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Solvation Effects on Electronic Excited States and Spectroscopy

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Understanding the photo-excitation processes and relevant spectroscopic data requires quantum mechanical description of molecular electronic structures. Moreover, as most of the photochemistry happens in solution, it is troublesome to exclude solvent effects in simulation of electronic spectra, *e.g.* UV/Vis spectra. A potentially very accurate strategy to compute excitation energies of molecules in solution consists of the inclusion of a large number of excplicit solvent molecules combined with a sampling over a statistically representative number of configurations to reproduce bulk and fluctuation effects. However, if this approach is used with accurate quantum mechanical methods, the sampling triggers, even for a relatively small number of explicit solvent molecules, high computational costs. Beside other effects, the most important solute-solvent interactions on the electronic excitations are generally of electrostatic origin and related to the solvent polarity. Recently, in our labratory, the well-known polarizable continuum model, COSMO is combined with *ab initio* ADC(2) method that is useful to describe electronic excitations in solution. Furthermore, to go beyond the continuum description of solute-solvent interactions, we have introduced an atomistic polarizable QM/MM method, PE-ADC(2) that retains the atomistic description of solute molecules and the solvent electrostatic effects, while comparing to full quantum mechanical calculations reduces the computational costs of simulation significantly.

In this practical, beside the conventional quantum chemistry methods, some of the recently developed methods that are designed to study electronic excitations in solutions will be introduced. We do not assume that every participant has done a computer simulation before. The practical will be conducted with TURBOMOLE program package and we will use computers that are equipted with Linux operating system. Participants will learn how to build initial molecular structures and how to find the optimized geometries and calculate the excitation energies in vacuum and within the polarizable continuum model. Afterwards, we will continue with setting up a polarizable QM/MM calculations for the same target systems and then pursue a workflow to visualize the UV/Vis spectra and natural transition orbitals to analyze the results. The role of solvatin and the best practices in order to do an appropriate quantum chemistry simulation will be discussed between the participants.