

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

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

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

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

(Po-Vers. 2013 | NatFak | Molecular Science (Master of Science) | Wahlpflichtmodul Molecular Science)

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### 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

Erstablesung: SS 2017, 1. Wdh.: WS 2017/2018

1. Prüfer: Andreas Göring

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### 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