Computational Chemistry 2 exercise 8 3.5.2019

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

here also

module load cp2k

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 or jsub –np 12 –mem 3G cp2k md-NaCl-water.in

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) Do a TDDFT Time Propagation simulation for a Be atom. See the manual of the example. Look the results in time and frequency domain. Do a one 40 fs run. That should be long enough.

2) Do a Linear Response TDDFT calculations for a water molecule. The manuals example need to modify a bit. In water there are 4 occupied states and one can use 30 empty states.