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

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

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

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#### 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)

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#### 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
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#### 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.)
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#### 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.

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#### 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

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Andreas Görling

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### 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