Computational Chemistry 2 exercise 6 26.4.2019

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 3G 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-examples directory. The GPAW manual is at page wiki.fysik.dtu.dk/gpaw

1) Make a bulk NaCl and a 2x2x2-(100) NaCl surface with the ag tool. It has a rock salt structure. What is the lattice parameter? You need to do first the bulk system and then enlarge the box in the surface direction in the xyz file. Note you can use PBC in all 3 directions. (this is easier since in the non-periodic direction there need to be points and to fix that is a bit tricky. It can be done with the center command). Do the surface relaxation. For the surface system 1 k-point is enough.

2) Add a water molecule to the system, both on top of Na and Cl. How the molecule is oriented? This can be done inside the ag with add atoms tool. This can also read molecules, like the water.xyz file.

3) more challenging exercise: Add bulk water to the system. This can be done inside the ag with add atoms tool. This can also read molecules, like the w32.xyz file. There are two water files w32-last.xyz and w64-last.xyz the lattice of these are 9.85 and 12.41 Å. What is the problem with these files. It is much more efficient to do the AIMD simulation with CP2K. There is an input file md-NaCl-water.in. Use that. It needs a coordinate file NaCl-water.xyz and the lattice should be in a CELL section in line starting ABC (in the md..in file). The simulation is now 1000 fs long (STEPS 1000) it is rather short but is takes some time. One can follow the dynamics with ag by ag NaCl-water-pos-1.xyz (the xyz file is one of the output files of CP2K). See also NaCl-water-1.ener for temperature etc.

One can follow the geometry of a GPAW calculation by making a .xyz file from the out file:

ag MgO-surf.out –o MgO-surf-opt.xyz

and then ag cnt-xxx.xyz (or if you want vmd cnt-xxx.xyz)

to run CP2K: module load cp2k and then jsub –np 12 -mem 2G