Homework6

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January 5, 2025

1 Band structure of silicon

Based on the data from the website and some articles, I set the coordinates of the 2 atoms in the primitive cell of FCC silicon crystal structure are:

```
set cell   5.13 5.13 0   0 5.13 5.13    5.13 0 5.13
atom Si01 silicon   -5.13   -5.13   -5.13
atom Si02 silicon   -2.565   -2.565   -2.565
```

1.1 k-point convergence

I run a python file to generate the command file of adding kpoints. It will generate 1.i to 8.i totally 8 files corresponding to the 8 shapes of the k points.

Then I get the total energy in the 8 output files and plot the figure also using python, the figure is:

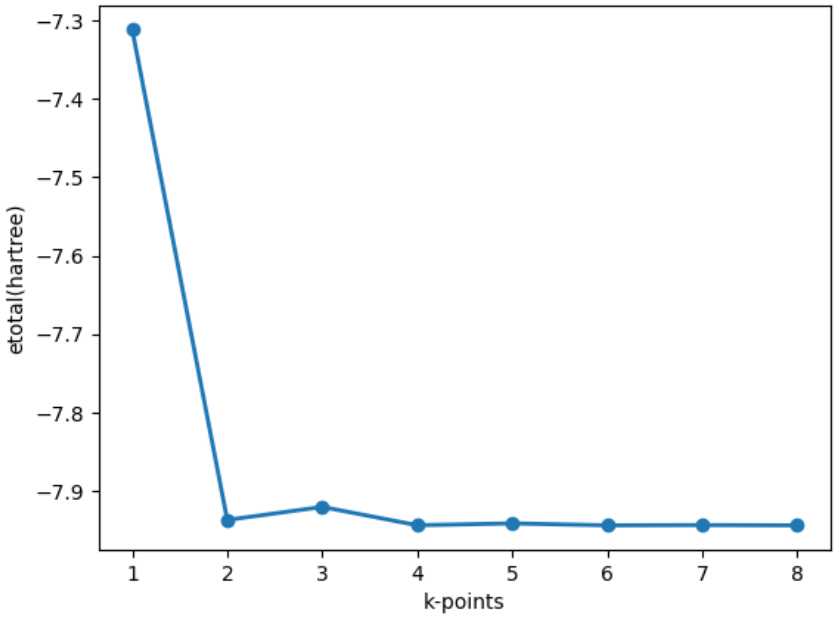

Figure 1: converged total energy with k points

You can see that the monotonicity is not particularly good. Because the 2*2*2 kpoints contain the 0 0 0 point but the 3 * 3 * 3 kpoints don't, so the 2 * 2 * 2 kpoints maybe better. And after 4 kpoints the energy could converge very well.

1.2 Non-SCF, band structure plot

In the reciprocal basis$\{\vec{b_1}, \vec{b_2}, \vec{b_3}\}$, the 3 point could be written as :

$$L : 0.5 \quad 0.5 \quad 0.5$$
$$\Gamma : 0.0 \quad 0.0 \quad 0.0$$
$$X : 0.5 \quad 0.0 \quad 0.5$$

And we first sample 100 points from L to Γ and then sample 100 points from Γ to X. Though there will be some points out of the first BZ, but the number of total sample points are still more than 100. I generate the way.i contains the add kpoint commends using python, then I use the run commend to get the eigenvalues of each point.

Then I use python to extract the eigenvalues from the way.out and plot the band structure pictures. I use the exact real wave vector in this figure, the length unit is bohr. You can see that the band structure is quite similar with the experimental results in [1] and the simulation results form [2].

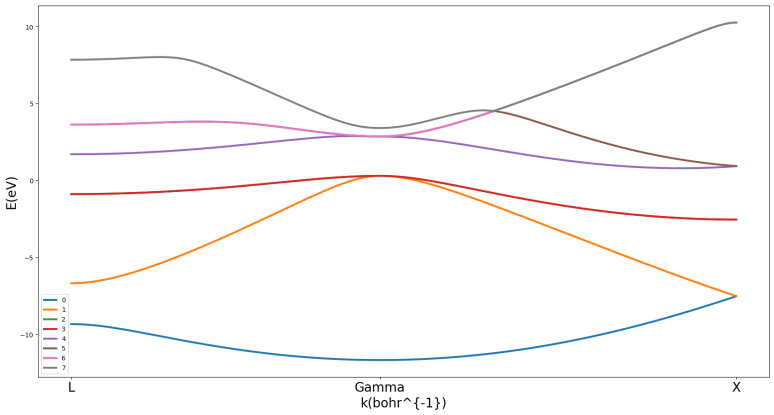

Figure 2: Band structure as $L \to \Gamma \to X$

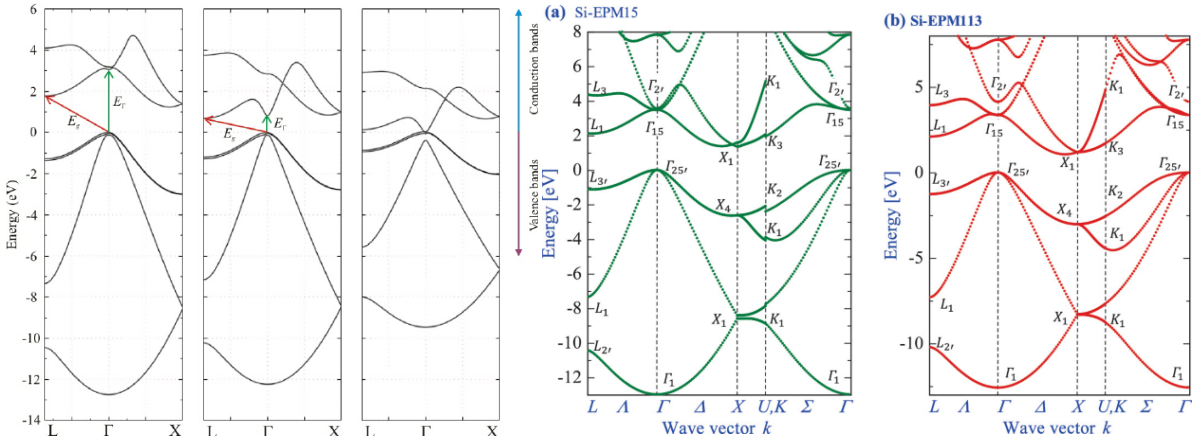

Figure 3: band structure from [1] in the left (the first figure), and [2] in the right.

SCF is called self-consistent field while non-SCF is non-self-consistent field. We only use the previously obtained density and do not update it, that is, we do not require the output density to be consistent with the input. The inderict band gap is is 0.5eV.

1.3 The effective mass

I write a python code to find the CBM then apply the polyfit on the local 11 points then I get the parameters and transfer it to SI units also using the python codes:

$$m_L^* \approx 0.952 m_e \tag{1}$$

It is a little similar to the literature result $0.91m_e$ from [3].

I make sure the variance of the fitting is about 10^{-10}.

References

[1] Filipe Oliveira. Photonic integrated circuit (pic) devices for inter- and intra-chip optical communication using gesn alloy layers grown on silicon substrates, 04 2011.

[2] Chihiro Hamaguchi. *Energy Band Structures of Semiconductors*, pages 1–63. Springer International Publishing, Cham, 2023.

[3] Martin A Green. Intrinsic concentration, effective densities of states, and effective mass in silicon. *Journal of Applied Physics*, 67(6):2944–2954, 1990.