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

Modulverantwortliche/r: Andreas Görling
 Lehrende: Andreas Görling

| | | |
|-----------------------------|------------------------|-----------------------|
| Startsemester: WS 2020/2021 | Dauer: 1 Semester | Turnus: jährlich (WS) |
| Präsenzzeit: 45 Std. | Eigenstudium: 105 Std. | Sprache: Englisch |

Lehrveranstaltungen:

Quantum Chemistry I (WS 2020/2021, Vorlesung mit Übung, 3 SWS, Andreas Görling et al.)

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!
- Quantum Chemistry I will be taught online (synchronous/asynchronous) until further notice
- 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)