Computational Chemistry 1, CHEM-E4110, Quantum chemistry Exercise 3 15.1.2019

1) Compute the correlation energy (no optimization) of water molecule using MP2 and CCSD(T) methods. Do some basis set extrapolation. Check which basis functions allow the automatic extrapolation. The geometry can be optimized with MP2.

2) Do a DFT calculation with PBE and PBE0 methods for water. Compare the correlation energy.

3) Find out how to do RI-MP2 calculation for say some of the methyl-phenols. (use PBE or similar optimized geom) here use jsub –np 6 –mem 4G orca …

4) Do a DLPNO-CCSD(T) calculation of a methyl-phenols. (do not optimize the structure, use DZ type basis) here use jsub –np 6 –mem 4G orca …

5) Do calculation of water dimer with LDA and MP2. Use aug- basis. What is the binding energy. Do the frequency calculations with LDA and PBE for water molecule and dimer. Compare the computer times.

6) Make an anhamonic analysis of a water molecule using the VPT2 method. (you can used PBE and TZ basis.)

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