[K3.6 | C3.5] *Molecular Simulations at Multiple Scales*	**Molecular Simulations at Multiple Scales**	**Wahlpflichtmodul**	**7 CP (insg.) = 210 h**		**4 SWS**
			Kontaktstudium 4 SWS / 60 h	**Selbststudium 150 h**	

Inhalte

This module provides students with a comprehensive introduction to molecular dynamics simulations, covering the theoretical background, fundamental mathematical derivations, and the practical application of molecular dynamics simulations using a commonly used software package. The lecture begins by discussing the underlying molecular interactions and how they are described in traditional atomistic force fields. Subsequently, statistical fundamentals and ensembles, as well as integrators, thermostats, barostats, cutoffs, Ewald sums, and basic analysis techniques for obtained trajectories are covered. Subsequently, coarse-grained force fields for simulating larger scales will be covered, as well as the combination of multiple resolutions in multiscale techniques such as QM/MM and AA/CG, and the transition to mesoscale models for even larger systems. Applications of the various simulation techniques will be discussed using current examples from research, with a focus on the successes, limitations, and synergies between the different methods. In addition, current developments toward machine-learned force fields will be discussed.

To reinforce and apply the lecture material, a theory exercise (first half of the course) and a computer lab (second half of the course) are held. In the theory exercise, the theoretical foundations and applied mathematical methods covered in the first half of the lecture are examined in greater detail to provide a deeper understanding of the topics. At the start of the second half of the course, which focuses on multiscale techniques and application examples of molecular dynamics simulations, students will conduct their first simulations in a computer lab. Here, students will learn how to use the widely used GROMACS software package (www.gromacs.org) and perform simulations of lipid membranes, proteins, and nucleic acids. In addition to the practical use of the GROMACS software package, the course also emphasizes the preparation, execution, and analysis of simulations, as well as suitable software packages for these tasks.

Lernergebnisse / Kompetenzziele

In this module, students learn the fundamentals of molecular dynamics simulations, ranging from the theoretical background and mathematical foundations to the different resolutions in atomistic, coarse-grained, and mesoscale models. In addition, they are introduced to multiscale simulation techniques such as QM/MM and AA/CG. Using modern application examples, the advantages of the various simulation techniques are demonstrated, and their limitations are explained. The computer lab provides hands-on training in the use of the GROMACS software package and gives students their first practical experience with the simulation of biomolecular ensembles.

Upon completion of the course, students should be able to assess the possibilities and limitations of applying molecular dynamics simulations to scientific questions and perform simple simulations.

Teilnahmevoraussetzungen für Modul bzw. für einzelne Lehrveranstaltungen des Moduls

None

Empfohlene Voraussetzungen

Basic knowledge of physical chemistry, organic or biochemistry, analysis, and linear algebra are recommended.

Organisatorisches

MSc Biochemistry: *This module does not count as one of the required practical modules.*

Zuordnung des Moduls (Studiengang / Fachbereich)	M.Sc. Chemie / FB14
Verwendbarkeit des Moduls für andere Studiengänge	M.Sc. Biochemistry, M.Sc. Computational Life and Natural Science (CLNS)(FB 12), M.Sc. Informatik (FB12), M.Sc. Biophysik (FB13)
Häufigkeit des Angebots	Once a year (in winter term)
Dauer des Moduls	1 Semester
Modulbeauftragte / Modulbeauftragter	Prof. Dr. Sebastian Thallmair
Studiennachweise/ ggf. als Prüfungsvorleistungen	
Teilnahmenachweise	Exercise/practical course: Regular and active attendance
Leistungsnachweise	Exercise/practical course: working on the exercises, presentation of exercise improves the final grade by 0.3, if passed.
Lehr- / Lernformen	Lecture, Exercises, Practical course
Unterrichts- / Prüfungssprache	Englisch
Modulprüfung	**Form / Dauer / ggf. Inhalt**
Modulabschlussprüfung bestehend aus:	Oral exam (30 min.) or written exam (120 min.) depending on the number of participants
kumulative Modulprüfung bestehend aus:	
Bildung der Modulnote bei kumulativen Modulprüfungen:	

	LV-Form	SWS	Semester CP			
			1	2	3	4
Molecular Simulations at Multiple Scales	L	2	*3*			
Exercises on Molecular Simulations at Multiple Scales	E	1	*2*			
Molecular Simulations in Practice	P	1	*2*			
SUMME		4	7			