Computational Chemistry 2 exercise 1 8.3.2019

All computations will be using the GPAW code. It has been implemented to Wihuri (wihuri.pub.chemistrylab.aalto.fi). You should have an own account in wihuri

You need to load the GPAW environment (save these)

module load ase
module load gpaw
module load gpaw-setups

to run the code (do not use more than 12 cores, 4 and 6 are also OK)

jsub –np 4 –mem 2G gpaw Cu.py

The cu.py can be any file that ends with .py (a python script file.) There are a lot of examples in the /home/kari/CC2-example directory. The GPAW manual is at page wiki.fysik.dtu.dk/gpaw

1) Compute the lattice parameter of Cu. (the lattice parameter that have the smallest energy). Use 8x8x8 k-points. (you can use Cu.py for very simple calculations and Cu-lattice.py will do it easier)

2) Test the convergence of Cu with respect of the k-points (use the minimum energy lattice parameter, again you can use Cu.py or Cu-k-points.py).

3) Draw Cu band structure in the Gamma-X direction (100 direction).

4) There is also a X-band-test.py program that produces a picture of the bands. It have to be run interactively: gpaw-python Cu-band-test.py

Extra) Repeat the same calculations for Si. (Hint: `si = bulk('Si', 'diamond',a=5.43`)