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The *Ab-initio* Study of Bulk Single Layer Defected Graphene towards Graphene Device

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ABSTRACT

Graphene is a promising new material for the construction of graphene devices because of its surface modification can be tuned the band gap. In this paper, the electronic and transport characteristics of defected graphene device are investigated. Both the electronic and transport characteristics are simulated using density functional theory (DFT). The band structures and transmission spectra are analyzed. The conductance and thermal conductance characteristic for both graphene is compared. From the simulation, it is found that the conductance, thermal conductance, and the I-V curves depend on the transmission spectrum of the graphene sheet or graphene device itself. The comparison between the defected graphene itself shows that the single layer with two vacancies shows better performance.

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1. INTRODUCTION

Graphene has gained so much interest since it was discovered in 2004 [1]. The research pertaining to its physical and electronic properties has been tremendous. The presence of the conical shape at the Dirac point makes graphene very competitive in electronics application. Due to the fact that graphene is a 2-dimentional (2D) material that has high ballistics electronic transport [1], many efforts have been done to show the great potential of graphene as sensing and detection device. Despite the outstanding properties, one cannot exclude the potential defect present on the graphene surface [2].

This honeycomb structure, one-atom-thick material consist of sp2-bonded carbon [3]. The normal perfect honeycomb structure is called pristine graphene. Whilst the unperfected honeycomb structure is called the defected graphene. There are several types of defect related to graphene according to Banhart *et.al* [4]. The defects can be extrinsic or intrinsic, where it can exist during growth or process. To the date, the interest of graphene has been overwhelming explored from the physical aspects to the electrical characteristics and design.

The interest of research also lingers in the topic of the conductance and the thermal conductance apart from the band structure, density of state (DOS), transmission spectrum and I-V curves. Such as the interface between metal and c-axis to the use of Raman spectrometer in measuring the readings of the conductance and thermal conductance [5],[6]. Jia Yang and co-workers [7] also conducted a research in thermal conductance but at the contact (electrodes) of the GFET. Research on types of defect was also done by some researchers such research on point-defect by Manoharan [8], Stone-Wales and lattice vacancy defect

by Dipankar Saha [9] and defects and dopant by Rani [10] where still the density of states and the transmission spectrum are amongst the favourite interest besides the I-V curves.

The motivation to do this study is to give a principal knowledge on how the defect affects the band structure and density of states and to analyze what really effect the transmission of carriers on graphene channel. It was explained thoroughly in [4], besides the different bond lengths from perfect graphene structure, single layer with other vacancies may also affect the electronic properties of graphene. But yet additional works need to be done using experiments or simulation to it.

In this work, we present the impact of various types of defect on single layer graphene sheets to observe the electronic properties of the graphene sheet. Then the performance of the graphene is analyzed in the form of graphene device. Here the transport characteristics of the defect are studied. In this paper the transmission spectrum, the thermal conductance and the conductance of single layer and single vacancy in single layer graphene is reported. The readings are taken at the 0 Fermi level energy at 300K (room temperature). The conductance and thermal conductance coefficient are also measured and analysed. It is hoped that the new finding resulted from this study may become another turning point in the development of highly performance biosensor to cater the emerging need of an advanced biomedical diagnostics device for healthcare and environmental applications. The next section will discuss the computational method including the software and calculation as well as the model of the simulated project.

2. RESEARCH METHOD

The research method is divided into two (2) main part. The first part is the software and calculation and the second part is the modelling.

2.1. Software and Calculation

The simulations are done using Atomistix Tool Kit (ATK) software from Quantum Wise. The software is chosen because it supports simulation in bulk and device system (bulk-nanodevice systems) such as transistors [11]. All calculations in the simulation are performed using the Density Functional Theory (DFT) methods [12], where the electronics and transport characteristics of various types of defect on graphene are simulated. The electronics properties of graphene sheets such as band structures and transmission spectra are calculated using the Recursion calculator. Similar methods are used to analyze the IV curves, the conductance and the thermal conductance. To solve the Poisson equation in the "electrode" calculations the multigrid techniques are used**.** All observed results are analyzed at the vicinity 0eV (Fermi level) at 300K temperature settings.

2.2. Model

The models are divided into two (2) section; 1) the bulk graphene sheet and 2) the graphene device as shown in Figure 1 and Figure 2. Identical configuration of different types of graphene with the same length and width are designed for the simulation purposes. The types of graphene are the single layer pristine (SLP), the single layer with a single vacancy (1 SV), the single layer with two vacancies (2 SV) and the single layer with Stone-Wales defect (SLSW).

Figure 1 shows the bulk graphene sheet with different types of the defect with the length of the graphene sheet is 13.55 Å and the width is 7.91 Å. The number of carbon atoms varies from 46 atoms to 48 carbon atoms depend on the type of defect. Figure2 shows the closed loop graphene device system. The red box indicates the source and drain whilst the green box indicates the gate. The length of the graphene is 13.55 Å and the width is 7.91 Å. The length of the source and drain is set to 4.92 Å. The dimension of the metal gate is set to 10.5 Å x 8.5 Å.

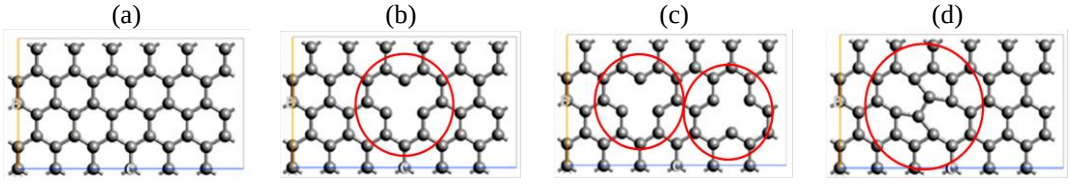

Figure 1. The identical configuration of different types of graphene where (a) SLP with 48 carbon atoms (b) 1 SV with 47 carbon atoms (c) 2 SV with 46 carbon atoms and (d) SLSW with 48 carbon atoms

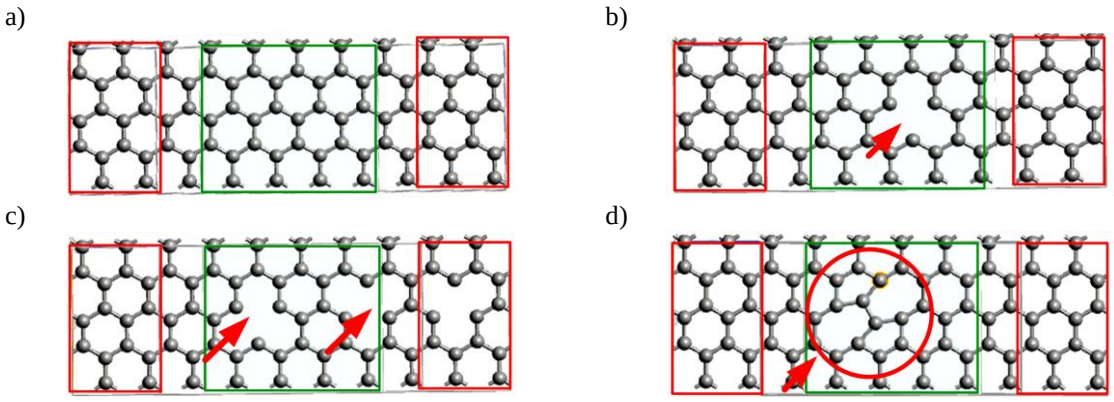

Figure 2. The identical configuration of single channel closed loop system where (a) SLP and (b) 1 SV (c) 2 SV and (d) SLSW defect. The arrow(s) in the figure shows the position of the missing atoms. Red box indicates the right and left electrode (source and drain) and the green box indicates the gates

3. RESULTS AND ANALYSIS

3.1. The electronic properties of graphene sheets

This section will discuss about the electronic properties of graphene sheets including the bandstructure, the DOS, the transmission spectrum together with the thermal conductance and the conductance. First, the analyses the band structures and the DOS of the SLP, 1 SV, 2 SV and SLSW are calculated at zero bias voltage. As for the band structures were simulated at point Γ (the center of Brillouin zone). The simulation comprises the axes of x, y, and z of the graphene sheet. Where the x represents the layer of the graphene sheet, the y represents the width of the graphene sheet and the z represents the length of the graphene sheet.

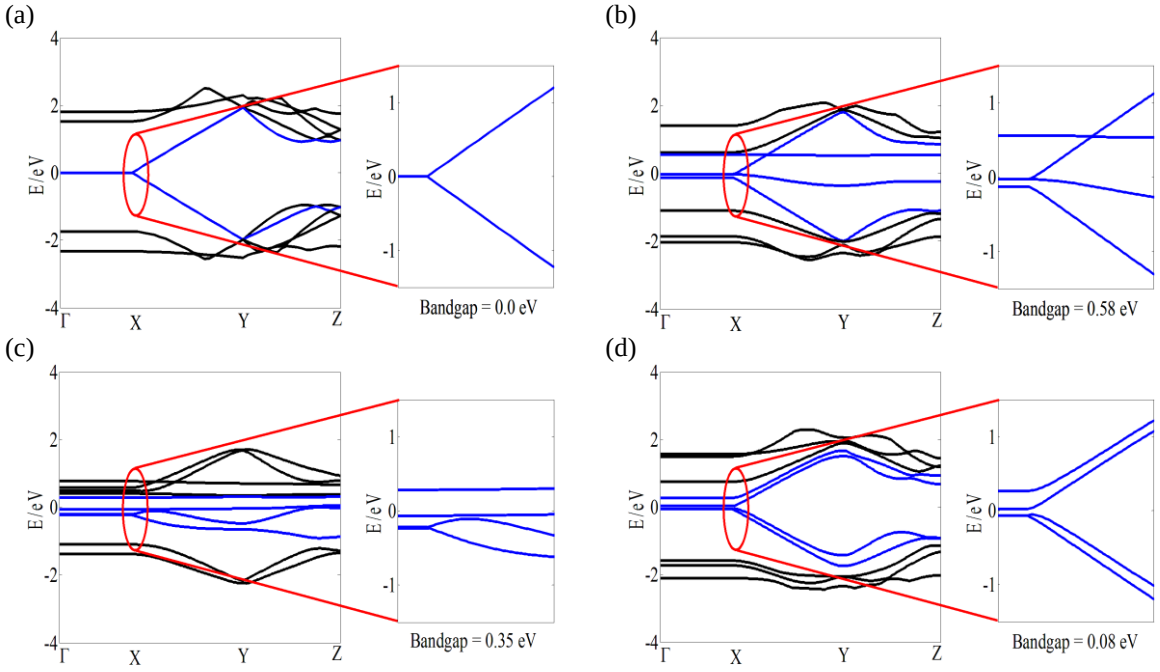

Figure 3. The band structures of the (a) SLP, (b) 1 SV, (c) 2 SV and (d) SLSW

Note that: The magnification (insets) are taken from the X point of the band structure. These insets show the conduction band and the valence band which the value of the bandgap is calculated respectively.

The band structure of the graphene sheets is shown in Figure 3 (a) – (d) which the bandgap is calculated at point X. Here it is clearly shown the changes in band structure in each types of graphene. The energy level for conductance band and valence band shifted (up and down from the 0 eV) respectively towards types of defect. The bandgap is 0.00 eV, 0.58eV, 0.35 eV and 0.08 eV for SLP, 1 SV, 2 SV and SLSW, respectively. The closing of bandgap near the Dirac point for SLP is confirming what has been report by Banhart *et.al* [4] and Allen and Warner [13], when there is no changing (doped, removed, added etc.) in the intrinsic carbon lattice. Continuing with the SLSW, the small bandgap in SLSW is due to the defect violate in the lattice symmetry bond at the graphene sheet [14]. As there is no missing or adding carbon atoms, but only the rotation of C-C bond at 90°.

When there is a missing atom in the carbon sheet as in 1 SV and 2 SV, the bandgap will widen open. This phenomenon is due to the free dangling bonds of the carbon atoms. Another criterion can be observed are the direct and indirect relation of the band structures. The SLP and the SLSW has a direct bandgap whilst the 1 SV and the 2 SV has the indirect bandgap. These results apparently proven to what had been reported by Balandin [5] that the graphene band gap can be tuned by defect.

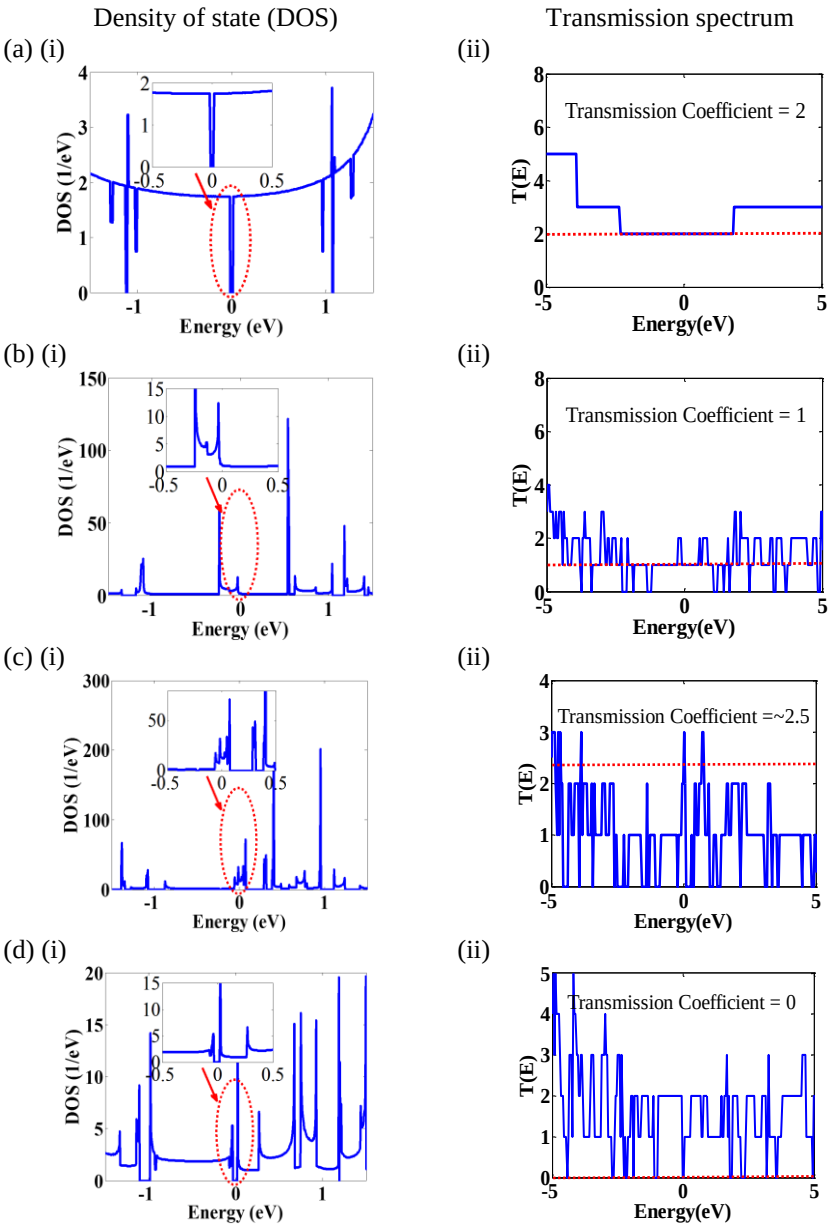

Figure 4. The density of state (DOS) (a)(i) – (d) (i) and the transmission spectrum (a) (ii) – (d) (ii) of the (a)(i) SLP, 1 SV, 2 SV and SLSW

Another feature for the electronic properties of bulks graphene is the DOS. The DOS of each graphene bulks are plotted and displayed in Figure 4 (a) (i) - (d) (i) respectively. The DOS of the SLP and the SLSW are clearly shown on the 0 eV^{-1} at vicinity 0 energy level. This situation connected to the band gap in the band structure explained earlier. The occupied valence and empty conduction bands meet at Dirac point means zero value at the DOS. With vanishing DOS at the Dirac point but no energy gap between the valence and conduction bands [13]. One interesting element for SLP, the DOS shows almost a symmetry form of DOS in the right and left x-axis of the diagram (Figure 4 (a) (i)). At the energy range around 1eV to 1.5eV, there are peaks arose at DOS value 3.2eV^{-1} and 3.5eV^{-1}.

The wide bandgap features in band structure affected the DOS in 1 SV and 2 SV. On this spot, the emergence of the gap state near the Fermi-energy level can be seen in Figure 4 (b) (i) - (c) (i). Unlike to the SLP or the SLSW, the DOS in the 1 SV and 2 SV shows, there are unpaired electrons in vicinity of vacancies thus resulting into spin polarized structure [10]. So, it is important of knowing the DOS to know the value of energy gap exist in material.

The analysis is then continued with the transmission spectrum. The transmission coefficient is 2, 1, 2.5 and 0 for SLP, 1 SV, 2 SV and SLSW respectively (Figure 4 (a) (ii) – (d) (ii)). The lower transmission coefficients may be responsible for the higher resistivity [15]. Since the electron scattering is not in the line form.

The last stage of the simulation is then continued with conductance and thermal conductance (Figure 5). Graphene exhibits unique electrical conductivity and thermal conductivity due to the large mobility carriers. As we can see the trend of the waveform for each pristine and defected graphene sheets are almost similar for the conductance and the thermal conductance. Figure 5 (a) shows the conductance coefficient for the 2 SV (G_g = 1.717e^{-4} S) shows 5.14% higher value compared to the SLP (G_g = 1.549e^{-4} S). The conductance coefficient for SLSW shows the least value at G_g = 3.84e^{-5} S and for the 1 SV, the conductance coefficient is G_g = 7.813e^{-5} S. The result shows that the electrons scattered do give impact with a long-range potential of conductance when the disorder is sufficiently large. And the result is assumed for the SLSW as there is no dangling atom in the sheet. All analysis is done at 0 Fermi level at 300K is measured at room temperature. The conductance coefficient shows that the 2 SV offers more carriers pass through the graphene materials compared to the SLP.

The last observation for graphene sheets are done for thermal conductance coefficient for all types of graphene. Proportionate to the conductance coefficient, the thermal conductance for the graphene sheets show different result. Figure 5 (b) shows clearly the thermal conductance for the SLP is much higher than the other three (3) types of defected graphene. The value of thermal conductance coefficient for the SLP is K_g = 1.136e^{-9} (W/K), for the 1 SV is K_g = 6.18e^{-10} (W/K), for the 2 SV is K_g = 7.709e^{-9} (W/K), and for the SLSW is K_g = 6.74e^{-10} (W/K). Which the 1 SV shows lowest thermal coefficient followed by the SLSW and the 2 SV. This is an agreement with the condition that the position and the magnitude of the thermal conductivity maximum will depend on the competition between the various scattering process (boundary, defect, phonon) [16]. For instance, the description of the thermal conductance is the measure of the heat passes in unit time through a plate of particular area and thickness when its opposite faces differ in temperature by one Kelvin.

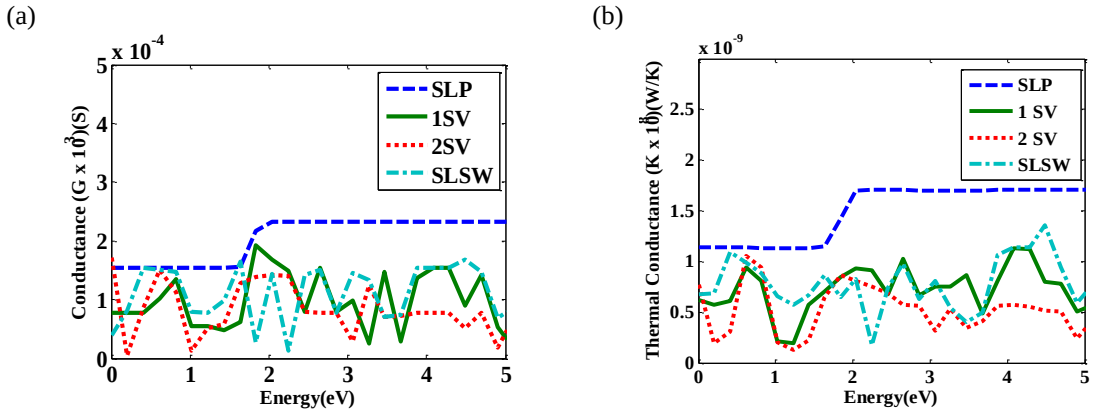

Figure 5. The transport characteristics (a) the conductance and (b) the thermal conductance

Note that**:** (G × 10e^{3})(S) is the conductance for graphene sheet with unit Siemens and (K × 10e^{8}) (W/K) is the total thermal conductance of graphene (total thermal conductance of phonons and thermal conductance of electrons) with unit Watt/Kelvin

3.2. Graphene device performance

This section will discuss about the graphene performance in device form. To compare the graphene device performance, the voltage bias is set at 2 V. The contact for the right electrodes and the left electrodes is assumed to be ideal contact. All the analysis are done at 0 Fermi level at 300 K temperature setting.

The transmission spectrum for graphene device is shown in Figure 6 (left). From the value of the transmission coefficient related to the type of defect on the graphene device, it shows that the 1 SV device is much more higher compared to other types of graphene device. Where the transmission spectrum coefficient itself reflect to the current-voltage curve at Figure 6 (right). The graphene device works well at the pristine graphene and the 1 SV at device level where we can see the saturated value of the I-V curves at the 1.8 V at 4.11 x 10^{4} nA and 4.09 x 10^{4} nA current value respectively. However the performance of graphene devices are deteriorated depending on the defect type on the graphene channel.

For the 2 SV, we can see the voltage is increased with the current value. But at the current value 1.46 x 10^{4} nA (at voltage value near 1.15 V), the performance of the graphene device started to decline. The same situation also happened to the SLSW graphene device. The performance of the graphene device starts to deteriorate shortly after 2.02 x 10^{4} nA even though we can see a smooth increment of voltage and current value before the breakdown of the graphene performance at 1.8 V. This results are predicted due to the transmission spectrum coefficient of the defected graphene devices that the value of transmission coefficient is approaching to zero (Figure 6 (left)). This results also an agreement to Manoharan [8] that even though defect induced the band gap, the carriers transport across the channel is not affected to it.

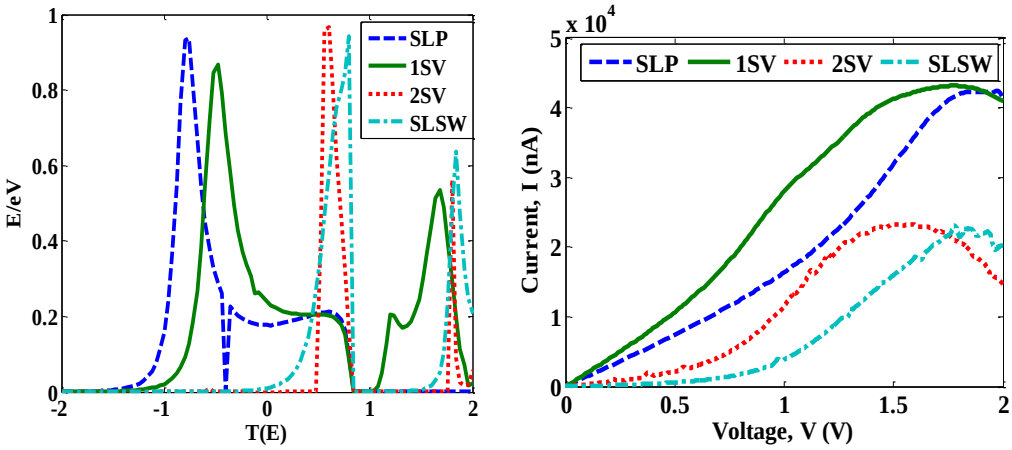

Figure 6. The transmission spectrum (left) and the current-voltage (right) characteristics of the SLP, the 1 SV, the 2 SV and the SLSW

The overall conclusion for simulation done for three (3) types of graphene defect and the pristine graphene sheet is tabulated in Table 1. From the table, it shows that the defect on graphene sheets do give impact to the band structure by shifted down to negative value. Then the transmission coefficient for pristine graphene sheet is slightly lower to the 2 SV**.** This effect the performance of the graphene sheet as a conductance and thermal conductance. The numbers of defect also influenced the potential energy of the graphene.

Table 1. The characteristics of single layer pristine, single layer with single vacancy, single layer with two vacancies and single layer with Stone-Wales defect simulated using Quantum Wise at ΔEF = 0 eV at T = 300K

	Band gap (eV)	Chemical Potential (eV)	Total Energy (eV)	Transmission Coefficient	Conductance Coefficient, G_g (S)	Thermal Conductance Coefficient, K_g (W/K)
SLP	0	-5.3786	-7588.118	2	1.549e^{-04}	1.136e^{-09}
1 SV	0.58	-5.2437	-7419.985	1	7.813e^{-05}	6.18e^{-10}
2 SV	0.35	-5.0440	-7251.884	2.5	1.717 e^{-04}	7.709e^{-10}
SLSW	0.08	-5.3325	-7590.471	0	3.84e^{-05}	6.74e^{-10}

SLP – Single Layer Pristine
1 SV – Single Layer with Single Vacancy
2 SV- Single Layer with Two vacancies
SLSW – Single Layer with Stone-Wales Defect

4. CONCLUSION

In this paper, we have considered an *ab-initio* study on single layer graphene in bulk and device form using Density Functional Theory (DFT) methods. Interestingly, we can see how the defect can manipulate the band structure and the density of states in the graphene sheets. Surprisingly even though the defect induced the band gaps in the density of states, the performance of the graphene especially in graphene device is not affected at all. What really matter is the transmission spectrum that shows how the carriers in graphene works. The transmission spectrum also give the reflection to the I-V curves in the graphene device. And yet it is still the pristine graphene device shows better performance compared to the defected graphene device. This problem occurs may be due to the short channel effect because of the lateral dimensions of the graphene channel is so small. To be fair, the comparison between the performances of defected graphene is also done, which it shows that the single layer with two vacancies it the best defects to be used as a graphene device.

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REFERENCES

[1] K. S. Novoselov, *et al.*, "Electric field effect in atomically thin carbon films," *Science*, vol/issue: 306(5696), pp. 666–669, 2004.
[2] L. D. Carr and M. T. Lusk, "Graphene gets designer defects," *Nat. Publ. Gr.*, vol/issue: 5(5), pp. 316–317, 2010.
[3] C. G. Lee, *et al.*, "Integration of reduced graphene oxide into organic field-effect transistors as conducting electrodes and as a metal modification layer," *Appl. Phys. Lett.*, vol/issue: 95(2), pp. 23304, 2009.
[4] F. Banhart, *et al.*, "Structural defects in graphene," *ACS Nano*, vol/issue: 5(1), pp. 26–41, 2011.
[5] A. A. Balandin, *et al.*, "Superior Thermal Conductivity of Single-Layer Graphene 2008," *Nano Lett.*, vol. 8, pp. 902–907, 2008.
[6] A. J. Schmidt, *et al.*, "Thermal conductance and phonon transmissivity of metal–graphite interfaces," *J. Appl. Phys.*, vol/issue: 107(10), pp. 104907, 2010.
[7] J. Yang, *et al.*, "Thermal conductance imaging of graphene contacts," *J. Appl. Phys.*, vol/issue: 116(2), pp. 23515, 2014.
[8] M. Manoharan and H. Mizuta, "Point defect-induced transport bandgap widening in the downscaled armchair graphene nanoribbon device," *Carbon N. Y.*, vol. 64, pp. 416–423, 2013.
[9] D. Saha, *et al.*, "Impact of Stone-Wales and lattice vacancy defects on the electro-thermal transport of the free standing structure of metallic ZGNR," *J. Comput. Electron.*, vol/issue: 13(4), pp. 862–871, 2014.
[10] P. Rani and R. Bhandari, "DFT Study of Defects in Graphene," no. i, pp. 237–239, 2013.
[11] *Atomistix ToolKit Manual (Version 13.8)*. .
[12] J. W. Jiang, *et al.*, "Minimum thermal conductance in graphene and boron nitride superlattice," *Appl. Phys. Lett.*, vol/issue: 99(4), pp. 43109, 2011.
[13] C. S. Allen and J. H. Warner, *Graphene*, no. 2009, 2013.
[14] L. A. Openov and A. I. Podlivaev, "Interaction of the Stone-Wales defects in graphene," *Phys. Solid State*, vol/issue: 57(7), pp. 1477–1481, 2015.
[15] J. Zhang, *et al.*, "Electronic and transport gaps of graphene opened by grain boundaries," *J. Appl. Phys.*, vol/issue: 112(5), 2012.
[16] J. P. Issi, *et al.*, "Electron and Phonon Transport in Graphene In and Out of The Bulk: in Physics of Graphene," Switzerland, Springer, 2014.

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