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| Modulbezeichnung: Theory (MSM-ME2) (Theory) | 15 ECTS | |
| Modulverantwortliche/r: | Andreas Görling | |
| Lehrende: | Bernd Meyer, Jannis Erhard, Wolfgang Hieringer, Andreas Görling | |
| Startsemester: SS 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 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)

Attendance in lab Course is compulsory!

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 Course is compulsory!

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

Attendance in lab Course is compulsory!

Handling of computer systems in science (SS 2020, Praktikum, 2 SWS, Wolfgang Hieringer et al.)

E. Practical Training in Computer Chemistry (2LAB)

Attendance in lab Course is compulsory!

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, 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).

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% oral examination

Prüfungssprache: Englisch

Erstablingung: WS 2020/2021, 1. Wdh.: SS 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 term