1. Installing packages

conda activate myproject

pip install seekpath

pip install natsort

pip install sumo

pip install cp2k-output-tools

2. Parsing the band structure output to .csv format

Go to the folder where you have the .bs file (calc/hyp or calc/exp) and run:

cp2k\_bs2csv filename.bs #change for your file

3. Understanding and completing the jupyter notebook

Try to do it yourself to obtain the plot and effective masses of electron and hole for your structure (the one after seekpath analysis – you might need to make an .xyz file out of it and convert it to .cif; if you have issues with the conversion of cell matrix to cell parameters you can use the jupyter notebook in the “structures” folder).

First plot the graph and try to think, from the graph, what you expect of the effective masses.

Then compute the effective masses and compare.

Reading:

https:/doi.org/10.1063/1.5108995

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