Computational Chemistry 2 exercise 4 29.3.2019

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

1-2) Estimate the CO molecules dissociation energy on Cu(111) surface. Now the unit cell need to be 2x2. You need to do 3 calculations CO, C and O on the surface. What error you will make if you put both C and O on the 2x2 surface.
3) Estimate Ag enrichment energy to Cu(111) and Cu(100) surfaces. You can make the cell by ag or take a look of the ener-agcu111.py file (/home/kari/CC2-example).
4) Carbon nanotubes (CNT) conductivity depend on their chirality. Make (10,10) and (10,0) CN tubes with ag tool or directly with python and plot their dos near Fermi energy. Note you need quite many k-point in tube direction. How about the other directions.