

|  |                              |
|--|------------------------------|
| <b>Modulbezeichnung:</b> Quantum Chemistry (CME1)<br>(Quantum Chemistry)         | <b>15 ECTS</b>               |
| Modulverantwortliche/r: Andreas Görling  |                              |
| Lehrende: Andreas Görling, Andreas Heßelmann, Wolfgang Hieringer, Christian Neiß |                              |
| Startsemester: WS 2019/2020  | Dauer: 2 Semester            |
| Präsenzzeit: 210 Std.  | Eigenstudium: 240 Std.       |
|  | Turnus: halbjährlich (WS+SS) |
|  | Sprache: Englisch            |

### Lehrveranstaltungen:

#### A. Quantum Chemistry I (2L, 1S)

Quantum Chemistry I / Quantenchemie I (WS 2019/2020, Vorlesung, 2 SWS, Andreas Görling)

Quantum Chemistry I - Exercises / Übung zur Quantenchemie I (WS 2019/2020, Übung, 1 SWS, Jannis Erhard et al.)

#### B. Quantum Chemistry II (2L, 1S)

Quantum Chemistry II (SS 2020, Vorlesung, 2 SWS, Andreas Görling)

Quantum Chemistry II (Seminar) (SS 2020, Übung, 1 SWS, Andreas Görling et al.)

#### C1. Scientific programming (2S)

Attendance in lab course is compulsory!

Scientific Programming / Wissenschaftliches Programmieren (WS 2019/2020, Praktikum, 2 SWS, Andreas Heßelmann et al.)

#### C2. Handling of computer systems in science (2S)

Attendance in lab course is compulsory!

Handling of computer systems in science (SS 2020, Praktikum, 2 SWS, Wolfgang Hieringer et al.)

#### C3. Training in computer chemistry (4LAB)

Attendance in lab course is compulsory!

Practical training in computer chemistry (SS 2020, Praktikum, 4 SWS, Andreas Görling et al.)

### Inhalt:

- Introduction to modern methods and the current research issues in the field of quantum and computer chemistry
- Basics of scientific programming and handling of computer systems in science
- Creating a self-written computer program to a problem situation in the field of quantum and computer chemistry, and demonstration of the functionality
- Practical studies on selected chapters of quantum and computer chemistry at an advanced level

### Lernziele und Kompetenzen:

Students

- sound knowledge in basic methods of quantum and computer chemistry
- are able to create computer programs for scientific purposes, to install and use scientific software on work stations and compute clusters
- apply quantum chemical methods to scientific questions under guidance.

### Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

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

[1] Chemie (Master of Science): 1-3. Semester

(Po-Vers. 2009 | NatFak | Chemie (Master of Science) | Wahlpflichtmodul | Quanten u. Computerchemie)

### Studien-/Prüfungsleistungen:

Quanten- und Computerchemie (Prüfungsnummer: 65301)

(englische Bezeichnung: Oral Examination or Examination (Klausur) on Quantum and Computer Chemistry)

Prüfungsleistung, schriftlich oder mündlich

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Oral examination (45 min) or alternative examination according to FAU Corona statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2020, 1. Wdh.: WS 2020/2021

1. Prüfer: Andreas Göring

---

**Organisatorisches:**

Module frequency: A and C1 in winter term; B, C2 und C3 in summer term

A/B: O45, 2 examiners (PL); C1: EX (SL); C2: EX (SL); C3: LAB (SL)

Calculation of the grade for the module: Result of the oral examination (100%)

**Bemerkungen:**

Module compatibility: M.Sc. Chemie (Mandatory elective module or Elective module) / M.Sc. Molecular Science (Elective module)