Computational Chemistry and Materials Modeling

Lab 2, due date is set in Canvas LMS

Topic: computational chemistry of molecules with DFT

Notes: Upload solution as a single file "YourName.zip". Provide absolute minimum of supporting info - no copies of work folders. Compare results with published experimental and theoretical data. Solution must be submitted as article-style report supplemented by required technical les: xyz- and cif-geometries, program run log- or out- files, extra figures etc. Be prepared to give a 5 min presentation of everything that you consider non trivial in your work.

Take a molecule consisting of at least 10 atoms and having a singlet ground state. Using DFT in vacuo and in a solvent:

- Optimize singlet geometry. Plot frontier orbitals and determine their energies. Calculate the HOMO-LUMO gap.
- Optimize Triplet state. Plot frontier orbitals and determine their energies. Calculate the HOMO-LUMO gap. Explain geometry changes relative to singlet. Determine ground state.
- Optimize geometry of cation/anion. Calculate IP/EA for both vertical and relaxed electron detachment/attachment.
- Calculate solvation energies of all the above states (including ground state).
- Compare IP/EA in vacuo and in the solvent.
- Calculate IR/Raman spectra and explain the nature of the most prominent spectroscopic features.
- Calculate deprotonation energy and proton affinity in vacuo and in the solvent.

Advanced (optional):

- Calculate 10-20 singlet excited states and plot the UV-Vis absorption spectrum. Explain the oscillator strength and nature of the lowest excited states in terms of MOs.
- Explain geometry changes of the relaxed S_1, T_1, cation/anion relative to the ground state. Calculate solvation energies of all the above states (including ground state).
- Optimize geometry of S_1 state (lowest excited singlet) and calculate the fluorescence energy and Stokes shift. Estimate the radiative lifetime of S_1 state.
- Optimize geometry of T_1 state (lowest energy triplet). Calculate the phosphorescence energy using both SCF and TDDFT approaches. Explain the nature of the T_1 state in terms of MOs.
- Compare IP/EA and singlet/triplet excitation energies in vacuo and in the solvent.

Sample solution: See Lab2 benzene.zip