Module: Molecular Dynamics

University/Department/Institute: Freie Universität Berlin/Department of Biology, Chemistry, Pharmacy/Institute of Chemistry and Biochemistry

Module supervisors: Lecturers of the module

Entrance Requirements: none

Goals of Qualification: Students know the basic concepts of classic molecular dynamics and are able to apply these to selected model systems of chemistry. They have acquired the numerical skills and necessary programming skills to run corresponding computer simulations.

Contents: Modeling of interactions between atoms with empirical potentials, simulation of dynamic processes in molecules with methods of classical mechanics, introduction to the numerical methods of molecular dynamics, basics of programming and acquisition of a programming language

Teaching methods	**Hours of attendance** (Hours per week)	**Forms of active participation**	**Workload** (hours)	
Lecture	2	-	Presence (L) Pre-, post-preparation (L) Presence (T) *Computer tutorial* *independent computer tutorial* Pre-, post-preparation (T) Exam preparation and examination	30 30 15 15 30 30
Tutorial	1	Contributions to topic related discussions, Presentation of selected simulation results		
Language offer of lecture		German		
Compulsory regular attendance		Lecture attendance is recommended, tutorial: yes		
Workload (total)		150 hours		5 CP
Length of module		One Semester		
Examination		Practical exam (simulation on the computer)		
Lecture is offered		Once per year		
Applicability		Bachelor study program Chemistry, Bachelor study program Biochemistry, Master study program Chemistry		