Computational Chemistry 2 exercise 3 22.3.2019

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

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

1) Compute Cu(111) surface relaxation using 1x1 unit cell and 5 atomic layers.

2) Compute the CO vibration frequency.

3) Compute CO molecule on Cu(111) surface. Now the unit cell need to be 2x2. The molecule is easiest to put on the surface by ag. Put the molecule on hollow site. What is the binding energy? (You need to compute the energy of the clean 2x2 surface and the CO molecule.)

4) A bit difficult one: Compute the vibrational frequency of the adsorbed CO molecule (only the CO molecule)

Python example of the Cu(111) surface:

```
from ase import Atoms
from gpaw import GPAW,FermiDirac,Mixer,restart
from ase.optimize import QuasiNewton
from ase.io import read,write
from ase import units
from ase.lattice.surface import fcc111

FD = 0.05
k = 3
hp = 0.20
cu = fcc111(symbol='Cu', size=[1, 1, 5],a=3.610, vacuum=8.000)

calc=(GPAW(h=hp, nbands=-12, xc='PBE',kpts=(k, k, 1), occupations=FermiDirac(FD),
      mixer=Mixer(beta=0.10, nmaxold=4, weight=90.0),
      convergence={'eigenstates': 5.0e-6, 'density': 1.0e-4}, txt='cu111-11.out'))

cu.set_calculator(calc)
energy=cu.get_potential_energy()

relax = QuasiNewton(cu, logfile='cu111-11.log')
relax.run(fmax=0.1)

cu.calc.write('Cu111-11.gpw')
```

Example of a vibrational computation of Cu(111) adsorbed CO molecule:

```
from ase import Atoms
from gpaw import GPAW,FermiDirac,Mixer,restart
from ase.io import read,write
from ase import units
from ase.vibrations import Vibrations
```

```
cu,calc=restart('Cu111-CO.gpw',txt='cu111-co-vib.out')

vib=Vibrations(cu,indices=[0,1],name='co-cu111-vib')
vib.run()
vib.summary(log='co-cu111-vib.log')
```