Module: Relativistic 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 have knowledge of the theory of relativity and its effects on the electronic structure of molecules. They can carry out simple relativistic quantum chemistry calculations and know a range of methods of approaching relativistic quantum chemistry.

Content: Special relativity theory; quantization and spin; Dirac equation for one-electron and multi-electron systems; methods of relativistic quantum chemistry; relativistic pseudopotentials

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
Seminar on the computer using special software	2	Working on problem sets and computer simulations		30 30 30
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		Not regularly		
Application		Master's program in Chemistry		