Calculation the Electrical Properties of Graphene-B/P Compound Sheets Using Density Functional Theory Calculations

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Abstract:

Present study concerns on the effect of B/P compound on the electrical properties of the pure graphene sheet. The calculations are including the electrical conductivity, thermal conductivity, I-V characteristic and transmission coefficient. These 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 pure graphene sheet GR1 still the largest, and for the doped, they are of the order of GR6 > GR5 > GR4. The I-V characteristis were analyzed, and the transmission coefficient of the pure graphene sheet is higher than that of doped graphene sheets.

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

حساب الخواص الكهربائية لأوراق كرافين- مركب بورون / فوسفور باستعمال حسابات نظرية دالة الكثافة

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الخلاصة:

تركز الدراسة الحالية على تأثير مركب بورون/ فوسفور على الخواص الكهربائية لورقة الكرافين النقية. تضمنت الحسابات كل من التوصيلية الكهربائية، التوصيلية الحرارية، مميزات تيار-فولتية (I-V) ومعامل الانتقال. اجريت الحسابات باستعمال برنامج GOLLUM . لقد وجدنا تخفيف جيد لأوراق الكرافين المدروسة والذي حصلنا عليه باستعمال دالة LDA/SZ ودالة DFT في برنامج SIESTA. ان التوصيلية الكهربائية والحرارية لورقة الكرافين النقي تبقى هي الاكبر، وبالنسبة للكرافين المطعم فأنها كانت بالترتيب GR6 > GR5 > GR4. حللت مميزات تيار- فولتية (I-V)، وان معامل الانتقال لورقة الكرافين النقي كان أعلى منه لأوراق الكرافين المطعمة.

الكلمات المفتاحية: ورقة كرافين، التوصيلية الكهربائية، التوصيلية الحرارية، مميزات تيار- فولتية و معامل الانتقال.

1. 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 used material since antiquity, a single graphene layer was not isolated and studied until relatively recently [1-3]. 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 [5-8]. 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, thin, and flexibility. These characteristics make graphene an excellent candidate for advanced applications in future electronics [7-9].

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 characteristis, conductance and transmission coefficient of pure GR1 and doped graphene sheets GR4, GR5 and GR6.

2. Theoretical Methods and Computational Details

The calculated properties of graphene sheets in figure 1 are carried out using density functional theory LDA/SZ basis sets method.

$$E_{XC}^{LDA}[\rho] = \int \rho(\vec{r})\, \epsilon_{XC}(\rho(\vec{r}))d\vec{r} \qquad (1)$$

$\rho(\vec{r})$ electrondensity ,$E_{XC}[\rho]$exchange-correlation energy

$$G=G_0\int_{-\infty}^{\infty} dE\; T(E)(-df(E)/dE) \qquad (2)$$

G The electrical conductance ,G_0 quantum of conductance ,$E_F$is the Fermi energy .

The structures of the studied sheets are designed at Gaussian View 5.0.8 program[10], the relaxation of the studied

30º.SEM images were obtained with Tescann-VegaII microscope.

structures was done using the SIESTA – trunk - 462 program [11], and all the calculations are carried out using GOLLUM program " version 1.0 " [12].

3. Result and Discussion:

Figure 1 illustrates the relaxed junctions of the suggested structures in this research, these structures are included a pure graphene sheet GR1 and the G-B/P (two lines, one line and dot) sheets as GR4, GR5 and GR6, respectively. We showed the addition of B and P atoms in pure graphene sheet to construct the doped graphene sheets has not effect on the structural properties of the structure, the C-C, C=C and C-H bonds remain in the same ranges of carbon rings structures[13,14].

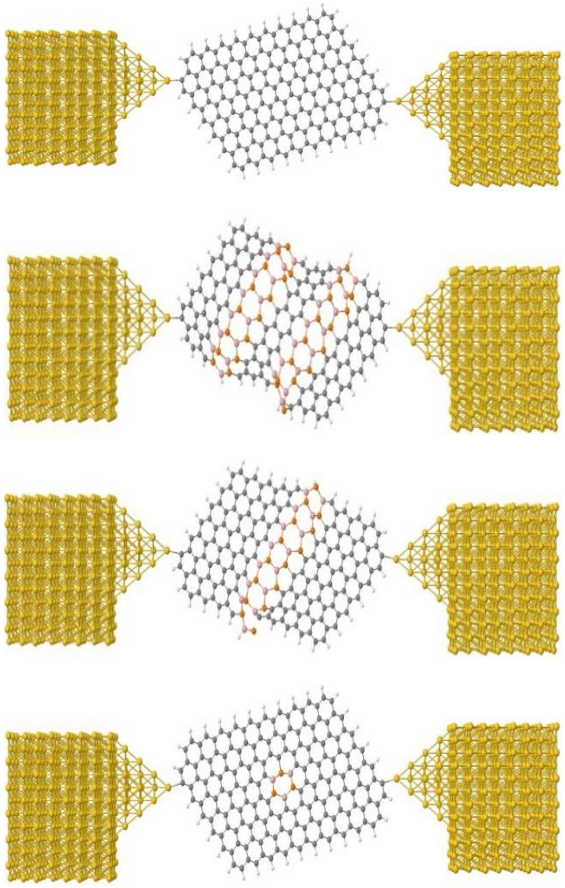

Figure1: The relaxed junctions of the studied graphene sheets. (Hydrogen(H)≡ white: Carbon (C)≡ gray: Boron (B)≡ violet: Phosphorus (P) ≡ orange)

Figure 2 shows that the electrical conductivity of the doped graphene sheets is in the order of GR6 > GR5 > GR4, the electrical conductivity of the sheet with dot doped ring in the middle of the sheet is the highest value 4.83 μs . This sheet has multi channels of electron transport in comparison with the two others. GR4 and GR5 have electrical conductivity equal to 3.27 μs and 1.04 μs, respectively. The reason of this result is due to that GR6 has small number of B and P atoms in comparison with GR4 and GR5. Increasing the number of B/P compounds in the sheet leads to decrease the electrical conductivity. Figure 2 showed the pure graphene sheet GR1 still has the largest value of electrical conductivity.

The form of the addition B/P compound in the sheet has a significant role in the electrical conductivity values. Graphene sheet with dot doped ring in the middle of the sheet has high electrical conductivity in comparison with the other doped sheets. In other words, the electrical conductivity of the pure paper GR1 is the largest compared with the rest of the doped sheets.

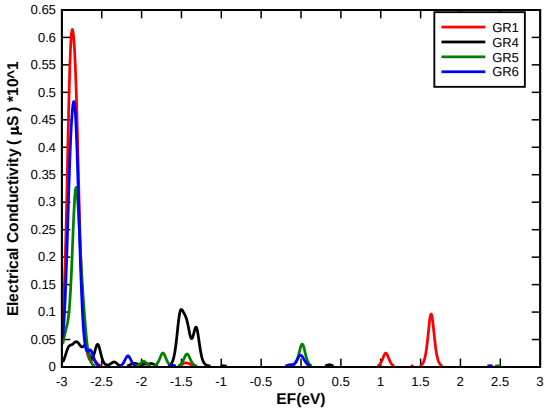

Figure 2: Electric conductivity in (μs) of the pure and doped graphene sheets

The effect of the B/P compound on the thermal conductivity of graphene sheets is shown in figure 3. The thermal conductivity of the doped graphene sheets has the same behavior of the electrical conductivity. GR6 of the dot B/P doping ring in the middle of the sheet has the highest value of thermal conductivity ($1.321*10^{-10}$ W / m. K), GR5 has $7.203*10^{-11}$ W / m. K and GR4 has thermal conductivity of $4.931*10^{-11}$ W / m. K. [15, 16]. Also, the pure graphene sheet GR1 has the higher value of thermal conductivity than the three doped sheets.

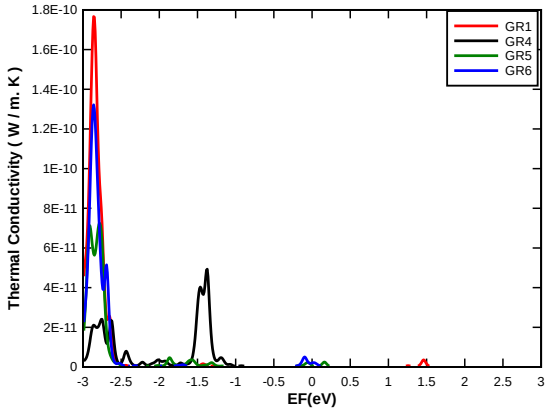

Figure 3: Thermal conductivity of the pure and doped graphene sheets

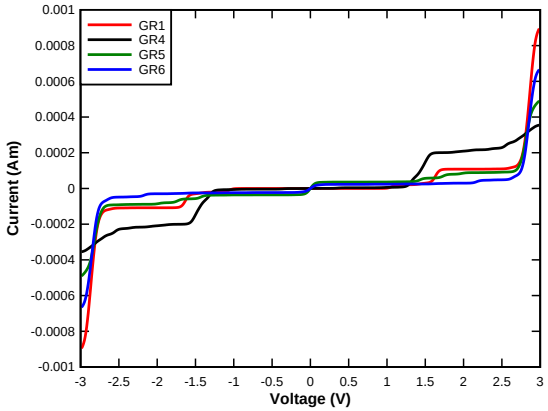

Figure 4: The I-V characteristic of the pure and doped graphene sheets

Figure 4 shows the analyze of the I-V characterization of the doped graphene sheets GR4, GR5 and GR6 with the one pure GR1. After each sheet inserted in between two gold contacts electrodes with a suitable anchor atom between the electrode and the sheet (figure 1), a bias voltage of 3 Volts was applied in the direction of the axis connecting both the anchor atoms. The Fermi level of the electrode was fixed and was considered lying in the middle of LUMO-HOMO gap. From figure 4, we observed that the GR6 (dot doping ring in the middle of the sheet) gave sensing behavior at 2.6 Volt bias voltage and -2.6 Volt reverse voltage. For GR4, the required bias voltage and reverse voltage for sensing are (1.25 and -1.25), and (1.5 and -1.5) Volts for GR5. A very valuable result obtained from above behavior, since this behavior reduces completely the high temperature effects that appear in the old macro devices. The I-V curve indicates to that the appropriate contact with the electrodes have rather limited effect on the sensing performance of the doped graphene sheets. current results since the lowering of the energy gap between the HOMO of the doped sheet and the Fermi level of the electrode in the forward and reverse bias [15, 17].

Figure 5 illustrates the relationship of the calculated values of the transmission coefficient of the three doped graphene sheets GR4, GR5 and GR6 with the pure GR1. We showed that the sheet with small number of B and P atoms as a dot doped ring in the middle of the sheet has the high value of transmission coefficient in comparison with the other doped sheets, this due to high number of open channels. In general, the transmission coefficient of the sheets has a wide range on energy scale. The pure GR1 without scattering region has a suitable transmission coefficient in a wide range of energy. In other words, The pure graphene sheet has higher value of transmission coefficient than that of the doped sheets. This could be ascribed to the effect of the B and P atoms, since the presence of these atoms cause rotation of the phenyl rings they are located and twist the paper of the graphene sheet, and that could affected the tuning between the energy channels or levels of the sheet and the electrodes result in a quantum destructive interference between the waves that propagate from the left electrode to the right electrode, which reduce the transmission coefficient. the results in figure 5 could be understand in terms of the impact of the number and the shape of the doping in the sheet[16, 17].

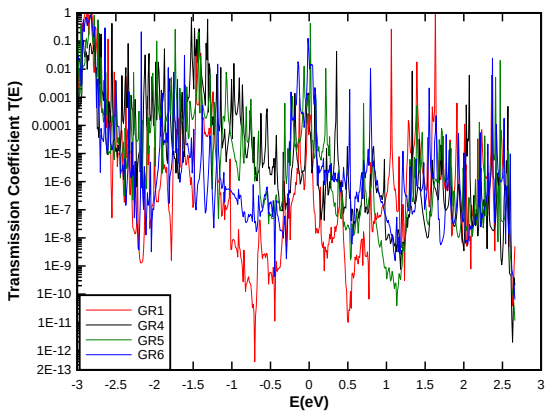

Figure 5: The transmission coefficient of the pure and doped graphene sheets

4. Conclusions

1. The electric conductivity , thermal conductivity and transmission coefficient are decrease when added the B and P atoms to grapheme as a doped .
2. The studied graphene sheets show I-V characteristics very much similar to sensing type. This behavior reduces completely the high temperature effects that appear in the old macro devices.
3. Pure graphene sheet has multi channels of electron transport, That means, the decreasing the number of B and P atoms in the sheet increases the number of channels that the electrons can pass and therefore gave the sheet high electrical and thermal conductivities..

5. Reference

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