**TUTORIAL WEEK 7**

**1. Results from optimization**

The results are available on the folders geo-opt and cell-opt.

You can save the last set of coordinates in the out file as an .xyz (with cell parameters) and then convert it to .cif using manage\_crystal.

Check for convergence and band gap in the out file.

Check if cell parameters changed significantly.

**2. Using seekpath to prepare a band structure calculation on CP2K**

Use the structure obtained from the last step of cell optimization.

Upload your structure to <https://www.materialscloud.org/work/tools/seekpath> (if you’re using .xyz, you will need to specify the cell parameters; if you use .cif it’s not necessary).

What is the suggested path?

As a test, upload separately your structure before any optimization and after geometry optimization. Does the path change?

*What you will need from seekpath*: suggested CP2K input coordinates (will consider the primitive cell); set of kpoints to be used. You will also need to take note on the lattice vectors in real and reciprocal space for later, when we will calculate the effective mass.

*What you need to add separately*: the scheme you want to use, some of the options are at gamma point, Monkhorst-Pack, etc.; and you also need to specify the grid, which at gamma point is 111, and for MP it can be 112, 113, 222 and so on. How do you decide it?

You can check an example of an input file for a band structure calculation on the folder bs-ex. Build your own input file and we will submit the calculation.

p.s.: you can also use pymatgen to get the primitive structure if you prefer, and you can install it with pip inside your conda environment: pip install pymatgen; open the .ipynb file on jupyter notebook to see an example.