

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 excited 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. Here you should add the available memory: `jsub -np 6 -mem 2G -smp orca h2o-tddft...inp`

3) Investigate the molecule size effect to the lowest excited state by doing TDDFT calculations of benzene, 2 fused benzenes (2ring) and 3 fused benzenes (antra). Here you should add the available memory: `jsub -np 12 -mem 4G -smp orca antra...inp`

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 its spin state. Usually there is 0 and 1, these should be -1 and 2. You can use the optimized structure). What happens to the excited states. Is this in agreement with the observation "Reduction of anthracene with alkali metals yields the deeply colored radical anion salts $M^+[\text{anthracene}]^-$ (M = Li, Na, K)."

6) Look at the intensities of the peaks of some of the molecules. Do they vary significantly. EXTRA: There is an 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 python/3.8-gpaw'`

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>