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|--------------------------------------------------------------------------|------------------------------------------------------------------------|------------------------------|
| <b>Modulbezeichnung: Quantum Chemistry (CME1)</b><br>(Quantum Chemistry) |                                                                        | <b>15 ECTS</b>               |
| Modulverantwortliche/r:                                                  | Andreas Görling                                                        |                              |
| Lehrende:                                                                | Andreas Görling, Wolfgang Hieringer, Andreas Heßelmann, Christian Neiß |                              |
| Startsemester: SS 2019                                                   | 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 2019, Vorlesung, 2 SWS, Andreas Görling et al.)

Quantum Chemistry II (Seminar) (SS 2019, 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 2019, Praktikum, 2 SWS, Wolfgang Hieringer et al.)

##### **C3. Training in computer chemistry (4LAB)**

Attendance in lab course is compulsory!

Practical Training in Computer Chemistry / Praktikum Computerchemie (WS 2019/2020, Praktikum, Andreas Görling et al.)

Practical training in computer chemistry (SS 2019, 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:

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

Erstabledung: WS 2019/2020, 1. Wdh.: SS 2020

1. Prüfer: Andreas Görling

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**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)