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

Modulverantwortliche/r: Petra Imhof

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

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

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**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)

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**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
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**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)

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**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

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**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