

3. Topic area Physical and Theoretical Chemistry

Module: Quantum Chemistry			
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 know the principles of the quantitative description of molecular structure using quantum mechanical methods of theoretical chemistry. They know the physical and mathematical principles of the relevant computer programs and can apply their knowledge to solve problem sets, independently or in a group.			
Content: <i>Ab initio</i> and semi-empirical methods of quantum chemistry; Hartree-Fock method; basis sets; density functional theory; introduction to correlation methods; potential energy surfaces for chemical reactions; introduction to the underlying algorithms of popular quantum chemistry programs			
Teaching and learning units	Attendance (Semester hours per week = SH)	Forms of active participation	Study time (hours)
Lecture	2	-	Attendance L 30 Preparation and follow-up L 30 Attendance T 30
Tutorial	2	Solving problem sets, contributing to discussions	Preparation and follow-up T 30 Examination preparation, examination 30
Language of instruction		German or English	
Compulsory regular attendance		Attendance recommended	
Study time, total hours		150 hours	5 CP
Duration of module		One semester	
Module offered		Every other semester	
Application		Master's program in Chemistry	