Modulbezeichnung:	**Theory (MSM-ME2)** (Theory)	**15 ECTS**
Modulverantwortliche/r:	Andreas Görling	
Lehrende:	Harald Lanig, Andreas Görling, Jannis Erhard, Bernd Meyer, Andreas Heßelmann	

Startsemester: WS 2016/2017	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 2016/2017, Vorlesung, 2 SWS, Andreas Görling)

Quantum Chemistry I - Exercises / Übung zur Quantenchemie I (WS 2016/2017, Übung, 1 SWS, Jannis Erhard et al.)

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.)

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

Modeling of Catalytic Processes (SS 2017, Vorlesung, 2 SWS, Bernd Meyer)

Modeling of Catalytic Processes (Praktikum) (SS 2017, Praktikum, 2 SWS, Bernd Meyer et al.)

C. Modeling of macromolecular compounds (2L/1S)

Polymer Modeling, Modeling of Macromolecular Compounds (SS 2017, Vorlesung mit Übung, Harald Lanig et al.)

D. Scientific programming (2LAB/1S)

Attendance in lab courses is compulsory!

Scientific Programming / Wissenschaftliches Programmieren (WS 2016/2017, Praktikum, 2 SWS, Andreas Heßelmann)

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

Attendance in lab courses is compulsory!

Handling of computer systems in science (SS 2017, Praktikum, 2 SWS, Andreas Heßelmann et al.)

F. Practical Training in Computer Chemistry (2LAB)

Attendance in lab courses is compulsory!

Practical Training in Computer Chemistry / Praktikum Computerchemie (WS 2016/2017, Praktikum, Andreas Görling et al.)

Practical training in computer chemistry (SS 2017, Praktikum, 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: Modeling of macromolecular compounds

Basic ideas of modeling biological and technical polymers; Monte-Carlo-techniques, quantitative structure-property relationships; molecular dynamics in polymers; homology modeling

D: Scientific programming using FORTRAN

E: Introduction to Linux systems;

F: 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).

Studien-/Prüfungsleistungen:

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

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 45
Anteil an der Berechnung der Modulnote: 100%
weitere Erläuterungen:
Assessment and examinations:
O45 (PL) + LAB (SL): oral examination (45 min, 2 examiners) + lab course protocol(s), ungraded
Calculation of the grade for the module: 100% from oral examination
Prüfungssprache: Englisch

Erstablegung: SS 2017, 1. Wdh.: WS 2017/2018
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:** summer term **D:** winter term **E:** summer term **F:** winter term