MMM Ex 5

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1 Setup

To be sure for the cutoff, I took the larger one of the suggested cutoff's for Si and C form SSSP (see Tab. 1). The crystalline structure of β-SiC is simple face centered cubic, hence `ibrav=2`. In the crystal there are two atoms in the cell, one Si and one C atom. This results in the following `&SYSTEM` settings:

```
&SYSTEM
  ibrav=2
  a=4.36
  nat=2
  ntyp=2
  ecutwfc=45.0d0,
  ecutrho=360.0d0,
  occupations='smearing'
  degauss=0.001
/
```

For the atom species, the provided files in `pseudo` directory were used, together with the respective masses of Si and C:

```
ATOMIC_SPECIES
  Si 28.0855 Si.pbe-n-rrkjus_psl.1.0.0.UPF
  C  12 C.pbe-n-kjpaw_psl.1.0.0.UPF
```

Finally the positions. The atoms form thetrahedrons, such that the center atom (in my case C) is centered in a sub cube of the cell (see Crystall Structure SiC)

```
ATOMIC_POSITIONS {alat}
  Si   0.0000000000d0   0.0000000000d0   0.0000000000d0
  C    0.2500000000d0   0.2500000000d0   0.2500000000d0
```

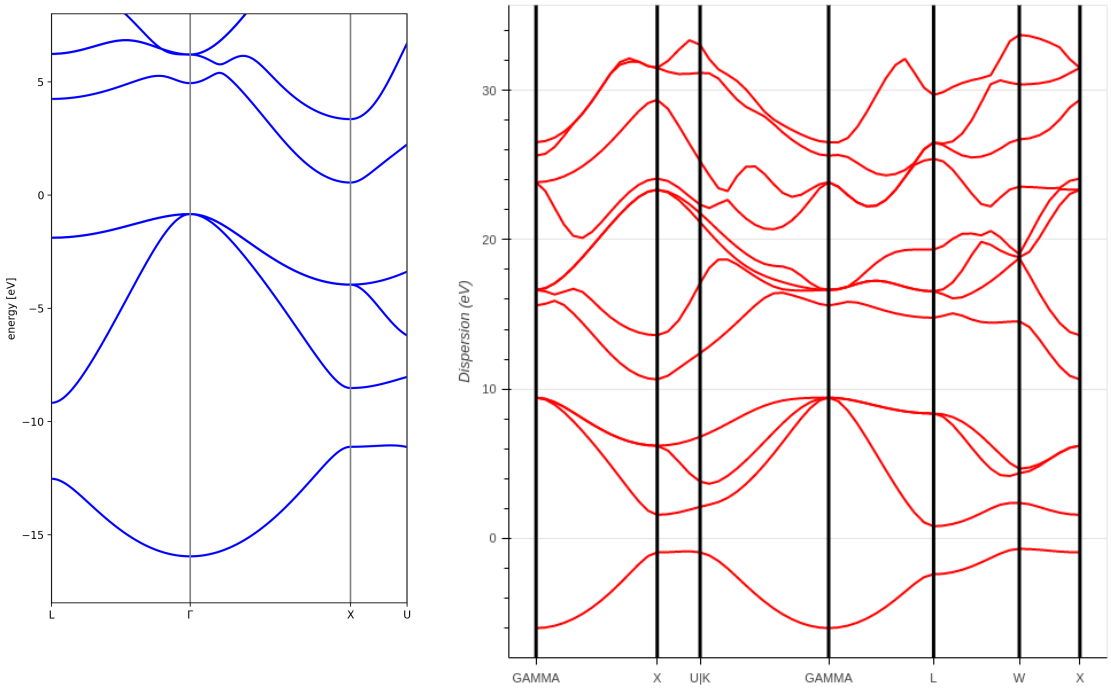
For the band structure calculation, we want to use the converged lattice parameter. This is $\|\mathbf{a1}\| * \texttt{alat} * 0.529177249 * \sqrt{2}$ because, the cell vector **a1** has been stretched in the optimization. We have to multiply it by `alat` because the cell vector is in cell coordinates. Then multiply by 0.529177249, the conversion rate from bohr to angstrom and finally multiply by $\sqrt{2}$ because **a1** originally had

	cutoff_wfc	cutoff_rho
Si	30.0	240.0
C	45.0	360.0

Table 1: Cutoff suggested by SSSP

two entries with amplitude 0.5. So to get the whole length, either take only the first entry of **a1** and multiply by two or the norm of a vector containing two such entries and multiplying by $\sqrt{2}$. ($\|\mathbf{a1} = (0.5, 0, 0.5)^\top\| = \sqrt{2} \cdot 0.5$).

I tried to run the same calculation with AiiDAlab but on my version there was only CSi id=24314 and id=51860 instead of id=mp-8062, suggested by the lecture nodes. As a consequence its not exactly the same structure. For example, the cell is triclinic instead of orthorhombic. Yet the structure around Gamma looks very similar but in at a different enegry level and a bit less streched out.



(a) Manual calculation (b) AiiDAlab reference

Figure 1: Resulting band structures