

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

Modulverantwortliche/r: Petra Imhof

Lehrende: Petra Imhof, Frank Beierlein, Harald Lanig, 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 distributions, Concepts of Information and Entropy;
- Thermodynamics of Monte-Carlo simulation and state-of-the art analyses 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 Algorithms 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

Erstablesung: 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!