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

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.)

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, 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

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)