

Band Structure Theory for Solid

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June 18, 2025

Abstract

This is a brief summary of the report in this semester.

1 Introduction

Here we first summarize the theory of Density functional theory in next section. Then we summarize the method of plane wave and pseudopotential technique in modern electronic structure theory. Finally, we use silicon band structure as an example to demonstrate the application of those methods in Quantum espresso.

2 Theory

2.1 Density Functional Theory

The total energy of a solid for a particular configuration of the ions is

$$E^{tot} = K^{ion} + U^{ion} + E^{ele} = K^{ion} + U^{ion} + [K^{ele} + U^{ion-ele} + U^{ele-ele}] \quad (1)$$

The K^{ion} and U^{ion} are kinetic energy and ion-ion repulsion energy. The U^{ion} can be calculated by Ewald summation method. We will focus on the electronic total energy.

Within DFT framework

$$K^{ele} = \sum_{\kappa} \langle \psi_{\kappa} | \frac{\hat{p}^2}{2m} | \psi_{\kappa} \rangle \quad (2)$$

$$U^{ion-ele} = \sum_k \langle \psi_{\kappa} | V^{ps}(\mathbf{r}) | \psi_{\kappa} \rangle \quad (3)$$

$$U^{ele-ele} = \frac{1}{2} \sum_{\kappa, \kappa'} \langle \psi_{\kappa} \psi_{\kappa'} | \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} | \psi_{\kappa} \psi_{\kappa'} \rangle + \mathcal{E}^{XC}[n(\mathbf{r})] \quad (4)$$

where $|\psi_{\kappa}\rangle$ is single-particle states obtained from a self-consistent solution. and $n(\mathbf{r})$ is the electron number density. κ is the compound index which includes both wave-vector \mathbf{k} and band index n .

$$n(\mathbf{r}) = \sum_{\kappa, \epsilon_{\kappa} < \epsilon_F} |\psi_{\kappa}(\mathbf{r})|^2 \quad (5)$$

where the summation is all occupied state with energy ϵ_{κ} below Fermi level ϵ_F . We adopt LDA for the exchange-correlation functional.

$$\mathcal{E}^{XC}[n(\mathbf{r})] = \int \epsilon^{XC}[n(\mathbf{r})] n(\mathbf{r}) d\mathbf{r} \quad (6)$$

The exchange-correlation potential is

$$\mathcal{V}^{XC} \equiv \frac{\delta \mathcal{E}^{xc}[n(\mathbf{r})]}{\delta n(\mathbf{r})} = \epsilon^{XC}[n(\mathbf{r})] + \frac{\partial \epsilon^{XC}[n(\mathbf{r})]}{\partial n(\mathbf{r})} n(\mathbf{r}) \quad (7)$$

The Kohn-Sham Equation is

$$\left[-\frac{\hat{p}^2}{2m} + V^{ps}(\mathbf{r}) + \frac{e^2 n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \mathcal{V}^{XC}(\mathbf{r}) \right] |\psi_\kappa\rangle = \epsilon_\kappa |\psi_\kappa\rangle \quad (8)$$

Multiplying this equation by $\langle \psi_\kappa |$ from left and sum over all occupied state, we get

$$\sum_{\kappa, \epsilon_\kappa < \epsilon_F} \epsilon_\kappa = \sum_{\kappa, \epsilon_\kappa < \epsilon_F} \langle \psi_\kappa | \frac{\hat{p}^2}{2m} + V^{ps}(\mathbf{r}) | \psi_\kappa \rangle + \int \int \frac{e^2 n(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + \int \mathcal{E}^{XC}(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} \quad (9)$$

We have to emphasize that this is not total electronic energy.

- the hartree energy is double counted
- the integral of exchange-correlation potential is not equal exchange-correlation energy .

$$E^{ele} = \sum_{\kappa, \epsilon_\kappa < \epsilon_F} \epsilon_\kappa - \frac{1}{2} \int \int \frac{e^2 n(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + \mathcal{E}^{XC}[n(\mathbf{r})] - \int \mathcal{V}^{XC}[n(\mathbf{r})] n(\mathbf{r}) d\mathbf{r} \quad (10)$$

2.1.1 Explicitly Result of Total Energy

For a periodic solid, the Fourier transformation of the density and the potentials provide a particularly convenient platform for evaluation of the various terms of the total energy. The Fourier transforms of the density and potential are given by

$$n(\mathbf{r}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} n(\mathbf{G}) \quad (11)$$

$$\Delta V^{XC}(\mathbf{r}) = \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \Delta V^{XC}(\mathbf{G}) \quad (12)$$

$$\int \Delta V^{XC}(\mathbf{r}) n(\mathbf{r}) d\mathbf{r} = V \sum_G \Delta V^{XC}(G) n(G) \quad (13)$$

$$\int \int \frac{e^2 n(\mathbf{r}) n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dr dr' \quad (14)$$

$$= \int dr n(\mathbf{r}) \left[\int \frac{n(\mathbf{r}')}{|r - r'|} dr' \right] \quad (15)$$

$$= \int dr n(\mathbf{r}) \left[\int \frac{\sum_G e^{iG'r'} n(G')}{|r - r'|} dr' \right] \quad (16)$$

$$= \int dr n(\mathbf{r}) \sum_{G'} n(G') e^{iG'r} \left[\int \frac{e^{iG'(r'-r)}}{|r - r'|} dr' \right] \quad (17)$$

$$= \int dr n(r) \sum_{G'} n(G') e^{iG'r} \frac{4\pi}{|G'|^2} \quad (18)$$

$$= \sum_{G'} \frac{4\pi}{|G'|^2} n(G') \int dr n(r) e^{iG'r} \quad (19)$$

$$= \sum_{G'} \frac{4\pi}{|G'|^2} |n(G)|^2 \quad (20)$$

3 Methods

3.1 Pseudopotential Method

(4.9 The pseudopotential.) There are two reason why we need pseudopotential. First of all, the contribution of valence states to total electron density is negligible within the core region and dominant beyond it. Secondly, the valence wavefunction oscillates very fast in core region in order to be orthogonal to core wavefunction, thus we need more plane wave basis to accurately describe this region. If we ignore core region and only focus on valence region, we can use less plane wave basis to describe the system.

3.1.1 Construction of Pseudopotential

In order to develop the pseudopotential for a specific atom, we consider it as an isolated atom. Let $\hat{H}^{(sp)}$ be the single particle Hamiltonian of atom. $|\psi^{(c)}\rangle$ and $|\psi^{(v)}\rangle$ be core and valence wavefunction respectively. They satisfy the Schrodinger equation:

$$\hat{H}^{(sp)} |\psi^{(c)}\rangle = \epsilon^{(c)} |\psi^{(c)}\rangle \quad (21)$$

$$\hat{H}^{(sp)} |\psi^{(v)}\rangle = \epsilon^{(v)} |\psi^{(v)}\rangle \quad (22)$$

Now let us define a new set of single-particle valence state $|\tilde{\phi}^v\rangle$, which satisfy the following equation

$$|\psi^{(v)}\rangle = |\tilde{\phi}^v\rangle - \sum_c \langle \psi^{(c)} | \tilde{\phi}^{(v)} \rangle |\psi^{(c)}\rangle \quad (23)$$

Let apply $\hat{H}^{(sp)}$ to equation 23.

$$\hat{H}^{(sp)} |\tilde{\phi}^v\rangle - \sum_c \epsilon^{(c)} \langle \psi^{(c)} | \tilde{\phi}^{(v)} \rangle |\psi^{(c)}\rangle = \epsilon^{(v)} \left[|\tilde{\phi}^v\rangle - \sum_c \langle \psi^{(c)} | \tilde{\phi}^{(v)} \rangle |\psi^{(c)}\rangle \right] \quad (24)$$

Rearranging equation, we find

$$\left[\hat{H}^{(sp)} + \sum_c (\epsilon^{(v)} - \epsilon^{(c)}) |\psi^{(c)}\rangle \langle \psi^{(c)}| \right] \tilde{\phi}^v = \epsilon^{(v)} |\tilde{\phi}^v\rangle \quad (25)$$

The wavefunction $|\tilde{\phi}^{(v)}\rangle$ have the same eigenvalue $\epsilon^{(v)}$ as valence wavefunction. But the new potential becombes

$$\tilde{V}^{ion} = V^{(sp)} + \sum_c (\epsilon^{(v)} - \epsilon^{(c)}) P^{(c)} \quad (26)$$

Finally the pseudopotential is not unique. Let define a new state $|\bar{\phi}^{(v)}\rangle$

$$|\bar{\phi}^{(v)}\rangle = |\tilde{\phi}^{(v)}\rangle + \sum_{c'} \gamma_{c'} |\psi^{(c')}\rangle \quad (27)$$

Then plug into equation 25, we find

$$\left[\hat{H}^{(sp)} + \sum_c (\epsilon^{(v)} - \epsilon^{(c)}) |\psi^{(c)}\rangle \langle \psi^{(c)}| \right] |\bar{\phi}^{(v)}\rangle - \left[\hat{H}^{(sp)} + \sum_c (\epsilon^{(v)} - \epsilon^{(c)}) |\psi^{(c)}\rangle \langle \psi^{(c)}| \right] \sum_{c'} \gamma_{c'} |\psi^{(c')}\rangle \quad (28)$$

$$= \epsilon^{(v)} |\bar{\phi}^{(v)}\rangle - \epsilon^{(v)} \sum_{c'} \gamma_{c'} |\psi^{(c')}\rangle \quad (29)$$

The second term in both sides is the same. We arrive at

$$\left[\hat{H}^{(sp)} + \sum_c (\epsilon^{(v)} - \epsilon^{(c)}) |\psi^{(c)}\rangle \langle \psi^{(c)}| \right] |\bar{\phi}^{(v)}\rangle = \epsilon^{(v)} |\bar{\phi}^{(v)}\rangle \quad (30)$$

3.1.2 Basic Steps in constructing a pseudopotential

1. Solve the all-electron Schrodinger equation for the isolated atom to obtain the all-electron wavefunctions and eigenvalues.

$$\hat{H}^{(sp)} |\psi^{(v)}\rangle = [\hat{F}^{sp} + V^{nuc}] |\psi^{(v)}\rangle = \epsilon^{(v)} |\psi^{(v)}\rangle \quad (31)$$

where \hat{F}^{sp} is operator in $\hat{H}^{(sp)}$ that contains all other terms except the external potential.

2. Choose a cutoff radius r_c . Construct the pseudo wavefunctions that match the all-electron wavefunctions outside the cutoff radius and are smoother inside.

$$\phi^{(v)}(r) = \psi^{(v)}(r) \quad \text{for } r > r_c \quad (32)$$

$$\phi^{(r)} \text{ is smooth, nodeless } r \leq r_c \quad (33)$$

$$\frac{d\phi^{(v)}(r)}{dr}, \frac{d^2\phi^{(v)}(r)}{dr^2} \text{ is continuous at } r_c \quad (34)$$

3. Normalize the pseudo-wavefunctions $\phi^{(v)}(r) \quad 0 \leq r \leq \infty$.
4. Invert the Schrodinger equation to obtain the pseudopotential $V^{ps}(r)$ that reproduces the pseudo-wavefunctions.

$$[\hat{F}^{sp} + V^{ps}] \phi^{(v)}(r) = \epsilon^{(v)} \phi^{(v)}(r) \implies V^{ps}(r) = \epsilon^{(v)} - \frac{\hat{F}^{sp} \phi^{(v)}(r)}{\phi^{(v)}(r)} \quad (35)$$

3.2 Plane Wave Basis

Let consider the single-particle equation which involve a pseudopotential

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V^{ps}(\mathbf{r}) \right] \tilde{\phi}_{\mathbf{k}}^{(n)}(r) = \epsilon_{\mathbf{k}}^{(n)} \tilde{\phi}_{\mathbf{k}}^{(n)}(r) \quad (36)$$

According to Bloch theorem, we can write the wavefunction as

$$\tilde{\phi}_{\mathbf{k}}^{(n)}(r) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}^{(n)}(r) \quad (37)$$

Where $u_{\mathbf{k}}^{(n)}(r)$ is a function with the periodicity of the lattice. We can expand $u_{\mathbf{k}}^{(n)}(r)$ in terms of plane waves

$$u_{\mathbf{k}}^{(n)}(r) = \sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} e^{i\mathbf{G}\cdot\mathbf{r}} \quad (38)$$

Where \mathbf{G} is a reciprocal lattice vector. Thus we have

$$\tilde{\phi}_{\mathbf{k}}^{(n)}(r) = \sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad (39)$$

Plug into the single-particle equation, we have

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V^{ps}(\mathbf{r}) \right] \sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} = \epsilon_{\mathbf{k}}^{(n)} \sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad (40)$$

Multiply both side by $e^{-i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}}$ and integrate over the volume of the crystal Ω , we have

$$\sum_{\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} \left[\frac{\hbar^2}{2m} |\mathbf{k} + \mathbf{G}|^2 \delta_{\mathbf{G},\mathbf{G}'} + \frac{1}{\Omega} \int d^3r V^{ps}(\mathbf{r}) e^{i(\mathbf{G}-\mathbf{G}')\cdot\mathbf{r}} \right] = \epsilon_{\mathbf{k}}^{(n)} c_{\mathbf{k}+\mathbf{G}'}^{(n)} \quad (41)$$

Now we have a matrix equation

$$\sum_{\mathbf{G}} H_{\mathbf{G}',\mathbf{G}} c_{\mathbf{k}+\mathbf{G}}^{(n)} = \epsilon_{\mathbf{k}}^{(n)} c_{\mathbf{k}+\mathbf{G}'}^{(n)} \quad (42)$$

3.2.1 Calculation of Matrix Elements

The kinetic energy term is easy to calculate

$$\langle \mathbf{k} + \mathbf{G}' | -\frac{\hbar^2}{2m} \nabla^2 | \mathbf{k} + \mathbf{G} \rangle = \frac{\hbar^2}{2m} |\mathbf{k} + \mathbf{G}|^2 \delta_{\mathbf{G},\mathbf{G}'} \quad (43)$$

The potential energy term is more complicated. The pseudopotential is given by

$$V^{ps}(\mathbf{r}) = \sum_{\mathbf{R}} \sum_{\alpha} \left(\sum_{i_{\alpha}} \tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{t}_{i_{\alpha}} - \mathbf{R}) \right) \quad (44)$$

Where $\tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{t}_{i_{\alpha}} - \mathbf{R})$ is the pseudopotential of the atom located at $\mathbf{t}_{i_{\alpha}} + \mathbf{R}$. Here \mathbf{R} is a lattice vector, $\mathbf{t}_{i_{\alpha}}$ is the position of atom i of type α in the unit cell. The Fourier transform of the pseudopotential is given by

$$V^{ps}(\mathbf{q}) = \frac{1}{\Omega} \int d^3r V^{ps}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \quad (45)$$

Plug in the expression of $V^{ps}(\mathbf{r})$, we have

$$V^{ps}(\mathbf{q}) = \frac{1}{\Omega} \int d^3r \sum_{\mathbf{R}} \sum_{\alpha} \left(\sum_{i_{\alpha}} \tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{t}_{i_{\alpha}} - \mathbf{R}) \right) e^{-i\mathbf{q} \cdot \mathbf{r}} \quad (46)$$

$$= \sum_{\alpha} \frac{1}{\Omega} \int d^3r \sum_{i_{\alpha}} \sum_R \tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{t}_{i_{\alpha}} - \mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{r}} \quad (47)$$

Change the variable $\mathbf{r}' = \mathbf{r} - \mathbf{t}_{i_{\alpha}}$, we have

$$V^{ps}(\mathbf{q}) = \sum_{\alpha} \frac{1}{\Omega} \int d^3r' \sum_{i_{\alpha}} \sum_R \tilde{V}_{\alpha}^{ion}(\mathbf{r}' - \mathbf{R}) e^{-i\mathbf{q} \cdot (\mathbf{r}' + \mathbf{t}_{i_{\alpha}})} \quad (48)$$

$$= \sum_{\alpha} \sum_{i_{\alpha}} e^{-i\mathbf{q} \cdot \mathbf{t}_{i_{\alpha}}} \left(\frac{1}{\Omega} \int d^3r' \sum_{\mathbf{R}} \tilde{V}_{\alpha}^{ion}(\mathbf{r}' - \mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{r}'} \right) \quad (49)$$

$$= \sum_{\alpha} \sum_{i_{\alpha}} e^{-i\mathbf{q} \cdot \mathbf{t}_{i_{\alpha}}} V_{\alpha}^{ion}(\mathbf{q}) \delta_{\mathbf{q}, \mathbf{G}} \quad (50)$$

$$= \sum_{\alpha} S_{\alpha}(\mathbf{q}) V_{\alpha}^{ion}(\mathbf{q}) \delta_{\mathbf{q}, \mathbf{G}} \quad (51)$$

Where $S_{\alpha}(\mathbf{q})$ is the structure factor of atom type α . The $V_{\alpha}^{ion}(\mathbf{q})$ is the Fourier transform of the ionic pseudopotential of atom type α $\sum_R \tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{R})$. We can interpret $\sum_R \tilde{V}_{\alpha}^{ion}(\mathbf{r} - \mathbf{R})$ as the potential generated by atom α with fractional position 0,0,0, and add all atom arranged with lattice. Finally we have the matrix element of the potential energy term

$$\langle \mathbf{k} + \mathbf{G}' | V^{ps} | \mathbf{k} + \mathbf{G} \rangle = \sum_{\alpha} S_{\alpha}(\mathbf{G} - \mathbf{G}') V_{\alpha}^{ion}(\mathbf{G} - \mathbf{G}') \quad (52)$$

3.2.2 Cutoff Energy

In practical calculation, we cannot include all plane waves in the expansion of wavefunction. The dimension of the matrix $H_{\mathbf{G}', \mathbf{G}}$ is $N_{bs} \times N_{bs}$. Here N_{bs} is the number of plane waves included.

We need to introduce a cutoff energy E_{cut} , and only include plane waves with kinetic energy less than E_{cut} .

$$\frac{|\mathbf{G}|^2}{2m} < E_{cut} \quad (53)$$

The number of plane waves N_{bs} increases as E_{cut} increases. When using the pseudopotential, $V_{\alpha}^{ion}(G)$ decays quickly as G increases. Thus we can use a relatively small E_{cut} to get converged results.

3.3 Special k-points

3.3.1 Motivation

We need to evaluate quantities like Equation 5

$$\bar{g} = \frac{1}{N} \sum_{\mathbf{k} \in BZ} g(\mathbf{k}) = \frac{V_{PUC}}{(2\pi)^3} \int g(\mathbf{k}) d\mathbf{k} \quad (54)$$

4 Results and Discussion

Here we will demonstrate the calculation of silicon band structure using Quantum ESPRESSO open source software.

4.1 SCF calculation

The input file is

```
1 &CONTROL
2   calculation = 'scf',
3   outdir = '.',
4   pseudo_dir = '.'
5 /
6
7 &SYSTEM
8  ibrav = 2,
9   cellldm(1) = 10.2076,
10  nat = 2,
11  ntyp = 1,
12  ecutwfc = 50,
13  nbnd = 8
14 /
15
16 &ELECTRONS
17 /
18
19 ATOMIC_SPECIES
20   Si 28.086 Si.UPF
21
22 ATOMIC_POSITIONS (alat)
23   Si 0.0 0.0 0.0
24   Si 0.25 0.25 0.25
25
26 K_POINTS (automatic)
27   6 6 6 0 0 0
```

Listing 1: silicon.in

Here the first section is control section, which controls our job. Here we set our calculation type to be which means do dft calculation. We set output directory and pseudopotential directory to be current directory.

4.1.1 pseudopotential

The pseudopotential used here is downloaded from

```
1 curl -o Si.UPF https://pseudopotentials.quantum-espresso.org/upf_files/
   Si.pz-vbc.UPF
```

UPF means Unified Pseudopotential Format, the information of pseudopotential is in header of pseudopotential files

```
1   <UPF version="2.0.1">
2 <PP_INFO>
3 Generated by new atomic code, or converted to UPF format
4 Author:
5 Generation date:
```

```

6 Pseudopotential type: NC
7 Element: Si
8 Functional: SLA PZ NOGX NOGC
9 Suggested minimum cutoff for wavefunctions: 0. Ry
10 Suggested minimum cutoff for charge density: 0. Ry
11 The Pseudo was generated with a Non-Relativistic Calculation
12 L component and cutoff radius for Local Potential: 0 0.0000
13 Valence configuration:
14 nl pn l occ Rcut Rcut US E pseu
15 3S 0 0 2.00 0.000 0.000 0.0000000
16 3P 0 1 2.00 0.000 0.000 0.0000000
17 Generation configuration: not available.
18 </PP_INFO>
19 <!--
20 END OF HUMAN READABLE SECTION

```

Listing 2: pseudopotential.header

The type of pseudopotential is NC means normal conserving . Functional: SLA PZ NOGX NOGC means we use Slater exchange + Perdew-Zunger correlation . NOGX ,NOGC means not using GGA.the valence configure is (3s,3p) orbital.

4.1.2 system

In system section, we set the lattice type and lattice parameters .nat means number of atom in cell,and ntype is the type of atoms.ecutwfc is cutoff energy and the unit is Ry (not hartree .1Ry=0.5 Hartree).nbnd is the number of eigenvalue we want to calculate.

4.1.3 others

ATOMIC_SPECIES ,Atomic.POSITIONS and K_POINTS is set.

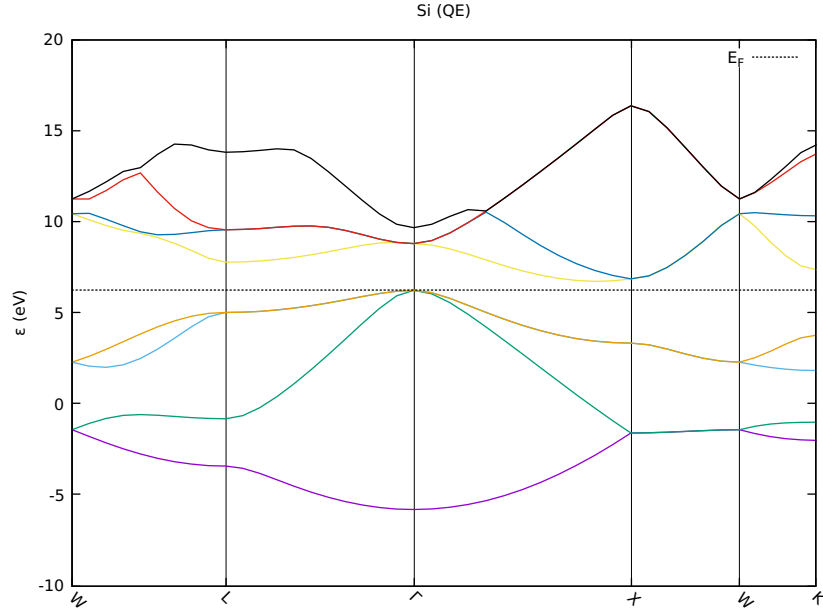
4.2 Band Structure Calculation

In band structure calculation ,we select k-points along high symemtry path other than we have set in scf calculation. We do not do scf in band structure calculateion ,just use the density in previous run .

```

1 &CONTROL
2 calculation = 'bands',
3 outdir = '.'
4 pseudo_dir = '.'
5 /
6
7 &SYSTEM
8 ibrav = 2,
9 celldm(1) = 10.2076,
10 nat = 2,
11 ntyp = 1,
12 ecutwfc = 50,
13 nbnd = 8
14 /
15
16 &ELECTRONS
17 /
18

```

```

19 ATOMIC_SPECIES
20   Si 28.086 Si.UPF
21
22 ATOMIC_POSITIONS (alat)
23   Si 0.0 0.0 0.0
24   Si 0.25 0.25 0.25
25
26
27 K_POINTS {crystal_b}
28 6
29 0.5      0.25      0.75      9  ! W
30 0.5      0.5       0.5       11 ! L
31 0         0         0        12 ! Gamma
32 0.5      0         0.5       6  ! X
33 0.5      0.25      0.75      5  ! W
34 0.375    0.375     0.75      0  ! K

```

Listing 3: band.in

here we change the calculation type into band. And the k-point become high symmetry points.

4.3 Plot of band structure

The tools we use to plot band structure is c2x

```

1 $ c2x --bands_gnu --title="Si (QE)" pwscf.xml Si.gnu
2 $ gnuplot -p Si.gnu

```

5 Conclusion

In this report we introduce the theory of plane-wave pseudopotential method used in morden electronic structure software. And calculate the silon band structure using open-source software Quantum ESPRESSO.

In the future ,we can do more things

- calculate more properties like density of state (DOS)
- Test the convergence of cutoff energy and kpoints in scf calculation.
- More details of construction of pseudopotential and k-point sampling is also need.
- Finally ,the implementation of code and extended to DSRG is a big project to do.