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Theoretical Study of Electronic and Electrical Properties of Pure and Doped Graphene Sheets

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Abstract*—The studied graphene sheets were design at Gaussian View 5.0.8 program and initially relaxed at Gaussian 09 program. The last relaxation of these structures was done using the SIESTA-trunk-462 program. All calculations are carried out using GOLLUM program. The results showed the presence of fluorine atoms in the sheet has not an effect on the geometrical parameters of carbon-carbon bonds. Pure graphene sheet has zero band gap and large electronic softness with higher electrical and thermal conductivities due to the multi channels of electron transport it has in comparison with the two doped graphene sheets, the presence of fluorine atoms in the rings leads to rise the energy gap and decrease the open channels of electron transfer, the electrical conductivity is linearly proportionality decreasing with the number of added fluorine atoms. The I-V characteristics of the studied graphene sheets was analyzed and observed resistance behavior for pure graphene sheet.*

***Keywords*—Graphene, Electrical Conductivity, Electronic Softness, I-V Curve.**

I. INTRODUCTION

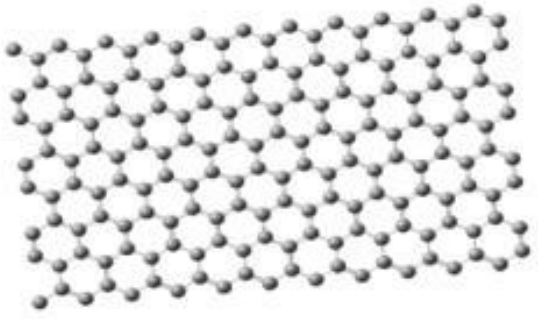
Graphene is a two-dimensional atomic layer of carbon atoms, the building block of the 3-D structure graphite. While graphite has been a well-known and utilized material since antiquity, a single graphene layer was not isolated and studied until relatively recently [1-3]. Graphene was generated by several 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 of pure GR1 and doped graphene sheets with different number of fluorine atoms GR2 and GR3.

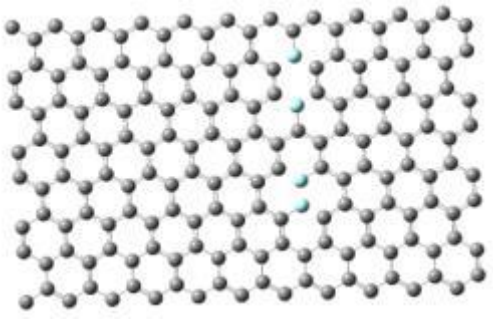
II. COMPUTATIONAL DETAILS

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 relaxation of the studied structures was initially done using Gaussian 09 package of programs and then using the SIESTA-trunk-462 program [11], all the calculations are carried out using GOLLUM program " version 1.0 " [12].

III. RESULTSAND DISCUSSION RESULTS



GR1



GR2

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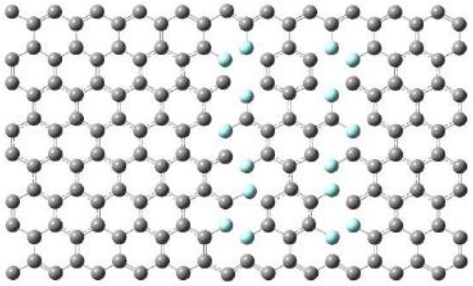

GR3

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

The three suggested relax structures in Fig. 1 are the pure graphene sheet GR1, the doped graphene with four fluorine F atoms GR2 and the doped graphene with sixteen fluorine F atoms GR3. We showed the addition of fluorine atoms in the pure graphene sheet to construct the doped graphene sheets has not an effect on the bonds C-C, C=C and C-C=C in the structure, these bonds are remain in the same ranges of carbon rings structures[13,14].

Fig. 2 shows the calculated values of total energy ET obtained from the relaxation of the studied structures. ET was decreased with adding the fluorine atoms in place of carbon atoms, it depends on the number of electrons in each structure, ET was decreased with increasing fluorine atoms in the sheet.

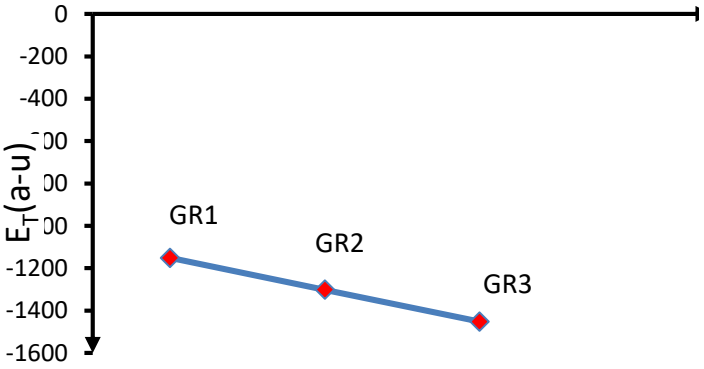

Fig.2: The total energy of therelax structures

Fig. 3 showed the calculated value of the energy gap Egof the pure graphene sheet GR1is the lowest (Eg= 0.0168 eV), this value was raised to (0.1109 and 0.0553) eV for GR2 and GR3, respectively. Eg is independent of the increasing of the number of fluorine atoms in the sheet, GR2 and GR3 are new molecular electronics have new electronic applications. Fig. 4 observed the electronegativity X of the studied sheets, it 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 illustrates the electronic softness S of the studied sheets, we showed the pure GR1 has the higher 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.

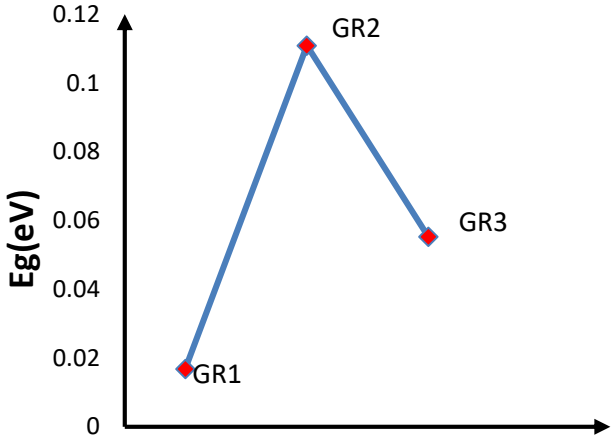

Fig. 3: The energy gap of the relax structures

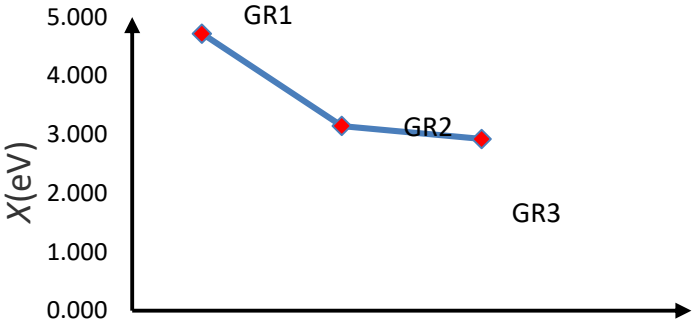

Fig. 4: The electronegativity of the relax structures

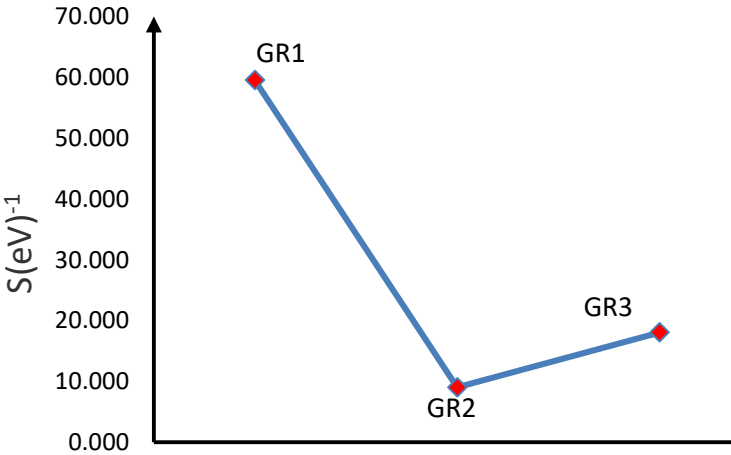

Fig. 5: The electronic softness of the relax structures

Fig.6 showed the electrical conductivity of all graphene sheets holds the stationary state approximately after (50) K in the range of temperature to (400) K. Generally, the pure GR1 has the higher electrical conductivity(2)µS dueto that the pure sheet has multi channels of electron

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transport in comparison with the two others. The electrical conductivity of GR2 is(0.897)µS and GR3 is (0.0519)µS, the presence of fluorine atoms in the rings decreased the open channels of electron transfer and therefore reduces the electrical conductivity of the sheet. The decreasing of the electrical conductivity is linearly proportionality with the increasing the number of added fluorine atoms.

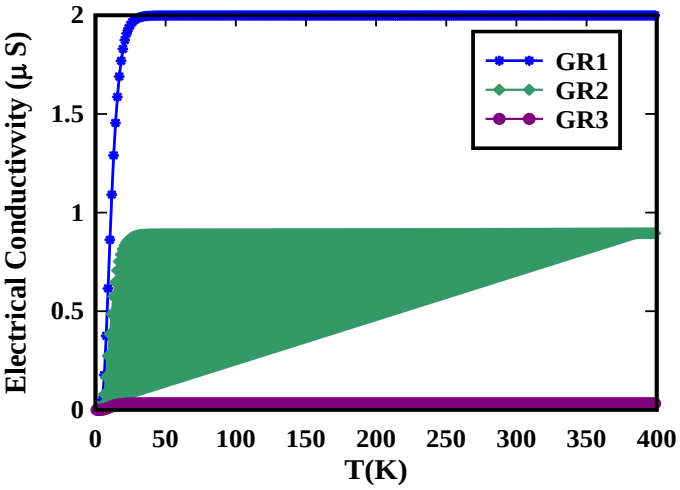

Fig.6: Electric conductivity in (µS) of the pure and doped graphene sheets.

Figure 7 declare the thermal conductivity of the studied graphene sheets has the same behavior of the electrical conductivity, it is increasing with increase of the temperature. At (300)K, GR1 has the higher thermal conductivity (1.141*10-9)W/m. K, GR2 has (5.153*10-10)W/m. K and GR3 has thermal conductivity of (3.710*10-11)W / m. K. Means, the increasing the number of fluorine atoms in the sheet decreases the number of open channels that the electrons can passthrogh and therefore, gave the sheet low electrical and thermal conductivities[15-17].

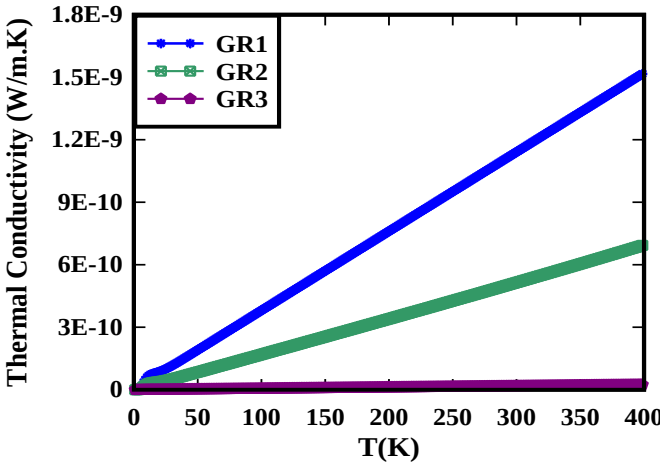

Fig.7: Thermal conductivity of the pure and doped graphene sheets.

Fig. 8 shows the I-V curve of the pure GR1 and doped GR2 and GR3 sheets. 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 V) 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 V), means GR1 has resistance behavior, after this value, we observed sensing behavior at (1.6 V) bias voltage and (-1.6V) 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.

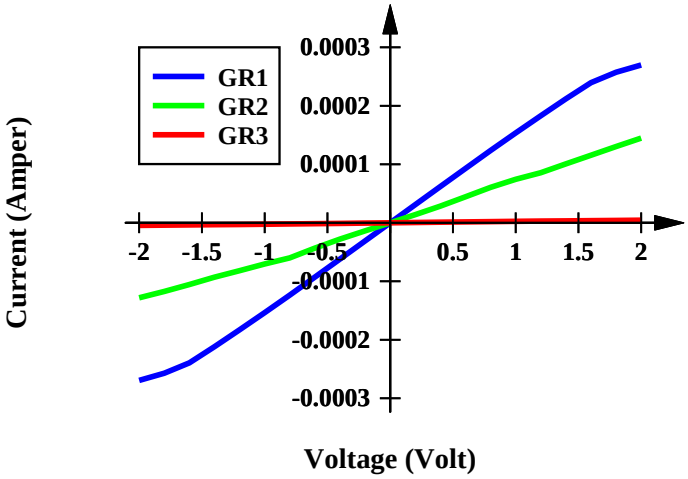

Fig.8: The I-V curve of the pure and doped grapheme sheets.

IV. CONCLUSION

From the above results in present study, one can conclude the following:

1. The number of the fluorine atoms added in the sheet has a significant role in the electrical conductivity values.
2. Pure graphene sheet has zero band gap with high electrical conductivity in comparison with the other doped sheets,the pure graphenehas the largest electrical conductivity multi channels of electron transport it has, the presence of more and more of fluorine atoms in the sheet decreases the

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number of channels that the electrons can pass through.

3. Thermal conductivity was decreased with increasing the number of fluorine atoms. Thermal conductivity has the same behavior of electrical conductivity.
4. Pure graphene sheet has the largest value of electronic softness in comparison with the doped sheets.
5. Pure graphene sheetshow I-V curve very much similar to resistance type. This behavior reduces completely the high temperature effects that appear in the old macro devices.

V. ACKNOWLEDGEMENTS

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