Computational Chemistry 2 exercise 5 5.4.2019

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) N doped CNT are rather good catalyst for hydrogen evolution. The whole reaction is rather complex but one can learn something by looking the hydrogen adsoption energy. Make a (10,0) CNT with one N dopant. The z-length should be 2 unit cells. Add a hydrogen atom on top of the N and a C next to the N. Use a neutral system and 2 or 4 k-points. You need to optimized the geometry. Which have lower energy. You can also do a calculation of H on a C far from N. Note the calculations take quite long. Look also the dos of these systems.
2) Make a bulk MgO and a 2x2x2-(100) MgO surface with the ag tool. It has a rock salt structure. What is the lattice parameter (A=4.21 Å). You need to do first the bulk system and then edit the box in the xyz file. You can use PBC in 2 or 3 directions. Compute the bulk electronic properties and do the surface relaxation. For the surface system 1 k-point is enough.
3) Add a Pt atom on the MgO surface. Where it likes to be (top of O, Mg or bridge, or hollow site).

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

ag –n 0:99 cnt-10x0-nh-2k.out –o cnt-10x0-nh-2k.xyz

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