Computational Chemistry 2 exercise 2 15.3.2019

All computations will be using the GPAW code. It has been implemented to Wihuri (wihuri.pub.chemistrylab.aalto.fi). 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 12 –mem 4G gpaw cu.py

to run the code interactively

gpaw-python cu_dos.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) Do a bulk calculations of Cu, Si and NaCl. Save the .gpw files and then compute the density of states of them. Use at least 12 k-points

2) Compute the s- p- and d-projected density of states of Cu, Si and NaCl. The examples can be done interactively (with gpaw-python command)

3) Do a calculation for P doped Si using 64 atom unit cell. The system relaxation is not needed.

4) Compute the s- p-projected density of states of Si63P. Do it also for P, Si far from P and Si next to P.