

---

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

Modulverantwortliche/r: Petra Imhof

Lehrende: Dirk Zahn, Harald Lanig, Frank Beierlein, Petra Imhof

---

Startsemester: WS 2020/2021	Dauer: 2 semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 90 Std.	Eigenstudium: 210 Std.	Sprache: Englisch

---

**Lehrveranstaltungen:**

All lectures and courses are online till further notice!

Modelling of Complex Systems (2V/1UE) (WS 2020/2021, Seminar, 3 SWS, Petra Imhof et al.)

Advanced Biomolecular Simulations (2V/1UE) (SS 2021, Seminar, 3 SWS, Petra Imhof)

---

**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: SS 2021, 1. Wdh.: WS 2021/2022

1. Prüfer: Petra Imhof

**Organisatorisches:**

Please note:

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

**Bemerkungen:**

Module compatibility:

- Lecture module **Molecular Modeling** within the **core module „Drug Discovery“** in M. Sc. Molecular LIFE Science