Iron ($(\boldsymbol{Fe})$

This article contains a simple experiment on how to determine the cutoff value, optimization of a structure, density of state, and band structure. I used iron (F_e) as training material. So, give your best idea for a science material.

1. **Enery Cutoff**

   Energy cutoff becomes important because it can affect the level of energy. The cutoff energy is also a calculation of the maximum momentum (k) of a wave function.

$$\Psi(r) = e^{i(\boldsymbol{G}+k)\boldsymbol{r}}$$

   And then, the values of cutoff wave function, cutoff charge, and k-points are determines a convergence. In this moment, I have calculate of energy cutoff by $15Ry$ until $50Ry$.

E_{cut}	Total Energy (1x1x1)	Total Energy (3x3x3)	Total Energy (5x5x5)
15	-111.8002303	-111.1938345	-111.1796668
20	-112.0423678	-111.6014353	-111.5874626
25	-112.0435553	-111.61731	-111.6040198
30	-112.0463185	-111.6189419	-111.6055984
35	-112.0466398	-111.6201405	-111.6067706
40	-112.0477115	-111.6207333	-111.607208
45	-112.0477765	-111.6207939	-111.6072604
50	-112.0477296	-111.6207662	-111.6072528

Table 1. The results of the calculation of total energy with different k points for each cutoff value

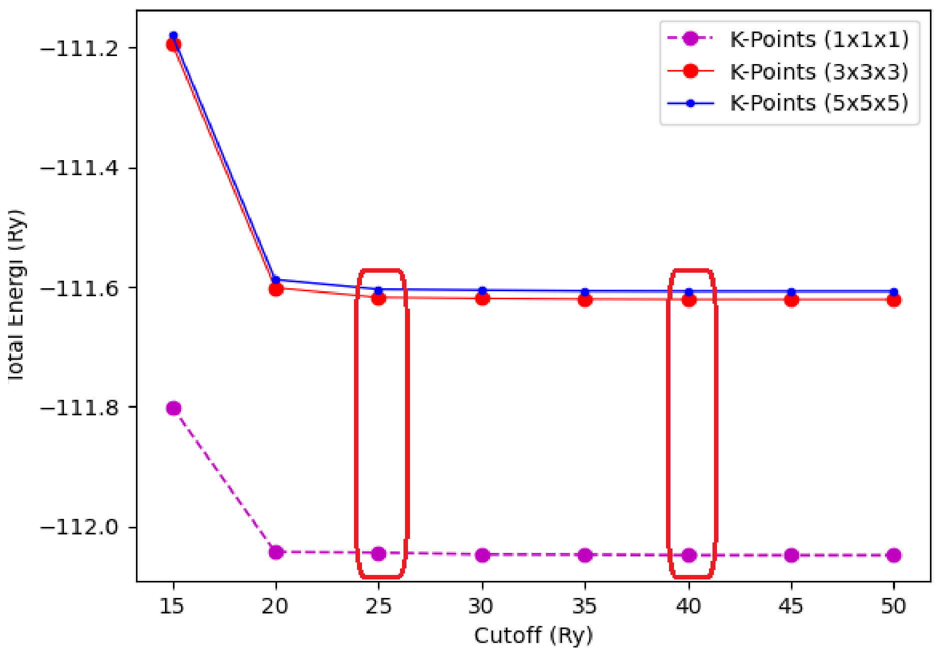

Figure 1. Total Energy Cutoff

2. Structure Optimization

In this section, the lowest total energy of the structure will be calculated

Computational parameters

$a = b = c = 2.2A - \dot{3}.6A$

$\alpha = \beta = \gamma = 90^0$

$E_{cut}(\Psi) = 40Ry$

$E_{cut}(\rho) = 400Ry$

$K - Points = 5 \times 5 \times 5$

a(A)	Total Energy (Ry)
2.2	-110.5322273
2.4	-111.2043451
2.6	-111.4691799
2.8	-111.5143175
3	-111.4534142
3.2	-111.348092
3.4	-111.2300403
3.6	-111.1148975

Table 2. Total energy of the various values

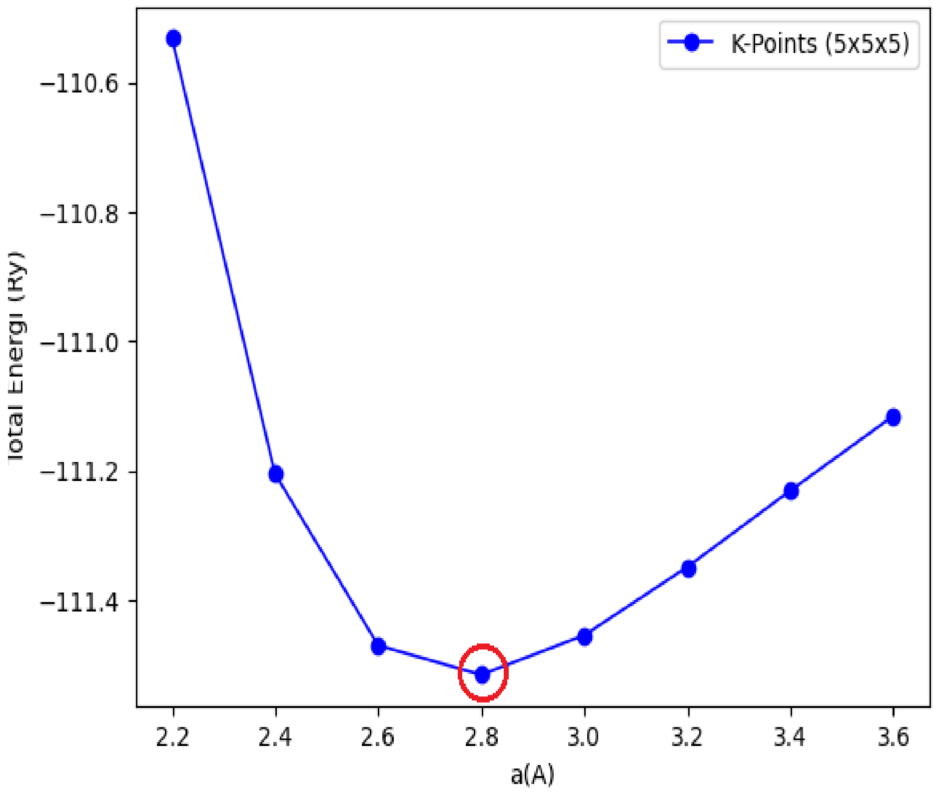

Figure 2. The minimum energy is $2.8\dot{A}$

3. Density of State

Density of state is the number of states of energy levels at a certain energy, meaning how the distribution of energy levels in a system. The simple way is to model it into a very large grid at each energy level.

Computationnal parameters

$a = b = c = 2.8\dot{A}$

$\alpha = \beta = \gamma = 90^0$

$E_{cut}(\Psi) = 25Ry$

$E_{cut}(\rho) = 22.5Ry$

$K - Points = 20 \times 20 \times 20$

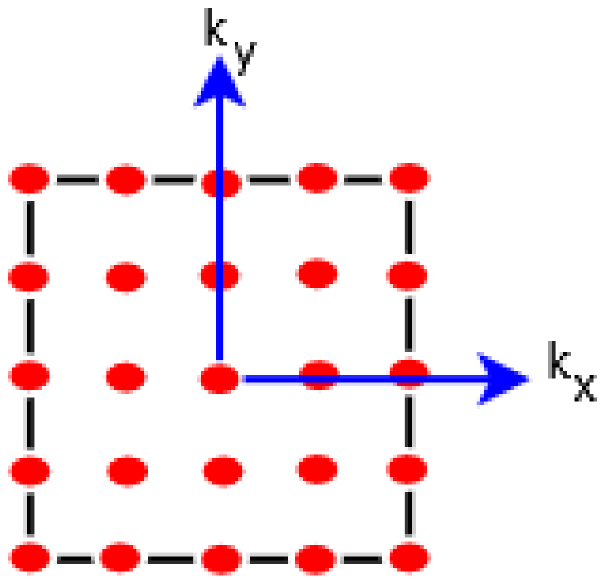

Figure 3. Energy grid on each level

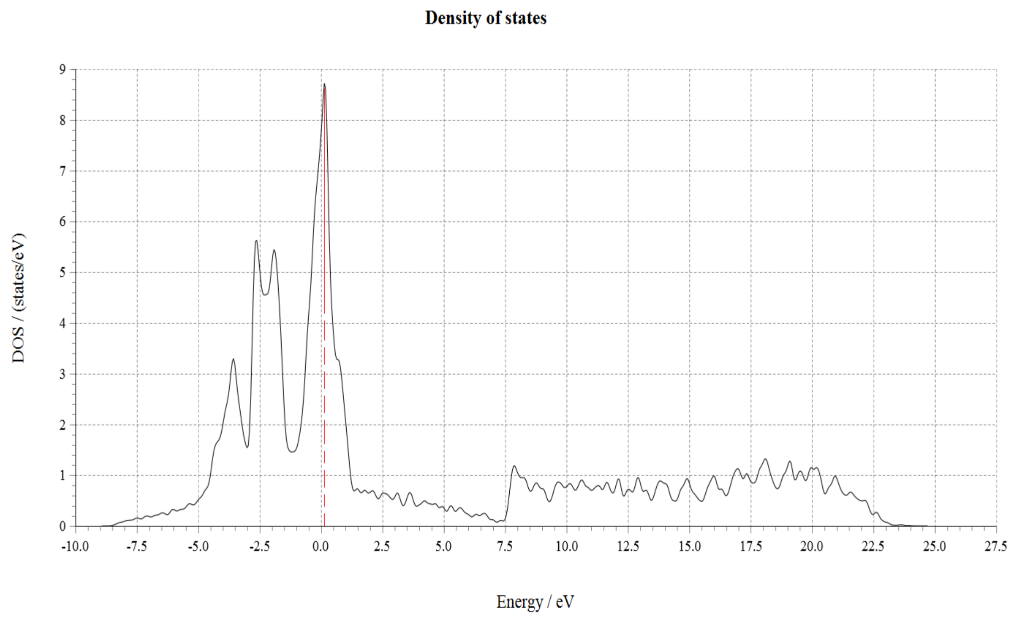

Figure 3. Distribution of energy levels

From the figure 2, it is explained that (F_e) is very conductive whose value is at $0eV - 7.5eV$. In addition, the right part of the red line (Fermi energy) is called the valence band, while the left part is known as the conduction band.

4. Band Structure

The last step in this experiment, we calculated of band structure. Band structure will show the value of the state of the energy level at a certain momentum. where the direction of the momentum is the Brillouin Zone (BZ).

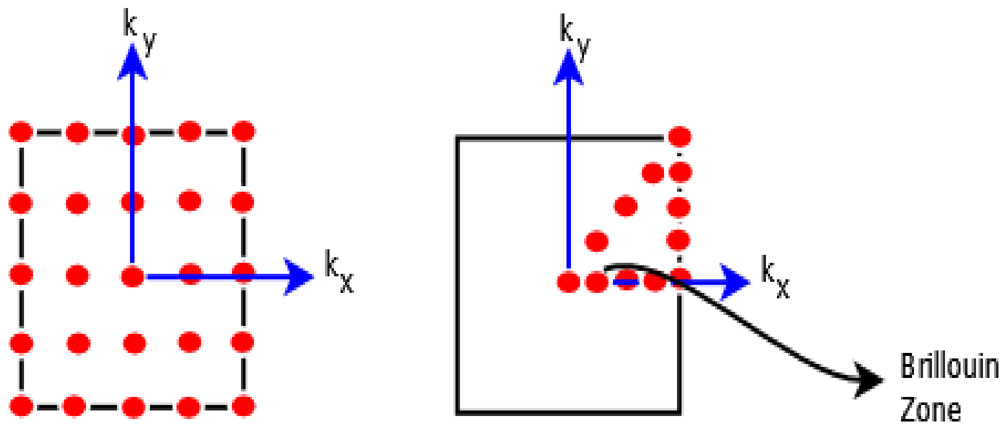

Figure 4. Grid difference between density of state and band structure

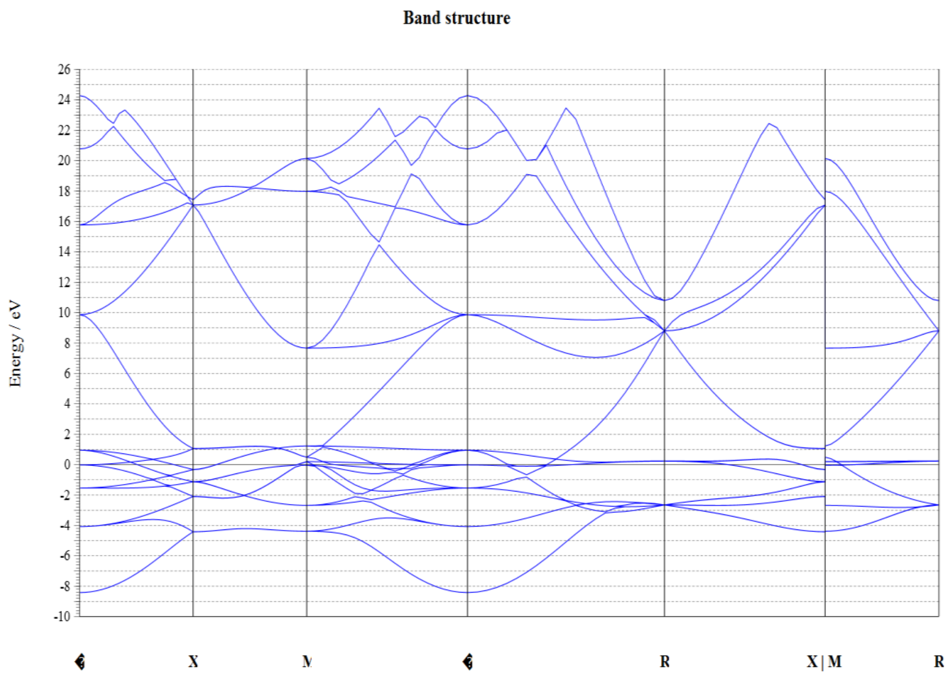

Figure 5. Band structure

It turns out, there are a lot of band structures that are able to pass the Fermi energy. This situation indicates that the iron (F_e) is a metal or a conductor.