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| <b>Modulbezeichnung:</b>    | <b>Theory (MSM-ME2)</b><br>(Theory)                                                | <b>15 ECTS</b>               |
| Modulverantwortliche/r:     | Andreas Görling                                                                    |                              |
| Lehrende:                   | Bernd Meyer, Jannis Erhard, Wolfgang Hieringer, Andreas Heßelmann, Andreas Görling |                              |
| Startsemester: WS 2017/2018 | 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 2017/2018, Vorlesung, 2 SWS, Andreas Görling)

Quantum Chemistry I - Exercises / Übung zur Quantenchemie I (WS 2017/2018, Übung, 1 SWS, Jannis Erhard et al.)

Quantum Chemistry II (SS 2018, Vorlesung, 2 SWS, Andreas Görling et al.)

Quantum Chemistry II (Seminar) (SS 2018, Übung, 1 SWS, Jannis Erhard et al.)

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

Modeling of Catalytic Processes (SS 2018, Vorlesung, 2 SWS, Bernd Meyer)

Modeling of Catalytic Processes (Praktikum) (SS 2018, Praktikum, 2 SWS, Bernd Meyer et al.)

##### **C. Scientific programming (2LAB/1S)**

Attendance in lab courses is compulsory!

Scientific Programming / Wissenschaftliches Programmieren (WS 2017/2018, 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 2018, 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 2017/2018, Praktikum, Andreas Görling et al.)

Practical training in computer chemistry (SS 2018, Praktikum, 4 SWS, 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: 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. 2007 | NatFak | Molecular Science (Master of Science) | alte Prüfungsordnungen | Masterprüfung | Wahlpflichtmodul Molecular Science)

**[2] Molecular Science (Master of Science)**

(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 2018, 1. Wdh.: WS 2018/2019

1. Prüfer: Andreas Görling

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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:** winter term **D:** summer term **E:** winter and summer term