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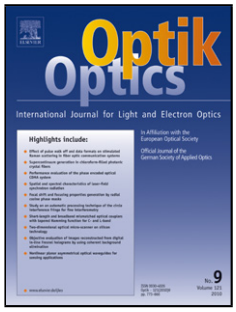

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Thermal and Electrical properties of Siligraphene and its derivatives

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Abstract

The electrical and optical properties of siligraphene have been investigated in this paper using semi-classical Boltzmann equation and the WIEN2K code based on density functional theory. We studied two configurations of siligraphene (g-SiC3 and g-SiC7 with different concentration of Silicon); our results show that these two configurations are semiconductor materials with a direct band gap. We find that the electrical properties of siligraphene changes as a function of silicon concentration. We also compared optical properties of two structures of siligraphene and we found that the electrical properties increases as a function of silicon concentration and decreases as function of temperature.

Keywords: semiconductors; ab initio calculations; siligraphene; electrical properties.

1. Introduction

The monolayer of graphene is one plan of graphite. Before 2004, the vision in science is synthesized experimentally a new material have structure with two dimensional and deduced their physical properties. This objective has been realized in the Centre for Mesoscopic and Nanotechnology of Manchester University, UK by A. Geim et al. [1-3]. This group used the micro-mechanical cleavage of graphite to produce graphene. Graphene has better physical properties compared to graphite due to its hexagonal structure which is bi-dimensional. Unlike graphite (3 dimensional), a carbon atom in

graphene is surrounded by three other atoms of carbon in planar sheet make just tree connection. The bond length between two carbon atoms (sp^2 bonded carbon atoms) has measured by Geim et al. using the transmission electron microscope (TEM) its equal 0.14nm.HC. Schniepp et al. and C. Berger et al. these two groups produced experimentally the isolate graphene [4-6]. The Recent research confirmed that graphene has high electron mobility [7-10]. The mechanical, electronic, optical and magnetic properties of graphene have been studied in these refs [11-16]. 2D materials emerge as potential systems for different applications such as nanoelectronics, [17-20] solar energy [21-22] and energy storage [23-25]. These 2D materials have both high mobility and a gap intrinsic charge carriers which makes them more efficient than silicon which is the basis of the current electronics industry. To date graphene (2D equivalent of graphite) are two-dimensional materials experiencing the greatest interest. While graphene suffers from a zero energy gap, our idea is to look for graphene-like materials may possess both properties (mobility and gap). In this work we propose a new 2D material emerge that can replace silicon in several industrial applications.

Pablo A. Denis to demonstrate that the band gap of graphene (monolayer or bilayer) can be opened with silicon, aluminium, phosphorus and sulfur dopping, also Pablo studied the mono and dual Doped Monolayer Graphene [26-27], the formation of band gap in graphene with silicon doped has been analyzed by MCS Escaño et al. MSS Azadeh et al. [28-29] also used doping technics by density functional calculation . Houmad et al. has been demonstration that it’s possible the opining the band gap of graphene with silicon doped, they finding that the optical conductivity increased as function silicon concentration [30-31]. Likewise, other methods to open the band gap of graphene are proposed like functionalization of graphene with hydrogen or molecule adsorptions [32-35]. The optical properties of graphene can also be improved when it is functionalized with organic molecules [36].

Recently until the siligraphene has a one derivatives of graphene, it’s the graphene doped or contained the silicon g-SiC7 or g-SiC3. The new 2D Silicon-Carbon has been fabricated experimental with single layer and bilayer by Lin [37]. The aim of this paper is to predict the optical properties and the electrical property of siligraphene, we used

density functional theory and semi-classical Boltzmann equation implanted in WIEN2K code, we show that siligraphene is a semiconductor with a small band gap and the electrical conductivity increased as function silicon concentration (g-SiC7; g-SiC3).

We show that siligraphene is a very promising 2D material with great impact that can lead to exceptional results in the field of solar energy and other application. Consequently, we push the experimental researches to discover this new 2D material (siligraphene) for using in solar cell application.

2. Computational details

Our calculations are based on Density functional theory (DFT) implanted in wien2k code [38] using generalized gradient approximation (GGA) [39], parameterized by PBE Perdew Burke Ernzerhof [40]. In this study the plane waves were determined using FP-LAPW [41] method, the space is divided into regions a spherical "muffin-tin" around the nucleus in which radial solutions of Schrödinger Equation and their energy derivatives are used as the basic functions, and an interstitial region between the muffin tins (MT). To study the electrical propriety of Siligraphene we used Boltzmann theory implanted in Boltztrap package [42] it's calculated as function of Temperature based on following equation:

$$\boldsymbol{\sigma_{\alpha\beta}(T;\mu) = \frac{1}{\Omega}\int \sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_{\mu}(T;\ \mu)}{\partial \varepsilon}\right]\partial\varepsilon}$$

The electrical conductivity$\boldsymbol{\sigma_{\alpha\beta}}$ is obtained with $\boldsymbol{\sigma_{\alpha\beta}(\varepsilon) = \frac{1}{N}\sum_{i,k}\sigma_{\alpha\beta}(i,K)\frac{\delta(\varepsilon-\varepsilon_{i,K})}{d\varepsilon}}$

α and β are the tensor indice $E_{i,j}$ is band structure and Ω is the number of k points that are sampled in the Brillouin zone . $\vartheta(k)$ is the band velocity, $\tau(k)$ is the relaxation time and f is Fermi function.

3. Results and discussions

3.1. Electronic properties

The effect of bonding structure and stoichiometry of the Silicon carbide monolayers as function of silicon and carbon concentration atoms on electronic properties of Silicon carbide has been reported by Z. Shi et al. [43].The super-cell of two

configurations of siligraphene SiC_7 and SiC3 are shown in Figures 1a and 1b. We are beginning our calculations by the relaxation of the structure of two type of Siligraphene, we show that the band length C-C and Si-C in SiC_7 is equal to 1.53A° and 1.7939A° respectively, and the value the band length C-C and Si-C for the second type of siligraphene (SiC_3) is equal to 1.7843A° and 1.4177A° respectively. The vacuum space in Z axis is also relaxed is equal 20A° this value avoid the interactions between two plans adjacent siligraphene.

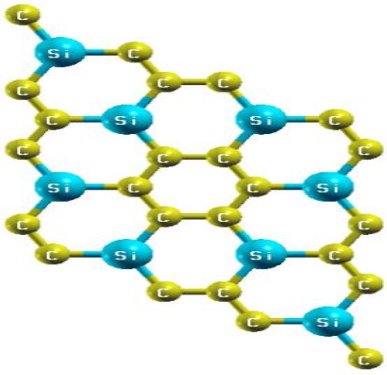


Figure 1a: The crystal structures of siligraphene SiC_3.

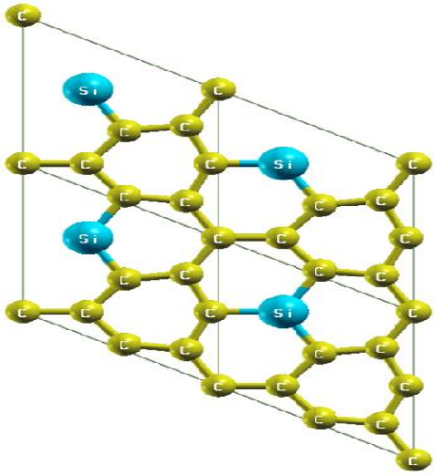


Figure 1a: The crystal structures of siligraphene SiC_7.

The band structure and density of states of two types of siligraphene SiC_3 and SiC_7 are presented in figure 2 and 3, our results show that these two configurations are semiconductor materials with direct band gap. The valence shell of Si atom is $3s^2 3p^2$ and the valence shell of C atom is $2s^2 2p^2$. We calculated the band gap energy of siligraphene SiC_3 and SiC_7, we obtained that the band gap energy of SiC_3 and SiC_7 are 0.0eV and

0.79eV respectively these values is in good argument with [44-45]. We established that the band gap is related to the concentration of silicon in hexagonal structure of graphene. We observed also the band gap of SiC_3 and SiC_7 is direct following K wave vector.

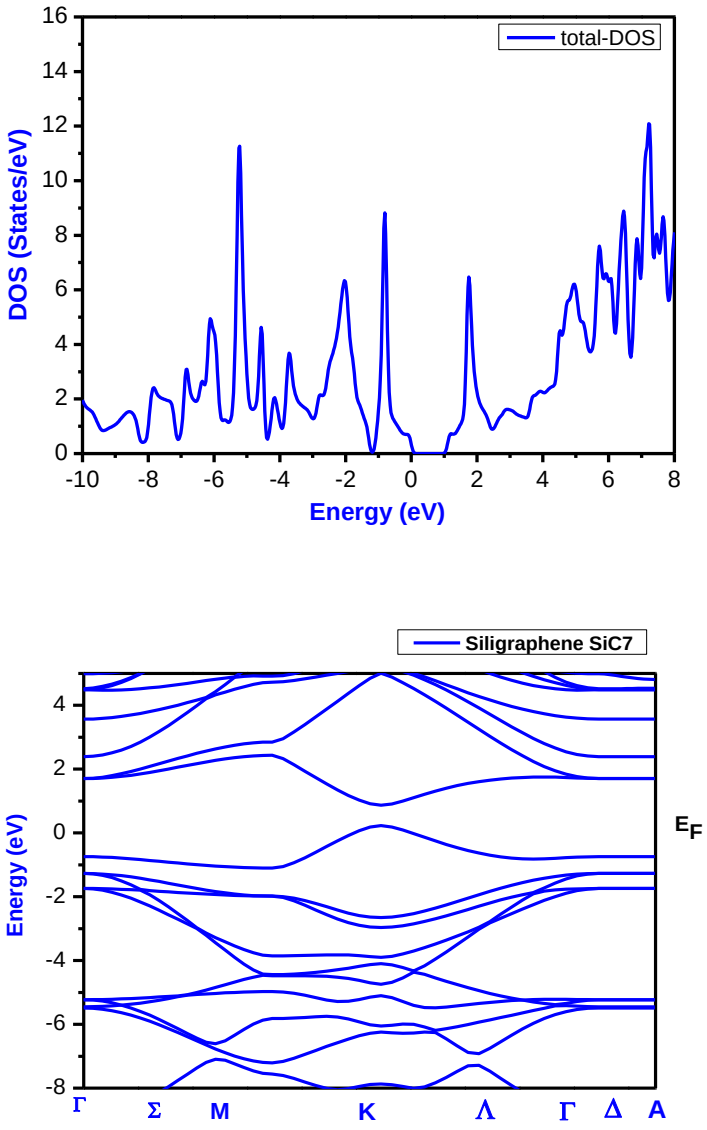
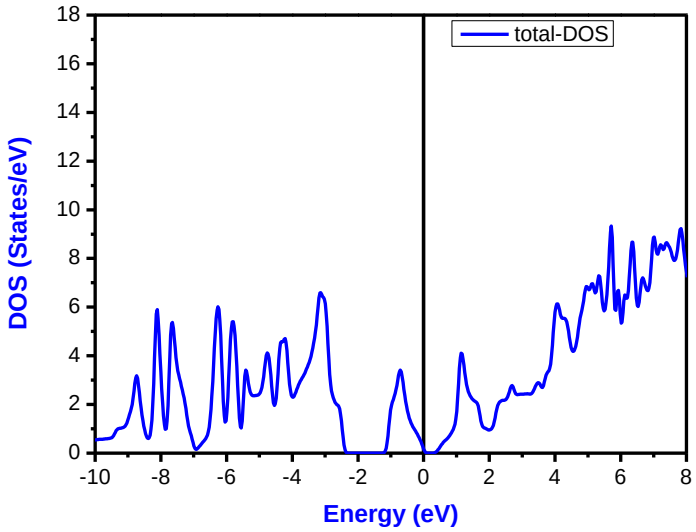


Figure 2: Band Structure and Density of states of Siligraphene SiC_7.



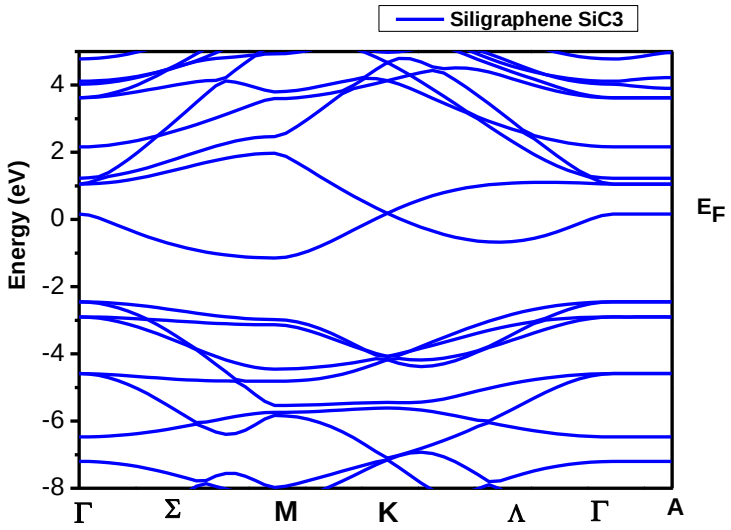


Figure 3: Band Structure and Density of states of Siligraphene SiC_3.

3.2. Optical properties

The character semi-metals of graphene has been limited to the directly application of graphene in solar cell application, this difficulty pause the scientists to resolute this problem's many idea has been established for example the functionalization of graphene with molecular or doping with atoms such as Silicon or germanium [46], the optical properties of graphene has been studied by Nair et al. [47], in particular the optical conductivity of graphene has been measured by Stauber et al. [48], The two groups established that graphene has a higher optical conductivity. The absorption coefficient is obtained with the following relation.

$$\alpha(\omega)=\frac{\sqrt{2}}{c}\omega\sqrt{-\varepsilon_1(\omega)+\sqrt{\varepsilon_1(\omega)^2+\varepsilon_2(\omega)^2}} \quad (4)$$

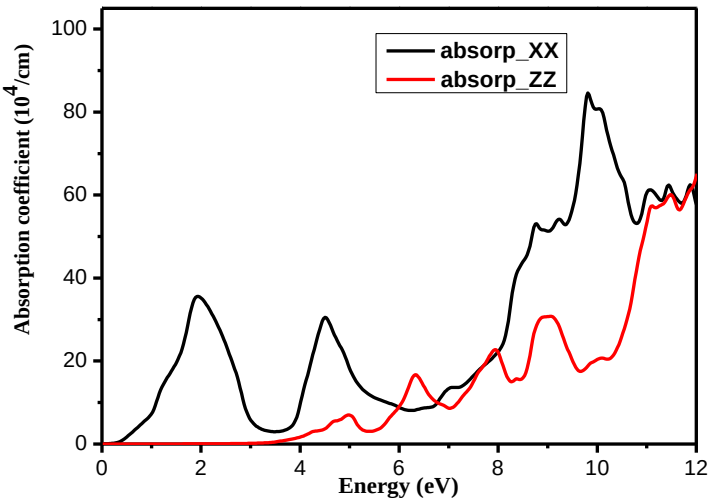


Figure 4: the absorption coefficient of Siligraphene (SiC_7) as function of photon energy in both direction xx and zz

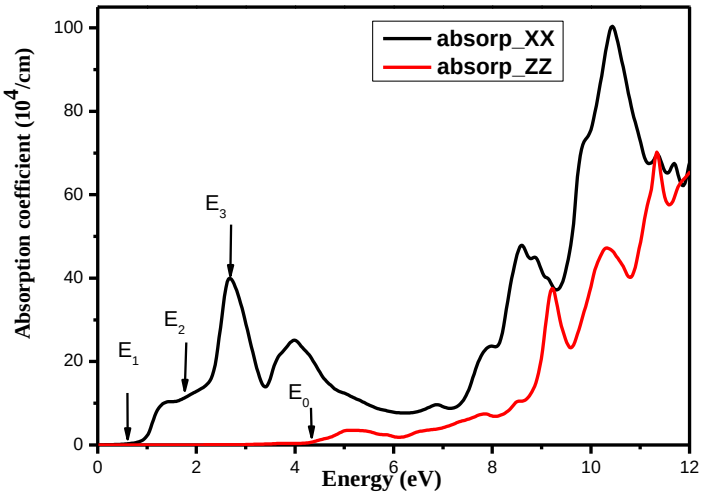


Figure 5: the absorption coefficient of Siligraphene (SiC_3) as function of photon energy in both direction xx and zz

The absorption coefficient of two siligraphene is shown Figure 4 and 5, we observe that the absorption coefficient for xx direction is different to zz direction this difference is due to anisotropy of siligraphene, we observe also that the absorption coefficient started firstly for SiC7 compared with SiC3 for two direction xx and zz because the band gap of SiC7 is lower than the band gap SiC3 therefore the first transition is in siligraphene SiC7 following K wave vector. The absorption coefficient of SiC7 started at energy equal 0.39eV for xx direction and 3.55eV for zz direction, but for siligraphene SiC3 is started at 0.511eV for xx direction and 4.34eV for zz direction.

3.2.1. Reflectivity spectrum R(ω)

The reflectivity of material plays an important role in a solar cell material application, the measurement of reflectivity of graphene has given 2.3%. Other experiment results obtained that reflectance of silicon surface decreased when the deposition of graphene on textured silicon surfaces, also it's possible the decreasing the reflectivity used the doping of graphene with boron and Nitrogen [49-50]. The reflectivity R(ω) is calculated with the Fresnel's formula:

$$R(\omega) = \left|\frac{\sqrt{\varepsilon(\omega)}-1}{\sqrt{\varepsilon(\omega)}+1}\right|^2 \quad (5)$$

In figure 6, we plot the reflectivity of siligraphene for two direction xx and zz we observe that reflectivity of siligraphene type SiC_7 is lower than SiC_3 we analyzed this result ofthe different concentration of silicon in two types.

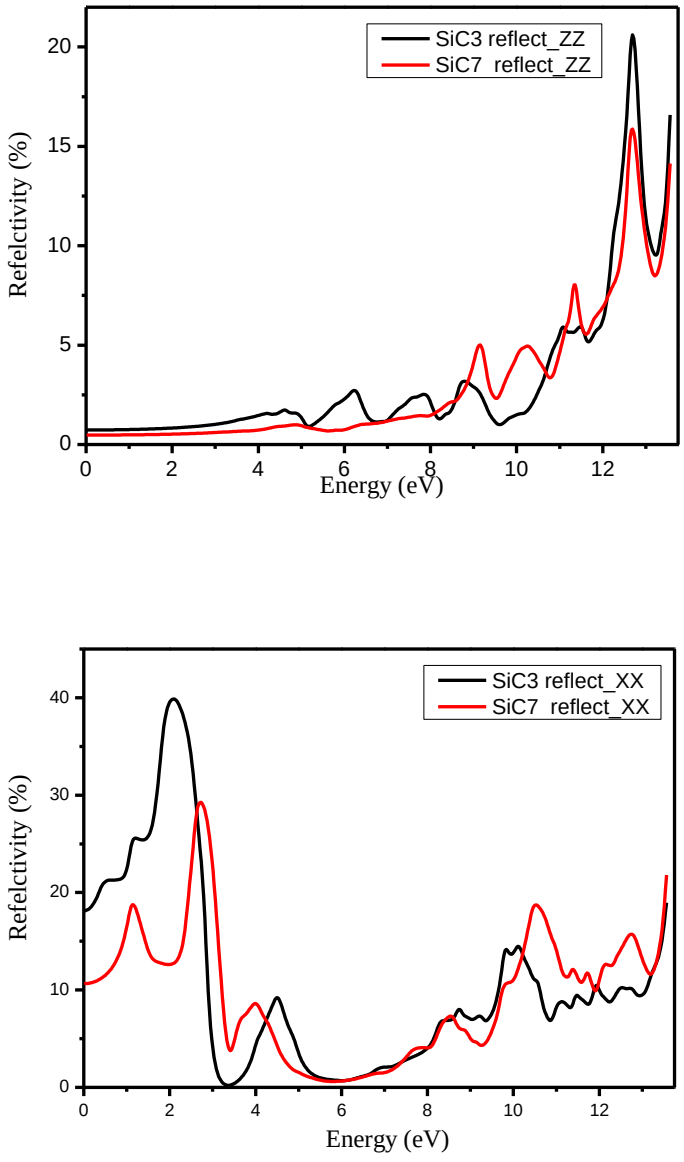
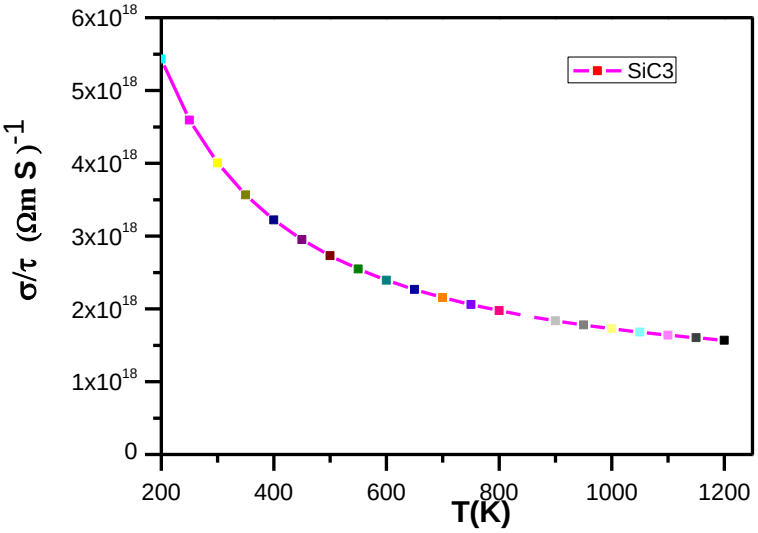


Figure 6: The reflectivity of siligraphene SiC7 and SiC3 as function of photon energy in both direction xx and zz

3.1.1. Electrical conductivity

The developments of solar cell material application are limited to yield of physical properties of absorbed material used in the cell l. The transport properties of graphene monolayer and bilayer are studied [51]; also the improving of the electrical conductivity of graphene with chemical doping (Potassium nitrate) is studied by khan et al.[52]. The platinum (Pt) metal adsorbates affect the properties of graphene and increasing their electrical conductivity [53]. At this time; we studied the electrical conductivity of siligraphene ($\boldsymbol{\sigma/\tau}$ is conductivity divided by time relaxations) based on the Boltzmann equation implanted in bolztrap package. We observe the difference between the electrical conductivity of siligraphene g-SiC3 and g-SiC7, the figure 6, shown that the electrical conductivity of g-SiC3 is better than the electrical conductivity g-SiC7 this difference is due to the difference of silicon concentration in siligraphene structure. We find also that the electrical conductivity of siligraphene decreases as function the temperature for g-SiC_3 and increasing for SiC_7 these results confirmed that g-SiC_7 is a semiconductor materials but g-SiC_3 is a conductors.



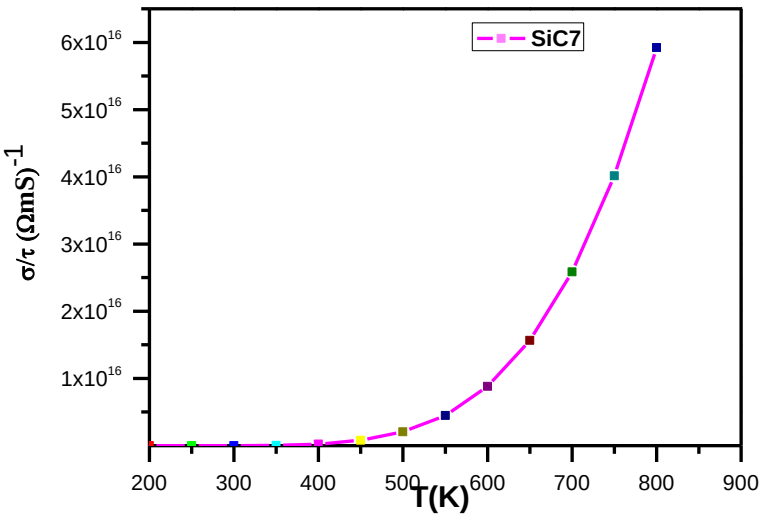
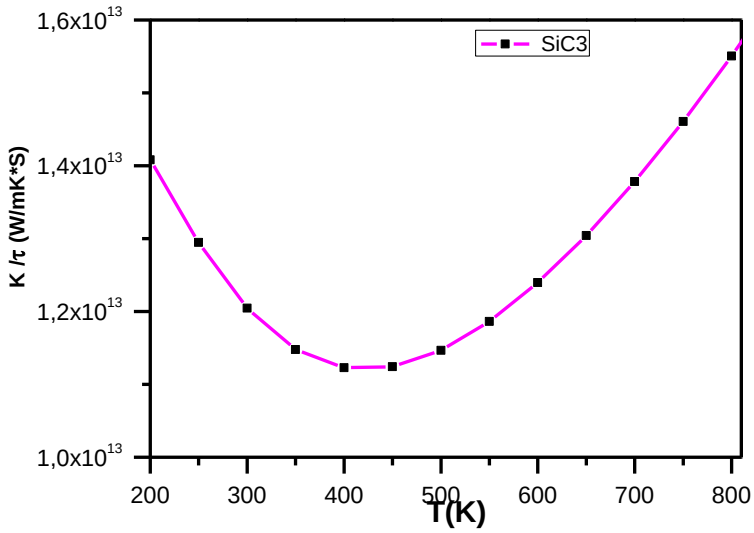


Figure 7: The electrical conductivity of siligraphene g-SiC_7 and g-SiC_3 as function temperature.

3.1.2. Thermal Property of siligraphene

The figure 8, show the thermal property of siligraphene SiC3 and SiC7 we observe that the siligraphene g-SiC3 has a better thermal property compared with siligraphene g-SiC7 ; also we obtained that thermal properties of g-SiC7 is increasing as function temperature but for g-SiC3 the thermal properties decreased as function temperature lower than 450 °K and become increasing for high temperature than 450 °K.



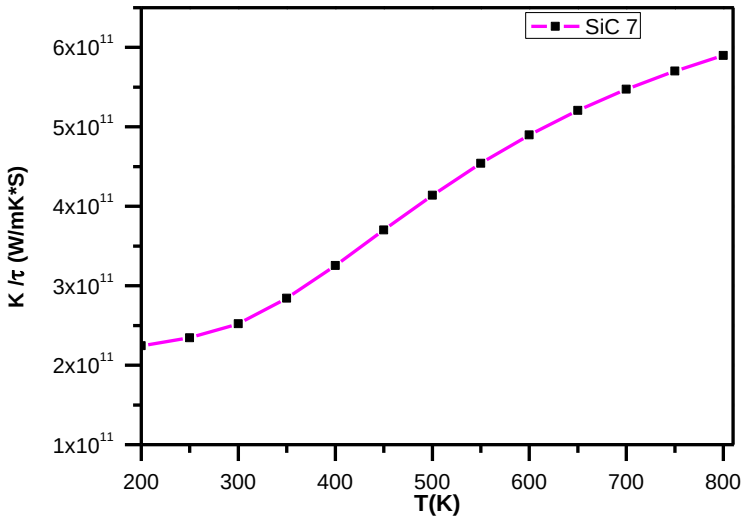


Figure 8: The thermal property of siligraphene g-SiC_7 and g-SiC_3 as function temperature.

4. Conclusion

The thermal, electrical property and optical properties of two structures of siligraphene are calculated within wien2k and Boltztrap packages. Our results predict that these two siligraphene have a direct band gap. We concluded that the optical properties

are depending to silicon concentration in siligraphene, and the reflectivity of SiC_7 is lower than the reflectivity of SiC_3 following xx and zz direction. Finally, we can observe that the electrical conductivity of g-SiC_3 is better than the electrical conductivity of g-SiC_7. We predict that siligraphene have the potential to use in solar cell application

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Notes

The authors declare no competing financial interest.

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