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**Modulbezeichnung:** Quantum Chemistry - Lab (CM-QC-Lab) 10 ECTS  
 (Quantum Chemistry - Lab)

Modulverantwortliche/r: Andreas Görling

Lehrende: Petra Imhof, Andreas Görling, Dirk Zahn, Christian Neiß, Bernd Meyer

Startsemester: WS 2021/2022

Dauer: 2 Semester

Turnus: jährlich (WS)

Präsenzzeit: 225 Std.

Eigenstudium: 75 Std.

Sprache: Englisch

### Lehrveranstaltungen:

**1. Scientific Programming 1 (5 SWS/Winter term):**

Quantum Chemistry - Lab / Scientific Programming (WS 2021/2022, Seminar, 5 SWS, Christian Neiß et al.)

**2. Scientific Programming 2 (5 SWS/Summer term):**

Quantum Chemistry - Lab / Scientific Programming (SS 2022, Seminar, 5 SWS, Christian Neiß et al.)

**3. Training in Applied Computational Chemistry (5 SWS/Winter or summer term):**

- Internship in one of the Theoretical Chemistry groups (Profs Görling, Imhof, B. Meyer, Zahn), time and place by agreement (Winter or summer term)
- Training has to be taken only once: in winter **or** in summer term (time and place by agreement)

Training in Applied Computational Chemistry (WS 2021/2022, Praktikum, 5 SWS, Anwesenheitspflicht, Andreas Görling et al.)

Training in Applied Computational Chemistry (SS 2022, Praktikum, 5 SWS, Anwesenheitspflicht, Andreas Görling et al.)

### Inhalt:

- Operating system Linux for high-performance computing (HPC)
- Scientific programming in Fortran and Python
- Using numerical and mathematical libraries/modules
- Introduction to parallel computing
- Exercises
- Programming project
- Training in applied computational chemistry

### Lernziele und Kompetenzen:

Students ....

- get familiar with Linux as operating system for HPC
- are able to create computer programs for scientific purposes
- can use numerical and mathematical libraries/modules in home-made programs
- obtain knowledge about basic parallelization paradigms
- apply quantum chemical methods to scientific questions under guidance

### Literatur:

- Stephen J. Chapman: Fortran for Scientists and Engineers, McGraw Hill 2017 (4th ed.)
- Bernd Klein: Einführung in Python 3, Hanser 2017 (3rd ed.)
- Stefan Gerlach: Computerphysik, Springer Spektrum 2019 (2nd ed.)

### Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

**[1] Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Chemistry (Master of Science) | Fachliche Wahlpflichtmodule | Quantum Chemistry | Quantum Chemistry laboratory)

**[2] Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Chemistry (Master of Science) | Ergänzende Wahlpflichtmodule | Quantum Chemistry | Quantum Chemistry laboratory)

**[3] Molecular Science (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Molecular Science (Master of Science) | Compulsory elective module | Quantum Chemistry | Quantum Chemistry laboratory)

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### Studien-/Prüfungsleistungen:

Quantum Chemistry Laboratory (Prüfungsnummer: 65081)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol: Successful implementation of the programming project (working program) including Lab report (ca. 5 pages)

Grading procedure: 100% Graded Computer Program

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Andreas Görling

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### Organisatorisches:

**Please note:**

- The core module "Quantum Chemistry" starts only in winter term!
- Students have to register for the module
- Registration / further information via StudOn

### Bemerkungen:

Module compatibility:

- Lab module within the **Core module** „Quantum Chemistry“ in M. Sc. Chemistry
- Lab module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science