Modulbezeichnung:	**Quantum Chemistry (CME1)** (Quantum Chemistry)	**15 ECTS**
Modulverantwortliche/r:	Andreas Görling	
Lehrende:	Christian Neiß, Andreas Heßelmann, Wolfgang Hieringer, Andreas Görling	

Startsemester: SS 2017	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 2017/2018, Vorlesung, 2 SWS, Andreas Görling)

Quantum Chemistry I - Exercises / Übung zur Quantenchemie I (WS 2017/2018, Übung, 1 SWS, Jannis Erhard et al.)

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

Quantum Chemistry II (SS 2017, Vorlesung, 2 SWS, Andreas Görling et al.)

Quantum Chemistry II (Seminar) (SS 2017, Übung, 1 SWS, Jannis Erhard et al.)

C1. Scientific programming (2S)

Attendance in lab course is compulsory!

Scientific Programming / Wissenschaftliches Programmieren (WS 2017/2018, 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 2017, Praktikum, 2 SWS, Andreas Heßelmann et al.)

C3. Training in computer chemistry (4LAB)

Attendance in lab course is compulsory!

Practical Training in Computer Chemistry / Praktikum Computerchemie (WS 2017/2018, Praktikum, Andreas Görling et al.)

Practical training in computer chemistry (SS 2017, Praktikum, 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:
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%)
Prüfungssprache: Englisch

Erstablegung: WS 2017/2018, 1. Wdh.: SS 2018
1. Prüfer: Andreas Görling

Organisatorisches:
Module frequency: A and C1 winter term; B, C2 und C3 summer term
Bemerkungen:
Module compatibility: M.Sc. Chemie / M.Sc. Molecular Science (Elective module)