Computational Chemistry 2, CHEM-E4225, Exercise 4 6.5.2021

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

to run it (in Wihuri) jsub -np 4 orca H2O.inp

There are a lot of example file in /home/kari/CC2-2021-example

To see what is in this dir type ls -l /home/kari/CC2-2021-example (ls is the list command)

you can copy the example files to your own directory: cp /home/kari/CC2-2021-example/h2o.inp .
(there is a dot at the end it is your working directory)

1-2) Do a TDDFT (with pbe and pbe0), CID and STEOM-CCSD calculation of a water, benzene and phenol. 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 25 min.

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).

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

5) Add an electron to anthracene (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)."

6) Look the intensities of the peaks of some of the molecules. Do they vary significantly. EXTRA: There is ASA tool (orca_asa) to visualize the adsorption spectra but I did not get it to work. You can try it.

ase-gui can be started with 'module load ase'

The instructions of Wihuri are included.

In the first time make your own directory in /home/kari/CC2-2021-results
mkdir /home/kari/CC2-2021-results/ossi (ossi should be your own name)
At end of exercise copy the results to your result dir: cp *out /home/kari/CC2-2021-results/ossi

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