sensing behavior at bias voltage of 2.6 Volt and -2.6 Volt reverse voltage.

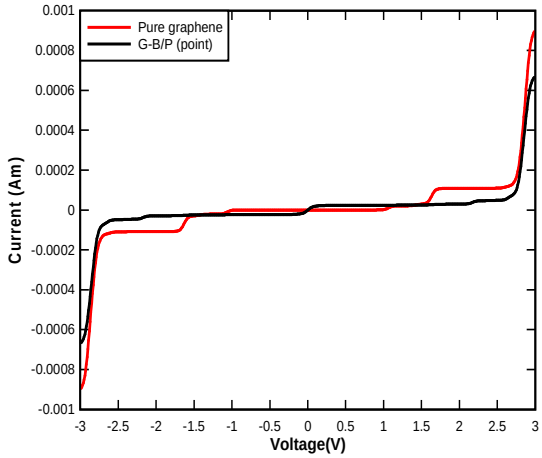


*Figure 4: The I-V characteristic of the pure graphene sheet and G-B/P (Point) sheet.*

The transmission coefficient of the two sheets under study was illustrated in figure 5. The transmission value of the pure graphene sheet is higher than that of G-B/P (Point)

sheet, and this could be a sign to the effect of the presence of B and P atoms in the sheet, B/P ring in the middle of the sheet causes a rotation of the phenylene rings it is located and leads to few twist in the paper of the graphene sheet[19,20].

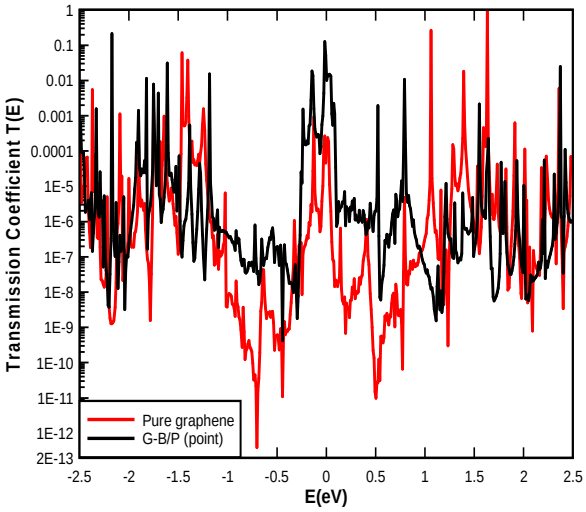


*Fig.5: The transmission coefficient of the pure graphene sheet and G-B/P (Point) sheet.*

## IV. CONCLUSIONS

The structures of the graphene sheets were designed at Gauss View 5.0.8. and relax by employing the LDA/SZ DFT at SIESTA – trunk - 462 of program. The results showed good relax done of the the studied sheets done by the above method. The electrical and the thermal conductivities of the pure graphene sheet are larger than that of the doped G-B/P (Point) sheet. This result is due to that the pure graphene sheet has multi channels of electron transport, the presence of B/P compound as a point in the middle of the sheet decreases the number of channels that the electrons can pass through. All pure and doped graphene sheets show I-V characteristics very much similar to sensing type. The transmission value of the pure graphene sheet is higher than that of G-B/P (Point) sheet.

## REFERENCES

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Journal of Science, Vol. 306, PP. 666–669, 2004.

[2] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Journal of Nature, Vol. 438, PP. 197–200, 2005.

[3] Y. Zhang, Y. Tan, H. L. Stormer, and P. Kim, Journal of Nature, Vol. 438, PP. 201–204, 2005.

[4] A. K. Geim and K. S. Novoselov, Journal of Nature Mater, Vol. 6, PP. 183–191, 2007.

[5] Ph. Avouris, Journal of Nano Lett., Vol. 10, PP. 4285–4294, 2010.

[6] P. R. Wallace, Journal of Physics Rev., Vol. 71, PP. 622–634, 1947.

[7] J. S. Moon, D. Curtis, M. Hu, D. Wong, C. McGuire, P. M. Campbell, G. Jernigan, J. L. Tedesco, B. VanMil, R. Myers-Ward, C. Eddy, Jr., and D. K. Gaskill, Journal of IEEE Electron Device Lett., Vol. 30, PP. 650–652, 2008.

[8] Y.-M. Lin, K. A. Jenkins, A. Valdes-Garcia, J. P. Small, D. B. Farmer, and P. Avouris, Journal of Nano Lett., Vol. 9, PP. 422–426, 2009.

[9] Y.-M. Lin, C. Dimitrakopoulos, K. A. Jenkins, D. B. Farmer, H.-Y. Chiu, A. Grill, and P. Avouris Journal of Science, Vol. 327, PP. 662, 2010.

[10] Ahmed N. A. Abdulwahhabb H.A. Mustafa.A.A. "Addition of Some Primary and Secondary Amines to Graphene Oxide, and Studying Their Effect on Increasing its Electrical Properties", Baghdad Science Journal Vol.13(1)2016.

[11] K. H. Al-Bayati, B. H. Al-Asaad,B. S.Hadi. "Study of the Inter-Particle Expectation Values for Inter and Outer Shell" Baghdad Science Journal,Vol.11,2,pp527-530, 2014.

[12] R. Dennington, T. Keith and J. Millam, "Gauss View 5.0.8", Semichem Inc, 2008.

[13] H.A. Abdulridha, S. N. Mazhir, H.I. Abbood, "Room Temperature Conductance of Graphene Sheet as a Function of Some Variables Using LAD/SZ Method", Advances in Physics Theories and Applications(iiste), Vol.52,pp28-32, 2016

[14] E. Artacho, J. Gale, A.Garc, J. Junquera, P.Ordej, D. anchez-Portal and J. Soler, "SIESTA-trunk-462", Fundaci on General Universidad Aut onoma de Madrid, 2013.

[15] J. Ferrer, C. Lambert, V. García-Suarez, S. Bailey, S. Hatef, D. Manrique, "GOLLUM version 1.0", Lancaster University, 2014.

[16] L. Pauling, "The Nature of the Chemical Bond", Cornell University Press, United States, 1960.

[17] F. Allen, D. Watson, L. Brammer, A. Orpen and R. Taylor, Journal of International Tables for Crystallography, Vol.C, PP.790-811, 2006.

[18] J. Soren and R. Morten, "Electronic and optical properties of graphene and graphene antidot structures", Master Thesis , University of Aalborg , 2013.

[19] F. Molitor, "Electronic properties of graphene Nanostructures", Ph.D. Thesis, ETH, 2010

[20] B. Ghavami, A. Ebrahimzadeh, Journal of Mesoscale and Nanoscale Physics, Vol.1, PP. 1-6, 2015.