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 files: 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 nontrivial in your work.*

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

- Optimize ground state geometry. Plot frontier orbitals and determine their energies. Calculate the HOMO-LUMO gap.
- 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.
- 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 ΔSCF and TDDFT approaches. Explain the nature of the T_1 state in terms of MOs.
- Optimize geometry of cation/anion. Calculate IP/EA for both vertical and relaxed electron detachment/attachment.
- 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).
- Compare IP/EA and singlet/triplet excitation energies in vacuo and in the solvent.
- Calculate IR/Raman spectra and explain nature of the most prominent spectroscopic features.
- Calculate deprotonation energy and proton affinity in vacuo and in the solvent.

Sample solution: See Lab2_benzene.zip