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**Modulbezeichnung:** Quantum Chemistry (CME1) 15 ECTS  
(Quantum Chemistry)

Modulverantwortliche/r: Andreas Görling

Lehrende: Christian Neiß, Wolfgang Hieringer, Andreas Görling

Startsemester: SS 2020

Dauer: 2 semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 210 Std.

Eigenstudium: 240 Std.

Sprache: Englisch

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#### Lehrveranstaltungen:

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

**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!

**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.)

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#### 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.
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#### 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)

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#### Studien-/Prüfungsleistungen:

Quanten- und Computerchemie (Prüfungsnummer: 65301)

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

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 45

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O45 (PL): Oral examination 45 min, 2 examiners,

EX (SL), EX (SL), LAB (SL)

Prüfungssprache: Englisch

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

1. Prüfer: Andreas Görling

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**Organisatorisches:**

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

Quantum Chemistry I/II: O45 (PL); Scientific Programming: EX (SL); Handling of computer systems:  
EX (SL); Training in Computer Chemistry: LAB (SL)

Grading procedure: Result of the oral examination (100%)

**Bemerkungen:**

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