Computational Chemistry and Materials Modeling
Lab 3, due date is set in Storion web page
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.*

The Lab work is separated into three parts: *practical part*, which includes all calculations; one-minute *oral presentation* and *written report*.

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

- (5%) Optimize singlet geometry. Plot frontier orbitals and determine their energies. Calculate the HOMO-LUMO gap.
- (15%) Optimize Triplet state. Plot frontier orbitals and determine their energies. Calculate the HOMO-LUMO gap. Explain geometry changes relative to singlet. Determine ground state.
- (10%) Optimize geometry of cation/anion. Calculate IP/EA for both vertical and relaxed electron detachment/attachment.
- (10%) Calculate solvation energies of all the above states (including ground state).
- (5%) Compare IP/EA in vacuo and in the solvent.
- (15%) Calculate IR/Raman spectra and explain the nature of the most prominent spectroscopic features.
- (10%) Calculate deprotonation energy and proton affinity in vacuo and in the solvent.

Advanced (optional):

- (+10%) 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.
- (+10%) 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).
- (+10%) 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.
- (+10%) 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.
- (+10%) Compare IP/EA and singlet/triplet excitation energies in vacuo and in the solvent.

Oral presentation. On the day of Lab report, you have to make a one-minute one-slide presentation with the main results of your work, which include the optimized structure of your selected molecule, information on stability, molecular orbitals and triplet/cation/anion state.

Lab report. Using the example of Lab report, you need to make your own, which includes all the results, their analysis and names of the input files. The following points are graded:

- (10%) Analysis of the results.
- (5%) Presence of input files names.
- (5%) Appropriate grammar and vocabulary.

Total grading: Practical work (70%) + Oral presentation (10%) + Written report (20%).

Sample solution: See Lab3 benzene.zip.