

An-Najah National University
Faculty of Graduate Studies

The Conductance Calculation of Silicene Field Effect Transistor

By

Fatima Hilal Heliel Maalee

Supervisor

Prof. Mohammad Elsaid

**This Thesis is Submitted in Partial Fulfillment of the Requirements for
the Degree of Master of Physics, Faculty of Graduate Studies, An-Najah
National University, Nablus, Palestine.**

2018

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This Thesis was Defended Successfully on 7\11\2018 approved by:

Defense Committee Members

Signature

- | | |
|---|-------|
| – Prof. Mohammad Khalil Elsaid / Supervisor | |
| – Dr. Hussein Shanak / External Examiner | |
| – Dr. Maen Ishtaiwi/ Internal Examiner | |

Dedication

For my mother and my father in the paradise, to my husband Ansar Nassar who supported me, to my affectionate brothers Ja'afer Maalee, Saed Maalee, Hassan Maalee, Muqdad Maalee and Mouhammad Maalee and dear sisters Jehan, Hala and Hedaya, from me biggest greetings and love. At last, to my darling son " Hakeem".

Acknowledgments

I would like to express my sincere thanks to my supervisor and instructor Prof. Mohammad Elsaid for his guidance, assistance, supervision and contribution of valuable suggestions. I can't forget to thank my colleagues Ayham Shaer and Mahmoud Ali for their help and especially in Mathematica computer program. Finally, I would like to thank all friends for providing encouragement and support.

الإقرار

أنا الموقعة أدناه، مقدمة الرسالة التي تحمل عنوان:

The Conductance Calculation of Silicene Field Effect Transistor

أقر بأن ما اشتملت عليه هذه الرسالة هي نتاج جهدي الخاص، باستثناء ما تمت الإشارة إليه حيثما ورد، وإن هذه الرسالة ككل، أو أي جزء منها لم يقدم من قبل لنيل أي درجة أو لقب علمي أو بحثي لدى أية مؤسسة تعليمية أو بحثية أخرى.

Declaration

The work provided in this thesis, unless otherwise referenced, is the research's own work, and has not been submitted elsewhere for any other degree or qualification.

Student's name:

اسم الطالبة:

Signature:

التوقيع:

Date:

التاريخ:

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List of Symbols and Abbreviations

E_g	Energy gap
a	Lattice constant
LB	Low buckled structure
2D	Two dimension material
FET	Field Effect Transistor
sp_2	Hybridization with three chemical bonds
sp_3	Hybridization with four chemical bonds
c	Speed of light
m_e	Mass of electron
DOS	Density Of State
E_f	Energy Fermi
\hbar	Reduced Planck's constant
v_f	Fermi velocity
i	Imaginary number
k_x, k_y	Component of wave vector
Δ	Energy difference between A and B sites in Silicene atom
Δ_{so}	Spin orbital gap energy
Δ_z	Energy difference between A and B sites in Silicene atom due to effect of external perpendicular electric field
Δ_{s,σ_z}	Energy gap equal to sum of Δ_z and Δ_{so}
Si	Silicon symbol
H	Hamiltonian matrix
I	Identity matrix
E_z	Electric field in z direction
F	Strength of electric field
d	Distance between sites A and B in Silicene atom

XII

E	Dispersion energy
n	Number of concentration
G	Conductivity of Silicene
$D(E)$	Density of states
$f(E)$	Fermi-Dirac distribution function
$M(E)$	Number of modes
$T(E)$	Transmission number
W	Width of channel in Field Effect Transistor
L	Length of channel in Field Effect Transistor
k_B	Boltzmann constant
T	Temperature in Kelvin
$\Gamma(n)$	Gamma function
$J_j(X)$	Complete Fermi-Dirac integral
q	Charge of electron
h	Planck's constant
$v_x(k)$	Carrier velocity
SOI	Spin Orbital Interaction
SOC	Spin Orbital Coupling
$H_n^{S_z}$	Hamiltonian matrix under effect of external electric field and Spin Orbital Interaction
$E_n^{S_z}$	Energy dispersion under effect of external electric field and Spin Orbital Interaction
k_+ / k_-	Dirac points
η	+/- for k_+ / k_- Dirac points
$\sigma_x, \sigma_y, \sigma_z$	Pauli matrices
s_z	Spin index +/- for spin up (\uparrow) and spin down (\downarrow),
V_g	Gate voltage
$\theta(E)$	Step function
m	Meter
s	Second

XIII

α	Ratio between Δ_z and Δ_{so}
TI	Topological insulator
BI	Band insulator
VSPM	Valley Spin-Polarized Metal

The Conductance Calculation of Silicene Field Effect Transistor

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Abstract

In this thesis, we have produced the number of carriers concentration expression of Silicene channel in Field Effect Transistor (FET) against gate voltage at various temperatures. Furthermore, we have also presented explicit analytical calculations for the conductance of Silicene 2D sheet, using Landauer's Formula, in the presence of an applied perpendicular electric field and the spin-orbital-interaction effect. The calculations show that the electric field and the SOI significantly affect the conductance, band structure and the density of state for the silicene used as a channel in the field effect transistor.

Chapter One

Introduction

1.1 Silicene, Graphene and other two dimension materials

Monolayer materials one of the most active research area of condensed matter physics. Silicene, is a single two-dimensional layer of silicon atoms in a honey comb lattice [1]. Similar to the graphene, silicon has a hexagonal buckled structure with two atoms per unit cell of lattice constant 3.82 \AA . The bulk silicon lattice constant is 0.78 \AA , as sketched figure (1.2) [2]. A natural question is whether other monolayer honey comb material purely made of one kind of atoms are possible. It is shown that monolayer honey comb system made of silicon, germanium and tin are possible, which are named silicene, germanene and stanene, respectively. Silicene is named after combination of silicon and suffix "ene" [3,4,5,6].

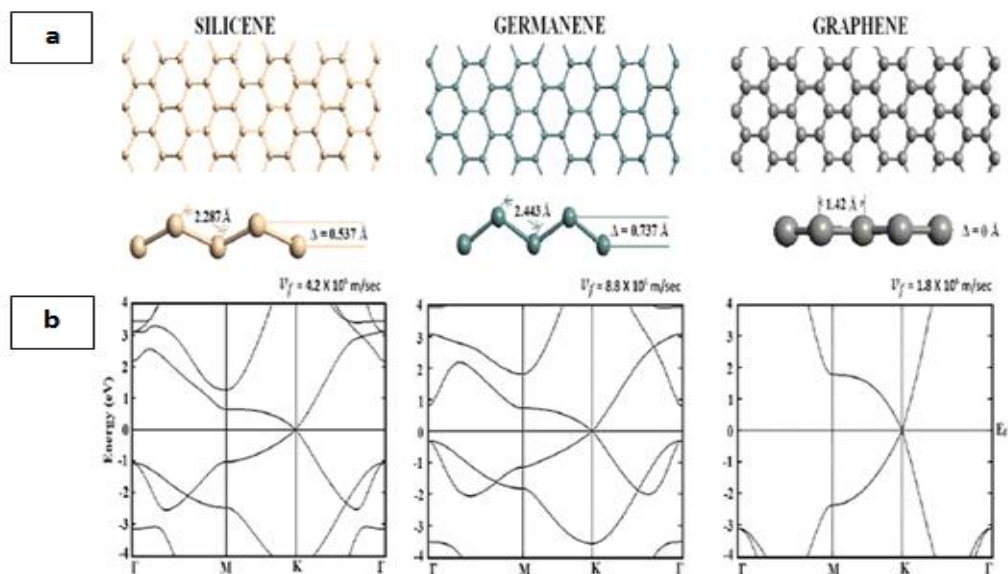


Figure (1.1) a) Buckled and unbuckled 2D materials, Silicene, Germanene, and Graphene monolayer. b) Band structure ($E - k$) of monolayer's diagrams of Silicene, Germanene, and Graphene monolayer [36].

Silicene, germanene and stanene are expected to be topological insulators. Topological insulator (TI) is a distinctive state of matter indexed by topological numbers, and characterized by an insulating gap in the bulk accompanied by topological protected gapless edges [7,8]. Thus the study of these topological insulators is very important since it has rich physics.

1.2 Comparison between Silicene and Graphene

One of the most attractive characteristics of graphene is ultra-high mobility at room temperature, comparable to the mobility of bulk silicon material which is currently used in the devices technology like our computers. This makes the graphene a very promising candidate material for high speed transistor electronic devices.

Due to the linear energy dispersion, the surface electron of the topological insulator behave as mass less Dirac fermions with transport properties different from those of the charge carrier in conventional metallic or semiconductor system [9]. In graphene, the low energy charge carrier are described by mass less Dirac equation where Fermi velocity plays the role of the light velocity. Due to the linear energy spectra, the normally incident electrons can tunnel through a potential barrier via Klein tunneling without reflection [10]. This is significant disadvantage for use of graphene and topological insulator as field effect transistors since the Klein tunneling leads to an appreciable off current and thus a poor on/off current ratio [11]. On the other hand the intrinsic spin-orbit interaction induced energy gap of silicene

$E_g \approx 0.34 eV$ is smaller than the minimum band gap requirement for transistor operation ($E_g \approx 0.8 eV$) [12, 13].

However, the band-gap of the silicon up to $800 meV$ donated by DFT calculation, since ionic radius of silicene is large in sp_3 hybridization implies a small buckling with structure more stable, it is noted that Si atoms favors sp_3 hybridization, whereas sp_2 hybridization for Silicene [14]. The main difference between the Silicene and Graphene lies in the fact that the planer Silicene unstable in contrast to Graphene [15]. This buckling has been reported in the range $0.36 A^\circ$ to $0.75 A^\circ$ [16, 17, 18]. The buckling structure can be turned by applying a perpendicular electric field, other group element, such as silicon and germanium, have also stable honey comb monolayer. Unlike planer graphene monolayer, the most stable silicene and germanene monolayer prefer allow-buckled (LB) structure, see figure (1.1). The electronic structure of the silicene and germanene are zero gap semi metallic, and their charge carrier are also mass less fermions when a vertical electric field is applied. The buckled structure that separates A and B atoms of the honeycomb lattice is in the transversal direction and provides the required gradient of the potential. The buckling parameter Δ_0 is defined as the vertical distance between the two planes of Si atoms as display shown in figure (1.2).

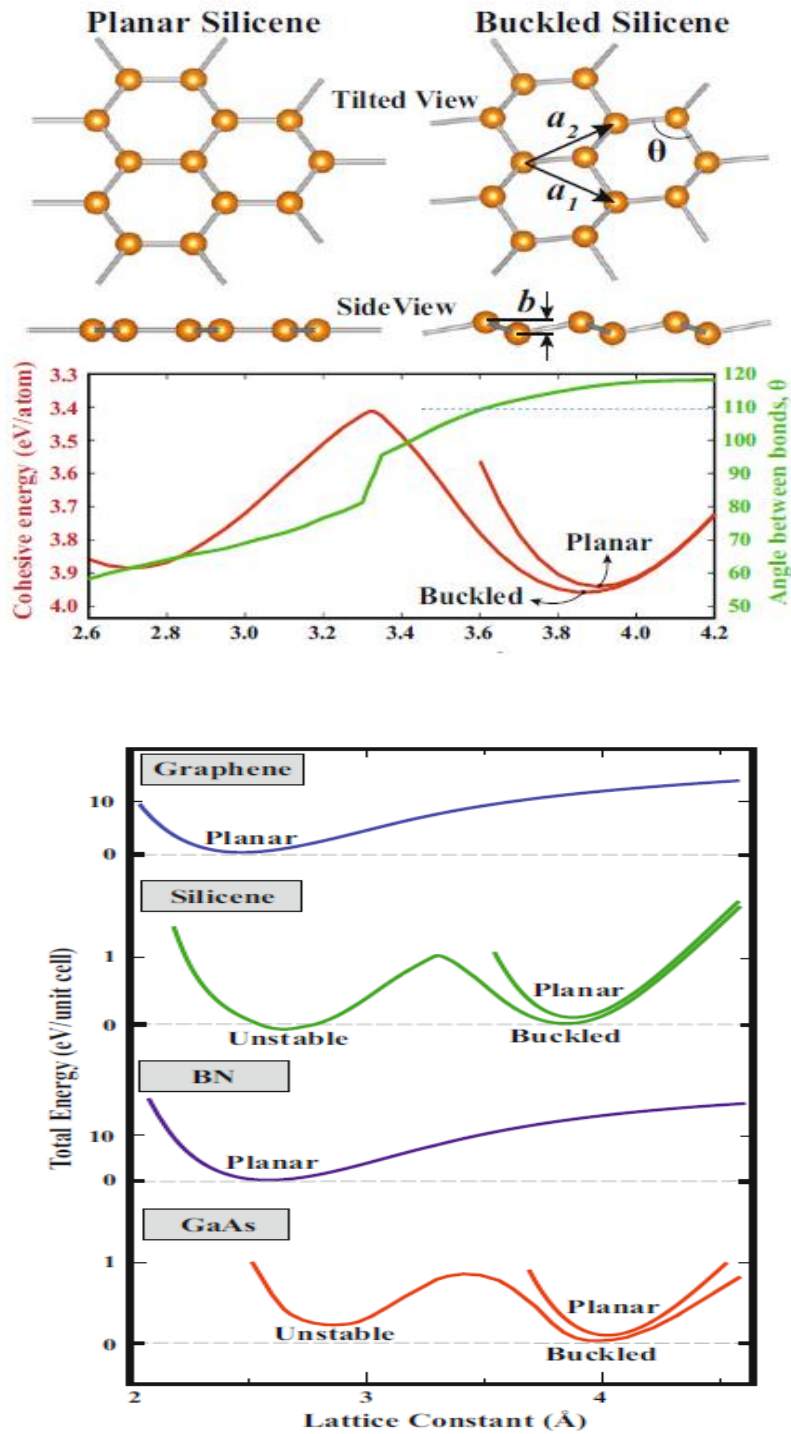


Figure (1.2) a: Silicene of planar and buckled silicene from tilted and side views. The bottom panel shows the variations of the cohesive energy (red solid line) and bond angle (green solid line) with respect to the lattice constant. The thin dashed blue line represents the ideal bond angle of sp^3 hybridization.

b: The total energy per unit cell versus the lattice constant for graphene, silicene, hexagonal BN sheet and GaAs sheet, zero of energy is set to the minimum energy of a stable configuration [43] .

1.3 Literature survey of Silicene Two Dimension Sheet

The original paper reporting the buckling of Si atoms was published in 1994 by Takeda and Shirashi [19]. As a result, the band structure can be controlled by an applied electric field that tunes the gap, as we mentioned in table (3.1). The modern electronic industry is built on a transistor designed from silicon not carbon. In 2007, a group of researchers published a theoretical paper and showed how the Silicene sheet transistor works [20]. Silicene was first predicted to the exists based on calculation in 1994 [21, 22]. It has high electrons mobility and also it has more advantage being easily integrated with the industrial silicon technology [23;27-29]. In the last years Silicene has been the object of many experimental and theoretical studies. For example, Silicene nanoribbons have been experimentally produced over Ag (110) surface by Padova et al [24]. Silicene nanosheet have been also synthesized by Xn et al [25]. And Silicene nanoribbons were successfully epitaxial grown on silver (110) and (100) surfaces by Lay [26].

Functionalized electronic properties of the Silicene based FET which is doped by Iodine and Fluorine could open a gap of 1.194 and 1.469 eV, doped Silicene sheet. These which are candidate as a FETs channel materials with tunable energy gap [1].

The new achievement in the field of 2D materials, divide the researcher community in two groups: one group support the graphene and another one in favors of Silicene [3].

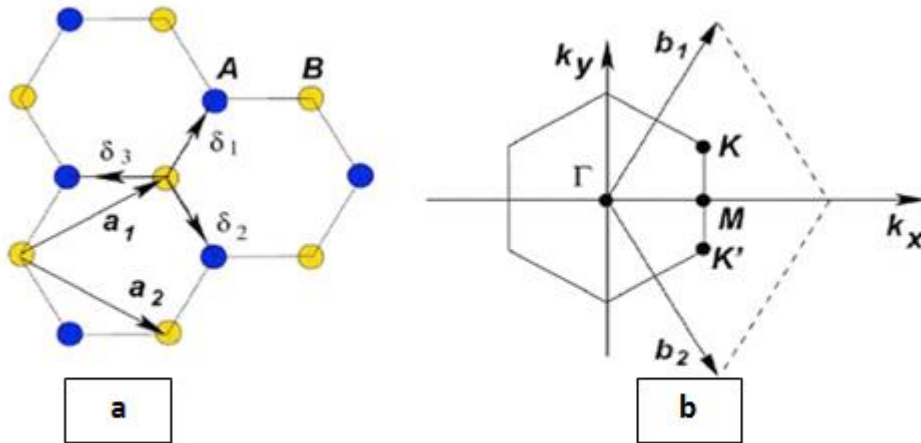


Figure (1.3) : a) Dirac space: The honeycomb structure, made of two fundamental lattice vectors \vec{a}_1 and \vec{a}_2 , consists of sublattices made of A and B. b) Reciprocal lattice is also a honeycomb lattice, which contains two inequivalent Dirac points \mathbf{k} and \mathbf{k}' [19].

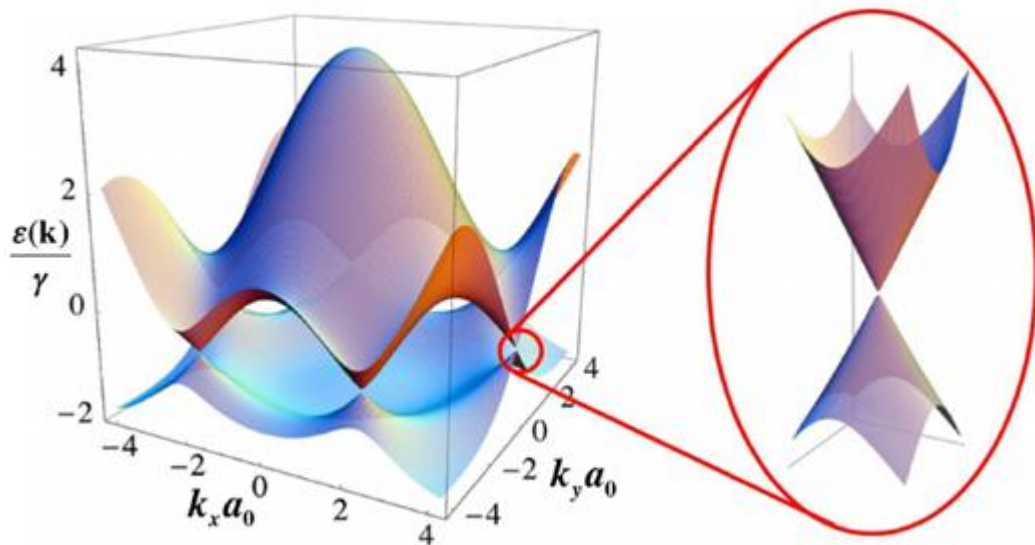
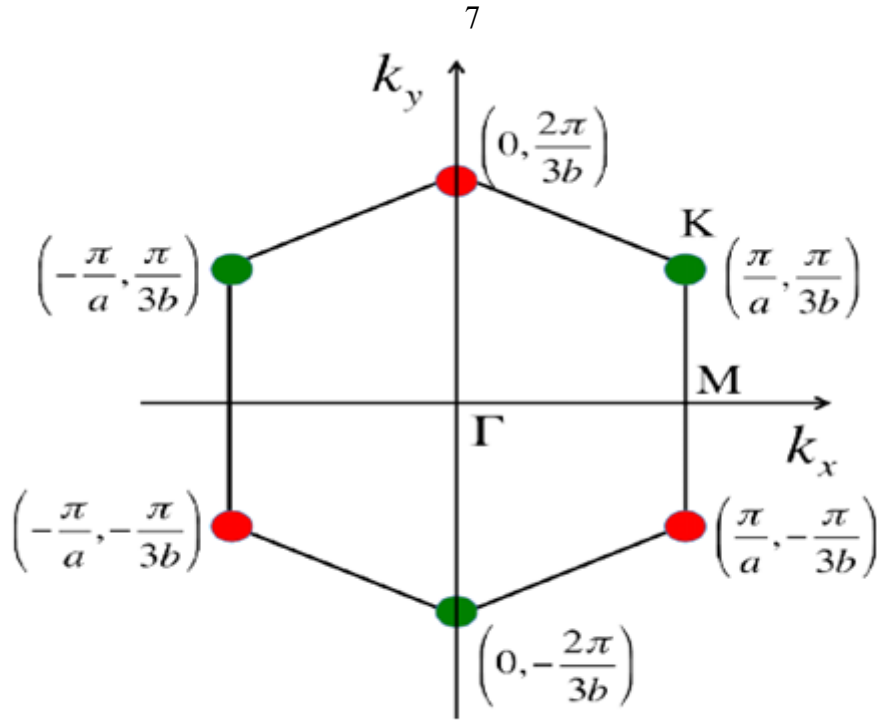


Figure (1.4) : The upper and lower bands of Graphene touch each other at the Dirac points, the vertices of the first Brillouin zone [19].



Figure(1.5): Graphene first Brillouin zone with Dirac points $k = \left(\frac{\pi}{a}, \frac{\pi}{3b}\right)$ and $k' = \left(\frac{\pi}{a}, -\frac{\pi}{3b}\right)$ [20].

Table (1.1) Some important parameter of selected 2D materials: Graphene, Silicene and Germanene [15, 19].

Parameter	Graphene	Silicene	Germanene
Lattice constant (a) (Å)	2.468	3.858	4.06
Bond Length (d) (Å)	1.424	2.232	2.341
Buckling Parameter (Δ_0) (Å)	0	0.42 – 0.45	0.69
Hopping Integral (t) (eV)	2.8	1.6	1.3
Energy Gap (E_g) (meV)	0.02	1.9	33
Fermi velocity (v_f) (10^6 ms^{-1})	1.01	0.65	0.62
Effective electron mass (m^*) (m_0)	0	0.001	0.007
λ_{so} (meV)	0.001	3.9	43
Rashba Interaction (meV)	0.00	0.7	10.7
ΔE (eV)	8.7	7.2	8.1
Buckled height (L) (Å)	0	0.23	0.33
\emptyset (Degree)	90	101.7	106.5

Chapter Two

Theory of Silicene

After discovery of graphene, as a two sp_2 bonded carbon atoms in two dimensional planner sheet in a honey comb lattice, which has fantastic electrical properties with zero band gap in the Dirac point [27,28,29]. Crystalline form of the silicon atoms arranged in a honey comb lattice with sp_3 bonded atoms called Silicene, as It has been observed by Nakano et al [30]. Theoretical calculations by Density Functional Theory (DFT) which show that the graphene is a 2D planner sheet of carbon atoms, while the silicene makes stable bounds in a semi two dimension buckled form as showing figure (1.1) [31, 32].

The atomic structure of graphene -was confirmed as two dimension in a honey comb lattice- consists from two carbon atoms in a unit cell, A and B, in the form of triangular sub lattice periodicity. Figure (1.2) show that the electron in Graphene behaves as mass less Dirac fermions due to the electron band structure near the Fermi level described by the dispersion relation between energy and momentum:

$$E^2=p^2c^2+m^2c^4 \quad \dots\dots\dots (1)$$

Where E is the energy, p is the momentum of the electron, m is the mass of body, and c the speed of electron. Here the energy is separated into two terms, first is kinetic energy and the second is rest energy of electron.

Figure (1.2) shows that the density of states (DOS) at the energy Fermi (E_f) is zero and the energy level and contribution of DOS below and above Fermi level. The conduction band and valence band touch other at symmetry point k , the point where valance and conduction bands touch other at E_f called Dirac points, and the charge at this point behaves like mass less Dirac fermions since the nature of these carrier obey relativistic Dirac-equation, as the figures (1.3, 1.4, 1.5)

2.1 Band Structure of Silicene

The dispersion relation of the Graphene as a 2D-material was derived explicitly by the help of tight-binding-method (TB). In various published works we refer the interested reader, for more details and + discussion to reference [33,34]. The behavior of the free electron near the origin ($k_x \approx k_y \approx 0$) in k -space is shown to be a relativistic Dirac behavior given by,

$$H_D = v_f \vec{\sigma} \cdot \vec{p} \quad \text{.....(2)}$$

The relativistic Hamiltonian in the presence of external electric field which describe the carrier structure of silicene around Dirac points, similar to that of graphene, **can** be written as [21, 22],

$$H = v_f \vec{\sigma} \cdot \vec{p} + \Delta \sigma_z \quad \text{.....(3)}$$

And in the matrix form as

$$H = \begin{bmatrix} \Delta & \hbar v_f (k_x - i k_y) \\ \hbar v_f (k_x + i k_y) & \Delta \end{bmatrix} \quad \text{.....(4)}$$

$$H = H_{\text{Graphene}} + \Delta \sigma_z \quad \text{.....(5)}$$

To find the Eigen energies, $E(k)$ of the silicene sheet, the determinant of the matrix H , should be vanish.

$$|H - EI| = 0 \quad \text{.....(6)}$$

$$\begin{vmatrix} -\Delta - E & \hbar v_f(k_x - ik_y) \\ \hbar v_f(k_x + ik_y) & \Delta - E \end{vmatrix} = 0 \quad \text{.....(7)}$$

$$-\Delta^2 + |E|^2 - \hbar^2 v_f^2 (k_x^2 + k_y^2) = 0 \quad \text{.....(8)}$$

This equation can lead to the energy result given by equation (10).

$$-\Delta^2 + |E|^2 = \hbar^2 v_f^2 |k|^2 \quad \text{.....(9)}$$

$$E = \pm \sqrt{\Delta^2 + \hbar^2 v_f^2 |k|^2} \quad \text{.....(10)}$$

Where k the momentum of charge carrier and v_f is Fermi velocity of charge carrier Dirac points, Δ is the energy difference between Si atoms on A and B sites, ($\Delta = F d$, F is strength of electric field and d is the distance between Si atoms along field direction), and $\hbar = 1.05 * 10^{-34}$ J.s is reduced Planck's constant. Due to the inversion symmetry between A and B sites like graphene, the energy dispersion relation in equation (10) in the absence of electric field when ($\Delta = F = 0$) becomes

$$E = \pm \hbar v_f |k| \quad \text{.....(11)}$$

2.2 Carrier Concentration in Silicene

The carrier concentration (n) in a band state of silicene sheet as a channel in FET is calculated by integrating the Fermi-Dirac distribution times density of state energy band as, $n = \int D(E) \cdot f(E) \cdot dE$ where $D(E)$ is Density of state and $f(E)$ is Fermi-Dirac distribution function. The density of state of silicene is calculated by converting the discrete continuum into integration form over k with respect of $E - k$ relation,

$$D(E) = \frac{wL}{4\pi^2} \int_{-\infty}^{\infty} \delta(E - E(k)) \cdot dE \quad \dots\dots\dots(12)$$

$$D(E) = \frac{wL}{4\pi^2} \int_{-\pi}^{\pi} d\theta \int_0^{\infty} k dk \cdot \delta(E - E(k)) \quad \dots\dots\dots(13)$$

Here the parameters W and L are the width and length of the channel in Field Effect Transistor (FET), and $\int dE \rightarrow \int d\theta \int k dk$ in 2D rectangular coordinates in k -space

The integration over θ is equal 2π and $E(k) = \sqrt{\hbar^2 v_f^2 k^2 + \Delta^2}$,

$$\text{So } \partial E(k) = \frac{2\hbar^2 v_f^2 k}{2E(k)} \partial k ; k = \frac{\sqrt{E(k)-\Delta^2}}{\hbar v_f} ; \partial k = \frac{1}{\hbar v_f} \frac{E(k) dE(k)}{\sqrt{E(k)-\Delta^2}}$$

$$D(E) = \frac{wL}{2\pi} \int \delta(E - E(k)) \cdot \frac{\sqrt{E(k)-\Delta^2}}{\hbar v_f} \cdot \frac{1}{\hbar v_f} \frac{E(k) dE(k)}{\sqrt{E(k)-\Delta^2}} \quad \dots\dots\dots(14)$$

$$D(E) = \frac{wL}{2\pi} \frac{1}{\hbar^2 v_f^2} |E| \quad \dots\dots\dots(15)$$

$$D(E) = \frac{2wL}{\pi \hbar^2 v_f^2} |E| \quad \dots\dots\dots(16)$$

The density of state in equation (15) should be multiplied by 2 include the spin and 2 for the degeneracies.

The total electron concentration of silicene equal to the density of state times the Fermi-Dirac distribution function

$$n = \int dE D(E) f(E) \theta(E) \quad \dots\dots\dots(17)$$

$$n = \int_0^\infty \frac{2wL}{\pi\hbar^2 v_f^2} |E|. \theta(|E| - \Delta). (1 + \text{Exp}(\frac{E-E_f}{(K_B T)}))^{-1} \quad \dots\dots\dots(18)$$

where $\theta(|E| - \Delta) = \begin{cases} 0, & \Delta > E > 0 \\ 1, & \text{otherwise} \end{cases}$

after performing the integrals by mathematica package program So equation (18) could be written as:

$$n = \frac{2wL}{\pi\hbar^2 v_f^2} (K_B T) \{ (K_B T). \Gamma(2). J_1(\eta) + \Delta. \Gamma(1). J_0(\eta) \} \quad \dots\dots\dots(19)$$

$$n = \frac{2wL}{\pi\hbar^2 v_f^2} \{ (K_B T)^2. J_1(\eta) + \Delta. (K_B T). J_0(\eta) \} \quad \dots\dots\dots(20)$$

Where $J_j(X) = \Gamma(j+1)^{-1} \int_0^\infty \frac{t^j dt}{(1+\text{Exp}(t-X))}$ is a Complete Fermi-Dirac integral and $\Gamma(n) = n(n-1)!$ is a Gamma Function.

2.3 The Conductivity of Silicene under the Effect of Electric Field.

To calculate the conductance of Silicene (G) channel between source and drain in a Field Effect Transistor (FET), as sketched in figure (1.6). We can take the Landauer's Formula, $G = \frac{2q^2}{h} \int_{-\infty}^\infty dE M(E) T(E). - \frac{\partial f(E)}{\partial E}$ [35].

In a ballistic transport $T(E) = 1$ and $M(E)$ is a number of modes, which is equal to,

$$M(E) = \sum_k \delta(E - E(k)) \frac{\pi\hbar}{L} |\mathcal{V}_x(k)| \quad \dots\dots\dots(21)$$

Where $v_x(k) = \partial E(k)/\hbar \partial k_x$ is a carrier velocity along the channel in x -direction

$$M(E) = \frac{w}{\pi\hbar} \sqrt{|E|^2 - \Delta^2} \quad \dots\dots\dots(22)$$

First, we will use the Landauer's formula to calculate the conductivity G , in absence of electric field ($\Delta = 0$) the number of mode in equation (10) becomes $M(E) = \frac{w}{\pi\hbar} |E|$

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^\infty dE |E| \frac{\partial}{\partial E} \left(\frac{1}{1+Exp\left(\frac{E+E_f}{(K_B T)}\right)} \right) - \int_0^\infty dE |E| \frac{\partial}{\partial E} \left(\frac{1}{1+Exp\left(\frac{E-E_f}{(K_B T)}\right)} \right) \right\} \quad \dots\dots\dots(23)$$

$$G = \frac{q^2 w (K_B T)}{\pi^2 \hbar^2 v_f} [J_{J_0}(-\eta) - J_0(\eta)] \quad \dots\dots\dots(24)$$

The details steps which lead to final analytical result of the conductance (G) in equation (24) for a channel made from a Silicene monolayer sheet, are shown explicitly in chapter three; Results and Discussion part.

Second, we switch on the electric field ($\Delta \neq 0$) and apply the same procedure to produce the conductance (G) of the Silicene channel as,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^\infty dE \sqrt{|E|^2 - \Delta^2} \frac{\partial}{\partial E} \left(\frac{1}{1+Exp\left(\frac{E+E_f}{(K_B T)}\right)} \right) - \int_0^\infty dE \sqrt{|E|^2 - \Delta^2} \frac{\partial}{\partial E} \left(\frac{1}{1+Exp\left(\frac{E-E_f}{(K_B T)}\right)} \right) \right\} \quad \dots\dots\dots(25)$$

By using Taylor series expansion technique, the quantity could be extended as $\sqrt{|E|^2 - \Delta^2}$ to obtain the conduction (G)

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^\infty dE \sqrt{|E|^2 - \Delta^2} \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}\left(\frac{E+E_f}{K_B T}\right)} \right) - \int_0^\infty dE \sqrt{|E|^2 - \Delta^2} \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}\left(\frac{E-E_f}{K_B T}\right)} \right) \right\} \quad \text{.....(26)}$$

Using Landauer's Formula and the definition of the complete Fermi-dirac formula $J_j(x)$, the conductance (G) of the Silicene channel after performing the integration by the help of mathematica symbolic package program is, given as :

$$G = \frac{q^2 w (K_B T)}{\pi^2 \hbar^2 v_f} [J_1(-\eta) - J_1(\eta)] \quad \text{.....(27)}$$

2.4 The conductivity of Silicene under effect of Spin Orbital Interaction (SOI)

Silicene is a honey comb structure of Silicene atoms sites on A and B, it is located from each other by $2L$ distance. The spin orbital interaction of Silicene is equal to 1.55 meV , and this value maybe make changes in the electronic properties for Silicene sheet in Field Effect Transistor (FET). However, (SOI) value measured in Graphene within limits of μeV which is not significant. In presence of spin orbital interaction (SOI) and external electric field perpendicular ($\Delta \neq 0$) to the Silicene sheet, and around k point the complete 2-D Hamiltonian can be written as [36].

$$H_\eta^{S_z} = \hbar v_f (\eta k_x \sigma_x + k_y \sigma_y) + \eta s_z \Delta_{so} \sigma_z + \Delta_z \sigma_z \quad \text{.....(28)}$$

Where v_f is a Fermi velocity of Dirac Fermions, η is +/- for k / k' dirac points, $(k_x, k_y) = \left(\frac{n\pi}{a}, \pm \frac{m\pi}{b} \right)$ are the components of wave vector where

+/- for k and k' relative to the Dirac points, $(\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices.

The spin index $s_z = + / -$ for spin up (\uparrow) and spin down (\downarrow), respectively. $\Delta_z = L E_z$, with $L = 0.23 \text{ \AA}$, here Δ_{so} represents the spin orbital gap with 3.9 meV for Silicene.

The energy spectrum has been obtained by diagonalizing from the Hamiltonian given by equation (2,16), as:

$$E_{\eta}^{s_z} = \pm \sqrt{\hbar^2 v_f^2 k^2 + (\Delta_z + \eta s_z \Delta_{so})^2} \quad \dots\dots\dots(29)$$

We noticed that the dispersion relation (10) and (29) for the silicene in the presence of electric field (Δ_z) and spin-orbit interaction (Δ_{so}) are similar under a simple linear direct shift: $\Delta_z \rightarrow \Delta + \eta s_z \Delta_{so}$ in equation (10).

Chapter Three

Results and Discussions

In this chapter we will give the main essential steps which produce the analytical results of conductance of Silicene and Graphene 2D material channels used in a Field Effect Transistor (FET). We show the dependence of the conductivity of electrons in silicene channel on the applied external electric field for varies temperature values. In addition, we show the effect of Spin-Orbit Interaction (SOI) term on the band structure and density of states on the silicene channel.

3.1 The Conductance calculations of Silicene in present of external perpendicular electric field

(3.1.1) Energy Dispersion of Silicene

The first point is study the electronic properties of materials looking at their band structure, as we say that Silicene's band gap can be opened at the Fermi level under influence of external electric field, where the electric field must be perpendicular to the plane of Silicene sheet. External electric field will break the inversion symmetry and open the band gap, since the potential at the atoms A and B are different, we can write;

$$\Delta = \alpha (V_A - V_B) \quad \text{.....(1)}$$

where α is the proportionality constant and (V_A, V_B) are the potential seen at the atoms (A, B) , when the field is applied, the difference potential becomes $(V_A - V_B) = F d$ where the F the field strength and d is the

distance between the atoms at the sites A and B, as we mentioned, the band gap can be evaluated:

$$E_g = 2 \Delta = 2 \alpha (V_A - V_B) = 2 \alpha F d = \alpha' F \quad \text{.....(2)}$$

The numerical values of the energy gap (E_g) of the silicene are listed in table (3.1) and also plotted in figure (3.1) for $\alpha' = 10.14$ (*meV per volt/nm*) taken from reference [37].

Table (3.1) : The energy band gap (E_g) of Silicene against the strength of the applied electric field along z-direction.

Electric Field (<i>volt/nm</i>)	Energy Band Gap (E_g)(<i>meV</i>)
-0.0078	-0.0261
0.2813	3.0090
0.5029	5.0330
0.9076	9.2490
1.0040	10.090
2.0740	21.050
3.0080	30.160
5.0030	50.570

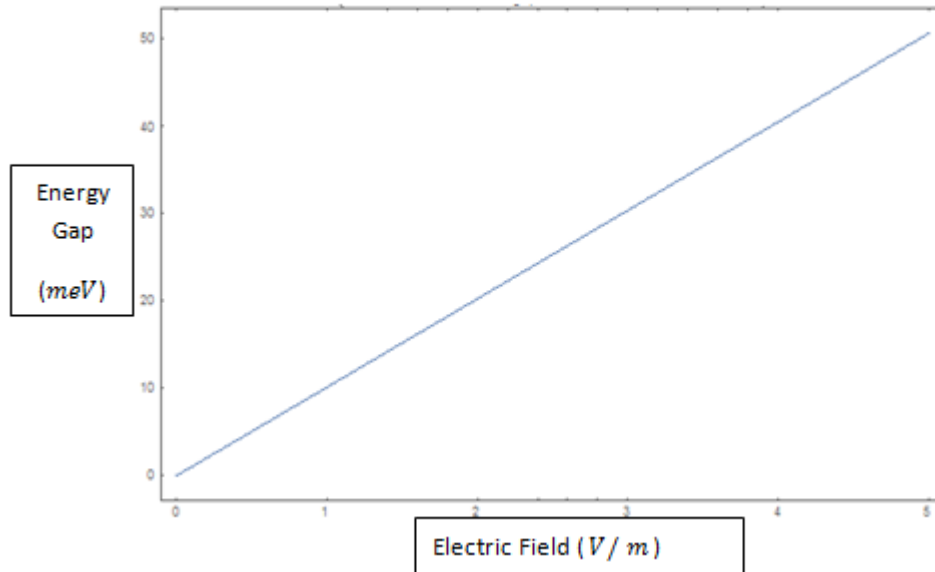


Figure (3.1) The variation of band gap (E_g) versus the strength of perpendicular external electric field to the plane of Silicene sheet.

To investigate the behavior of the silicene band structure and energy gap on the momentum (\vec{k}) and electric field (Δ), we have used the dispersion relation

$$|E| = \pm \sqrt{|\Delta|^2 + \hbar^2 v_f^2 |k|^2} \quad \text{.....(3)}$$

To list the calculated numerical energy gap at various gate voltage.

The computed result are also displayed in table (3.2) and figure (3.2) to display the band structure of the silicene.

In equation (3), k is the momentum of charge carrier and v_f is Fermi velocity of charge carrier at Dirac points, Δ is the energy difference between Si atoms on A and B sites, ($\Delta = F d$), F is strength of electric field and d is the distance between Si atoms along field direction), and $\hbar = 1.05 \times 10^{-34}$ J.s is the reduced Planck's constant. Due to the inversion symmetry in A and B sites like graphene and ($\Delta = 0$) the energy dispersion becomes

$$E = \pm \hbar v_f |k| \quad \text{.....(4)}$$

In equation (4), it is possible to make non-zero Δ in graphene by chemical doping, but it's difficult task. Another way to create $\Delta \neq 0$ in the material is by including the Spin-Orbit-Interaction effect. The value of Δ is found to be zero for the graphene and about 1.55 meV for silicene [38, 39].

Table (3.2) The values of energy band gap (E_g) with $|\vec{k}|$ values at different gate voltages, in absence electric field ($V_{g2} = 0$) and presence perpendicular electric field ($V_{g2} \neq 0$).

$k - vector$ 1×10^8 (m^{-1})	E_n (meV)				
	$V_{g2} = 0$	$V_{g2} = 0.1$	$V_{g2} = 0.2$	$V_{g2} = 0.5$	$V_{g2} = 1.0$
-8.033	724.9	715.1	720.5	741.2	872.2
-6.066	554.5	541.3	539.5	588.0	733.5
-3.033	283.0	272.5	288.5	367.8	578.1
0	5.263	48.08	97.97	250.5	498.5
3.033	264.1	278.9	272.7	370.2	572.5
6.066	560.8	550.8	558.5	588.0	737.2
3.033	718.6	705.7	714.2	755.6	874.0

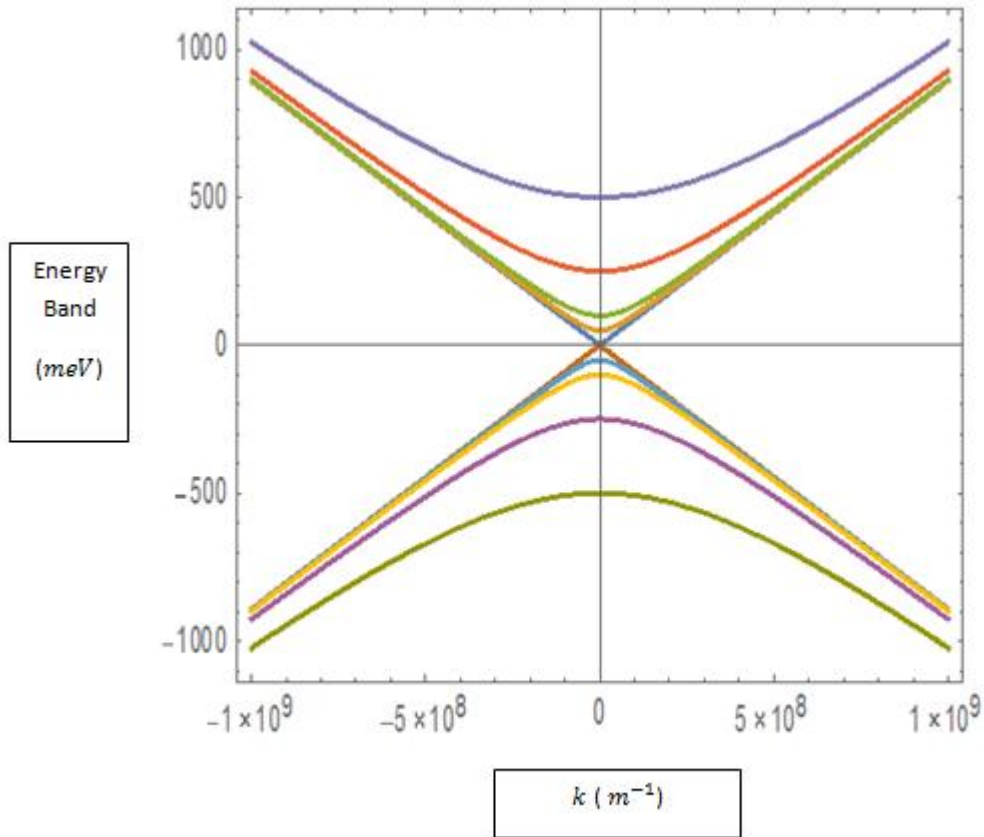


Figure (3.2): ($E - k$) Band structure of Silicene in absence and presence of a perpendicular electric field: energy gap (E_g) against k - values.

In this figure, we show the band structure of Silicene for difference gate voltage (V_g) where $\Delta = \frac{q}{2} (V_{g2} - V_{g1})$, here $V_{g2} - V_{g1}$ is gate voltage at the Field Effect Transistor (FET), and q is electron charge. We have noticed that band gap of silicene increases with gate voltage in presence of the perpendicular electric field. For $\Delta = 0$ case, the band gap of silicene and graphene have the same behavior with also band gap ($E_g = 0$). Although, small difference due to Fermi velocity of the two materials.

3.1.2: Carrier Concentration of Silicene

To show the behavior of the carrier concentration of Silicene and the effect of electric field, we have to find the relation of the concentration (n) to the gate voltage (V_g). For this purpose, we can start from equation (2.6),

$$n = \int dE D(E) f(E) \theta(E) \quad \text{.....(5)}$$

$$n = \int_0^\infty \frac{2wL}{\pi \hbar^2 v_f^2} |E|. \theta(|E| - \Delta). (1 + \text{Exp}(\frac{E-E_f}{K_B T}))^{-1} dE \quad \text{.....(6)}$$

where $\theta(|E| - \Delta) = \begin{cases} 0, & \Delta > E > 0 \\ 1, & \text{other} \end{cases}$

by changing variables as $\eta = \frac{E_f - \Delta}{K_B T}$ and $X = \frac{E - \Delta}{K_B T}$

equation (6) can be obtained as :

$$n = \frac{2wL}{\pi \hbar^2 v_f^2} K_B T \left\{ \int_0^\infty \frac{(K_B T) X dX}{(1 + \text{Exp}(X - \eta))} + \int_0^\infty \frac{\Delta dX}{(1 + \text{Exp}(X - \eta))} \right\} \quad \text{.....(7)}$$

in equation (7), the first term is the complete Fermi-Dirac integral with first order $j = 1$, and the second term with zero order j .

Where the complete Fermi-Dirac integral is given by the standard expression $J_j(X) = \Gamma(j + 1)^{-1} \int_0^\infty \frac{t^j dt}{(1 + \text{Exp}(t - X))}$

So equation (3.7) could be rewritten as:

$$n = \frac{2wL}{\pi \hbar^2 v_f^2} K_B T \left\{ K_B T. \Gamma(2). J_1(\eta) + \Delta. \Gamma(1). J_0(\eta) \right\} \quad \text{.....(8)}$$

equivalently,

$$n = \frac{2wL}{\pi \hbar^2 v_f^2} \left\{ (K_B T)^2. J_1(\eta) + \Delta. (K_B T). J_0(\eta) \right\} \quad \text{.....(9)}$$

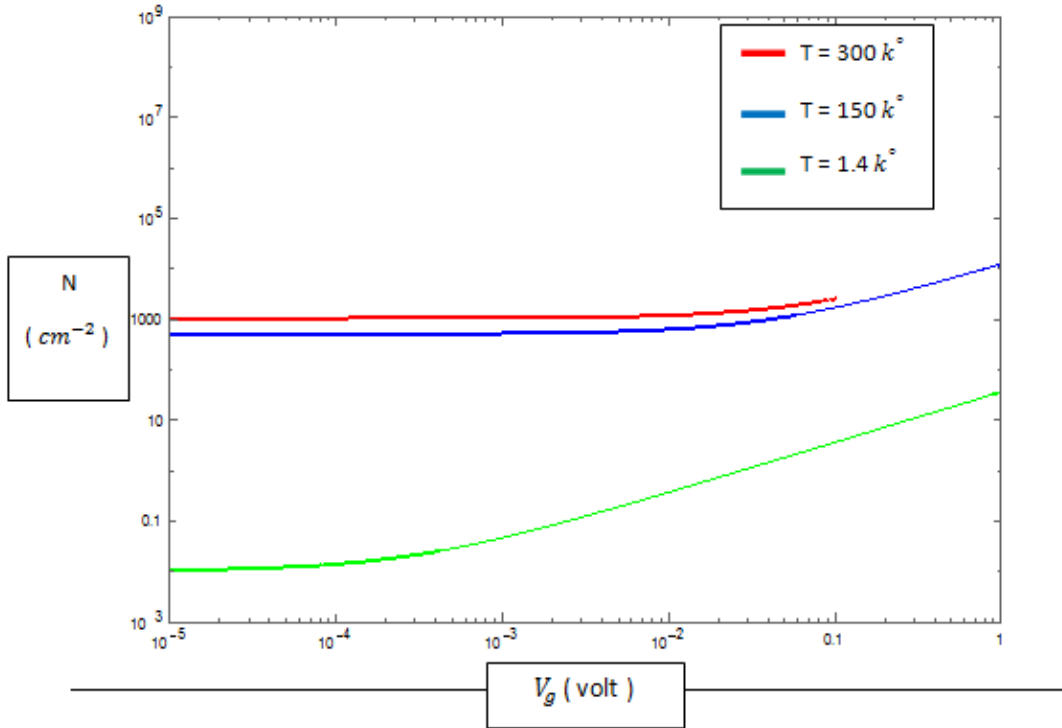


Figure (3.3): The total carrier concentration of Silicene - in absence of electric field - versus gate voltage at different temperature $T = 300\text{ K}^\circ$, $T = 150\text{ K}^\circ$ and $T = 1.4\text{ K}^\circ$.

The above figure (3.3) shows the electron concentration of Silicene has been increasing dramatically with increase the temperature. This behavior is in agreement with the analytical expression of number of electron concentration (n) given in equation (3.9) the number of electron concentration (n) is linearly proportional with the temperature.

3.1.3: The Conductivity of Silicene:

To calculate the conductance of Silicene (G) channel between the source (S) and the drain (D) in a Field Effect Transistor (FET), we can use the Landauer's formula;

$$G = \frac{2q^2}{h} \int_{-\infty}^{\infty} dE M(E)T(E). \left(-\frac{\partial f(E)}{\partial E}\right) \dots\dots(10)$$

where q is the electron charge $q = 1.6 \times 10^{-19}\text{ C}$, and $h = 6.626 \times 10^{-36}\text{ Js}$ is a Plank's constant. Here, the electron transport in the channel is assumed

to be ballistic tunneling process $T(E) = 1$, the number of modes ($M(E)$) that are above the cut-off at the energy E in the transition channel could be expressed as:

$$M(E) = \sum_k \delta(E - E(k)) \frac{\pi \hbar}{L} |\mathcal{V}_x(k)| \quad \dots\dots\dots(11)$$

$$M(E) = \frac{w L}{(2\pi)^2} \int \delta(E - E(k)) \frac{\pi \hbar}{L} |\mathcal{V}_x(k)| \quad \dots\dots\dots(12)$$

Where $\mathcal{V}_x(k)$ is the carrier velocity of charge in the channel in x - direction

$$\mathcal{V}_x(k) = \partial E(k) / \hbar \partial k_x = \frac{1}{\hbar} \frac{\partial \left(\sqrt{\hbar^2 v_f^2 k^2 + \Delta^2} \right)}{\partial k_x} \quad \dots\dots\dots(13)$$

$$\mathcal{V}_x(k) = \frac{\hbar v_f^2 k_x}{\sqrt{\hbar^2 v_f^2 k^2 + \Delta^2}} \quad \dots\dots\dots(14)$$

Substituting equation (14) in equation (12), we have the expression for the number of modes as:

$$M(E) = \frac{w \hbar^2 v_f^2}{4\pi^2} \int_{-\pi}^{\pi} \cos^2 \theta d\theta \int_0^{\infty} \frac{\delta(E - E(k))}{E(k)} k^2 dk \quad \dots\dots\dots(15)$$

$$\int_{-\pi}^{\pi} \cos^2 \theta d\theta = 2\pi, \text{ and } \int_0^{\infty} \frac{\delta(E - E(k))}{E(k)} k^2 dk = \frac{1}{\hbar^2 v_f^2} \sqrt{|E|^2 - \Delta^2}$$

$$M(E) = \frac{w}{\pi \hbar v_f} \sqrt{|E|^2 - \Delta^2} \quad \dots\dots\dots(16)$$

For zero electric field ($\Delta = 0$), the number of modes model of Graphene would be similar to the number of modes model of the Silicene. However, it's value different in the Silicene due to a different Fermi velocity of its carrier. Therefore, the number of modes in Silicene in absence of field can obtained as:

$$M(E) = \frac{w}{\pi \hbar v_f} |E| \quad \dots\dots\dots(17)$$

We will use Landauer's formula to calculate the conductivity (G) with considering the number of modes $M(E)$ as equation (17) to have,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \int_{-\infty}^{\infty} dE |E| \frac{\partial (1 + \text{Exp}(\frac{E-E_f}{K_B T}))^{-1}}{\partial E} \dots\dots\dots(18)$$

$$\text{Here, } -\frac{\partial f(E)}{\partial E} = \frac{e^{\frac{E-E_f}{K_B T}}}{\left(1 + e^{\frac{E-E_f}{K_B T}}\right)^2} \dots\dots\dots(19)$$

Substituting the derivation of Fermi Dirac function equation (19) into equation (18), we get:

$$G = \frac{2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^{\infty} dE |E| \frac{e^{\frac{-E-E_f}{K_B T}}}{\left(1 + e^{\frac{-E-E_f}{K_B T}}\right)^2} + \int_0^{\infty} dE |E| \frac{e^{\frac{E-E_f}{K_B T}}}{\left(1 + e^{\frac{E-E_f}{K_B T}}\right)^2} \right\} \dots\dots\dots(20)$$

Equation (20) can be rewritten as,

$$G = \frac{2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^{\infty} dE |E| \frac{e^{\frac{+E+E_f}{K_B T}}}{\left(1 + e^{\frac{+E+E_f}{K_B T}}\right)^2} + \int_0^{\infty} dE |E| \frac{e^{\frac{E-E_f}{K_B T}}}{\left(1 + e^{\frac{E-E_f}{K_B T}}\right)^2} \right\} \dots\dots\dots(21)$$

We noticed that equation (21) can be written as a derivation of Fermi-Dirac Distribution function with negative sign of E_f ,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^{\infty} dE |E| \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}(\frac{E+E_f}{K_B T})} \right) - \int_0^{\infty} dE |E| \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}(\frac{E-E_f}{K_B T})} \right) \right\} \dots\dots\dots(22)$$

The first and second terms in the previous equation can be integrated by parts, as : $u = E$ and $\partial v = dE \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}(\frac{E-E_f}{K_B T})} \right)$

We arrive to a final expression for the conductance,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ - \int_0^\infty \frac{dE}{1 + \text{Exp}\left(\frac{E+E_f}{K_B T}\right)} + \int_0^\infty \frac{dE}{1 + \text{Exp}\left(\frac{E-E_f}{K_B T}\right)} \right\} \quad \text{.....(23)}$$

Suppose, $\eta = \frac{E_f - \Delta}{K_B T}$ and $X = \frac{E - \Delta}{K_B T}$

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ - \int_0^\infty \frac{K_B T dX}{(1 + \text{Exp}(X + \eta))} + \int_0^\infty \frac{K_B T dX}{(1 + \text{Exp}(X - \eta))} \right\} \quad \text{.....(24)}$$

The terms in equations (3.24) represent the Complete Fermi-Dirac Distribution function $\mathcal{J}_j(X)$, similar to equation (3.7), to obtain the closed expression for the conductance as,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ K_B T \cdot \Gamma(1) \cdot \mathcal{J}_0(-\eta) - K_B T \cdot \Gamma(1) \cdot \mathcal{J}_0(\eta) \right\} \quad \text{.....(25)}$$

$$G = \frac{q^2 w K_B T}{\pi \hbar^2 v_f} \left\{ \mathcal{J}_0(-\eta) - \mathcal{J}_0(\eta) \right\} \quad \text{.....(26)}$$

Equation (26) describes the conductance of Silicene for zero gate voltage ($V_g = 0$) in absence of external electric field

($\Delta = \vec{E} \cdot \vec{L} = \frac{q}{2} (V_{g2} - V_{g1})$). When we use the Silicene as channel of Field Effect Transistor, the conductance of channel does not goes to zero gate voltage, unlike other materials, as we show in figure (3.4).

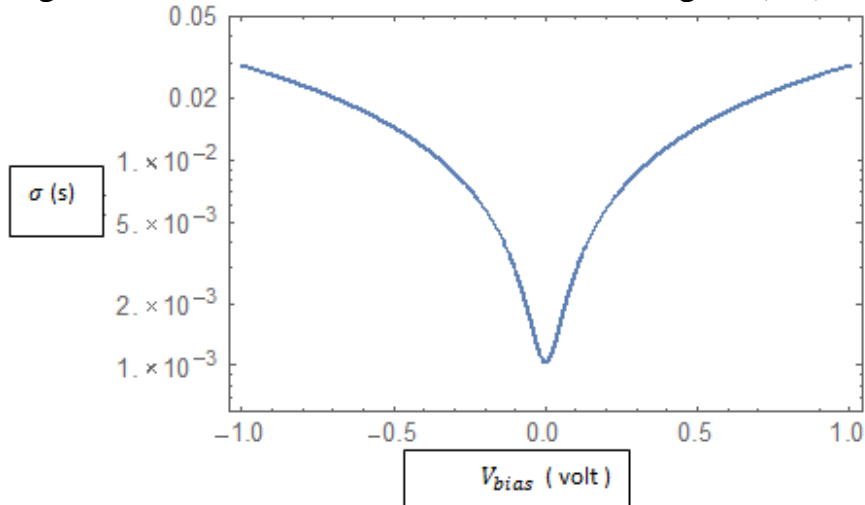


Figure (3.4): The analytical conductivity of Silicene against the bias voltage for zero external electric field, ($V_g = 0$).

Now, we consider the conductance of silicene in a Field Effect Transistor (FET) under effect of external perpendicular electric field ($V_g \neq 0$).

We will follow almost the same procedure to arrive to an analytical expression for the conductance (G). The number of modes in equation (16) ($M(E) = \frac{w}{\pi \hbar v_f} \sqrt{|E|^2 - \Delta^2}$) is taken. We can substitute $M(E)$ in Landauer's Formula, and expand $\sqrt{|E|^2 - \Delta^2}$ as : $|\frac{E^2}{2\Delta} - \Delta|$ by using Taylor expansion. This approximation is valid when $E^2 \ll 2\Delta$, and we know that Fermi Dirac Function always limit the conductance into few $K_B T$ and this confined Fermi energy which is 25.8 meV at room temperature. Therefore, the energy E is also confined to few $K_B T$, if we consider $\Delta > 500 \mu eV$, the difference between $\sqrt{|E|^2 - \Delta^2}$ and $|\frac{E^2}{2\Delta} - \Delta|$ is 1 % (it is fails when temperature decreasing). Therefore, the approximation is very good $\Delta > 500 \mu eV$ and $E^2 > 1 meV$.

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ \int_0^\infty dE \left| \frac{E^2}{2\Delta} - \Delta \right| \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}\left(\frac{E+E_f}{K_B T}\right)} \right) - \int_0^\infty dE \left| \frac{E^2}{2\Delta} - \Delta \right| \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}\left(\frac{E-E_f}{K_B T}\right)} \right) \right\} \quad \dots\dots(26)$$

Let us put : $u = \frac{E^2}{2\Delta} - \Delta$

$$\text{And } \partial v = dE \int_0^\infty dE \left| \frac{E^2}{2\Delta} - \Delta \right| \frac{\partial}{\partial E} \left(\frac{1}{1 + \text{Exp}\left(\frac{E-E_f}{K_B T}\right)} \right)$$

The first term in equation (26) is integrated by parts, the second term could be integrated in the same way but replace E_f with negative sign, equation (26) becomes

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ -\frac{1}{\Delta} \int_0^\infty \frac{EdE}{1+\text{Exp}\left(\frac{E+E_f}{c}\right)} + \frac{1}{\Delta} \int_0^\infty \frac{EdE}{1+\text{Exp}\left(\frac{E-E_f}{K_B T}\right)} \right\} \quad \text{Making change}$$

of variables , $\eta = \frac{E_f - \Delta}{K_B T}$ and $X = \frac{E - \Delta}{K_B T}$

Equation (26) could be obtained as,

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \left\{ -\frac{(K_B T)^2}{\Delta} \int_0^\infty \frac{K_B T dX}{(1+\text{Exp}(X+\eta))} + \frac{(K_B T)^2}{\Delta} \int_0^\infty \frac{K_B T dX}{(1+\text{Exp}(X-\eta))} \right\} \quad \dots\dots\dots(28)$$

Here , the first and second terms in equation (28) represent the Complete Fermi-Dirac function $\mathcal{J}_j(X)$ with first order ($j = 1$) to give the final analytical form expression for (G) as :

$$G = \frac{-2q^2}{h} \frac{w}{\pi \hbar v_f} \cdot -\frac{(K_B T)^2}{\Delta} \left\{ \Gamma(2) \cdot \mathcal{J}_0(-\eta) - \Gamma(2) \cdot \mathcal{J}_0(\eta) \right\} \quad \dots\dots\dots(29)$$

$$G = \frac{q^2 w (K_B T)^2}{\Delta \pi^2 \hbar^2 v_f} \left\{ \mathcal{J}_0(-\eta) - \mathcal{J}_0(\eta) \right\} \quad \dots\dots\dots(30)$$

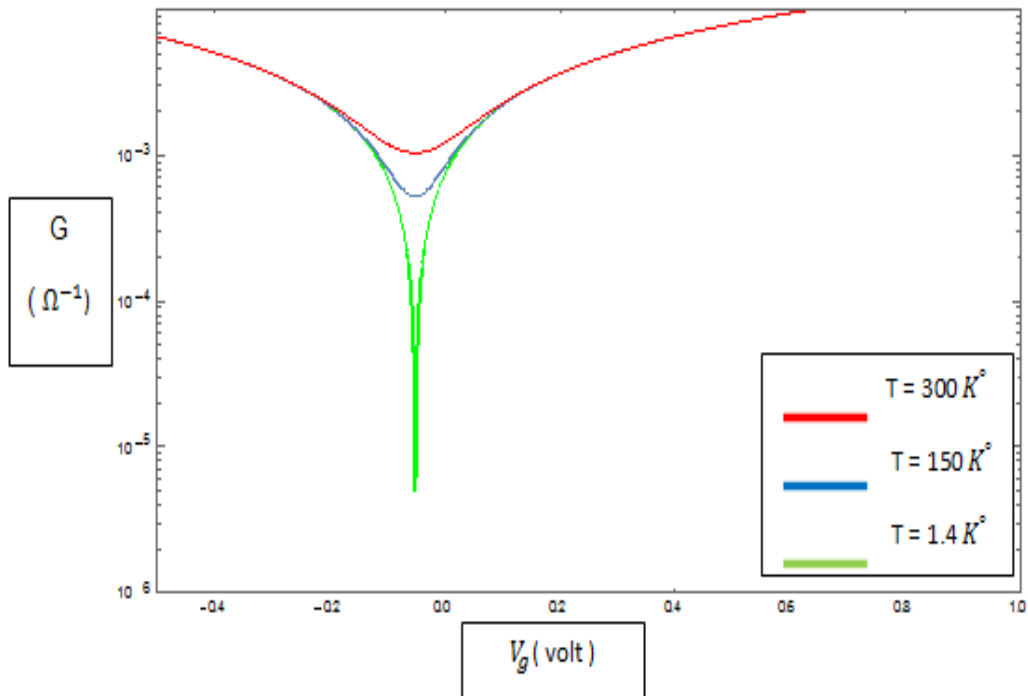


Figure (3.5): The conductance of Silicene versus gate voltage, at various temperatures.

Figure (3.5) shows the behavior of the conductance of Silicene on the effect of external electric field in the Field Effect Transistor (FET). It is clear that conductance (G) increasing with increase the gate voltage in the different temperature (T). Increasing as the minimum conductance increases with temperature.

For a single layer of Graphene, with zero band gap structure and linear dispersion relation ($E = \hbar v_f |k|$), the conductance of Graphene can be written as equation (26) : $G = \frac{q^2 w (K_B T)}{\pi^2 \hbar^2 v_f} \{ J_0(-\eta) - J_0(\eta) \}$, where $v_f = 1 \times 10^6$ m/s.

3.2 The Conductance calculations of Silicene in presence of external perpendicular electric field and effect of Spin Orbital Interaction (SOI)

In this part, we will derive and investigate the effect of spin orbital interaction on the conductivity of Silicene channel in Field Effect Transistor (FET). We start by taking the Hamiltonian of Silicene under effect of external electric field and consider the Spin Orbital Interaction (SOI).

$$H_{\eta}^{S_z} = \hbar v_f \begin{bmatrix} 0 & \eta k_x \\ \eta k_x & 0 \end{bmatrix} + \hbar v_f \begin{bmatrix} 0 & -i k_y \\ i k_y & 0 \end{bmatrix} + \begin{bmatrix} \eta \Delta_{so} & 0 \\ 0 & -\eta \Delta_{so} \end{bmatrix} + \begin{bmatrix} \Delta_z & 0 \\ 0 & -\Delta_z \end{bmatrix} \quad \dots\dots\dots(31)$$

$$H_{\eta}^{S_z} = \begin{bmatrix} \eta \Delta_{so} + \Delta_z & \hbar v_f (\eta k_x - i k_y) \\ \hbar v_f (\eta k_x + i k_y) & -\eta \Delta_{so} - \Delta_z \end{bmatrix} \quad \dots\dots\dots(32)$$

3.2.1 Calculation of dispersion energy under effect of external electric field and Spin Orbital Interaction (SOI):

To calculate the energy value ($E_{\eta}^{S_z}$), we take the determinant of Hamiltonian

$$|H_{\eta}^{S_z} - IE_{\eta}^{S_z}| = 0$$

$$\begin{vmatrix} \eta \Delta_{so} + \Delta_z & \hbar v_f (\eta k_x - i k_y) \\ \hbar v_f (\eta k_x + i k_y) & -\eta \Delta_{so} - \Delta_z \end{vmatrix} - \begin{vmatrix} E_{\eta}^{S_z} & 0 \\ 0 & E_{\eta}^{S_z} \end{vmatrix} = 0 \quad \dots\dots\dots(33)$$

$$-\eta \Delta_{so} + \Delta_z)^2 + |E_{\eta}^{S_z}| = \hbar^2 v_f^2 \eta^2 |k|^2 \quad \dots\dots\dots(34)$$

$$E_{\eta}^{S_z} = \pm \sqrt{\hbar^2 v_f^2 \eta^2 |k|^2 + (\eta \Delta_{so} + \Delta_z)^2} \quad \dots\dots\dots(35)$$

$$E_{\eta}^{S_z} = \pm \sqrt{\hbar^2 v_f^2 \eta^2 |k|^2 + \Delta_{s,\sigma_z}^2} \quad \dots\dots\dots(36)$$

Where $\Delta_{s,\sigma_z} = \eta \Delta_{so} + \Delta_z$

Equation (36) for silicene can be produced from (3) by replacing Δ_z by $\eta \Delta_{so} + \Delta_z$.

Here, \hbar is Planck's constant, v_f is a Fermi velocity of Dirac Fermions, η is +/- for k_+ / k_- Dirac points, (k_x, k_y) are the components of wave vector relative to the Dirac points. $(\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices which are equal $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, respectively. The spin index $S_z = +$ /- for spin up (\uparrow) and spin down (\downarrow), respectively. $\Delta_z = L E_z$, with $L = 0.23 \text{ \AA}^\circ$ is a band gap produced by external perpendicular electric field, here $\Delta_{so} = 3.9 \text{ meV}$ represents the spin orbital gap with 3.9 meV for Silicene, as table (1.1).

3.2.2 Calculation of carrier concentration of Silicene under effect of external electric field and Spin Orbital Interaction:

From equation (2.4), we can derive the density of state $D(E) = \sum_k \delta(E - E(k))$

$$D(E) = \frac{wL}{4\pi^2} \int_{-\infty}^{\infty} \delta(E - E_{\eta}^{S_z}(K)) \cdot \theta(E - E_{\eta}^{S_z}(K)) dE_{\eta}^{S_z} \dots\dots\dots(37)$$

$$= \frac{wL}{4\pi^2} \int_{-\infty}^{\infty} \delta(E - E_{\eta}^{S_z}(K)) \cdot \theta(E - E_{\eta}^{S_z}(K)) \cdot E_{\eta}^{S_z}(K) dE_{\eta}^{S_z} \dots\dots\dots(38)$$

$$D(E) = \frac{wL}{2\pi} \frac{1}{\hbar^2 v_f^2} |E| \theta(E - E(K)) \dots\dots\dots(39)$$

To calculate the number of carriers, and conductance of Silicene, we can apply the same procedure described in section (3.1)

$$n = \int dE D(E) f(E) \theta(E) \dots\dots\dots(40)$$

$$n = \int_0^{\infty} \frac{2wL}{\pi \hbar^2 v_f^2} |E_{\eta}^{S_z}| \cdot \theta(E_{\eta}^{S_z} - \Delta_{S,\sigma_z}) \cdot (1 + \text{Exp}(\frac{E-E_f}{K_B T}))^{-1} dE_{\eta}^{S_z} \dots\dots\dots(41)$$

$$n = \frac{2wL}{\pi \hbar^2 v_f^2} \{ (K_B T)^2 \cdot J_1(\eta) + \Delta_{S,\sigma_z} \cdot (K_B T) \cdot J_0(\eta) \} \dots\dots\dots(42)$$

where $\eta = \frac{E_f - \Delta_{S,\sigma_z}}{K_B T}$, $E_f = 25.8 \text{ meV}$ and $\Delta_{S0} = 3.9 \text{ meV}$, at Room temperature ($T = 300 \text{ K}^\circ$) [28].

3.2.3 Conductance calculation of Silicene under effect of external electric field and Spin Orbital Interaction:

Number of modes $M(E) = \sum_k \delta(E - E(k)) \frac{\pi \hbar}{L} |\mathcal{V}_x(k)|$ and dispersion relation

$$E_{\eta}^{S_z} = \pm \sqrt{\hbar^2 v_f^2 \eta^2 |K|^2 + \Delta_{S,\sigma_z}^2} \dots\dots\dots(43)$$

$$\text{so, } M(E) = \frac{w}{\pi \hbar v_f} \sqrt{|E|^2 - \Delta_{S,\sigma_z}^2} \dots\dots\dots(44)$$

the conductance of Silicene

$$G = \frac{2q^2}{h} \int_{-\infty}^{\infty} dE M(E) T(E) \cdot -\frac{\partial f(E)}{\partial E} \quad \dots\dots\dots(45)$$

$$G = \frac{q^2 w (K_B T)^2}{\Delta_{S,\sigma_Z} \pi^2 \hbar^2 v_f} \{ \mathcal{J}_0(-\eta) - \mathcal{J}_0(\eta) \} \quad \dots\dots\dots(46)$$

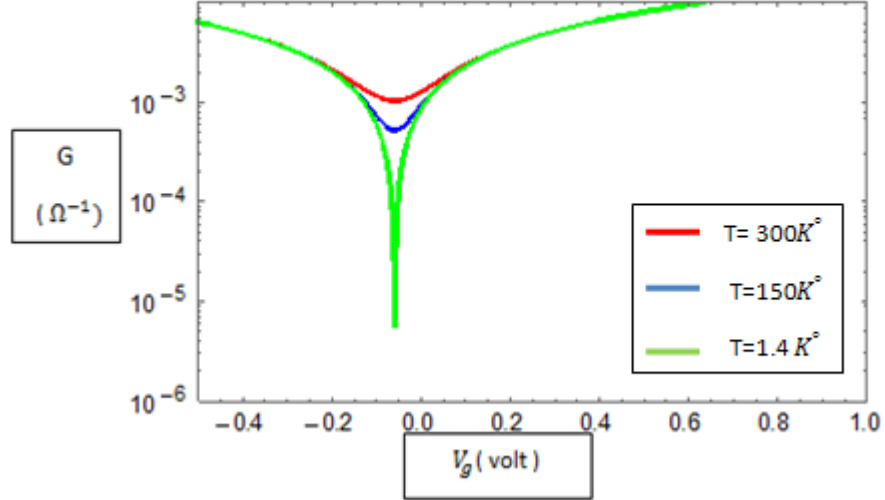


Figure (3.6): The conductance of Silicene under effect of SOI and external electric field.

We note that the conductance of Silicene under effect of Spin Orbital Interaction (SOI) has slightly different to the conductivity of Silicene when we hide the effect of (SOI), due to the effect in Spin Orbital band gap Δ_{S,σ_Z} . Recently, many theoretical works had calculated the band structure of Silicene using Density Functional Theory(DFT), which includes the effect of Spin Orbital Coupling (SOC) and external perpendicular electric field. The Spin Orbital band gap reach to 1.5 meV and it can be rise to 2.9 meV under strain [28].

We back to equation (15) in chapter two, the Hamiltonian contained two tunable parameter Δ_z and Δ_{so} , so we have three very interesting cases (i) $\Delta_z < \Delta_{so}$, (ii) $\Delta_z = \Delta_{so}$, and (iii) $\Delta_z > \Delta_{so}$.

$$H_{\eta}^{S_z} = v_f (\eta k_x \sigma_x + k_y \sigma_y) - \frac{1}{2} \eta \Delta_{so} \sigma_z + \frac{1}{2} \Delta_z \sigma_z \quad \dots\dots\dots(47)$$

The physical quantities in the electron Hamiltonian in equation (47) are defined as follow: The first term in the previous equation for Dirac electrons with velocity v_f (we take $\hbar = 1$), the second term is SOC with SOC band gap Δ_{SO} , the last term represent the perpendicular electric field E_z . Rashba SOC is included to the intrinsic SOC , as the Rashba SOC in order of ten times smaller than the intrinsic SOC, we can neglect it [28]. The Eigen values are evaluated from above Hamiltonian to be:

$$E_{\eta}^{S_z} = \pm \sqrt{v_f^2 |k|^2 + \frac{1}{4} (\Delta_z - \eta \sigma_z \Delta_{SO})^2} \quad \dots\dots\dots(48)$$

Equation (48) can be parameterized as follows:

$$E_{\eta}^{S_z} = \pm \sqrt{\hbar^2 v_f^2 \eta^2 |K|^2 + \frac{1}{4} (\Delta_z - \eta \sigma \Delta_{SO})^2} \quad \dots\dots\dots(49)$$

$$\frac{E_{\eta}^{S_z}}{\Delta_{SO}} = \pm \sqrt{\frac{\hbar^2 v_f^2 \eta^2 |K|^2}{\Delta_{SO}} + \frac{1}{4} \left(\frac{\Delta_z}{\Delta_{SO}} - \eta \sigma \right)^2} \quad \dots\dots\dots(50)$$

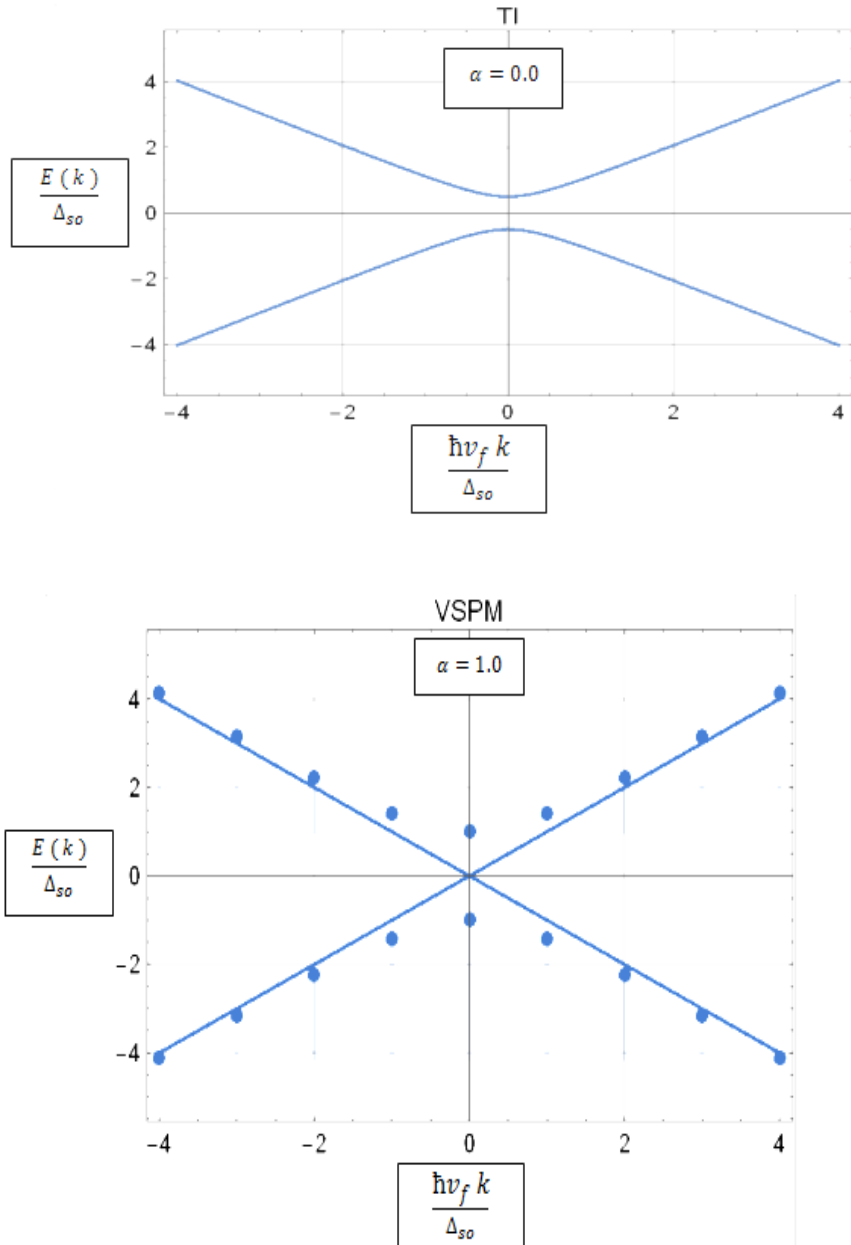
Let's assume $Y \rightarrow \frac{E_{\eta}^{S_z}}{\Delta_{SO}}$, $X \rightarrow \frac{\hbar^2 v_f^2 \eta^2 |K|^2}{\Delta_{SO}}$ and $\alpha = \frac{\Delta_z}{\Delta_{SO}}$

$$Y = \pm \sqrt{X^2 + \frac{1}{4} (\alpha - \eta \sigma)^2} \quad \dots\dots\dots(51)$$

This equation could be represented by the factor of (α). As we mentioned previously, where $\alpha = \frac{\Delta_z}{\Delta_{SO}}$, we have three cases $\alpha < 1$, $\alpha = 1$ and $\alpha > 1$.

These cases are plotted in figure (3.2.2). For the value of $\Delta_z = 0.5 \Delta_{SO}$ ($\alpha < 1$), the band spin-split reversed at the k points and spin up-down, which it is vary, in this state the band spin-split described as a topological insulator (TI) . when $\Delta_z = \Delta_{SO}$ ($\alpha = 1$) at this critical point, the gap of one spin-split

bands is closed to the Dirac point ($E_g = 0$) where the others is gaped ($E_g \neq 0$). This is called a valley spin-polarized metal (VSPM)[40, 41, 42].



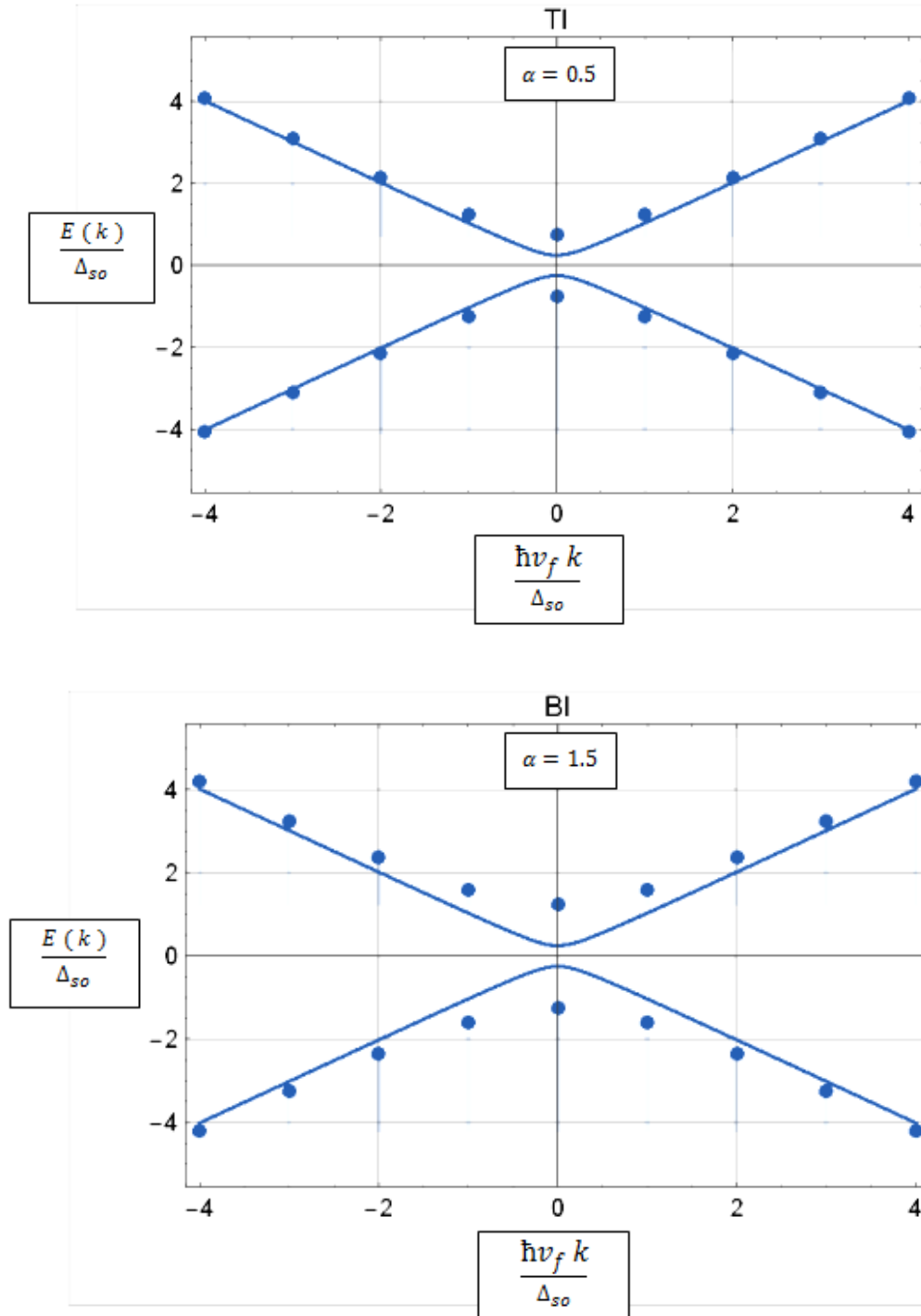


Figure (3.7): Electronic band structure of Silicene at k Dirac point, at three regions: TI, VSPM and BI.

If $E_z = 0 \rightarrow \frac{\Delta_z}{\Delta_{so}} = 0$ ($\alpha = 0$) in this case, the spin-split is one gap edge no further jump since the density of state. The following formula of density of state

$$N(E) = \sum_{\sigma,\eta} N_{\sigma,\eta}(E) \quad \dots\dots\dots(52)$$

$$\text{Where } N_{\sigma,\eta}(E) = \frac{|E|}{2\pi\hbar^2 v_f^2} \theta(2|E| - \Delta_{\sigma,\eta}) \quad \dots\dots\dots(53)$$

And $\Delta_{\sigma,\eta} = \Delta_z - \eta\sigma \Delta_{so}$ with $\sigma = \pm$ index of spin up and down for k, k' Dirac points, respectively.

Equation (52) can be formulated :

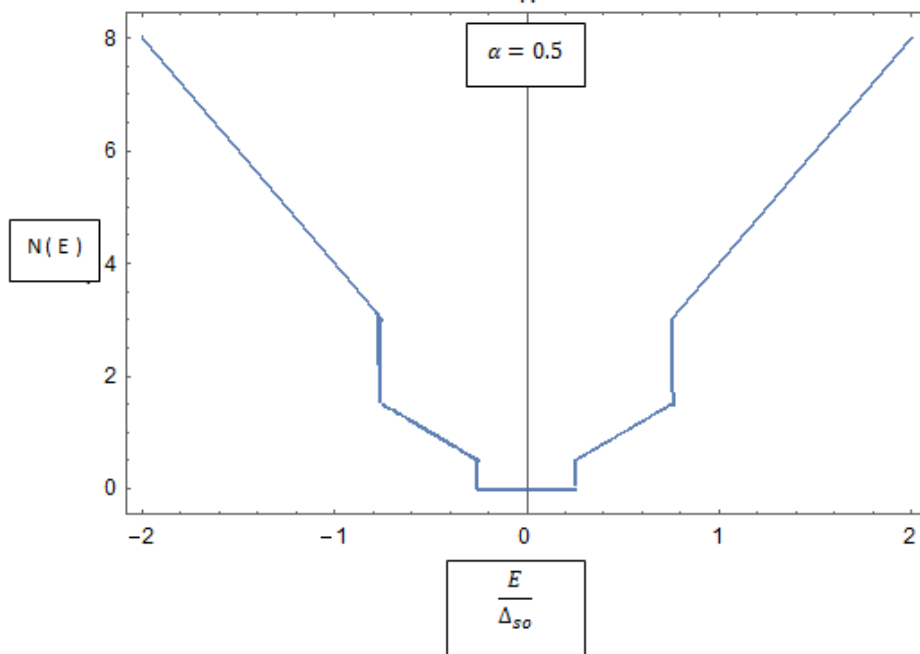
$$\frac{N_{\sigma,\eta}(E)}{\Delta_{so}} = \frac{|E|}{2\pi\hbar^2 v_f^2} \frac{1}{\Delta_{so}} \theta(2 \frac{|E|}{\Delta_{so}} - \frac{\Delta_z}{\Delta_{so}} - \sigma \eta) \quad \dots\dots\dots(54)$$

If we assume $\frac{|E|}{2\pi\hbar^2 v_f^2} \frac{1}{\Delta_{so}} = ee$ and $\alpha = \frac{\Delta_z}{\Delta_{so}}$ equation (51) becomes

$$N(E) = \sum_{\sigma,\eta} \frac{1}{2\pi\hbar^2 v_f^2} (ee) \theta(2|ee| - \alpha - \sigma \eta) \quad \dots\dots\dots(55)$$

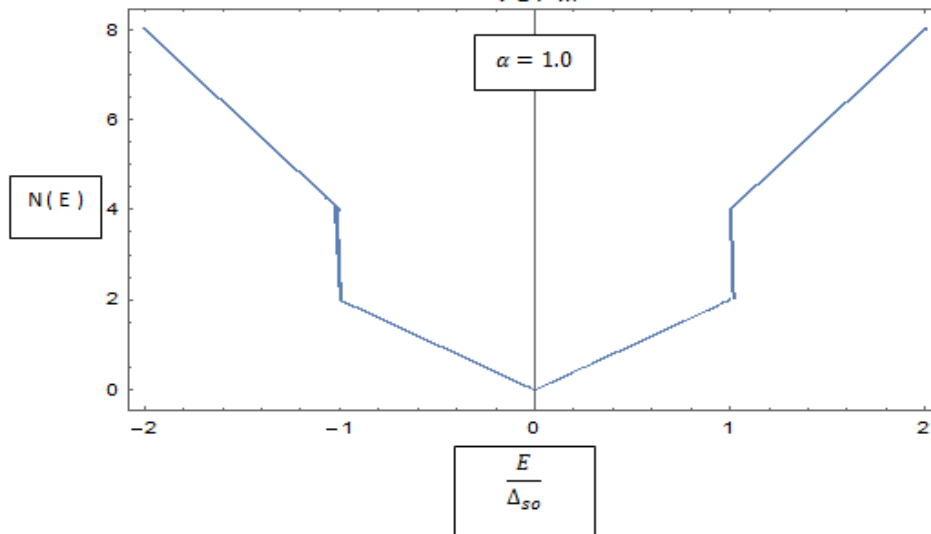
A plot of the energy band shows in the figure (3.7) which the solid curve () indicate the gap for spin up and dashed line (-----) for the gap of spin down at k point.

TI



$\frac{E}{\Delta_{SO}}$
$\frac{E}{\Delta_{SO}}$

VSPM



Chapter Four

Conclusion

In this work, we have considered a field effect transistor (FET) with a channel made from a Silicene material. We have presented in details the derivation of carrier concentration expression relation of Silicene. the dependence of sheet concentration on the gate voltage at difference temperature had been calculated numerically and displayed.

In addition, the conductance of the Silicene monolayer as a channel had been studied. We have investigated the effects of both the external applied gate voltage and spin-orbit interaction (SOI) on the density of state and the conductance of the Silicene as a 2D nonmaterial sheet channel in the field effect transistor (FET).

Our computed results show the significance of the effect of temperature, external gate voltage and spin-orbit interaction (SOI) on tuning the material properties of the Silicene nonmaterial sheet.

References

- (1) Sadeghi, H, **Journal of Nanoscience and Nanotechnology**, Volume 14 : 4178-4184 (2014).
- (2) Lew Yan Voon L. C, Zhu J, and Schwingen U, ***Silicene: Recent theoretical advances***, **Applied Physics Review** 3, 040802(2016).
- (3) Gian G. Guzmán-Verri and L. C. Lew Yan Voon. ***Electronic structure of silicon-based nanostructures***, **Phys. Rev. B** 76, 075131 (2007).
- (4) Gahangirov, S. Topsakal, M and Akturk, E et al. ***Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium***, **Phys Rev Lett.** 102:236804 (2009).
- (5) Ouyang, FP. Peng. SL and Liu, ZF et al. ***Bandgap opening in graphene antidot lattices: the missing half***, **ACS Nano** 5: 4023-30 (2011).
- (6) Pardo, V and Pickett, WE. ***Half-Metallic Semi-Dirac-Point Generated by Quantum Confinement in TiO₂/VO₂ Nanostructures***, **Phys. Rev. Lett.** 102 166803 (2009).
- (7) M. Z. Hasan and C. L. Kane, ***Colloquium: Topological insulators***, **Rev. Mod. Phys.** 82, 3045 (2010).
- (8) K. S. Novoselov, A. K. Geim, S. V. Morozoo, D. Jiang, M. L. Katsnelson, L. V. Griyorieva, S. V. Dubonos, A. A. Firsov, ***Two-dimensional gas of massless Dirac fermions in graphene***. **Nature** 438,197 (2005).
- (9) Xiao-Liang Qi and Shou-Cheng Zhang. ***Topological insulators and superconductors***, **Rev. Mod. Phys.** 83, 1057 (2011).

- (10) C. Bai, X. Zhang, *Electronic structures of silicon nanoribbons*, **Phys. Rev. B** **76**, 075403 (2007).
- (11) H. Min, J. E. Hill, N. A. Sinitsyn, B. R. Sahu, L. Kleinman, A. H. MacDonald, *Charge and Spin Transport in Disordered Graphene-Based Materials*, **Phys. Rev. B** **74**, 165310 (2006).
- (12) Y. Yao, F. Ye, X-L. Qi, S-C. Zhang, Z. Fang, *Spin-orbit gap of graphene: First-principles calculations*, **Phys. Rev. B** **75**, 041401 (R) (2007).
- (13) A. O' hare, F. Kusmartsev, and K. I. Kugel, *A Stable "Flat" Form of Two-Dimensional Crystals: Could Graphene, Silicene, Germanene Be Minigap Semiconductors?* **Nano Lett.** **12**, 1045 (2012).
- (14) C. Bai, X. Zhang, *Analytic approach to the ground-state energy of charged anyon gases*, **Phys. Rev. B** **76**, 075403 (2007).
- (15) F. Schwierz, *Graphene transistor*. **Nat. Nanotechnol.** **5**, 487-496 (2010).
- (16) Huang, W. Kang, and L. Yang, *Electronic Structure and Quasiparticle Band Gap of Silicene Structures*, **arXiv:1212.2305** (2012).
- (17) P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M. C. Asensio, A. Resta, 13. Ealet, and G. Le Lay, *Silicene: Compelling Experimental Evidence for Graphenelike Two-Dimensional Silicon*, **Phys. Rev. Lett.** **108**, 155501 (2012).
- (18) C. Kamal, A. Chakrabarti, A. Banerjee and S. Deb, *Silicene Beyond Mono-layers - Different Stacking Configurations and Their Properties*, **arXiv: 1210.4733** (2012).

- (19) M.I. Katsnelson, *Graphene: Carbon in Two Dimensions* (Cambridge University Press, Cambridge, 2012).
- (20) Sadeghi H, Redoute J. M, Lai D. T. H, Ahmadi M. T, Ismail R, *Smart Nano-Micro Material and Devices*, Vol. 8204, 820420. 2011 SPIE. CCC code: 0277-786X/11/\$18. Doi: 10.1117/12.903196.
- (21) Kyozauro Takeda and Kenji Shiraishi, *Theoretical possibility of stage corrugation in Si and Ge analogs of graphite*, *Phys. Rev.* **50**, 14916 (1994).
- (22) S. Cahangirov, M. Topsakal, E. Aktürk, H. Şahin, and S. Ciraci, *Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium*, *Phys. Rev. Lett.* **102**, 236804 (2009).
- (23) Suman Chowdhury, Santu Baidya, Dhani Nafday, Soumyajyoti Haldar, Mukul Kabir, Biplab Sanyal, Tanusri Saha-Dasgupta, Debnarayan Jana, Abhijit Mookerjee, *A real-space study of random extended defects in solids: Application to disordered Stone–Wales defects in graphene*, *Physics E* **61**, 191- 197 (2014).
- (24) Paola De Padova, Paolo Perfetti, Bruno Olivieri, Claudio Quaresima, Carlo Ottaviani and Guy Le Lay. *1D graphene-like silicon systems: silicene nano-ribbons*, *Phys. Condens. Matter* **24**, 223001 (2012).
- (25) Mingsheng Xu, Tao Liang, Minmin Shi, and Hongzheng Chen. *Graphene-Like Two-Dimensional Materials*, *Chem. Rev.* **113**, 3766-3798 (2013).

- (26) B. Lalmi, H. Oughaddou, H. Enriquez, A. Kara, S. Vizzini, B. Ealet, B. Aufray, Appl. *First-principles calculation of intrinsic carrier mobility of silicene* , **Phys. Lett.** **97** 223109 (2010).
- (27) S. Cahangirov, M. Topsakal, E. Akturk, H. Sahin, S. Ciraci, *Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium*, **Phys. Rev. Lett.** **102**, 236804 (2009).
- (28) Y. Ding, J. N. Appl. *Electronic structures of silicon nanoribbons*, **Phys. Lett.** **95** 083115 (2009).
- (29) G. Le Lay, B. Aufray, C. Léandri, H. Oughaddou, J. P. Biberian, P. De Padova, M. E. Dávila, B. Ealet, A. Kara. *Physics and chemistry of silicene nano-ribbons*, **Volume 256**, 524-529 (2009).
- (30) H. Nakano, T. Mitsuoka, M. Harada, K. Horibuchi, H. Nozaki, N. Takahashi, T. Nonaka, Y. Seno, and H. Nakamura, *Angew. Soft synthesis of single-crystal silicon monolayer sheets*, **Chem. Int. Ed.** **45**, 6303 (2006).
- (31) J. M. Solar, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejón, and D. Sanchez-Portal, *J. The SIESTA Method for ab Initio Order-N Materials Simulation*, **Phys.: Condens. Matter** **14**, 2745 (2002).
- (32) S. Cahangirov, M. Topsakal, E. Akturk, H. Sahin, and S. Ciraci, *Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium*, **Phys. Rev. Lett.** **102**, 236804 (2009).
- (33) J. B. Oostinga, H. B. Heersche, X. Liu, A. F. Morpurgo and L. M. K. Vandersypen, *Gate-induced insulating state in bilayer graphene devices*. **Nature Mater.** **7**, 151 (2008).

- (34) P. R. Wallace, *The Band Theory of Graphite*, *Phys. Rev.* **71**, 622 (1947).
- (35) S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge University Press New York, US (2005).
- (36) I. Ahmed, M. Tahir, K. Sabeeh, *Prediction of topological Nernst effect in silicene and similar 2D materials*, arXiv:1402.6113v1 [cond-mat.mes-hall].
- (37) C. Kamal, *cond-mat.mes-hall*, arXiv: 1202.2636v1.
- (38) Y. Yao, F. Ye, X. L. Qi, S. C. Zhang, and Z. Fang, *Spin-orbit gap of graphene: First-principles calculations*, *Phys. Rev. B* **75**, 041401 (2007).
- (39) C. C. Liu, W. Feng, and Y. Yao, *Quantum Spin Hall Effect in Silicene and Two-Dimensional Germanium*, *Phys. Rev. Lett.*, **107**, 076802 (2011).
- (40) N. D. Drummond, V. Zolyomi, V. I. Fal'ko, *Electrically tunable band gap in Silicene*, *Phys. Rev. B* **85**, 075423 (2012).
- (41) Z. Ni, Q. Liu, K. Tang, J. Zhou, R. Qin, Z. Gao, D. Yin, J. Lu, *Tunable bandgap in silicene and germanene*, *Nano Lett.* **12** 113 (2012).
- (42) M. Ezawa, *A topological insulator and helical zero mode in silicene under an inhomogeneous electric field*, *New J. Phys.* **14**, 033003 (2012).
- (43) Sahin, H., Cahangirov, S., Topsakal, M., Bekaroglu, E., Aktürk, E., Senger, R.T., Ciraci, *Monolayer honeycomb structures of group-IV*

elements and III-V binary compounds: First-principles calculations,
Phys. Rev. B **80**, 155453 (2009).

(44) Tao, L. et al. *Silicene field-effect transistors operating at room temperature*. **Nat. Nanotech.** **10**, 227-231 (2015).

جامعة النجاح الوطنية

كلية الدراسات العليا

حسابات الموصليه للترانسستور (FET) المصنع من مادة السيليسين

إعداد

فاطمة هلال هليل معالي

إشراف

أ.د. محمد السعيد

قدمت هذه الأطروحة استكمالاً لمتطلبات الحصول على درجة الماجستير في الفيزياء في كلية الدراسات العليا في جامعة النجاح الوطنية – نابلس.

2018

ب
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المخلص

قمنا في هذه الأطروحة بحساب تركيز النواقل الموجودة في صفيحة السيلييسين المستعملة كقناة توصيل في قطعة الترانسسستور (FET) واعتمادها على جهد البوابه (V_g) و درجة الحرارة. تم ايضاً عرض حسابات تحليلية وتفصيلية لموصلية الصفيحة باستخدام صيغة لانداور (Landauer) وتحت تأثير مجال كهربائي خارجي و عامودي على الصفيحة والأخذ بعين الاعتبار التأثير الناتج عن ظاهرة التفاعل ما بين حركتي الالكترون: المغزلية والمدارية. أظهرت نتائج الدراسة أهمية تأثير العاملين المذكورين على الخواص المادية لصفحة السيلييسين مثل: الموصلية والحزم البنونية وكثافة المستويات.