Modulbezeichnung: **Quantum Chemistry (CM-QC)** **10 ECTS**
(Quantum Chemistry)

Modulverantwortliche/r: Andreas Görling
Lehrende: Andreas Görling, Christian Neiß

Startsemester: WS 2021/2022 | Dauer: 2 Semester | Turnus: jährlich (WS)
Präsenzzeit: 90 Std. | Eigenstudium: 210 Std. | Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry - WS:

Winter Term:

1. Quantum Chemistry 1 (2V)
2. Quantum Chemistry 1 Seminar (1S)

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

Quantum Chemistry - SS:

Summer Term:

3. Quantum Chemistry 2 (2V)
4. Quantum Chemistry 2 Seminar (1S)

Quantum Chemistry 2 (SS 2022, Vorlesung mit Übung, 3 SWS, Andreas Görling)

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, basic linear algebra

Inhalt:

- Introduction to modern methods and current research issues in the field of quantum and computer chemistry
- Hartree-Fock, DFT, Many Body Perturbation Theory
- Configuration Interaction, Second Quantization, Coupled Cluster
- TD-HF, TD-DFT, RPA

Lernziele und Kompetenzen:

Students ...

- obtain sound knowledge in basic and advanced 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.)

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

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

[1] **Molecular Science (Master of Science): ab 1. Semester**
(Po-Vers. 2020w | NatFak | Molecular Science (Master of Science) | Compulsory elective module | Quantum Chemistry | Quantum Chemistry)

Dieses Modul ist daneben auch in den Studienfächern "Chemistry (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Quantum Chemistry (Prüfungsnummer: 65071)
Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 30
Anteil an der Berechnung der Modulnote: 100%
weitere Erläuterungen:
O30 (PL): Oral Examination (30 minutes) or alternative examination according to FAU Corona Statutes!
Prüfungssprache: Englisch

Erstablegung: SS 2022, 1. Wdh.: WS 2022/2023
1. Prüfer: Andreas Görling

Organisatorisches:

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

Bemerkungen:

Module compatibility:

- Lecture module within the **Core module** „Quantum Chemistry“ in M. Sc. Chemistry (students of M.Sc. Chemistry have to choose 2 Core Modules out of 4: Inorganic, Organic, Physical and Quantum Chemistry)
- Lecture module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science