7. Topic area Theoretical Chemistry

<table>
<tr><td colspan="3">Module: Quantum Chemistry: Correlation Methods</td><td></td></tr>
<tr><td colspan="4">University/department/institute: Freie Universität Berlin/Department of Biology, Chemistry and Pharmacy/Institute of Chemistry and Biochemistry</td></tr>
<tr><td colspan="4">Responsible for the module: module lecturers</td></tr>
<tr><td colspan="4">Admission requirements: none</td></tr>
<tr><td colspan="4">Qualification aims: The students have detailed knowledge of the theoretical principles of quantum chemistry correlation methods. They are familiar with quantum chemical program packages, can independently carry out quantum chemical correlation calculations for simple systems and prepare computer-aided visualizations of the calculated data.</td></tr>
<tr><td colspan="4">Content: Molecular Hamiltonian operator and electronic wave functions; Gaussian basis sets and pseudopotentials; the Hartree-Fock theory and the correlation methods based on it. Introduction to quantum chemical program packages and computer-aided visualization of the data calculated</td></tr>
<tr><td>Teaching and learning units</td><td>Attendance
(Semester hours per week = SH)</td><td>Forms of active participation</td><td>Study time
(hours)</td></tr>
<tr><td>Lecture</td><td>2</td><td>-</td><td rowspan="2">Attendance L 30
Preparation and follow-up L 30
Attendance SPC 30
Preparation and follow-up SPC 30
Examination preparation, examination 30</td></tr>
<tr><td>Seminar on the computer using special software</td><td>2</td><td>Working on problem sets and computer simulations</td></tr>
<tr><td colspan="2">Language of instruction</td><td colspan="2">German or English</td></tr>
<tr><td colspan="2">Compulsory regular attendance</td><td colspan="2">Lecture: attendance recommended; seminar: yes</td></tr>
<tr><td colspan="2">Study time, total hours</td><td>150 hours</td><td>5 CP</td></tr>
<tr><td colspan="2">Duration of module</td><td colspan="2">One semester</td></tr>
<tr><td colspan="2">Module offered</td><td colspan="2">Every third semester</td></tr>
<tr><td colspan="2">Application</td><td colspan="2">Master’s program in Chemistry</td></tr>
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