Computational Chemistry 2, CHEM-E4225, Exercise 4 17.11.2022

To run Orca you need to load it: module load orca

to run it (in mylly2) jsub orca H2O.inp for more memory

jsub -mem 2400M orca phenol-ccsd-exited.inp

for cp2k: jsub -np 24 cp2k md-NaCl-water-28.inp

There are a lot of example file in /home/kari/CC2-2022-examples

To see what is in this dir type ls -l /home/kari/CC2-2022-examples (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2022-examples/h2o.inp . (there is a dot at the end it is your working directory)

1) Do a short (0.5 ps) AIMD simulation of NaCl-water system using the CP2K code. How the waters are oriented around the Cl- (or Na+). Here the simulation time is so short that it may be difficult to see the orientation in detail. These simulations will take some hours. (The input file for CP2K is md-NaCl-water-28.inp use 24 cores. The CP2K have to be loaded with command module load cp2k, use ase gui to visualize the NaCl-water-28-pos-1.xyz file) Look the NaCl-water-28-1.ener file for the temperature. You can plot the temp with gnuplot: first gnuplot then inside gnuplot plot 'NaCl-water-28-1.ener' u 2:4 w l

You need two files: md-NaCl-water-28.in and NaCl-water-28.xyz There are also longer simulation files on examples dir if you like to analyse them.

2) Do a TDDFT (with pbe and pbe0), CID and STEOM-CCSD calculation of a water, benzene and phenol. (for ccsd see phenol-ccsd-exited.inp, these calculations need more memory, see above) Compare the exited state energies. See also if there are states that are combinations of several KS or HF states. Which of these methods are closest to CCSD. Note the CCSD calculations will take up to 10 min. Look the intensities of the peaks of some of the molecules. Do they vary significantly.

3) Investigate the molecule size effect to the lowest exited state by doing TDDFT calculations of benzene, 2 fused benzenes (2ring) and 3 fused benzenes (antra). Use more memory (2400M)

4) Try the stddft methods for the anthracene. Is that faster than the TDDFT.

5) Add an electron to anthracene (you need to edit the xyzfile line. The two numbers in it means the charge of the molecule and it spin state. Usually there is 0 and 1, these should be -1 and 2. You can use the optimized structure). What happen to the exited states. Is this in agreement with the observation "Reduction of anthracene with alkali metals yields the deeply colored radical anion salts M^+[anthracene]$^-$ (M = Li, Na, K)."

ase gui can be started with 'module load python'

The instructions of mylly2 are included.

In the first time make your own directory in /home/kari/CC2-2022-results
mkdir /home/kari/CC2-2022-results/ossi (ossi should be your own name)
At end of exercise copy the results to your result dir: cp *out /home/kari/CC2-2022-results/ossi

Orca input library: https://sites.google.com/site/orcainputlibrary/home