

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

#### 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)