Modulbezeichnung: **Molecular Modeling (DD-MM)** **10 ECTS**
(Molecular Modeling)

Modulverantwortliche/r: Petra Imhof
Lehrende: Frank Beierlein, Harald Lanig, Petra Imhof, Dirk Zahn

Startsemester: SS 2022	Dauer: 2 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 90 Std.	Eigenstudium: 210 Std.	Sprache: Englisch

Lehrveranstaltungen:

All lectures and courses are online in winter term 2020/2021!
Advanced Biomolecular Simulations (2V/1UE) (SS 2022, Seminar, 3 SWS, Petra Imhof)
Modelling of Complex Systems (2V/1UE) (WS 2022/2023, Seminar, 3 SWS, Petra Imhof et al.)

Inhalt:

WS:

- Rationalizing Complex Systems from Statistics: Probability distributi-ons, Concepts of Information and Entropy;
- Thermodynamics of Monte-Carlo simulation and state-of-the art ana-lyses of transition pathways;
- Molecular dynamics simulations of complex systems: data evaluation and reduction to key information.

SS:

- Model building and setup of first-guess configurations;
- Enhanced sampling techniques to tackle manifolds of configurations and to find reaction paths;
- Machine-learning and prediction of real-world properties from molecular data.

Lernziele und Kompetenzen:

Students

- master the basics of molecular modelling,
- are able to select and apply from a wide range of different simulation techniques the one that is relevant and suitable for different problems,
- can analyse, evaluate and present data and results,
- monitor and control their own progress.

Literatur:

- B. Smit, D. Frenkel: Understanding Molecular Simulation: From Algo-rithms to Applications
- A. Leach: Molecular Modelling: Principles and Applications

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. 2020w | NatFak | Molecular Science (Master of Science) | MolSc Module LIFE | Studienrichtung Drug Discovery | Molecular Modeling)

Studien-/Prüfungsleistungen:

Molecular Modeling (Prüfungsnummer: 30671)
Prüfungsleistung, Klausur, Dauer (in Minuten): 90
Anteil an der Berechnung der Modulnote: 100%
weitere Erläuterungen:
W90(PL): Written examination (90 minutes) or alternative examination according to FAU Corona Statutes!
Prüfungssprache: Englisch

Erstablegung: WS 2022/2023, 1. Wdh.: SS 2023
1. Prüfer: Petra Imhof

Organisatorisches:

Please note:

- Molecular Modeling will be taught online!
- Students have to register for the module examination (check registration periods on meinCampus)!
- Registration/further information via StudOn!

Bemerkungen:

Please note: The core module **"Drug Discovery"** has to be taken as a whole!