Density Functional Theory Calculations of Electronic and Electrical Properties of Pure Graphene and Fluorine Graphene Sheets

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الخلاصة

تم استعمال برنامج Gaussian View 5.0.8 لتصميم رقائق الكرافين النقي GR1 والمطعمة بالفلور GR2 وGR3. ان استرخاء هذه التراكيب قد تم باستعمال برنامج SIESTA- 462. ان جميع الحسابات تم اجراؤها باستعمال برنامج Gollum. تبين النتائج ان وجود ذرات الفلور في الرقيقة ليس له تأثير على المعاملات الهندسية لأواصر كاربون-كاربون. ان الكرافين النقي يملك فجوة طاقة صفرية ومرونة الكترونية عالية مع توصيلية كهربائية وحرارية عاليتين نتيجة امتلاكه قنوات متعددة لنقل الالكترون بالمقارنة مع الرقيقتين المطعمتين، ان وجود ذرات الفلور في الحلقات قاد الى رفع فجوة الطاقة ونقصان القنوات المفتوحة لنقل الالكترون، ان التوصيلية الكهربائية تتناسب تناقصا» خطيا» مع عدد ذرات الفلور المضافة، تم تحليل منحني تيار- فولتية لرقائق الكرافين المدروسة، تبين النتائج أن رقيقة الكرافين النقي تسلك كمقاومة نقية.

الكلمات المفتاحية

الكرافين، التوصيلية الكهربائية، المرونة الالكترونية، منحني تيار- فولتية.

Abstract

Gaussian View 5.0.8 code was used to design the pure graphene sheet GR1 and the fluorine doped samples GR2 and GR3. The relaxation of these structures was done using the SIESTA-trunk-462 code. All calculations are carried out using GOLLUM code. The result shows the presence of fluorine atoms in the sheet has no effect on the geometrical parameters of carbon-carbon bonds. Pure graphene sheet has zero band gap, high electronic softness and high electrical and thermal conductivities due to the multi channels of electron transport in comparison with the two doped graphene sheets. The presence of fluorine atoms in the rings leads to raise the energy gap and decrease the open channels of electron transfer. The electrical conductivity is decreasing linearly proportional to the number of added fluorine atoms, the I-V curve of the studied graphene sheets is analyzed, the result shows that the pure graphene sheet behave as pure resistance.

Keywords

Graphene, Electrical Conductivity, Electronic Softness, I-V Curve.

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 utilized 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 ofgraphene 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, thinness, and flexibility. These characteristics make graphene an excellent candidate for advanced applications in future electronics [7-9].

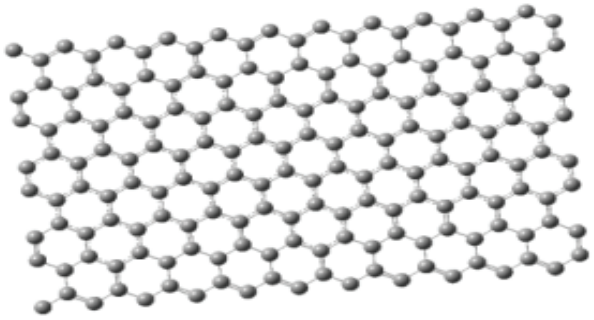
In particular, the potential of graphene in high-speed analog electronics is currently being extensively explored [3,6,8]. In current paper, we discuss briefly the basic electronic structure and transport properties, I-V characteristic, conductance and transmission coefficient of pure GR1 and doped graphene sheets with different number of fluorine atoms GR2 and GR3.

2. Computational Details

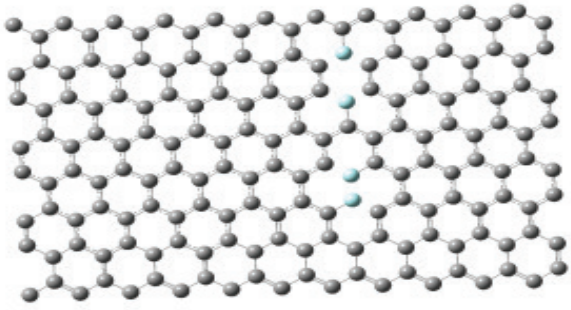
The calculated properties of graphene sheets in figure 1 are carried out using density functional theory LDA/SZ basis sets method. The structures of the studied sheets are designed at Gaussian View 5.0.8 program [10], the relax was initially done using Austin Model 1 at Gaussian 09 package of programs and then using the SIESTA-trunk-462 program [11], and all the calculations are carried out using GOLLUM program " version 1.0 " [12].

3. Results and Discussion

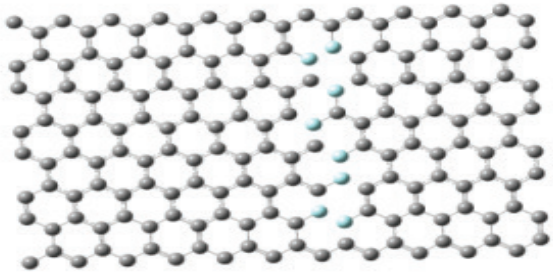
Fig. (1) illustrated the suggested relax structures, GR1 is the pure graphene sheet, GR2 is the doped graphene with four fluorine atoms and GR3 is the doped graphene with eight fluorine atoms. We can see that from Fig 1 the addition of fluorine atoms in the pure graphene sheet to construct the doped graphene sheets has not an effect on the C-C, C=C and C-C=C bonds in the structure, these bonds are remain in the same ranges of carbon rings structures [13,14]. Fig. (2) shows the total energy ET obtained from the relax structures was decreased with adding the fluorine atoms in place of carbon atoms. ET depends on the number of electrons in each sheet, it was decreased with increasing fluorine atoms in the sheet.



GR1



GR2



GR3

Fig (1): The relax structure (Carbon (C)≡ gray: Fluorine (F) ≡ green).

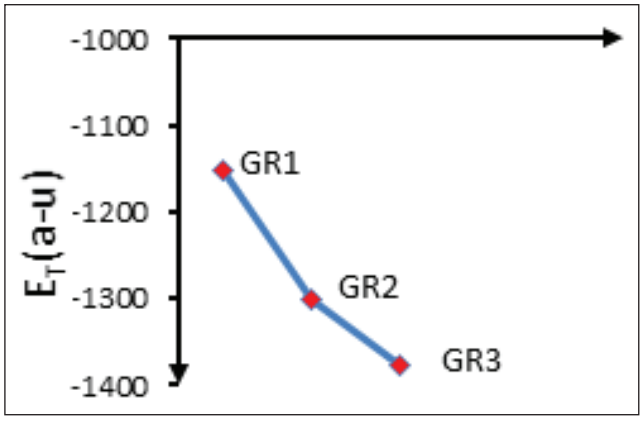


Fig (2): The total energy of the relax structures

The resultant energy gap (Eg) in Fig. (3) shows the pure graphene sheet GR1has the lowest value (0.0168 eV), this value was raised to (0.1109 eV and 0.2677 eV) for GR2 and GR3, respectively. (Eg) is linearly increased with increasing the number of fluorine atoms in the sheet, means, GR2 and GR3 are new molecular electronics have new properties in electronic applications. Fig. (4) observed the electronegativity X is in the order of GR1 > GR2 > GR3, this corresponds to the results of ionization energy IE and electron affinity EA, where IE and EA are in the order of GR1 > GR2 > GR3. Fig (5). shows the pure GR1 has the higher electronic softness S, the increasing of electronic softness is the main future as a sign for that band gap goes to be rather soft and lowering the resistance of the structure to lose an electron.

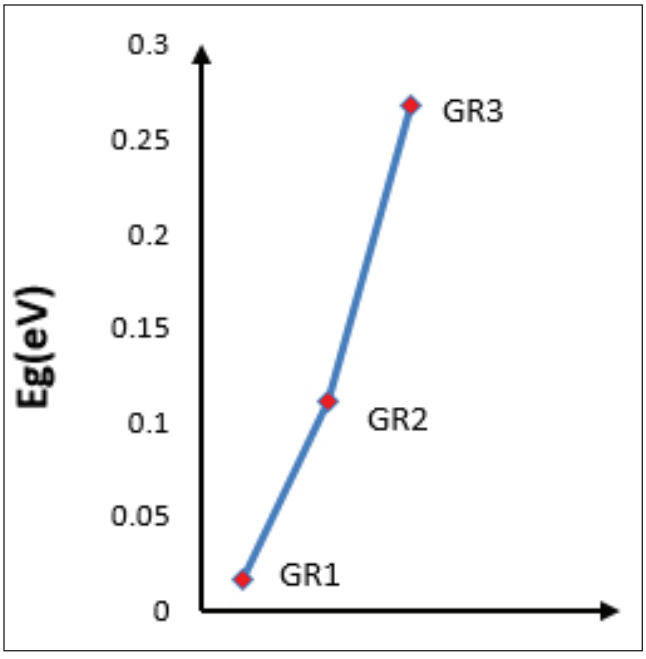


Fig. (3): The energy gap of the relax structures

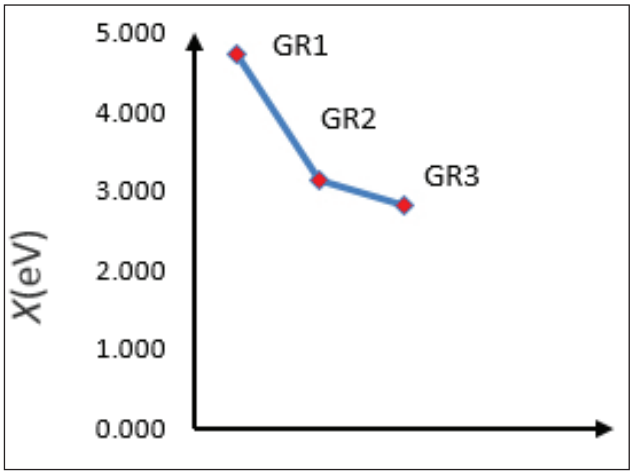


Fig. (4): The electronegativity of the relax structures

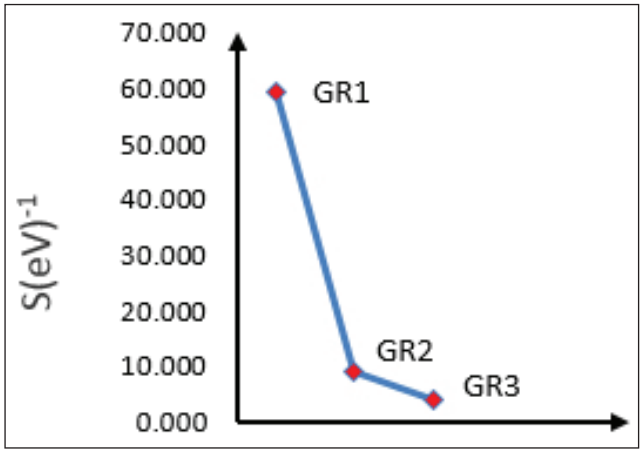


Fig (5): The electronegativity of the relax structures

Fig. (6) shows the electrical conductivity of all graphene sheets holds the stationary state after (50) K in the range of temperature to (400) K. On the other hand, GR1 has the higher electrical conductivity (2) µS, this sheet has multi channels of electron transport in comparison with the two others. The electrical conductivity of GR2 is (0.882) µS and GR3 is (0.202) µS, the presence of fluorine atoms in the rings decreased the open channels of electron transfer and therefore reduced the electrical conductivity of the sheet. The decreasing of the electrical conductivity is linearly proportionality with the number of added fluorine atoms.

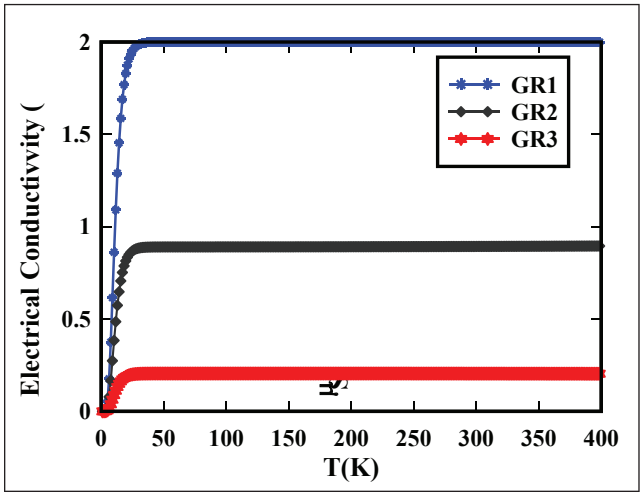


Fig. (6): Electric conductivity in (µS) of the pure and doped graphene sheets.

The thermal conductivity of the graphene sheets has the same behavior of the electrical conductivity; it is increase with temperature increasing. At (300) K, GR1 has the higher value of thermal conductivity (1.141x10-9) W / m. K, but GR2 has (5.153x10-10) W / m. K and GR3 has thermal conductivity of (1.149x10-10) W / m. K. That means, the increasing the number of fluorine atoms in the sheet decreases the number of open channels that the electrons can pass and therefore gave the sheet low electrical and thermal conductivities, as seen in Fig (7) [15-19].

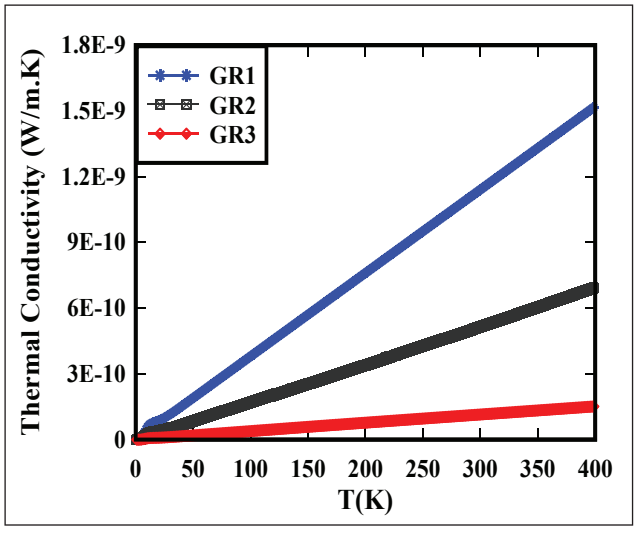


Fig (7): Thermal conductivity of the pure and doped graphene sheets.

The analysis of I-V curve of our samples are shown in Fig. (8). After each sheet inserted in between two gold contacts electrodes with a suitable anchor atom between the electrode and the sheet, a bias voltage of (2) 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 I-V curve, for GR1 we observed a linear relationship between the current and the voltage reaches to (1.6) Volt, means GR1 has resistance behavior, after this value we observed sensing behavior at (1.6) Volt bias voltage and (-1.6) Volt reverse voltage. The response of the I-V curve was reduced with adding the fluorine atoms in the sheet. This responsively was lowered with increasing the number of fluorine atoms, as seen for GR2 and GR3. 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.

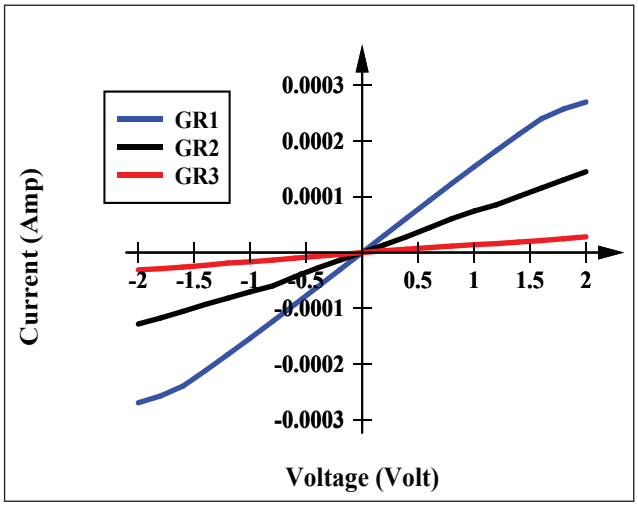


Fig (8): The I-V curve of the pure and doped graphene sheets.

4. Conclusions

From the results in present study, one can conclude that the number of the addition of fluorine atoms in the sheet has a significant role in the electrical conductivity values. Pure graphene sheet has zero band gap with high electrical conductivity in comparison with the other doped sheets. The electrical conductivity of the pure graphene is the largest because it has multi channels of electron transport, the presence of more and more of fluorine atoms in the sheet decreases the number of channels that the electrons can pass through. Thermal conductivity was decreased with increasing the number of fluorine atoms. Thermal conductivity has the same behavior of electrical

conductivity. Pure graphene has the largest value of electronic softness in comparison with the doped sheets.

Pure graphene sheet show I-V curve very much similar to resistance type. This behavior reduces completely the high temperature effects that appear in the old macro devices.

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