SCPY 394: Advanced Physics Laboratory II
Lab 6: Density Functional Theory (DFT) calculation

Dulyawat Boonvut, 6205110

November 23, 2022

1 Objective

1. To find lattice constants of aluminum and silicon.
2. To obtain a density state representation from a band structure from different materials.
3. To study van Hove singularity from the band structures of the different materials.

2 Density Functional Theory (DFT)

Density functional theory (DFT) uses a **density functional** instead of a typical wave function. Using the density functional, material properties can be determined. With the appropriate density functional, ground state energy can be determined by the variational principle.

3 Calculation Process using DFT

The density function is usually determined by **self-consistent method** which an initial density functional is constructed from a non-interactive system and the corresponding energy will be calculated. The density function will be reconstructed and used for a calculation repeatedly until the energy converges to a specific value.

The used model in the experiment is **muffin-tin orbital model**, which atom is inside the *muffin tin*. Spherical harmonics as a basis function will contribute to the density function to obtain the ground state energy using a self-consistent method.

Each material has a unique lattice constant. The lattice constant can be obtained using the self-consistent method. For different samples of lattice constant, cohesive energy is obtained for the number of iterations. We can then determine the actual value of the lattice constant by considering the lowest cohesive energy.

The obtained lattice constant will be used to obtain a band structure. the density of state (DOS) - energy graph will be shown also.

The experiment focuses on the materials: *aluminum* and *silicon*. Their lattice constants are obtained and their band structures afterward. The van Hove singularities of both materials, which are represented as spikes in the DOS graph, are observed.

4 Results

4.1 Result of aluminum

4.1.1 Lattice constant

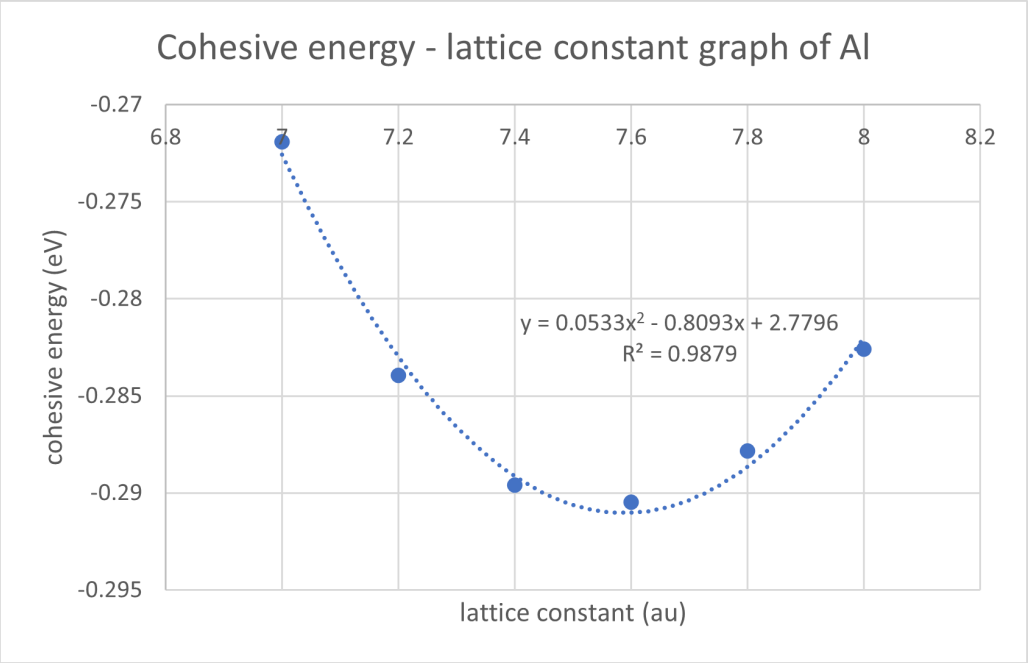

Figure 1: Lattice constant - cohesive energy graph of aluminum

From figure 1, the lattice constant of aluminum corresponding to the lowest cohesive energy is

$$a_{Al} = 7.597 \text{ au} = 4.019 \text{ Å} \tag{1}$$

The obtained aluminum lattice constant is approximately close to $a = 404.95$ pm $= 4.0495$ Å from `https://periodictable.com/Elements/013/data.html`.

4.1.2 Density of state

from figure 6 An amount of peculiar peaks along the continuous line of graph 6 represent **van Hove singularities**. The van Hove singularities show possible state of the material since number of state is rapidly changing.

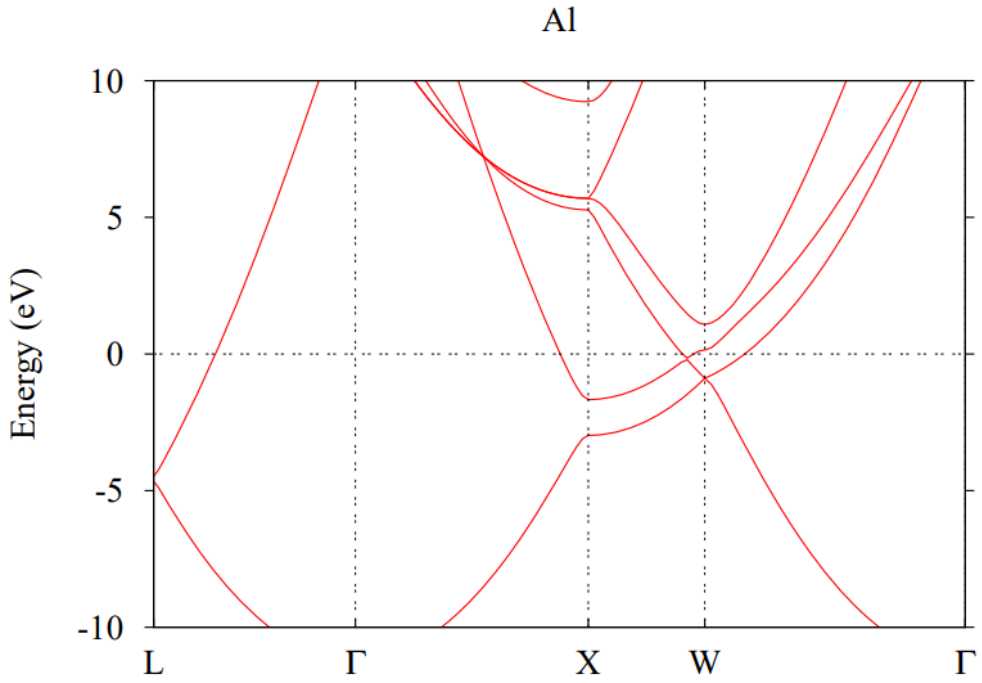

Figure 2: Aluminum band structure

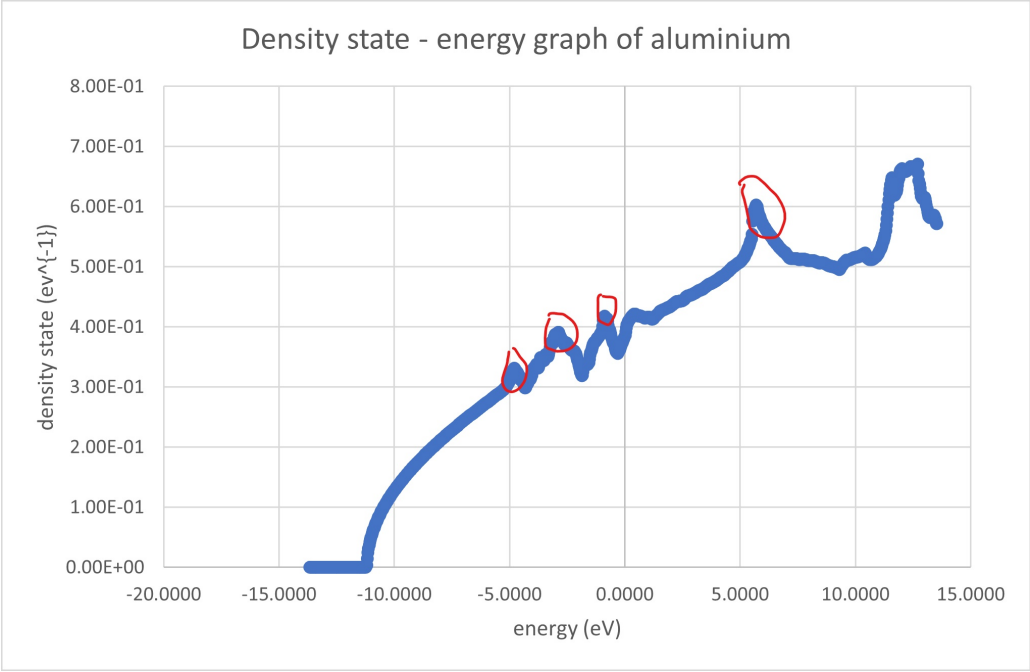

Figure 3: Density state - energy graph of aluminum. The red circles are van Hove singularities.

4.2 Result of silicon

4.2.1 Lattice constant

From figure 4, the lattice constant of silicon corresponding to the lowest cohesive energy is approximately

$$a_{Si} = 10.27 \text{ au} = 5.5458 \text{ Å} \tag{2}$$

The obtained silicon lattice constant is approximately close to $a = 543.09$ pm $= 5.4309$ Å from `https://periodictable.com/Elements/014/data.html`.

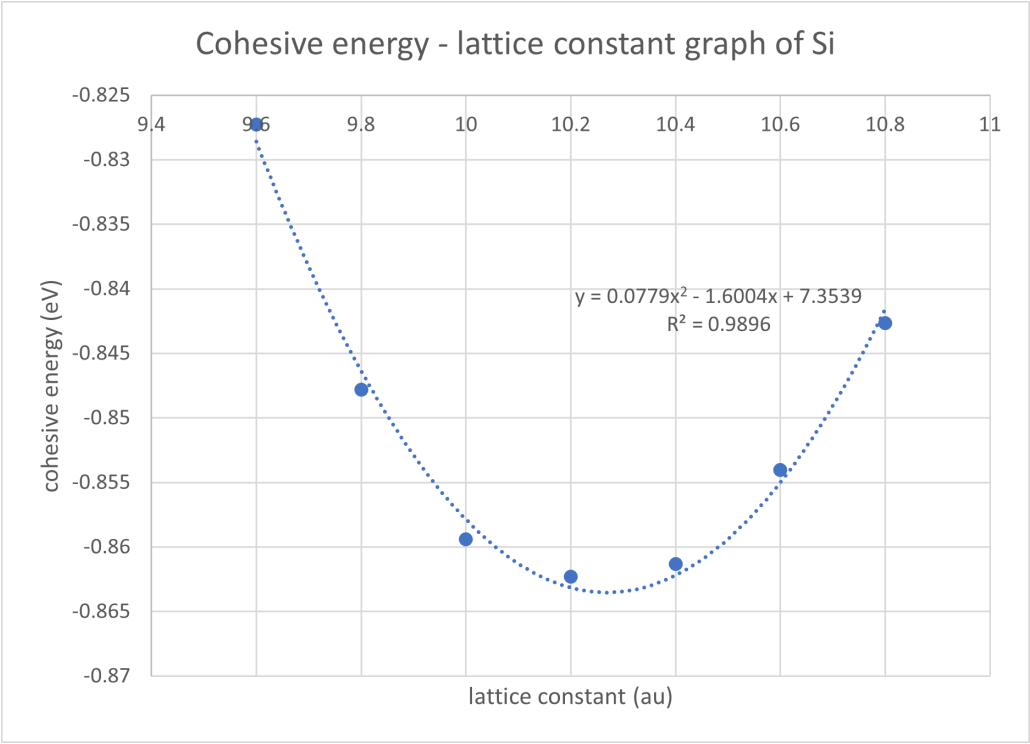

Figure 4: Lattice constant - cohesive energy graph of silicon

4.2.2 Density of state

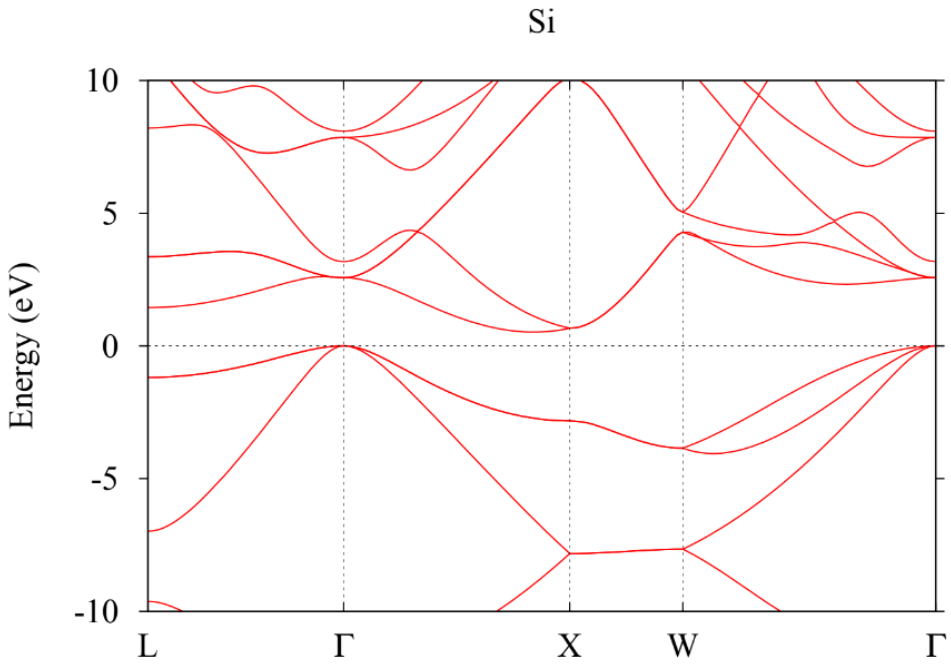

Figure 5: Silicon band structure

from figure 6 From a silicon band structure, the van Hove singularities are shown as peaks in the band structure.

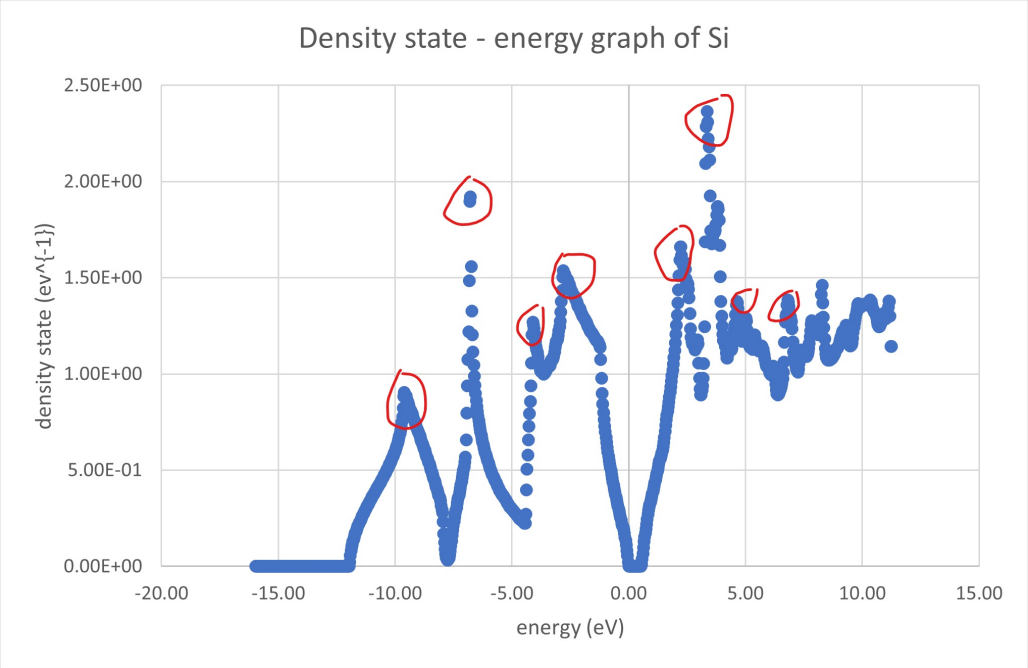

Figure 6: Density state - energy graph of silicon. The red circles are van Hove singularities.

4.3 Comparison of the results obtained from the aluminum and the silicon

Contrary to the aluminum DOS graph, there are a huge amount of van Hove singularities in the silicon DOS graph.

5 Conclusion

The experiment is to use density functional theory (DFT) to obtain the lattice constants of aluminum and silicon along with their band structure and visualization of the density of state (DOS). The computed lattice constant of aluminum is $a_{Al} = 4.019$ Å and one of silicon is $a_{Si} = 5.5458$ Å. The band structures and DOS graph of both materials are constructed. The van Hove singularities are determined in both DOS graphs. From both DOS graph, there are a huge amount of van Hove singularities in the silicon DOS graph than one from the aluminum.