
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
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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.)
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Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Chemistry (Master of Science) | Wahlmodule | Quantum Chemistry 1)

[2] **Data Science (Master of Science)**

(Po-Vers. 2021w | Gesamtkonto | Anwendungsfach | Chemistry | Quantum Chemistry 1)

[3] **Molecular Science (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Molecular Science (Master of Science) | Elective modules | Quantum Chemistry 1)

Studien-/Prüfungsleistungen:

Quantum Chemistry 1 (Prüfungsnummer: 65591)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral Examination (20 minutes, not graded: pass/fail) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Andreas Görling

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)