Modulbezeichnung:	**Quantum Chemistry - Lab (CM-QC-Lab)** (Quantum Chemistry - Lab)	**10 ECTS**
Modulverantwortliche/r:	Andreas Görling	
Lehrende:	Bernd Meyer, Christian Neiß, Andreas Görling, Petra Imhof, Dirk Zahn	

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)

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

Erstablegung: SS 2022, 1. Wdh.: WS 2022/2023
1. Prüfer: Andreas Görling

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