Computational Chemistry 1, CHEM-E4110, Quantum chemistry Exercise 5 22.1.2019

1) Find out how you can add point charges to Orca calculation. (Chapter 6.1.3) and do a water dimer calculation so that one of the waters has been replaced with point charges. Use charges of -0.834 for O and 0.417 for H. Why you shouldn't optimize the structure?

2) Do a solvation calculation of Na^{+}, Ca^{2+}, Al^{3+}, Cl- and Na+$(H_2O)_6$ in water and hexane. Compare the solvation energies, CPCM Dielectric + Free-energy (cav+disp) .

3) Do an ab initio molecular dynamics calculation of Cl- or Na+ in 31 water molecules using CP2K code. The input and .xyz files are in /home/kari/CC-example. To run the CP2K code type jsub –np 12 –smp cp2k md-w31-cl.inp you need to load the CP2K code before: module load cp2k (instructions are also in run-cp2k). Warning this takes (with 12 cores) almost 2 hours. Use vmd or ag to see the w31-cl-pos-1.xyz file. See how the temperature and potential energy behaves (from the w31-xx-1.ener file.)

4) Complete any of the unfinished exercises.

   The instructions of Wihuri are included. Also example files of the exercises are included.