Import module

[E1.8]	Modeling and Simulation of Biomolecules	Compulsory elective module	6 CP (total) = 180 h		4 SWS
			Contact hours 4 SWS / 60 h	Independent study 120 h	

Content

Lecture: Review of probability theory; Primer in equilibrium statistical mechanics, with review of the necessary classical mechanics and mathematics. Highlights on structures as free energy minimizer; Introduction to stochastic phenomena. Gaussian noise, Brownian motion, diffusion (Fokker-Planck equation); Two state systems: from Ion channels to cooperative binding; Kramer's theory for thermally activated processes. Protein folding; Numerical simulations. Euler algorithm for Brownian motion.

Tutorial: In order to deepen the lecture material, the lecture is accompanied by a practical exercise and independent literature work.

Introduction to MD + equilibrium MD; Molecular dynamics. Scales in time and space. Atomistic and coarse-grained MD; Biophysical Interactions, all-atom force fields and coarse grain force field (Martini); Production code and parallel computing. Introduction to GROMACS; predicting biophysical properties; Periodic boundary conditions. Ewald's summation for electrostatics; Thermostats & Barostats; visualizing biophysical systems; Molecular simulations of biological systems.

Learning outcomes and skills

Understand the basic principles of equilibrium and out-of-equilibrium statistical mechanics.

Understand the principles of molecular dynamics simulations and the technical details involved in the setup of MD simulations. Perform basic molecular dynamics simulations of biological systems. Calculate biophysical properties of biomolecules to help the interpretation of the experimental data.

Admissions requirements/Conditions for participation in the module/courses

None

Recommended prior knowledge

Basic knowledge of thermodynamics and statistics.

Organizational details

Import module, the registration and cancellation deadlines of the Bachelor's/Master's Biophysics regulations apply. (The exam requires online **registration**, no later than **seven days** before the exam date. You can withdraw up to one working day before the exam date without giving reasons.)

Module allocation (degree programme/faculty)	Master Biophysics / FB13
Eligibility of the module for other courses	Master Chemistry / FB14, Master Biochemistry / FB14
Module offered	summer semester
Duration	1 semester
Module coordinator	Prof. Hummer
Course requirements for credits	
Participation record	Tutorial: Regular and active participation, processing of the tutorials
Coursework	Written exam (90 min.)
Forms of teaching / learning	lecture, tutorial
Language teaching and instruction	English
Module assessment	**Form / duration / content, if applicable**
Final module assessment	None
Cumulative module assessment consisting of	
Composition of the module grade for cumulative module assessment	

	Mode of teaching / study	Semester hours per week	Semester CP			
			1	2	3	4
Modeling and simulation of biomolecules	L	2		3		
Modeling and simulation of biomolecules	T	2		3		
TOTAL		4		6		