FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

Modulbezeichnung:	**Theory (MSM-ME2)** (Theory)	**15 ECTS**
Modulverantwortliche/r:	Andreas Görling	
Lehrende:	Andreas Görling, Wolfgang Hieringer, Andreas Heßelmann, Bernd Meyer	

Startsemester: WS 2019/2020	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.)
Quantum Chemistry II (SS 2020, Vorlesung, 2 SWS, Andreas Görling)
Quantum Chemistry II (Seminar) (SS 2020, Übung, 1 SWS, Andreas Görling et al.)

B. Modeling of catalytic processes (2L/1S)

Modeling of Catalytic Processes (SS 2020, Vorlesung, 2 SWS, Bernd Meyer)
Modeling of Catalytic Processes (Praktikum) (SS 2020, Praktikum, 2 SWS, Bernd Meyer et al.)

C. Scientific programming (2LAB/1S)

Attendance in lab courses is compulsory!
Scientific Programming / Wissenschaftliches Programmieren (WS 2019/2020, Praktikum, 2 SWS, Andreas Heßelmann et al.)

D. Handling of computer systems in science (2LAB/1S)

Attendance in lab courses is compulsory!
Handling of computer systems in science (SS 2020, Praktikum, 2 SWS, Wolfgang Hieringer et al.)

E. Practical Training in Computer Chemistry (4LAB)

Attendance in lab courses is compulsory!
Practical Training in Computer Chemistry / Praktikum Computerchemie (WS 2019/2020, Praktikum, Andreas Görling et al.)
Practical training in computer chemistry (SS 2020, Praktikum, 4 SWS, Andreas Görling et al.)

Inhalt:

A: Quantum Chemistry I:

Consolidation of the mathematical backgrounds in quantum chemistry, Hertree-Fock method, configuration interactions; density functional theory and its application to molecular systems

B: Modeling of catalytic processes

Introduction to the theoretical concepts and methods to study catalytic processes: energetic, kinetics and dynamics of adsorbates, reactivity of surfaces; transition state theory, microkinetic modeling, kinetic Monte-Carlo techniques, molecular dynamics

C: Lab course: Scientific programming using FORTRAN
D: Lab course: Introduction to Linux systems;
E: Lab course: application of modern modeling techniques to investigate molecular systems

Lernziele und Kompetenzen:

The students

- get experience with advanced knowledge and techniques in theoretical chemistry
- are able to utilize advanced computer-based techniques to model research related problems in the field of chemistry, biochemistry, catalysis and material science
- learn to operate Linux-based and large-scale computing systems
- are able to summarize and to interpret theoretical calculations in written form (lab report).

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

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

[1] **Molecular Science (Master of Science)**
(Po-Vers. 2013 | NatFak | Molecular Science (Master of Science) | Wahlpflichtmodul Molecular Science)

Studien-/Prüfungsleistungen:

Theorie und Modellierung - Theory (Prüfungsnummer: 30802)
(englische Bezeichnung: Theory and Modelling - Theory)

Prüfungsleistung, schriftlich oder mündlich
Anteil an der Berechnung der Modulnote: 10%
weitere Erläuterungen:
Assessment and examinations: Oral examination (45 min) or alternative examination according to FAU Corona statutes!
Prüfungssprache: Englisch

Erstablegung: SS 2020, 1. Wdh.: WS 2020/2021
1. Prüfer: Andreas Görling

Organisatorisches:

Intended stage in the degree course: Mandatory Elective Module (Wahlpflichtmodul) or Elective Module (Wahlmodul), semester 1-3
Frequency of offer: Annually, **A:** winter term **B:** summer term **C:** winter term **D:** summer term **E:** winter and summer term