Module: Density Functional Theory	
University/department/institute: Freie Universität Berlin/Department of Biology, Chemistry and Pharmacy/Institute of Chemistry and Biochemistry	
Responsible for the module: module lecturers	
Admission requirements: none	
Qualification aims: The students have detailed knowledge of the theoretical principles of ground-state and excited-states density functional theory. They are familiar with quantum chemical program packages, can apply density functional theory confidently and carry out structural optimization and frequency analyzes.	
Content: Principles of density functional theory; development of exchange-correlation functions; application fields and precision of different density functional methods; molecular properties and excited states described by time-dependent density functional theory. Algorithms to optimize molecular structure and frequency analysis. Introduction to quantum chemical program packages focusing on density functional methods and computer-aided interpretation of the data calculated	

Teaching and learning units	**Attendance** (Semester hours per week = SH)	**Forms of active participation**	**Study time** (hours)	
Lecture	2	-	Attendance L Preparation and follow-up L Attendance SPC Preparation and follow-up SPC Examination preparation, examination	30 30 30 30 30
Seminar on the computer using special software	2	Working on problem sets and computer simulations		
Language of instruction		German or English		
Compulsory regular attendance		Lecture: attendance recommended; seminar: yes		
Study time, total hours		150 hours		5 CP
Duration of module		One semester		
Module offered		Every third semester		
Application		Master's program in Chemistry		