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

Modulverantwortliche/r: Andreas Görling

Lehrende: Andreas Görling, Christian Neiß, Andreas Heßelmann, Wolfgang Hieringer

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Startsemester: WS 2019/2020	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)**

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.)

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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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**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)