

Density Functional Theory concept and determine Germanium solid properties

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Jun 20 2023

Abstract

In quantum mechanics many bodies problems cannot be solved analytically from Schrodinger equation direct. Moreover, when we use Schrodinger equation to solve it numerically by descrtizing the space of $3N$ dimension where N is quantum particles number, then its data cannot be include in any super computer due to its very huge complexity addition to its huge time need to finish the calculation. However, There are some methods that could be used to approximate the system such as density functional theory and pseudopotential calculation. By density functional theory (*DFT*) the problem could be solved by using an approximation to the charge density and then the equation will be solved depends on the charge density. Also, by pseudopotential method the wavefunction could be approximate inside the core by some smooth function with some properties to be consistence with the origin wavefunction solution. In this article, the concept of *DFT* had been introduced include some useful theorems. Then, some properties of germanium semiconductor *Ge* had been determined by using Quantum Espresso software based on *DFT* and pseudo-potential files.

1 Introduction

Schrodinger equation for multiple interacted bodies systems cannot be solved analytically. Unfortunately, numerical solution need to much memory and time to find the eigenvalue and eigenfunction of the Hamiltonian operator for the non interacting particles. The Hamiltonian operator can be written as [Cottenier et al., 2002]:

$$\begin{aligned} \bar{H} = & - \sum_{i=1} \frac{\hbar^2}{2M_i} \nabla_{R_i}^2 - \sum_{i=1} \frac{\hbar^2}{2m} \nabla_i^2 \\ & - \frac{1}{4\pi\epsilon_0} \sum_{i,j} \frac{e^2 Z_i}{|\vec{r}_i - \vec{R}_j|} + \frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \\ & + \frac{1}{8\pi\epsilon_0} \sum_{i \neq j} \frac{e^2 Z_i Z_j}{|\vec{R}_i - \vec{R}_j|} \end{aligned} \quad (1)$$

Where M_i , m are the mass of the atoms and the electrons respectively, Z_i the atom charge and R_i , r_i are the position of the atoms and electrons respectively. So, the first two terms represent the kinetic energy of atoms and electrons respectively, third term is for the potential energy between electrons and atoms, fourth term is the electrons interaction potential energy and the last term for the potential energies between atoms. But since equa-

tion 1 is hard to solve, we need to make some approximation and use some theorems and software to solve it for a specific complex system.

2 Approximations

In this section many approximation may be used to simplify equation 1.

2.1 The Born-Oppenheimer approximation

Since the nuclei is much heavier than electrons, so is can be assumed to be fixed. Which mean that its kinetic energy is about zero. Farther more, we can now say that the last term of equation 1 is some constant. Then, the Hamiltonian can be reduced to [Cottenier et al., 2002]:

$$\hat{H} = \hat{T} + \hat{V} + V_{ext} \quad (2)$$

Where \hat{T} is the electrons kinetic energy, \hat{V} is the electrons interaction potential and V_{ext} is the external potential from the nuclei.

2.2 Density Functional approximation (Kohn-Sham equation)

In this approximation we can use the density of electrons to solve Schrodinger equation depends on the theorems of Hohenberg and Kohn [Baerends, 2001] that say the expected value of the wave function Ψ could be written as a density functional $\Psi[\rho]$. And since for any operator \hat{O} the expected value is depends on the wave function $\langle \Psi[\rho] | \hat{O} | \Psi[\rho] \rangle$ so the operator itself could be written as a density functional. So, the Hamiltonian operator can be written as a density functional as the relation:

$$\langle \Psi | \hat{H} | \Psi \rangle = E[\rho] \quad (3)$$

Now once can use Kohn-Sham equation to deal with the problem [Yang et al., 2009].

$$E[\rho] = T[\rho] + V_{ext}[\rho] + V_{e-e}[\rho] + V_{xc}[\rho] \quad (4)$$

Where $T[\rho]$ is the kinetic energy, $V_{ext}[\rho]$ the external potential energy comes from the nuclei, $V_{e-e}[\rho]$ the electrons interaction potential and $V_{xc}[\rho]$ the exchange correlation potential which is like an error come due to the approximation of taking non interacting electrons model, we will talk about xc in coming section 2.3. So, this equation based on dealing with the electrons as non interacting particle so we solve initially for this fictitious system and write the wave function as the form:

$$\Psi(r_1, r_2, \dots, r_N) = |\phi_1(r_1), \phi_2(r_2), \dots, \phi_N(r_N)| \quad (5)$$

And the Hamiltonian operator could be written as the relation:

$$\hat{H} = \sum_{i=1}^N \hat{h}_i \quad (6)$$

Where \hat{h}_i operator could be written as the Schrodinger-like Kohn-Sham equation:

$$\hat{h}_i = \frac{\hbar^2}{2m} \nabla_i^2 + V_{e-e} + V_{ext} + V_{xc} \quad (7)$$

Where the operators terms are as the following [Cottenier et al., 2002]:

- The Hetree potential

$$V_{e-e} = \frac{e^2}{4\pi\epsilon_0} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' \quad (8)$$

- The external potential:

$$V_{ext} = \frac{e^2}{4\pi\epsilon_0} \sum_{i=1}^N \frac{Z_i}{|\vec{R}_i - \vec{r}|} \quad (9)$$

- The exchange correlation potential which is the functional derivative of the exchange correlation energy:

$$V_{xc} = \frac{\delta E_{xc}[\rho]}{\delta \rho} \quad (10)$$

Finally, the density could be find by the relation:

$$\rho(r) = \sum_{i=1}^N |\phi_i(r)|^2 \quad (11)$$

So, we can use Poisson's equation to write equation 8 as the following:

$$\nabla^2 V_{e-e}(\vec{r}) = 4\pi\epsilon_0 \rho(\vec{r}) \quad (12)$$

Then, the problem could be solved as the following [Cottenier et al., 2002]:

- Make an initial guess of the electrons density $\rho(r)$
- Solve the Kohn-Sham equation with the Hamiltonian [equation 7] to find the eigenfunction for each electrons:

$$\hat{h}_i \phi_i = \epsilon_i \phi_i \quad (13)$$

- calculate the new density from the equation 11. Now, this new value will be compared with the previous one and the accepted value will be used when it converge.

2.3 Local Density Approximation

In this approximation we will discuss the importance to include the term $E_{xc}[\rho]$ or $V_{xc}[\rho]$ in the Hamiltonian operator. First of all, in equation 4 we can see that without the last term correction there is a wrong description of the system with just one electron, so it will provide the self interaction electrons. Addition to that, it will describe how electrons avoid each other due to Pauli exclusion principle (exchange energy x) and also the repulsion between electrons (correlation energy c).

Now, from equation 7 we can note that the exchange correlation potential (V_{xc}) does not known till now. So, here we need to do another approximation which will be the local density approximation (LDA) [Cottenier et al., 2002]. From this approximation we can get E_{xc}^{LDA} as the relation:

$$E_{xc}^{LDA} = \int \rho(\vec{r}) \epsilon_{xc}(\rho(\vec{r})) d\vec{r} \quad (14)$$

Where the function $\epsilon_{xc}(\rho(\vec{r}))$ is the exchange correlation energy by electron for the homogeneous electron gas that could be written as [Harrison, 2003]:

$$\epsilon_{xc}(\rho(\vec{r})) = \epsilon_x(\rho(\vec{r})) + \epsilon_c(\rho(\vec{r})) \quad (15)$$

$$\epsilon_x(\rho(\vec{r})) = -C\rho^{1/3} \quad (16)$$

And the correlation function could be calculated by quantum Monte Carlo method.

3 Pseudo-potential Method

In this method there are several approximation that help us to eliminate some complex computational calculations that need more memory space and huge time to do that calculations. For instance, we know that the atoms which contain a large number of electrons will have valence electrons and core electrons. Fortunately, the core electrons are more localized and we can ignore including them in quantum calculations and replace them by an effective potential that approximate the effect on the valence electrons and do the calculations for just the valence electrons. [Sholl and Steckel, 2022].

Now, we can approximate the wavefunction inside the core to be more smoother since in general it will contains many oscillations. In general, using $\phi_i(r) = r\psi_i(r)$ and do some correction in the potential to use the effective potential to make Schrodinger equation as the form:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}\right)\psi_i(r) = \epsilon_i\psi_i(r) \quad (17)$$

And the wavefunction of the valence electron could be written as an expansion of the core states addition to a smooth function (say $|\phi\rangle$). Then the valence state $|\psi\rangle$ could be written as the following:

$$|\psi\rangle = |\phi\rangle - \sum_n^{core} \langle\chi_n|\phi\rangle |\chi_n\rangle \quad (18)$$

Where $|\chi_n\rangle$ are the core states. Now, apply the Hamiltonian operator and knowing that $\hat{H}|\psi\rangle = E|\psi\rangle$:

$$\hat{H}\left(|\phi\rangle - \sum_n^{core} \langle\chi_n|\phi\rangle |\chi_n\rangle\right) = E\left(|\phi\rangle - \sum_n^{core} \langle\chi_n|\phi\rangle |\chi_n\rangle\right) \quad (19)$$

Simplifying equation and substitute $\hat{H}|\chi_n\rangle = E_n|\chi_n\rangle$ 19 to get:

$$\hat{H}|\phi\rangle + \sum_n^{core} (E - E_n) \langle\chi_n|\phi\rangle |\chi_n\rangle = E|\phi\rangle \quad (20)$$

Finally, we can write equation 20 as the form:

$$(\hat{H} + \hat{V}_{nl})|\phi\rangle = E|\phi\rangle \quad (21)$$

Now, the extra potential \hat{V}_{nl} depending on n and l states due to the spherical symmetry. Since the E energy for the valence state and E_n energy for the core state we can say that $E_n > E$. So, \hat{V}_{nl} is a repulsive potential. [Kresse and Joubert, 1999].

3.1 Norm-Conserving Pseudo-potential

The norm conserving pseudo-potential allow us to use the smooth state inside the core (for $r < r_c$). Then we have the relations:

1. real and pseudo state have the same value outside the cutoff r_c .

$$\psi_{nl}^{AE}(r) = \psi_{nl}^{PS}(r) \text{ for } r > r_c \quad (22)$$

Where $\psi_{nl}^{AE}(r)$ and $\psi_{nl}^{PS}(r)$ are the all electron state and pseudo-potential state respectively.

2. The probability of the probability density function of real and pseudo states are the same inside the cutoff.

$$\int_0^R |\phi_{nl}^{AE}(r)|^2 r^2 dr = \int_0^R |\phi_{nl}^{PS}(r)|^2 r^2 dr \text{ for } R < r_c \quad (23)$$

where we here use $r\phi_{nl}(r) = \psi_{nl}(r)$.

3. The real and pseudo state have the same eigenvalues.

$$E_{nl}^{PS} = E_{nl}^{AL} \quad (24)$$

[Reis et al., 2003].

After that, to get the norm conserving pseudo-potential we need to do the following steps

1. Solve the all electron atomic system and decide which are core and which are valence.
2. Generate the pseudo-potential V_{nl} for the valence state. This generation could be done using Kerker method which have been done by construct the pseudo state by a function $e^{p(r)}$ where $p(r)$ is a 4th order polynomial which will matching with the true solution and its derivatives at r_c .
3. After that, we can get $V_{nl}(r)$ from the inverse of Schrodinger equation as the relation:

$$V_{nl,total}(r) = \epsilon - \left[\frac{l(l+1)}{2r^2} - \frac{\frac{d^2}{dr^2}\phi_{nl}^{PS}(r)}{\phi_{nl}^{PS}(r)} \right] \quad (25)$$

Where also here we use $\psi(r) = r\phi(r)$.

4. Finally, the pseudopotential will be:

$$V_{nl} = V_{nl,total} - V_{Hxc}^{PS} \quad (26)$$

Where V_{Hxc}^{PS} comes from the Hartree and exchange-correlation terms.

3.2 Semi-local Pseudo-potential

Now from the equations 20 and 21, knowing that $|\chi_n\rangle$ are the core state and it is spherical symmetry since it will finally replace the potential of a nucleus. So, we can write the pseudo-potential operator as the relation:

$$\hat{V}_{SL} = \sum_{lm} |Y_{lm}\rangle V_{nl}(r) \langle Y_{lm}| \quad (27)$$

Where $|Y_{nl}\rangle$ is the spherical harmonic state. Now, consider the plane wave state $|k\rangle = e^{i\vec{k}\cdot\vec{r}}$. We can see that the semi-local pseudo-potential create several problems on the plane wave. We can see it by some straightforward algebra:

$$\begin{aligned} \langle k | \hat{V}_{SL} | k' \rangle &= \frac{1}{\Omega} \sum_{lm} \int \int e^{-i\vec{k}\cdot\vec{r}} \\ &\quad \times Y_{lm}^*(\theta, \phi) V_{nl}(r) Y_{lm}(\theta', \phi') \\ &\quad \times e^{i\vec{k}'\cdot\vec{r}} r^2 dr d\Omega' d\Omega \end{aligned} \quad (28)$$

Using series expansion of the exponential and the theorem of the summation of spherical harmonic respectively:

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r}) \quad (29)$$

$$\sum_m Y_{lm}^*(\hat{k}') Y_{lm}(\hat{k}) = \frac{2l+1}{4\pi} P_l(\cos(\theta_{\vec{k}\vec{k}'})) \quad (30)$$

Where $j_l(kr)$ is Bessel function and $P_l(\cos(\theta_{\vec{k}\vec{k}'}))$ is Legendre polynomial function. Substitute equation 29 in 28 and using equation 30 to get the final relation:

$$\begin{aligned} \langle k | \hat{V}_{SL} | k' \rangle &= \frac{4\pi}{\Omega} \sum_l (2l+1) \int j_l(kr) j_l(k'r) \\ &\quad \times P_l(\cos(\theta_{\vec{k}\vec{k}'})) V_l(r) r^2 dr \end{aligned} \quad (31)$$

3.3 The Kleinman-Bylander Transformation

As we see in [sec 3.2] the semi-local pseudo-potential have some difficulty due to its locality on the radial coordinate. So, Kleinman and Bylander define a non-local pseudo-potential that depends on the radial part and do an action on the pseudo-state as same as the semi-local pseudo-potential as equation [eq: 32]

$$\hat{V}_l^{NL} |\phi_{lm}^{PS}\rangle = \hat{V}_l^{SL} |\phi_{lm}^{PS}\rangle \quad (32)$$

So, we need to find the pseudo wave function ϕ_{lm}^{PS} correspond with the pseudo-potential. We can construct the local part V_L which is a complete arbitrary function that has a long range behavior of the real potential, and subtract it from the semi-local pseudo-potential to get the

non-local part V_{NL} . This non-local operator could be construct as the relation:

$$\hat{V}_{NL} = \sum_l \hat{V}_l^{NL} = \sum_{lm} \frac{|\hat{V}_l^{SL} \phi_{lm}^{PS}\rangle \langle \phi_{lm}^{PS} \hat{V}_l^{SL}|}{\langle \phi_{lm}^{PS} | \hat{V}_l^{SL} | \phi_{lm}^{PS} \rangle} \quad (33)$$

So, using equation [eq: 33] and affect the non-local pseudo-potential on the pseudo state then it will be as [eq: 34]

$$\begin{aligned} \hat{V}_l^{NL} |\phi_{lm}^{PS}\rangle &= \frac{\hat{V}_l^{SL} |\phi_{lm}^{PS}\rangle \langle \phi_{lm}^{PS} | \hat{V}_l^{SL} | \phi_{lm}^{PS} \rangle}{\langle \phi_{lm}^{PS} | \hat{V}_l^{SL} | \phi_{lm}^{PS} \rangle} \\ &= \hat{V}_l^{SL} |\phi_{lm}^{PS}\rangle \end{aligned} \quad (34)$$

Which is consist with the equation [eq: 32]

In plane wave representation, by finding the expectation value of the non-local pseudo-potential (ie. $\langle k | \hat{V}_l^{NL} | k \rangle$), we can get the matrix element as the equation [eq: 35]:

$$\langle k | \hat{V}_l^{NL} | k' \rangle = \frac{\langle k | \hat{V}_l^{SL} \phi_{lm}^{PS} \rangle \langle \phi_{lm}^{PS} \hat{V}_l^{SL} | k' \rangle}{\langle \phi_{lm}^{PS} | \hat{V}_l^{SL} | \phi_{lm}^{PS} \rangle} \quad (35)$$

[Gonze et al., 1991]

4 Quantum Espresso calculation

Quantum Espresso is an open source software use the density functional theory concepts, plane wave and pseudo-potential files for each atom for doing the calculations of the electronic and molecule structure or solids [Quantum ESPRESSO, 2022]. This calculation determine the molecules properties such as its energy bands, energy gap and k points in Brillouin zone. In the next subsections I do some calculation for the Germanium semiconductor and determine its properties. [Hung et al., 2022].

4.1 Germanium Semiconductor

The semiconductors are materials that have a lot of special properties such as its conductivity, resistivity relation with temperature. In this article the Germanium semiconductor (*Ge*) had been selected to do some calculation to its properties using quantum espresso software. Knowing some of the basic properties of *Ge* like the atomic number which is 32, and the mass unit is 72.64u where *u* is the mass unit.

4.1.1 Quantum Espresso Input Data for Ge

In this subsection, the input data for the Germanium that used in quantum espresso software input files had been inserted below. software. [Hung et al., 2022] And the properties in the input file are:

1. Type of Bravais lattice: face center cubic (*FCC*) as figure [fig: 4.1.1].
2. number of atom per unit cell: 2 atom per unit cell.
3. number of types of atoms per unit cell: 1 type per unit cell.
4. The cutoff energy of the plane wave function: 40 Ry.
5. The cutoff energy of the plane wave with expansion of charge density: 160 Ry.
6. The atomic position in the crystal for 2 atoms are: (0.00.00.0), (0.250.250.25). in a unit of the lattice vector. And the magnitude of the lattice vector here will be $10.677a$ where a is Bohr radius.
7. The K points had been considered automatic to be the values: 444000 which means that there are 64 k points 4 points for each direction in the reciprocal lattice and without shifting in the origin of the k points.

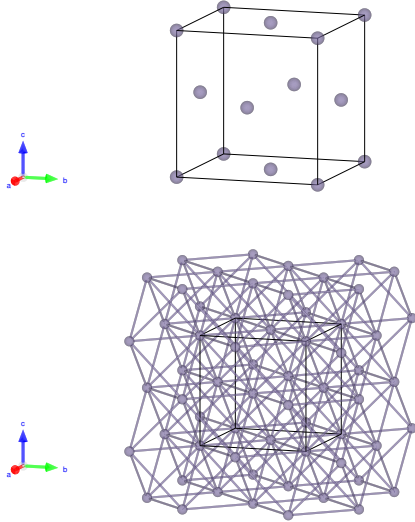


Figure 1: Germanium (*Ge*) *FCC* Bravais lattice structure using VESTA software to plot the 3D structure of the germanium atoms. The upper figure shows the *FCC* lattice structure with atomic position on the compound cell (cubic cell). The other figure shows many cells of *Ge* *FCC* lattice with its bonds.

4.1.2 Results for Ge

In this subsection, the results that come from Quantum Espresso calculation for the *FCC* lattice of the *Ge* semiconductor had been included. The following sections have all output results for the calculations.

4.1.2.1 Stable lattice constant region

In this section, the stable range of the lattice constant had been calculated by calculation the total energy from quantum espresso software with different lattice constant value and plot the relation between total energy and lattice constant. Then, the stable region will be at a small range around the minimum energy of the plotted relation. The stable region shown in figure [fig: 4.1.2.1]

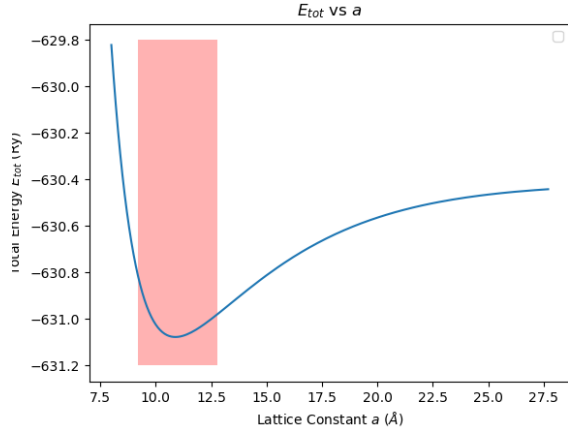


Figure 2: The relation between total energy E_{tot} in Rydberg *Ry* and lattice constant a in angstrom \AA by using python code and quantum espresso calculation to plot the relation of 160 points. The stable region will be around the minimum which is shown in the red rectangle

From the relation in [fig: 4.1.2.1] the minimum value of total energy is at approximate lattice constant a and its energy E_{tot} :

$$\begin{aligned} a &= 10.9 \text{ \AA} \\ E_{tot} &= -631.07707821 Ry \end{aligned} \quad (36)$$

We here can take any value that is close to the lattice constant at the minimum in the stable region. So, the value of the lattice constant which had been taken is:

$$a = 10.677 \text{ \AA} \quad (37)$$

4.1.2.2 Energy and k values

The first results shows the convergence total energy value of the solid in the equation [eq: 38]:

$$E_{total} = -631.05551434 Ry \quad (38)$$

And the calculated energy bands gap E_g could be calculated from the highest occupied level E_H and lowest occupies levels E_L and the difference between them will be the calculated energy band gap of the Germanium in

the equation [eq: 39]:

$$\begin{aligned} E_H &= 8.4370eV \\ E_L &= 8.7647eV \\ E_g &= 0.3277eV \end{aligned} \quad (39)$$

Then, the total K-points in the Brillouin zone with its weight factor in the Cartesian coordinate had been calculated and written in the following tables below [tables: 1, 2, 3] where each table have 20 k points values of the total 60 k points.

Table 1: the Cartesian coordinate value of each k point with its weight factor (1-20 k points)

K point value	Weight factor
(-0.0625000, 0.0625000, 0.0625000)	0.007812
(-0.1875000, 0.1875000, -0.0625000)	0.023437
(-0.3125000, 0.3125000, -0.1875000)	0.023437
(-0.4375000, 0.4375000, -0.3125000)	0.023437
(0.4375000, -0.4375000, 0.5625000)	0.023437
(0.3125000, -0.3125000, 0.4375000)	0.023437
(0.1875000, -0.1875000, 0.3125000)	0.023437
(0.0625000, -0.0625000, 0.1875000)	0.023437
(-0.0625000, 0.3125000, 0.0625000)	0.023437
(-0.1875000, 0.4375000, -0.0625000)	0.046875
(-0.3125000, 0.5625000, -0.1875000)	0.046875
(0.5625000, -0.3125000, 0.6875000)	0.046875
(0.4375000, -0.1875000, 0.5625000)	0.046875
(0.3125000, -0.0625000, 0.4375000)	0.046875
(0.1875000, 0.0625000, 0.3125000)	0.046875
(-0.0625000, 0.5625000, 0.0625000)	0.023437
(-0.1875000, 0.6875000, -0.0625000)	0.046875
(0.6875000, -0.1875000, 0.8125000)	0.046875
(0.5625000, -0.0625000, 0.6875000)	0.046875
(0.4375000, 0.0625000, 0.5625000)	0.046875

Table 2: the Cartesian coordinate value of each k point with its weight factor (21-40 k points)

K point value	Weight factor
(0.3125000, 0.1875000, 0.4375000)	0.046875
(-0.0625000, 0.8125000, 0.0625000)	0.023437
(0.8125000, -0.0625000, 0.9375000)	0.046875
(0.6875000, 0.0625000, 0.8125000)	0.046875
(0.5625000, 0.1875000, 0.6875000)	0.046875
(0.4375000, 0.3125000, 0.5625000)	0.046875
(-0.0625000, -0.9375000, 0.0625000)	0.023437
(-0.1875000, -0.8125000, -0.0625000)	0.046875
(-0.3125000, -0.6875000, -0.1875000)	0.046875
(-0.0625000, -0.6875000, 0.0625000)	0.023437
(-0.1875000, -0.5625000, -0.0625000)	0.046875
(-0.0625000, -0.4375000, 0.0625000)	0.023437
(-0.1875000, 0.1875000, 0.1875000)	0.007812
(-0.3125000, 0.3125000, 0.0625000)	0.023437
(-0.4375000, 0.4375000, -0.0625000)	0.023437
(0.4375000, -0.4375000, 0.8125000)	0.023437
(0.3125000, -0.3125000, 0.6875000)	0.023437
(0.1875000, -0.1875000, 0.5625000)	0.023437
(-0.1875000, 0.4375000, 0.1875000)	0.023437
(-0.3125000, 0.5625000, 0.0625000)	0.046875

Table 3: the Cartesian coordinate value of each k point with its weight factor (41-60 k points)

K point value	Weight factor
(0.5625000, -0.3125000, 0.9375000)	0.046875
(0.4375000, -0.1875000, 0.8125000)	0.046875
(0.3125000, -0.0625000, 0.6875000)	0.046875
(-0.1875000, 0.6875000, 0.1875000)	0.023437
(0.6875000, -0.1875000, 1.0625000)	0.046875
(0.5625000, -0.0625000, 0.9375000)	0.046875
(0.4375000, 0.0625000, 0.8125000)	0.046875
(-0.1875000, -1.0625000, 0.1875000)	0.023437
(-0.3125000, -0.9375000, 0.0625000)	0.046875
(-0.1875000, -0.8125000, 0.1875000)	0.023437
(-0.3125000, 0.3125000, 0.3125000)	0.007812
(-0.4375000, 0.4375000, 0.1875000)	0.023437
(0.4375000, -0.4375000, 1.0625000)	0.023437
(0.3125000, -0.3125000, 0.9375000)	0.023437
(-0.3125000, 0.5625000, 0.3125000)	0.023437
(0.5625000, -0.3125000, 1.1875000)	0.046875
(0.4375000, -0.1875000, 1.0625000)	0.046875
(-0.3125000, -1.1875000, 0.3125000)	0.023437
(-0.4375000, 0.4375000, 0.4375000)	0.007812
(0.4375000, -0.4375000, 1.3125000)	0.023437

These k values then had been used to determine the energy bands gap.

4.1.2.3 Energy Bands

In this section, the energy bands for each k points had been calculated. The result of the first 10 energy bands for each k point had been plotted in figure [fig: 3].

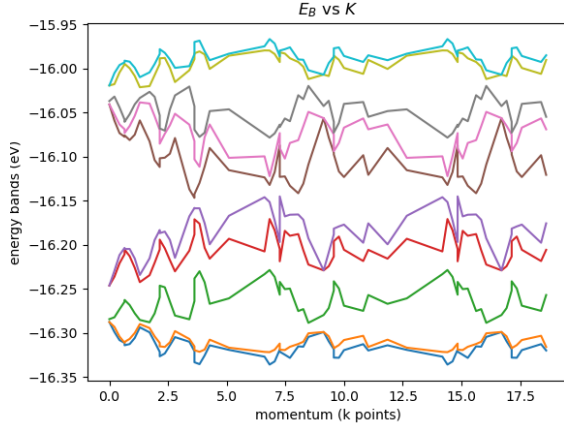


Figure 3: The relation between energy bands and wave vector for first 10 energy bands values

And the result of the next 10 energy bands had been plotted in figure [fig: 4].

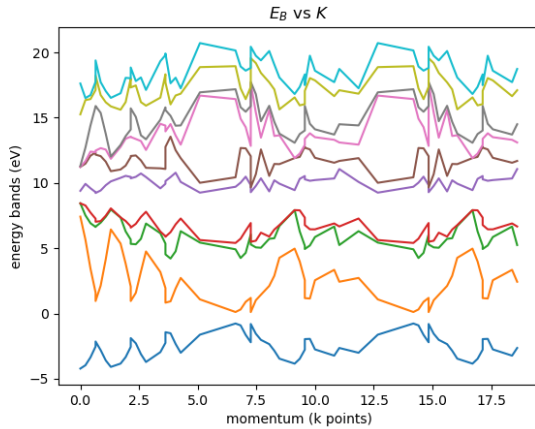


Figure 4: The relation between energy bands and wave vector for last 10 energy bands values

The combination of both of the two plotted figures [3 and 4] which is the total energy band value had been plotted in figure [fig: 5].

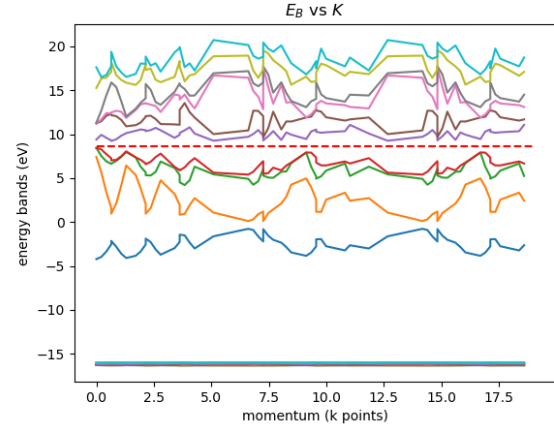


Figure 5: The relation between energy bands and wave vector total energy bands values. The red horizontal line splits the figure between the valence states and conducting states

From figure [fig: 5] we can determine the energy bands up which are the difference between the valence state and the conducting states. The red line position that split the valence state from the conducting state had been determined from the maximum and minimum of the valence state and conducting state respectively from [eq: 39].

5 Conclusion

In the complex systems in quantum mechanics for molecules and solids particles we cannot solve Schrodinger equation neither analytically nor numerically. So, density functional theory and pseudopotential methods could be use in these systems to simplify the system and approximate some of the system properties such as the total energy, energy bands or the bands gap for solids. In Quantum Espresso calculation there are some useful results based on density functional theory, plane wave and pseudo-potential methods. In our results the relation E_{tot} vs a had been plotted in [fig: 4.1.2.1] and the stable region could be determined. Moreover, the k points and total energy could be found in [tables: 1, 2, 3] and [eq: 38] respectively. However, there are some problems on the calculation of the energy bands gap. Since the calculated value is shown in [eq: 39] but the true value of the bands gap for Germanium is $E_g = 0.7\text{eV}$ so there is a big difference in the calculation of bands gap using this software.

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