Studying Solvation Effects on Electronic Excited States and Spectra with Computational Chemistry

Quantum Chemistry Group of Bochum

In this hands-on module, participants will learn how to calculate with computational chemistry methods molecular structures, spectra, and reaction energies in vacuum and solution. We will use the TURBOMOLE and the COSMOconf and COSMOtherm program packages with graphical user interfaces, use Density Functional Theory (DFT) and calculate acid constants (pK_a) e.g. in aqueous solution. If time allows, we may in addition look at electronic excitation energies (UV/Vis spectra) and solvent shifts in these spectra.

Participants will in this module how to

- build initial molecular structures on a computer and how to optimize their structures with DFT
- compute vibrational spectra and visualize normal modes,
- include solvent effects with implicit solvent models
- calculate (de-)protonation energies and acid constants (pK_a)