Modeling UV/Vis Spectroscopy of Solvated Systems Through QM/MM

Overview:

Hybrid quantum mechanics/molecular mechanics (QM/MM) is a computational approach that combines the accuracy of quantum mechanical calculations with the sampling efficiency of molecular mechanics simulations. This methodology is particularly useful for studying complex systems, such as solvated systems, where the presence of a solvent significantly influences the behavior of the solutes. The system is divided into two parts: a QM region that includes the solute and possibly a small number of vicinal molecules, while the remainder fraction of the simulated system is described by a molecular mechanics force field. This division is possible because the spectral response in the large majority of cases arises from the solute, not from the solvent. Therefore, the solute must be accurately described in all its degrees of freedom, while the remainder of the system can be treated at a lower level of theory. The most challenging aspect of QM/MM models is the definition of the solute-solvent coupling term. After being set, it can be inserted into the solute's QM Hamiltonian through explicit terms, thus permitting the exploitation of the quantum chemistry machinery to obtain the desired properties in the same way as they are calculated for isolated systems. The QM/MM approach allows us to take full advantage of decades of research and development of QM methods for isolated systems and of MM methods for large systems, to enable the accurate and computationally efficient simulation of large systems.

Learning goal:

The workshop aims to equip participants with a foundational understanding of QM/MM simulations, as well as practical skills in applying these methods to model electronic spectra of solvated systems.

Course Structure:

- Introduction:
  Brief overview of QM/MM simulations, DFT methods, and molecular mechanics force field.
- Tutorials:
  General tutorials on applying QM/MM coupled with Molecular Dynamics (MD) for modeling electronic spectra. Emphasis on systems of varying complexity in different environments.

Prerequisites:

- Familiarity with basic MD and DFT techniques is recommended for an enriched learning experience.

Venue: University of Duisburg-Essen, Faculty of Physics, AG Kuiper,
Lotharstr. 1
47057 Duisburg, Germany
Office: MD 263
Closest Tram Station: Zoo/Uni Duisburg

Duration of the course: 24 May 2024, from 10:00am-4:00pm.

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