Density Function Theory Calculations of Graphene Sheet

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Abstract:

We investigated the electrical properties of Graphene Sheet by employing the B3LYP/DFT at SIESTA – trunk - 462 of program, and calculated by employing the LDA calculations using the Gollum software . We showed that the studied Graphene Sheet has small energy band gap. Graphene Sheet has high values of ionization potential and electron affinity. It has small value of electrochemical hardness and large value of electronic softness. The calculated density of states and the observed nonzero density of states indicates a finite number of states. The I-V characteristic and conductance curves showed high value of conductivity. Pure Graphene Sheet is suggest that may make it a suitable for thermoelectric applications.

Keywords: Graphene Sheet, Energy gap, I-V characteristic, conductance and transmission coefficient.

حسابات نظرية دالة الكثافة للكرافين شيت

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الخلاصة:

تم فحص الخواص الكهربائية للكرافين شيت بتطبيق نظرية دالة الكثافة ذات المعاملات الثلاث في برنامج SIESTA وحساب تلك الخواص بتطبيق حسابات تقريب الكثافة الموضعية باستعمال برنامج Gollum. لقد لاحظنا ان الكرافين شيت قيد الدراسة يمتلك فجوة طاقة صغيرة . كما أنه يمتلك جهد تأين وألفة الكترونية عاليتين. أن الكرافين شيت له صلادة كهروكيميائية صغيرة ومرونة الكترونية كبيرة. أن كثافة الحالات المحسوبة واللاصفرية تشير الى العدد المناسب للحالات. أن منحنيات خصائص تيار- فولتية و التوصيلية تبين ان الكرافين شيت يمتلك قيمة عالية للتوصيلية. تبين النتائج أن الكرافين شيت النقي مناسب جدا" للتطبيقات الكهرو حرارية.

الكلمات المفتاحية: كرافين شيت، فجوة الطاقة، مميزات تيار- فولتية، التوصيلية، معامل الانتقال.

1. Introduction

Graphene is an allotrope of carbon in the form of a two-dimensional , atomic-scale, hexagonal lattice in which one atom forms each vertex. It is the basic structural element of other allotropes , and its is a

particularly intriguing two-dimensional structure with the quasi-relativistic dispersion law that has recently burst into the solid state physics. In 2004, researchers of Manchester University (UK) have succeeded to manufacture a monoatomic graphite layer graphene on an insulating substrate [1,2,3,4,5]. This technological breakthrough has attracted a great deal of attention of leading experimental and theoretical groups over the world. In a very short time, a new area of research the study of graphene-based structures has emerged and become one of key research directions in the material science and condensed matter physics, The reason for this is exceptional properties of graphene that make this material highly interesting from the point of view of both fundamental physics and potential applications [1]. Most prominently, the carbon-based nanoelectronics. A.Geim and K. Novoselov were awarded the Nobel Prize 2010 for the discovery of graphene.

There have been several reviews discussing the topic of graphene in recent years. Many are theoretically oriented, with Castro Neto et al.'s review of the electronic properties as a prominent example [6] and a more focused review of the electronic transport properties [7]. Experimental reviews, to name only a few, include detailed discussions of synthesis [8] and Raman characterization methods [9], of transport mechanisms [10, 11], of relevant applications of graphene such as transistors and the related bandgap engineering [12], and of graphene optoelectronic technologies [13]. We feel, however, that the literature is lacking a comprehensive overview of all major recent experimental results related to graphene and its applications.

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) – LDA] level with Single Zeta (SZ) basis sets, All calculations were carried out using the SIESTA – trunk - 462 program [14] , GOLLUM program " version 1.0 " [15] and Gaussian View 5.0.8 [16] .

3. Results and Discussion

Chart 1 represents the relaxation structure of Graphene Sheet design at Gauss View 5.0.8. and relax by employing the B3LYP/DFT at SIESTA – trunk - 462 of program. Table 1 shows the result of the relaxation of the Graphene Sheet included the total energy ET in a. u, LUMO-HOMO energy gap Eg in eV, ionization energy IE and electron affinity EA in eV, electrochemical hardness in eV, electronic softness S in (eV)-1, chemical potential K in eV, electronegativity K and electrophilic index W in eV. As seen in table 1, The HOMO and LUMO are closest to each other, in other words, the valence band and the conduction band are closest to the Fermi level and thus determine the energy band gap, and therefore, the electrical conductivity of the Graphene Sheet. The calculated energy band gap is 0.035 eV, this may an indication to that the highest band is partially filled and this taking on the properties of both the valence and the conduction bands. The very lower HOMO-LUMO band gap in the Pure Graphene Sheet indicate that when the Sheet is connected in a device, then a better electron injection process can be expected. The Graphene Sheet under study has high values of IE and EA, these values are main futures which gave us the ability to interact the two ends of the Sheet to two electrodes through suitable anchor atoms.

The results showed that the Graphene Sheet has small value of and large value of S. The lowering of electrochemical hardness is the main future as a sign for that band gap goes to be rather soft and therefore lowering the resistance of the Graphene Sheet to lose electrons. The calculated electronegativity and electrophilic index refer to that the Graphene Sheet can interacts with other species in the medium, high electrophilicity means large escaping tendency.

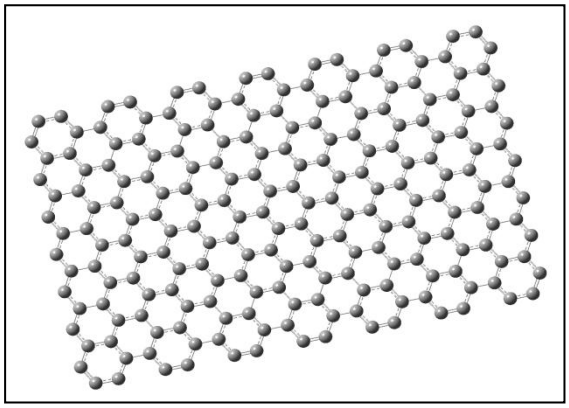

Figure 1: The relax structure of Graphene Sheet

Table 1: The results of the relaxation of the Graphene Sheet

Homo (ev)	Lumo (ev)	E_T (ev)	E_g (ev)	IE (ev)
-6.709	-6.674	-32250.4	0.035	6.709

EA (ev)	η (ev)	S $(ev)^{-1}$	K (ev)	X (ev)	W (ev)
6.675	0.017	28.860	-6.692	6.692	1292.437

The density of states governs many physical properties and consequently plays an important role in solid state physics. It is important to be able to predict how the density of states will behave for different nanostructure geometries. The density of states of a system describes the number of states per interval of energy at each energy level that are available to be occupied.

The distribution of energy between identical particles depends in part upon how many available states there are in a given energy interval. The density of states of Pure Graphene Sheet as a function of Fermi energy were calculated by employing the DFT-B3LYP/6-31G level of theory and shown in figure 2. The observed nonzero density of states indicates a finite number of states. This is likely in the presence of local potential fluctuations in the Graphene Sheet. From the distribution of the density of states in figure 2, we can estimate a characteristic amplitude of the fluctuations of 5 eV.

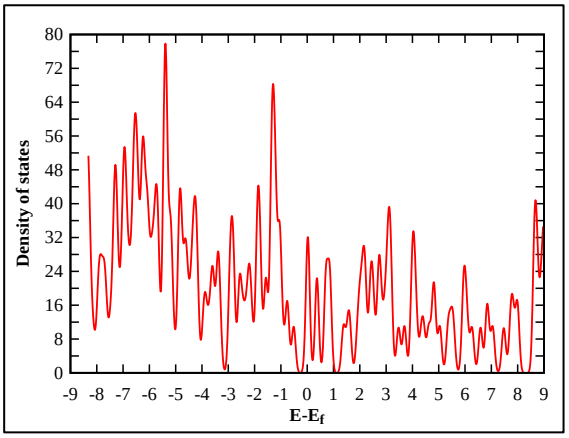

Figure 2: The density of states of Graphene Sheet

The analyze of the current-voltage characterization of the Pure Graphene Sheet is done by employing the LDA calculations and carried out using the Gollum software. In this calculation, the Graphene Sheet is inserted in between two carbon contacts electrodes with a suitable anchor atom between the electrode and the Sheet. Provision has been taken to make straight the Graphene Sheet in such a way that the two electrodes will be in one axis. Then bias voltage is applied in the direction of the axis connecting both the anchor atoms. The resulting I-V characteristic and conductance curves obtained for the Pure Graphene Sheet are shown in figures 3 and 4, respectively. For the resolution of calculation, the Fermi level of the electrode was fixed and was

considered lying in the middle of HOMO-LUMO gap. From Figure 3, it is clear that Graphene Sheet shows characteristics very much similar to rectification type and the required bias voltage for rectification decrease in 1.1 V. The Pure Graphene Sheet Shows high electric conductivity in energy range (-1.75 to 1.75) eV, the maximum value of conductivity (dI / dV) is 5.9 μs [17].

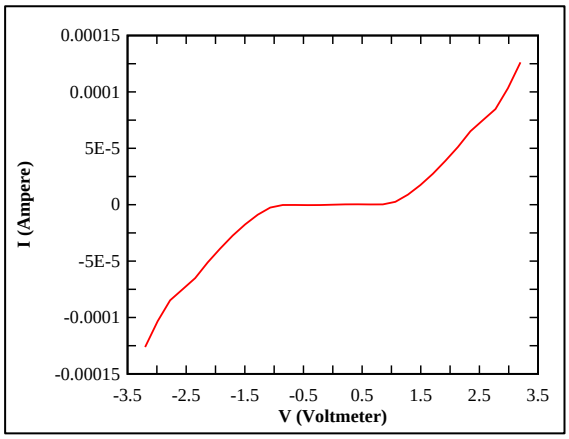

Figure 3: The I-V characteristic of Graphene Sheet

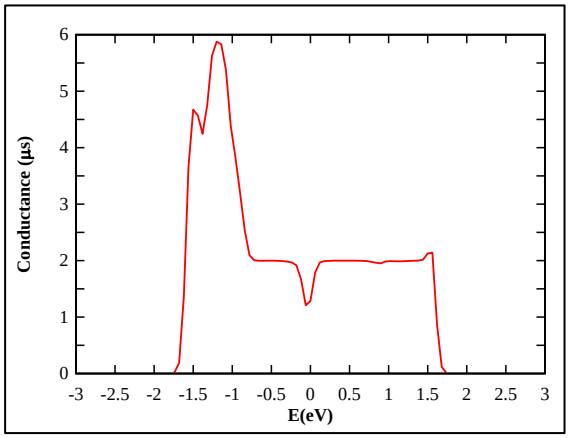

Figure 4: The room temperature conductance of Graphene Sheet

The figure of merit is a dimensionless property represents the characterization of thermoelectric performance of a material. It depends on the thermal conductivities attributed to electrons and phonons. The total thermal conductivity in figure 6 and the calculated value of figure of merit in Figure 5 for Pure Graphene Sheet are suggest that may make it suitable for thermoelectric applications. The combination of geometrical structuring makes it possible to optimize both electronic and phononic transport properties of the considered Graphene Sheet which have already been realized with existing fabrication technology. The calculated value of figure of merit is the aim for efficient thermo electrics and good candidates for technological applications. Thermal conductivity is a physical quantity of a material that conducts heat. The overall trend of thermal conductivity spectra shows that more transfer of heat takes place in the range (-1.5 to 1.5) eV Fermi energy. The thermal conductivity has contributions from the phonons and electrons. The average thermal conductivity of Pure Graphene is 3.2 E -9 W/m. K at 300 K, as illustrated in Figure 6.

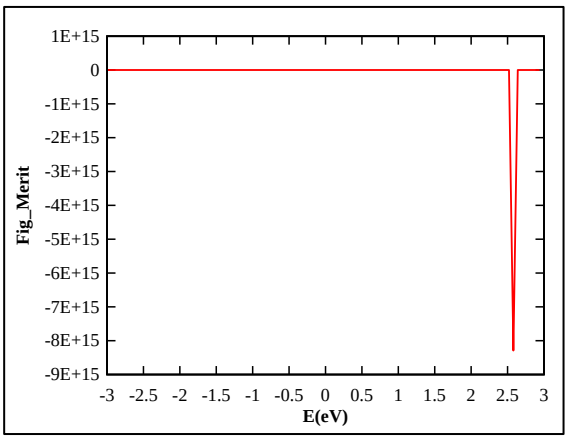

Figure 5: The Figure of Merit of Graphene Sheet

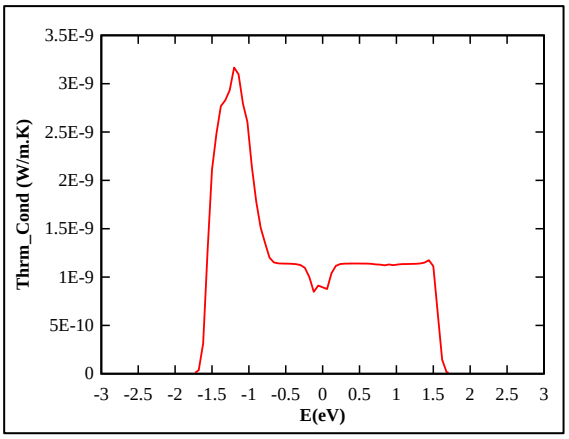

Figure 6: The thermal conductivity as a function of Fermi level of Graphene Sheet

The main thermoelectric transport property in material is the Seebeck coefficient. It is related to the fact that electrons carry both heat and charge. The diffusion of the electron depends on temperature gradient present in the material which creates the opposite electric field and hence voltage known as Seebeck voltage. The trend of the spectra in the Seebeck coefficient and electronic conductivity depends on the Seebeck voltage. Its magnitude and sign are correlated with an asymmetry distribution of electrons around the Fermi level. The asymmetric energy distribution of electrons moving in the material related to the Fermi energy gives a greater value of Seebeck coefficient. From Figure 7 the Pure Graphene Sheet shows same contribution of electron and hole concentrations, it shows a maximum value of Seebeck coefficient of about 330 μ V / K at 300 K. Figure 8 shows the transmission coefficient of the studied Pure Graphene Sheet[17].

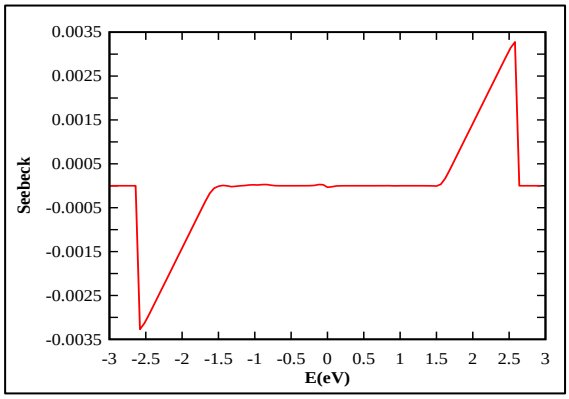

Figure 7: The Seebeck coefficients as a function of Fermi level of Graphene Sheet

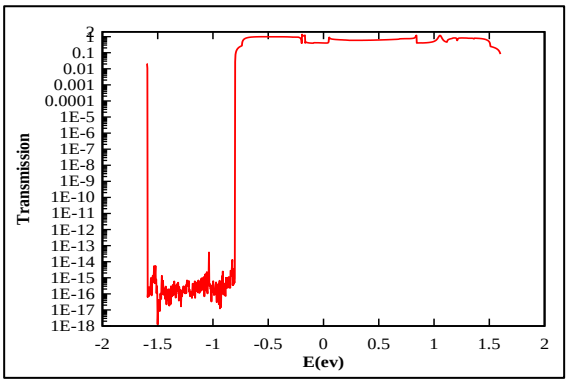

Figure 8: The transmission of Graphene Sheet

4. Result and Discussion:

Graphene Sheet was design at Gauss View 5.0.8. and relax by employing the B3LYP/DFT at SIESTA – trunk - 462 of program, the electrical properties were calculated by employing the LDA calculations and carried out using the Gollum software. From the results, one can conclud:

1- The relax structure under study has 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- Total energy is few, and thus be of transmission electron valence band to conduction band easier and its energy band gap is 0.035 eV .

3- The Graphene Sheet under study has high values of IE and EA, so it has small value of electrochemical hardness η and large value of electronic softness S . These results are correspond to the small resultant energy band gap.

4- The calculations of the density of states and the observed nonzero density of states indicates a finite number of states. This is likely in the presence of local potential fluctuations in the Graphene Sheet .

5- The I-V characteristic and conductance curves showed high electric conductivity, and the highest

value of conductivity of the Graphene Sheet is 5.9 μs.

6- By calculation, the total thermal conductivity, the value of figure of merit, the Seebeck coefficient and the transmission coefficient for Pure Graphene Sheet are suggest that may make it suitable for thermoelectric applications.

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