# Study of the effect of configuration of GR-Ge-GR sandwich sheets on their electronic applications

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## Abstract

*Current study deals with the effect of the configuration of GR-Ge-GR sandwich sheets on their electronic applications. The electrical properties was calculated by using GOLLUM program. The results showed good relax of the sandwich structures was obtained using GGA/DZP- DFT at SIESTA - trunk - 462 of program. We showed the electric conductance at room temperature of the sandwich sheets is an indication to designing different configurations of two dimension sandwich materials gave different electronic applications, so the sandwich structures can take place in many electronic applications according to temperature variations. Moreover, the configuration of the sandwich sheets is an important in calculating of thermal conductivity. On the other hand, some structures of GR-Ge-GR sheets appeared contribution of electron concentration and other are appearing contribution of hole concentration at Fermi energy. The results showed the I-V characteristics of the studied structures refer to variety in the application of the sandwich sheets as electronic devices.*

**Keywords:** *Sandwich sheets, Electric conductance, Thermal conductivity and I-V curve.*

## 1. Introduction

The discovery of Graphene as a two dimension material is the key point to a large amount of new and exciting physics [1]. Mermin-Wagner theorem states that a two dimension crystal cannot exhibit long-range order at any finite temperature, but the remark that a single sheet of atoms is stable was at present fairly a surprise[2].

Nelson and Peliti in 1987 [3] showed the an-harmonic coupling between in-plane and out-of-plane lattice vibrations is significance for the stability of a membrane, without this an-harmonic coupling the membrane would be fully wrinkled. As a result of this an-harmonic coupling, the membrane becomes overall more or less plane, but the membrane displays strong intrinsic waves that are characterized by a power-law behavior of the atomic-displacement correlations functions. The system remains approximately two dimensional and approximately crystalline[4-6]. At least for rigid systems, such as Graphene, this means that one can safely use the term "two dimensional crystal" for any practical resolution [5].

Experimental studies have shown that freely Graphene is indeed undulated [7]. The notable rise of Graphene has incited many scientists to search for alternative two dimension materials. The examination of this new two dimension materials has hardly begun, its potentials have not yet completely materialized, and the degree of its potential for new physics and devices remains largely unemployed. Silicene and Germanium are the most obvious alternatives group IV elements for Graphene [8, 9].

Germanene, Silicene and Graphene share a number of a typical and stimulating electronic properties. However, a few differences between Germanene and Silicene on the one hand and Graphene on the other hand. Firstly, the honeycomb lattice of Graphene is fully planar, while the honeycomb lattices of Germanene and Silicene are predicted to be buckled [10-12]. Secondly, Germanene and Silicene have a much stronger spin-orbit coupling due to the larger atomic number of germanium and silicon in comparison to carbon. A small buckling will increase the spin-orbit coupling by orders of magnitude [5]. The spin-orbit coupling results in the opening of a small band gap at the Dirac points in the interior of the material, topological protected gapless helical modes at the edges of the two dimensional material and a quantum spin Hall effect which is characterized by spin current transport via the edges modes [13, 14]. The spin-orbit gap in Graphene, Silicene and Germanene are < 0.05 meV, 1.55 meV and 23.9 meV, respectively [15-19]. This worth that the quantum spin Hall state is only experimentally easy to get for Silicene and Germanene [20, 21]. In this study we focuses on designing two dimensions GR-Ge-GR as sandwich sheets and study of the effect of the configuration of Ge sheet in between the two GR sheets to investigate the electrical properties of the new sandwich sheets.

## 2. Method

GGA/DZP density functional theory was used to calculating the electrical properties of the two dimension GR-Ge-GR sandwich sheets by employing the GOLLUM program " version 1.0 " [22] . The relax structures were carried out using SIESTA-trunk-462 program [23]. A vacuum space of 10 Å along the x direction in which the structures are not periodic to avoid the possible interactions between the periodically repeated unit cells. The Brillouin zone integration is sampled using Monkhorst-Pack grid of 1 × 1 × 1 k-points for structural relaxations, electronic properties, and charge transfer calculations. The density mesh cut-off is set to be 200 Hartree, and the structures are allowed to fully relax until the force on each atom becomes less than 0.04 eV/Å.

## 3. Results and Discussion

Fig. 1 illustrates the geometrical optimization of Graphene-Germanene-Graphene GR-Ge-GR as sandwich two dimension structures. GR-Ge-GR structure is one monolayer of Germanene sheet was inserted in between two monolayer of Graphene sheets. Initially, the location of Ge sheet between the two GR sheets was tested to reaches the geometrical optimization of the structure at the ground state energy. This process was repeated for ten suitable positions. Then the electrical properties were calculated for the ten structures of GR-Ge-GR sandwich.

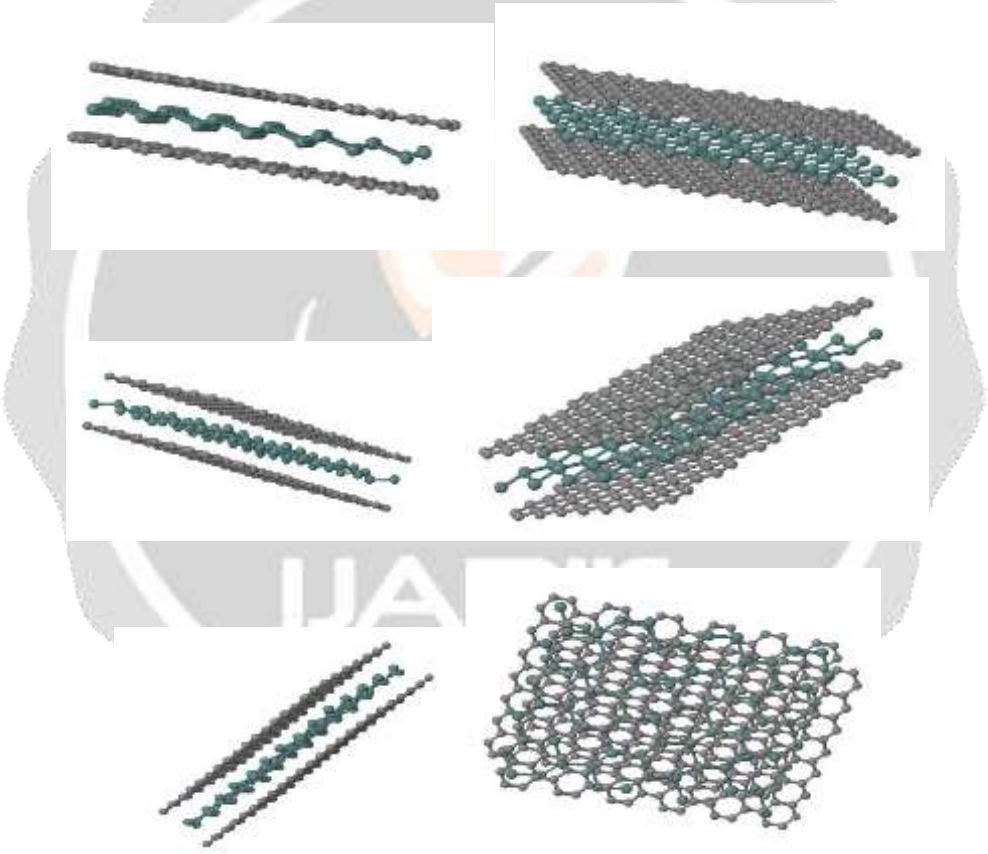

**Fig. 1: The relax structure of GR-Ge-GR sandwich**

### 3.1 Electric Conductance

Fig. 2 illustrates the electric conductance at room temperature for the structures GR-Ge-GR as a function of energy. At $E_F$=0, structures 10 and 1 have the highest conductance ( 0.0946 and 0.0754) S, respectively. The lowest value of conductance was measured for structure 2 ( 0.000281 S). The electric conductance for the structures 3,4 and 5 are (0.00133, 0.00781 and 0.000535) S, respectively. Structures 6 and 7 were appeared electric conductance of ( 0.041and 0.026) S, respectively, while the structures 8 and 9 are appeared electric conductance at $E_F$=0 equal to ( 0.0239 and 0.0311) S, respectively. In simple statement, the order of electric conductance for the studied structures at Fermi level is as:

10 > 1> 6 > 9 > 7 > 8 > 4 > 3 > 5 > 2

Above result can be discussed in terms of the location of Ge sheet between the two GR sheets in which the location play a significant role in an electron transmission, the result refers to different electronic applications can be found for the sandwich GR-Ge-GR structures depending on the location of the Ge monolayer sheet between the GR sheets.

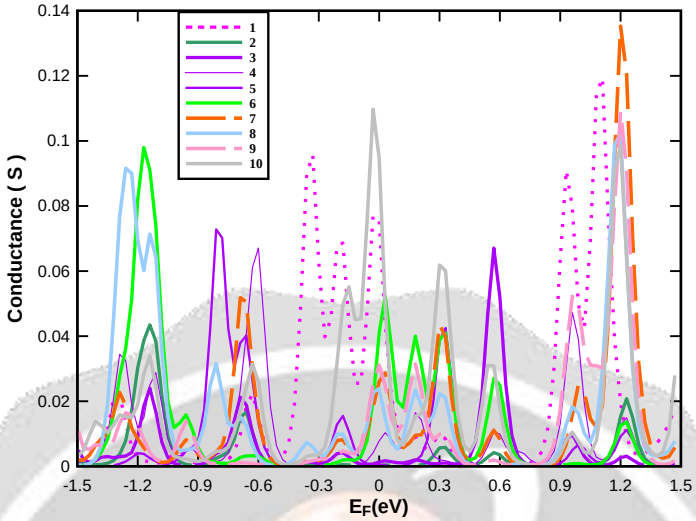


**Fig. 2: Electric conductance of GR-Ge-GR sandwich sheets**

### 3.2 Thermal Conductivity

Fig. 3 illustrates the calculated values of thermal conductivity of the ten structures of GR-Ge-GR sandwich sheets as a function of energy (-1.5 to 1.5) eV. In general, all the structures have low values of thermal conductivity, the lowest value is $4.429*10^{-14}$ W/m. K for structure 2 at $E_F$=0 and the highest is $5.795*10^{-12}$ W/m. K for structure 1. Structure 10 has also high thermal conductivity $5.753*10^{-12}$ W/m. K at $E_F$=0. Different values of thermal conductivity for the other structures were calculated at Fermi energy as follow: 3($3.344*10^{-13}$ W/m. K), 4($1.081*10^{-12}$ W/m. K), 5($5.468*10^{-13}$ W/m. K), 6($2.205*10^{-12}$ W/m. K), 7($5.123*10^{-12}$ W/m. K), 8($1.836*10^{-12}$ W/m. K) and 9($4.453*10^{-12}$ W/m. K). Above results indicate to an importance of the configuration of the sandwich sheets in calculating of thermal conductivity.

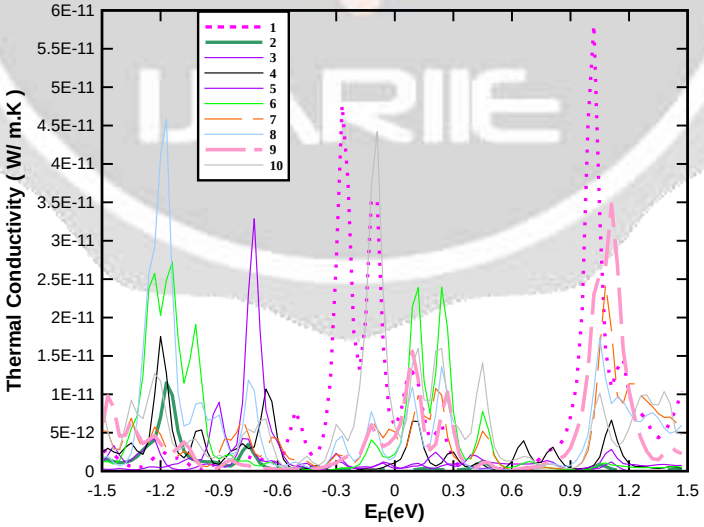


**Fig. 3: Thermal conductivity of GR-Ge-GR sandwich sheets**

### 3.3 I-V Curve

The effect of the configuration of the GR-Ge-GR sandwich sheet on the I-V characteristic was measured and drawn in Fig. 4. We showed the structures of GR-Ge-GR sandwich sheets were appeared different values of voltage for sensing depending on the configuration form for each one. Structures 1 and 10 were observed sensing at -0.45 V and 0.45 V reverse and bias voltages, while low sensing were observed for structures 2 and 3 at -1 V and 1 V reverse

and bias voltages. The structures 6-9 were appeared obvious sensing at -1.13 V and 1.13 V reverse and bias voltages. Generally, the variance in I-V curves for the studied structures refer to variety in the application of the sandwich sheets as electronic devices.

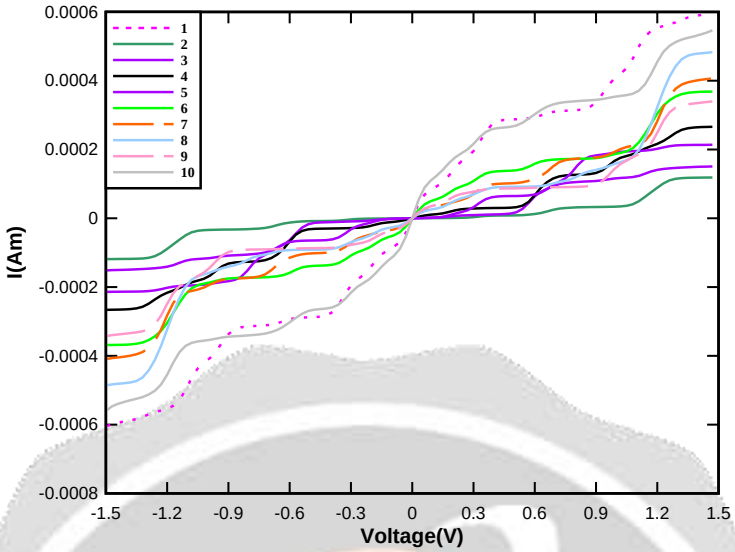


**Fig. 4: I-V characteristic of GR-Ge-GR sandwich sheets**

### 3.4 Seebeck coefficient

The behavior of the Seebeck coefficient for the GR-Ge-GR sheets at room temperature was shown in Fig. 5. The spectra of the Seebeck coefficient for all structures were observed different values along the energy range (-1.5 to 1.5 ) eV, but at Fermi level $E_F$=0 only the structures 1, 5, 8, 9 and 10 were appeared positive values of Seebeck coefficient. This result refers to that these structures appeared contribution of electrons concentration. The other structures are appearing contribution of holes concentration at Fermi energy.

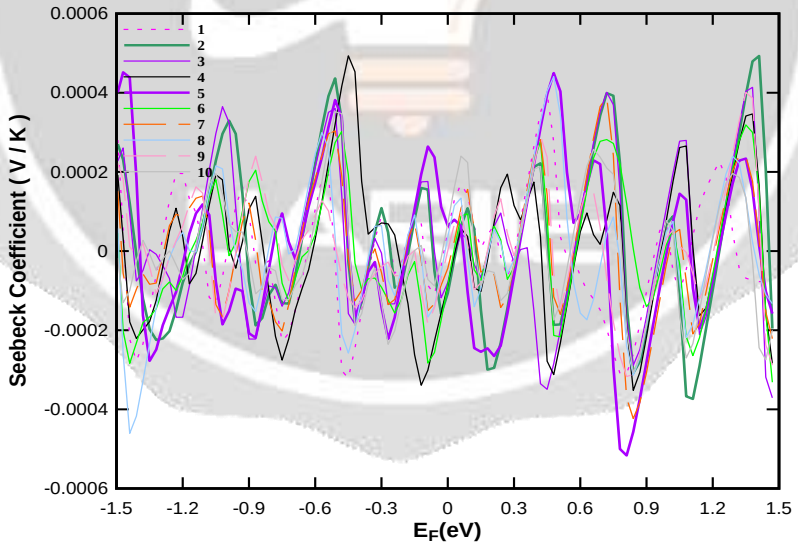


**Fig. 5: Seebeck coefficient of GR-Ge-GR sandwich sheets**

### 3.5 Figure of Merit

Fig. 6 illustrates the figure of merit for the GR-Ge-GR sandwich sheets. The results in mentioned Fig. are depending on the electric conductance, thermal conductivity and Seebeck coefficient for the structures, and therefore, the values of figure of merit at Fermi level are corresponding to previous calculations. The structures 1 and 10 were appeared the highest values of figure of merit at Fermi level in comparison with the others.

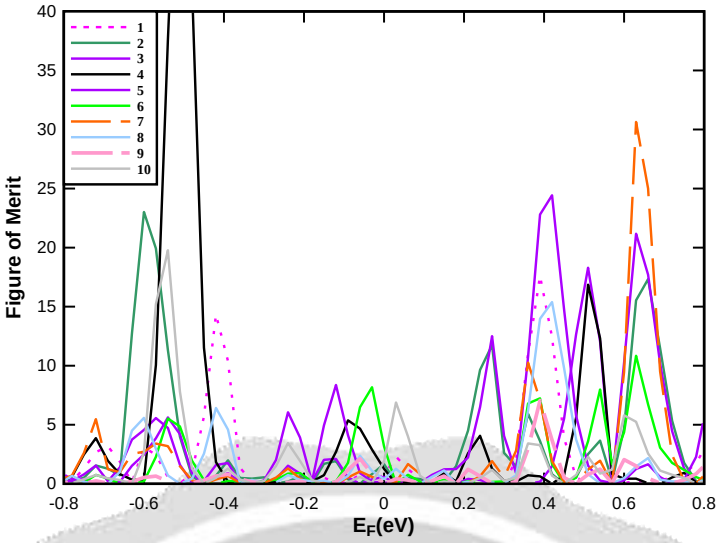


**Fig. 6: Figure of Merit for GR-Ge-GR sandwich sheets**

## Conclusions

From the results, one can conclude that the location of Ge sheet between the two GR sheets play significant role in an electron transmission. We showed the electric conductance at room temperature of the ten sandwich sheets is an indication to designing different configurations of two dimension sandwich materials gave different electronic applications, so the sandwich structures can take place in many electronic applications according to temperature variations. Moreover, the thermal conductivity at T=300 K indicates to an importance of the configuration of the sandwich sheets in calculating of thermal conductivity. On the other hand, some structures of GR-Ge-GR sheets appeared contribution of electron concentration and other structures are appearing contribution of hole concentration at Fermi energy. The results showed the I-V characteristics of the studied structures refer to variety in the application of the sandwich sheets as electronic devices.

## References

[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666 Geim A K and Novoselov K S 2007 Nat. Mater. 6 183

[2] Mermin N D 1968 Phys. Rev. 176 250

[3] Nelson D R and Peliti L 1987 J. Physique 48 1085

[4] Fasolino A, Los J H and Katsnelson M I 2007 Nat. Mater. 6 858

[5] Katsnelson M I and Fasolino A 2013 Acc. Chem. Res. 46 97

[6] Katsnelson M I 2012 Graphene: Carbon in Two Dimensions (Cambridge:Cambridge University Press) Chapter 9

[7] Mozorov S V, Novoselov K S, Katsnelson M I, Schedin F, Ponomarenko L A, Jiang D and Geim A K 2006 Phys. Rev. Lett. 97 016801

[8] Le Lay G, Salomon E, Angot T, Dᴗvila M E 2015 Micro- and Nanotechnology Sensors, Systems, and Applications VII (Proc. of SPIE vol 9467) ed T George et al p 94670U-1

[9] Le Lay G, Salomon E, De Padova P, Layet J-M and Angot T 2014 Aust. J. Chem. 67 1370–2

[10] Takeda K and Shiraishi K 1994 Phys. Rev. B 50 14916

[11] Guzmن-Verri G G and Lew Yan Voon L C 2007 Phys. Rev. B 76 075131

[12] Cahangirov S, Topsakal M, Aktürk E, Şahin H and Ciraci S 2009 Phys. Rev. Lett. 102 236804

[13] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 146802

[14] Kane C L and Mele E J 2005 Phys. Rev. Lett. 95 226801

[15] Boettger J C and Trickey S B 2007 Phys. Rev. B 75 121402

[16] Gmitra M, Konschur S, Ertler C, Ambrosch-Draxl C and Fabian J 2009 Phys. Rev. B 80 235431

[17] Abdelouahed S, Ernst A, Henk J, Maznichenko I V and Mertig I 2010 Phys. Rev. B 82 125424

[18] Liu C-C, Feng W and Yao Y 2011 Phys. Rev. Lett. 107 076802

[19] Ye X-S, Shao Z-G, Zhao H, Yang L and Wang C-L 2014 RSC Adv. 4 21216

[20] Han W, Kawakami R K, Gmitra M and Fabian J 2014 Nat. Nanotechnol. 9 794–807

[21] Konschuh S, Gmitra M and Fabian J 2010 Phys. Rev. B. 82 245412

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

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