Module: Theoretical Chemistry

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 and methods of theoretical chemistry. They are able to use time-independent and time-dependent quantum mechanical methods for selected model systems of chemistry and have acquired the numeric skills to run computer simulations. In this way they have acquired an understanding for the characteristics of molecules and chemical reactions.

Contents: mathematical depiction of time-independent and time-dependent quantum mechanics, solving quantum mechanical one – particle problems (free particles, harmonic oscillators, hydrogen atoms), core dynamics (oscillation and rotation), core movement of multi-atom molecules, time-dependent and time-independent perturbation theory, selected numerical solution methods for the calculation of time-dependent quantum mechanics

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		English		
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		