

First-Principle Calculations

Lab Report 4

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Procedure:

1. Download and unzip t4.zip from the google classroom
2. Open t4 (renamed here as "Lab") in terminal by right clicking/ manually changing directory from home user
3. Open README file in terminal using '*cat*' command
4. As per instruction, open the input files for aluminum and silicon in '*vi*' editor and change *pseudo directory* and *output directory*

Here are the input files:

<i>al.scf.in</i>	<i>si.scf.in</i>
<i>al.dos1.in</i>	<i>si.dos1.in</i>
<i>al.dos2.in</i>	<i>si.dos2.in</i>

5. The first step is to perform the self-consistent field calculation after the structural optimization.

Importance :

SCF calculations enhance the electronic structure by iteratively solving the Schrödinger equation to determine the electronic wave function that minimises energy after optimising the geometry of a molecular system. This stage addresses the dynamic interaction between electron-electron and electron-nucleus interactions, which is necessary to fully describe electron dispersion. The SCF calculation accurately predicts molecular energies, electronic spectra, and reaction routes by matching the electronic configuration to the molecule's ground state. Thus, post-structural optimisation SCF calculations improve quantum chemical simulation reliability and molecular behaviour knowledge in various chemical and biological situations.

```
pw.x < al.scf.in > al.scf.out
```

```
pw.x < si.scf.in > si.scf.out
```

6. Calculate the non-self-consistent field using a denser k-mesh:

Importance :

A denser k-mesh in a non-self-consistent field (NSCF) calculation is important for figuring out the electronic structure of things in condensed matter physics and materials research. The k-mesh controls discontinuous Brillouin zone sampling, affecting electronic structure computations. A denser k-mesh in NSCF calculations provides more exact information regarding electronic band structures, density of states, and other features. When studying subtle energy level shifts, band crossings, or material energy gaps, this increased granularity is essential. A finer k-mesh represents the electronic structure better, helping researchers describe the material's behaviour and forecast its electrical and optical properties.

```
pw.x < al.band1.in > al.band1.out  
pw.x < si.band1.in > si.band1.out
```

7. For the conversion of data to x-y format, perform:

Importance of 'bands.x':

The bands.x module in Quantum ESPRESSO analyses and visualises electronic band structures, which are essential to understanding material electronic characteristics. Bands.x generates band structure graphs of electron energy levels as a function of momentum after a self-consistent field calculation. This visualisation helps characterise the material's electrical behaviour by identifying band gaps, dispersion, and Fermi surfaces. Bands.x helps researchers understand how electrical structure affects conductivity, optical characteristics, and performance. In conclusion, bands.x in Quantum ESPRESSO helps scientists and engineers create and optimise materials for numerous purposes by interpreting and communicating electronic structural information.

```
bands.x < al.band2.in > al.band2.out  
bands.x < si.band2.in > si.band2.out
```

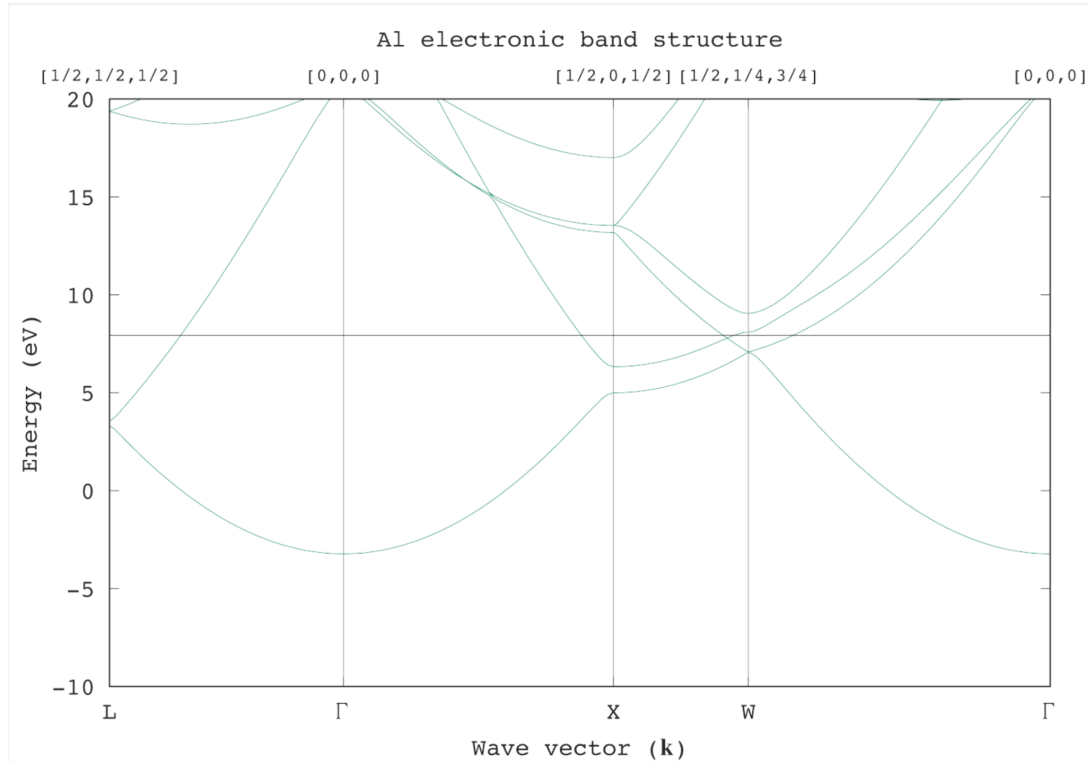
8. After the above calculations, there will be '*bands.that.gnu*' generated, from which we will get information about the band structure along the specified path. (the path mentioned here is a L- Γ -X-W- Γ)

```
0.5 0.5 0.5 50  
0.0 0.0 0.0 50  
0.5 0.0 0.5 50  
0.5 0.25 0.75 50  
0.0 0.0 0.0 50
```

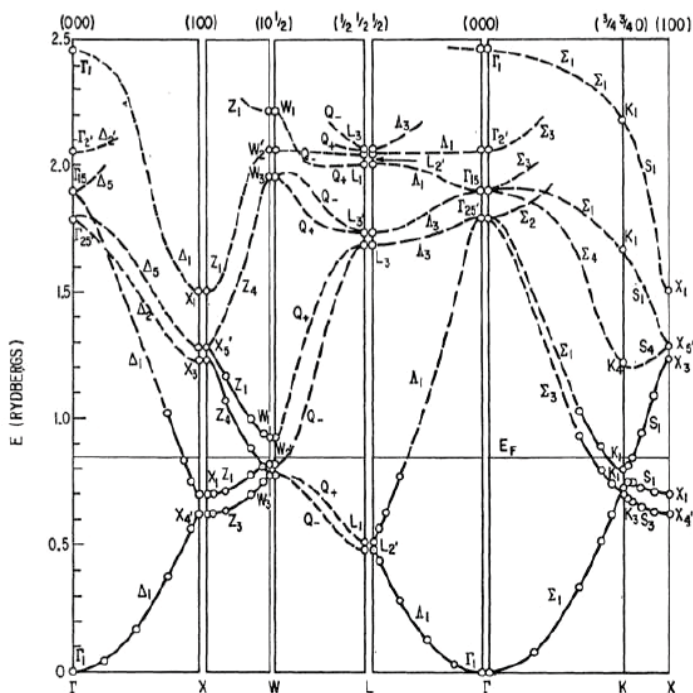
9. Use the given script in the folder '*gnuplot*' to get well annotated band structure from the '*bands.dat.gnu*' files for the respective elements
10. Compare the electronic band structure that is generated from the above calculations with the one available in the literature.

Observations:

A. Band Structure of Aluminium :

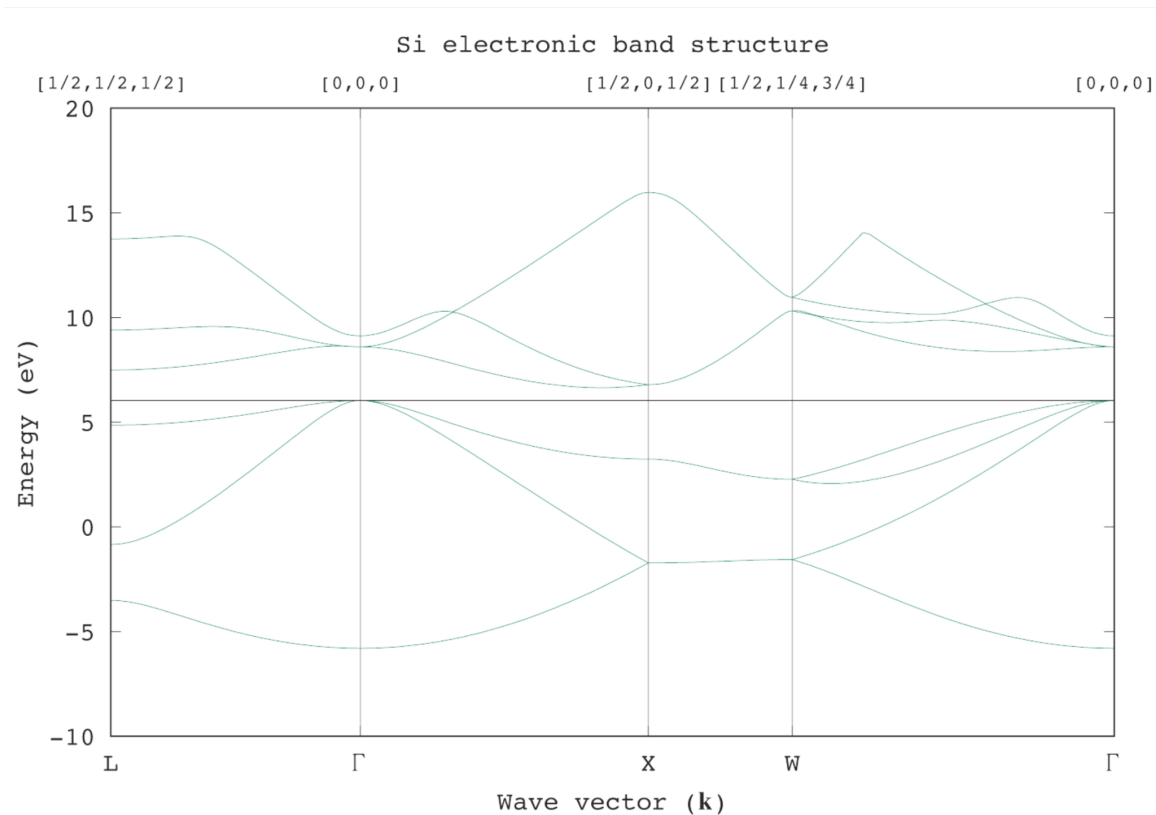


Literature Band Structure :

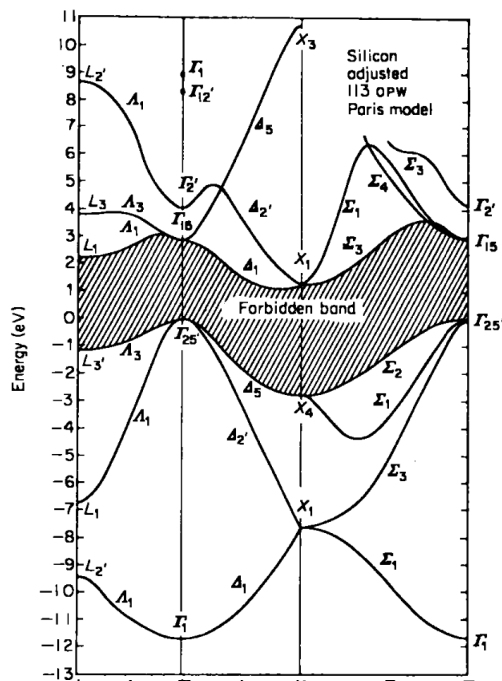


The aluminium band structure is comparable to the one determined using the aforementioned method.

B. Band Structure of Silicon:



Literature Band Structure of Silicon:



Based on the literature, we can conclude that:

- Calculated bandgap : 0.60 eV
- Literature bandgap : 1.12 eV
- Possible Reasons:

First-principles DFT (Quantum ESPRESSO) estimations of silicon's bandgap may differ from literature values due to DFT's limitations and approximations. The exchange-correlation

functional describes electron-electron interactions in DFT, and its choice affects outcomes. Choosing pseudopotentials, basis sets, and treating electron correlation effects may also cause inconsistencies. The indirect bandgap of silicon further complicates predictions. Experimental circumstances, temperature, and pressure can also cause discrepancies in literature data. Calibration concerns include aligning computational and experimental reference energy, which can further cause variances. The difference in computational and literature bandgap values emphasises the necessity to carefully analyse methodological factors and DFT technique flaws.

NOTE : All the input files and calculations are attached to the report in the respective folders.