Electronic and Molecular Structure Theory (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
7 RC	9 CP	270 h	2. Semester	Each SuS	1 Semester
Courses a) Lectures b) Exercises c) Integrated computer practical			**Contact hours** a+b) 3 SWS c) 5 SWS	**Self-Study** a) 30 h b) 75 h c) 75 h	**Group size** 10-20 Students

Prerequisites

Learning outcomes

a+b) After completing this course students will have basic knowledge of modern wavefunction-based computational electronic and molecular structure methods and how these methods can be applied to solve typical problems in structure determination, spectroscopy, and the investigation of mechanisms and energetics of chemical reactions. Furthermore, they will know how to judge the accuracy and reliability of such methods.

c) They will be familiar with software for electronic structure calculations, know how apply modern electronic structure methods to practical problems and how to analyze, visualize and present results of electronic and molecular structure calculations.

Content

a+b) The course starts with basic principles for quantum mechanical many-particle systems and how their wavefunctions can be described in compact ways and then discusses a variety of modern wavefunction methods and their application:

- Pauli principle and Slater determinants
- Particle number representation (second quantization)
- Hartree-Fock and Multiconfigurational Self-Consistent Field methods
- Single- and Multiconfigurational Configuration Interaction methods
- Single- and Multireference Perturbation Theory
- Coupled-Cluster Methods
- Explicitly Correlated F12 Methods
- Response Theory approach to excitation energies and spectra
- Basis set convergence and basis set extrapolation
- Thermochemistry protocols

c) Application of electronic structure methods to determine molecular structures, energy differences between conformers, barriers for interconversion, vibrational spectra (IR and Raman), characterization of electronically excited states, optical spectra (UV-Vis), accurate reaction energies and intermolecular binding energies.

Teaching methods

a+b) Lectures and exercises with problems for self-studying, Q&A and discussion sessions with presentations given by the participants, Moodle course with online material.
c) Computational hands-on projects to be solved on own laptops and/or a computer lab with different software packages, done partially in supervised sessions and partially as self-study.

Mode of assessment

a+b) submission and grading of the solution sheets for the exercises and a final oral end-of-semester exam
c) submission and grading of reports of the computational hands-on projects

Requirements for the award of credit points

c) successful acceptance of the reports for the computational hands-on projects and

a+b) passing the oral end-of-semester exam
Module applicability M.Sc. iMOS and M.Sc. Chemistry
Weight of the mark for the final score According to CP
Module coordinator and lecturer(s) C. Haettig
Further information