Computational chemistry II assignments Oct. 2019

Essay assignment

Explain the following aspects (choose 3)

E1) The basis set: what type of basis functions there are and what is the logic behind them. Why we need basis functions? What kind of function you should use? What is the idea of basis set interpolation?

E2) Explain the general ideas of wave function based post-HF methods. What is correlation energy, explain the CI (or CC) methods and MPn method (you do not need to go deep into the math.) Explain the general idea of the DFT. List some of the problems of DFT and why it is still very popular method. What can you say of the formal computational scaling of these methods and how this correspond to scaling of practical scaling of slightly approximated similar methods?

E3) How can you estimate the Gibbs Free energy using quantum chemical methods. What kind of systems these calculations are valid and why? What is the advance of AIMD methods for Free energy calculations?

E4) In Machine Learning the overfitting is a key problem. What it means and how the training and test set are related to that? What is a good quality criterion of a ML model? We can choose several ML models but why we need to optimize a chosen ML method?

Computational assignments (choose 4)

C1) Investigate the correlation energy of water molecule using MP2 and DZ, TZ and QZ basis. Use also some interpolation method. Do also CCSD and CCSD(T) calculations. Here two basis are enough. Estimate the value of the full correlation energy.

C2) Compute the binding energy and Free energy of water dimer at 100 K, 300 K and 500 K. What can you say of the bonding? Use MP2 level of theory. Think what basis to use.

C3) Compute the IR spectra for benzene, toluene and phenol. Decide what theory and basis to use. Compare to the experimental spectra. In benzene and toluene try to find the corresponding high intensity peaks. Which experimental peaks are probably overtones. The orca_mapspc is useful. Note that phenol is difficult and the detailed assignment is not needed. Why the highest frequency peak of phenol is so broad. A good experimental database: https://sdbs.db.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

C4) Investigate the solvation effect of methanol molecule. Decide what theory and basis to use. Do the calculations in gas phase, toluene and water. Report the change in dipole moment, vibrational frequencies, IR intensities and the solvation energy. Do a vibration calculation of water tetramer (it is a planar ring, square. You should start from the optimized coord since the convergence is slow). What you can say of the O-H stretching frequencies compared to the solvation calculation of a single water molecule.

C5) Do a 5 ps (5000 steps) AIMD simulation of HCl in water using the CP2K code. How the waters are oriented around the Cl- and what happen to HCl molecule. These simulations will take easily a day. (there is an input file for CP2K md-w31-hcl.inp use 12 cores. The CP2K is loaded with command module load cp2k, use ase-gui or vmd to visualize the w31-hcl-pos-1.xyz file) Look the w31-hcl-1.ener file for the temperature.

will continue ….

C6) I try to add a ML problem. Stay tuned.

You should do **3 E assignments** and **4 C assignments** from the total list above. You will get 5 p. form the each of the theoretical assignments and 4 p. form the computational ones.

Each E assignment report should be at least 3 pages and C assignment around 3 pages (you can and should use some figures or screen captures) and there should be 1.5-2 pages of text. All material you find can be used but do not copy directly any source, like Wikipedia. Please use at least some references especially in the E assignments. When returning the assignments, put your NAME, STUDENT NUMBER to the filename. You can return the E and C assignments on two different files. If you return them individually put the assignment name on the filename (like ..E1.pdf or ..C3.docx). Most common formats are OK. pdf is recommended.

Return the answers to the MyCourses folder. I would hope to get them latest **at end of Nov. 2021.**