Computational Chemistry 1, CHEM-E4110, Quantum chemistry Exercise 4 18.1.2019

1) Do a water (and methanol) calculations with HF and PBE (using TZ basis, optimize the structure). Compare the Mulliken and Lowdin charges. Compare also the dipole moments.

2) (A bit difficult thing). Try to plot the some of the orbitals (MO) of CH2=CH2 (or water). Use the %plot tool to store the cube file (Format Cube) and the VMD to visualize them. In VMD use the Graphics Representation isosurface. The scan the isovalue to see different density values. Use either Solid Surface or Wireframe. Find also how to plot the electron density. (see also the orca_plot tool)

3) Go to the water dimer calculation and compute the free energy difference at room temp (295 K). Note you need the free energy of the monomer. Try to do it also at 100 K and 500 K.

4) Do calculation of water molecule using two solvents, water and THF using the CPMD model with SMD and without it. Compare the dielectric energy, the solvation energy, dipole moment, and vibrational frequencies.

extra) Do a bond scan calculation for OH bond of methanol. (The scan window could be 0.8 – 1.2 Å). Try to fit a parable (a*(r-r0)**2+E0, here r0 is the minimum bond distance and E0 the min energy) and a third order polynomial (b*(r-r0)**3+a(r-r0)**2+E0). Is the real potential anharmonic.

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