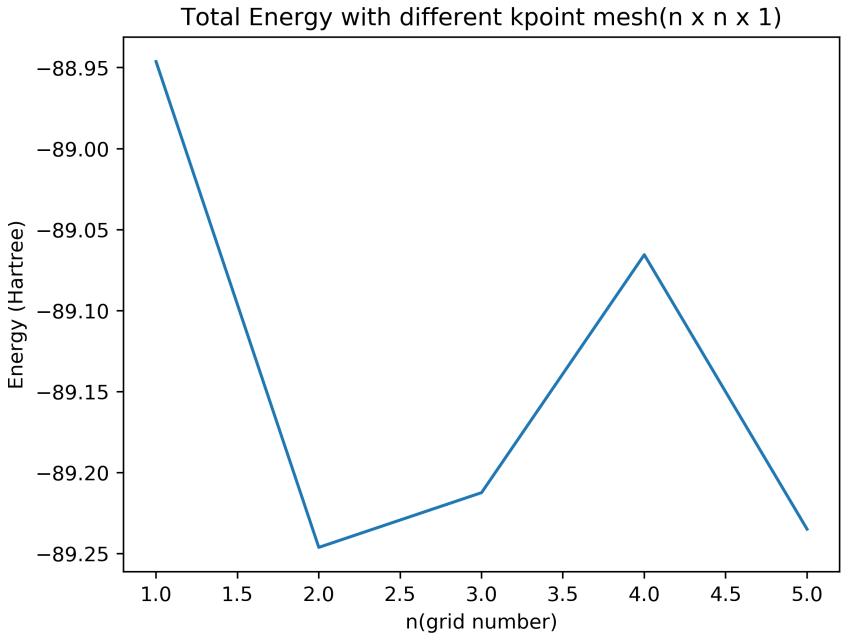
1. The Band Structure of MoS_2

Miao Wangqian

1.1. MP Sampling

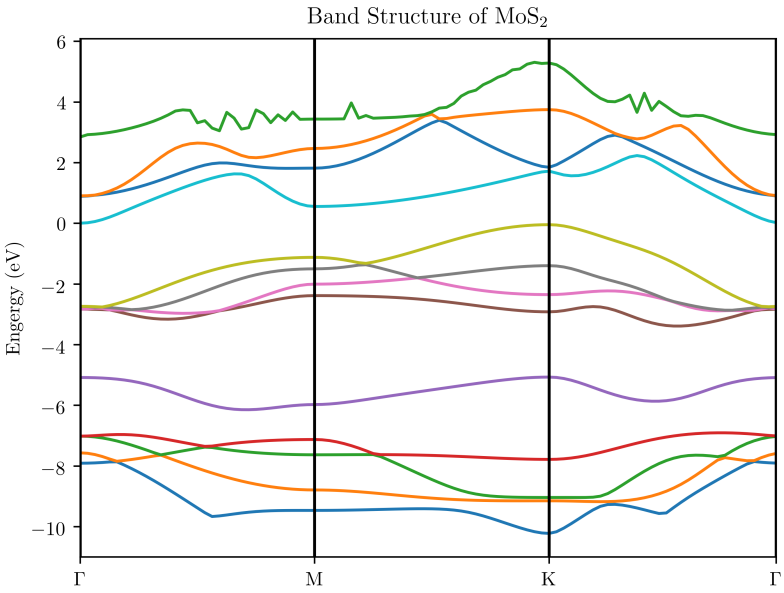
When we use the MP sampling method to do the ground energy calculation, the result is as following.



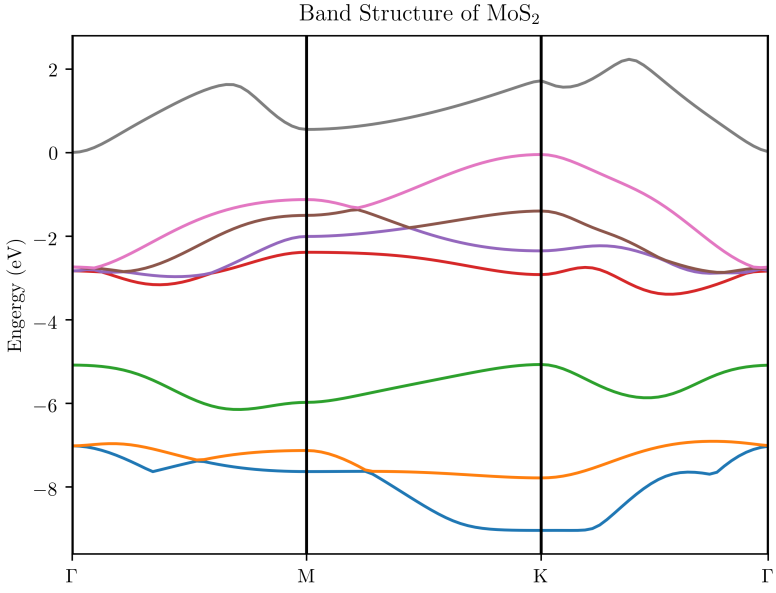
1.2. Band Structure

```
# create band.i
python k_sample.py
# run qbox
qb.x < bandstructure.in > band.out
# plot
python band.py
```

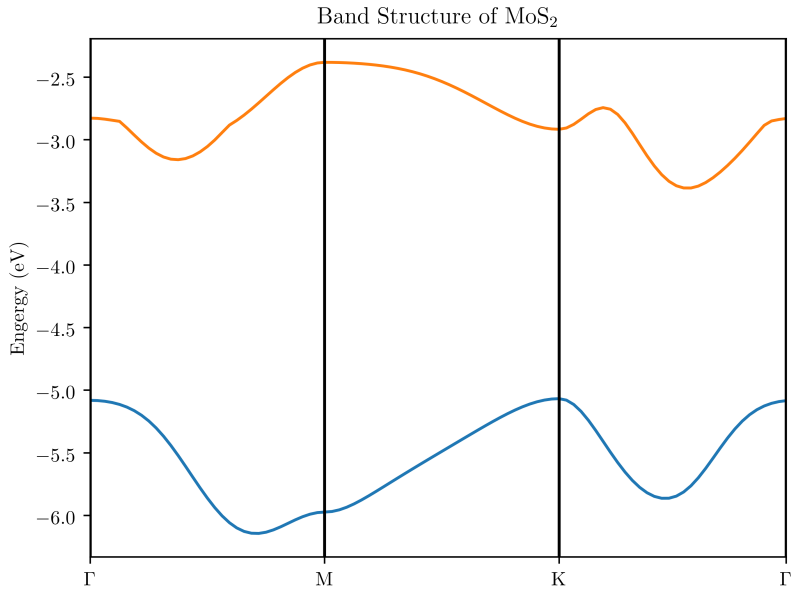
The band structure in the path $\Gamma \to M \to K \to \Gamma$ is as following, which is consistent with reference[1].
The overview of total bands is as following:



Eight bands near fermi surface is as following (The green one is the top of valence band and the red one is the bottom of conduction band):



Two bands near fermi surface (The blue one is the valence band and the orange one is the conduction band):



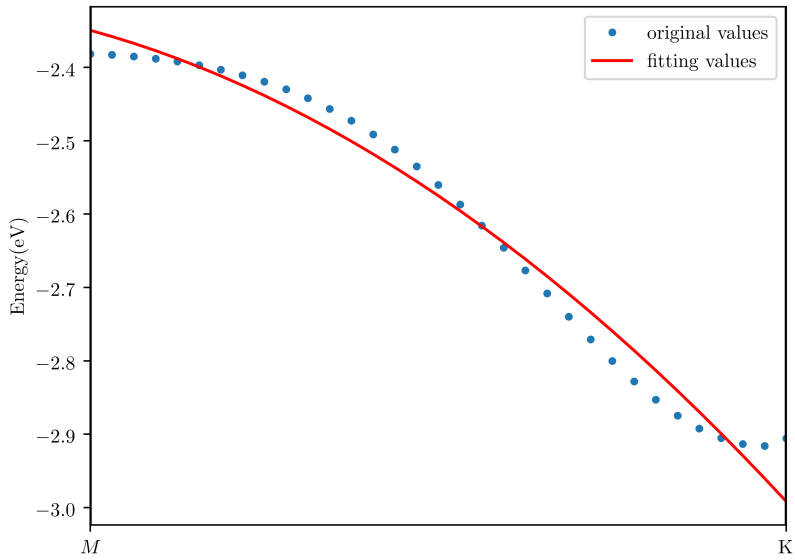
The band gap at K point is around 2.1 eV as shown in the picture above.

1.3. Effective Mass

The equation to calculate effective mass is as following:

$$m_{\text{eff}} = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2} \right)^{-1}$$

The effective mass along the path $M \rightarrow K$ is -4.51×10^{-30} kg. However, the effective mass at the K is almost zero.



1.4. Reference

[1] Electronic structure of a single MoS2 monolayer, Eugene S. Kadantsevab, Pawel Hawrylakb https://doi.org/10.1016/j.ssc.2012.02.005