

Modulbezeichnung: Quantum Chemistry I (QuantCh-1) **5 ECTS**
(Quantum Chemistry I)

Modulverantwortliche/r: Andreas Görling

Lehrende: Andreas Görling

Startsemester: WS 2021/2022

Dauer: 1 Semester

Turnus: jährlich (WS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry 1 (WS 2021/2022, Vorlesung mit Übung, Andreas Görling et al.)

Empfohlene Voraussetzungen:

Required Qualifications:

- good knowledge of basic quantum mechanics: axioms of QM, application to simple systems (particle in a box, harmonic oscillator, rigid rotator)
- good knowledge in mathematics: differential calculus of functions of several variables, linear algebra

Inhalt:

- Mathematical concepts and current research issues in the field of quantum and computer chemistry
- Hartree-Fock, DFT

Lernziele und Kompetenzen:

Students ...

- obtain sound knowledge in basic methods of quantum chemistry
- are able to solve mathematical problems occurring in quantum chemistry
- are able to understand and assess scientific reports in the field of quantum chemistry

Literatur:

- Attila Szabo, Neil S. Ostlund: Modern Quantum Chemistry, Dover 1996
- Frank Jensen: Introduction to Computational Chemistry, Wiley 2017 (3rd ed.)
- Ira N. Levine: Quantum Chemistry, Pearson 2016 (7th ed.)

Organisatorisches:

- The elective module "Quantum Chemistry I" will be taught only in winter term!
- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)