title of module	Research practical in the focal point program theoretical chemistry

credit points	14	***available in semester(s)***	3
hours per week	14	***compact course***	☒

lecturer(s)	J. Behler, C. Hättig, D. Marx
teaching methods	computer lab course (15 hours per week), this course takes place in the third semester
evaluation of learning progress	active participation in practical, feedback during and on the virtual experiments, feedback on written and oral lab reports by teaching assistants
mode of examination	lab report of the virtual experiments (75 %) and 45 min. oral presentation of the results (25 %)
learning objectives	planning of a research project, advanced knowledge of the use of computational methods employed in state-of-the-art research in order to understand the properties of (bio)molecular systems, critical assessment of the scope and limitations of various approaches/approximations in theoretical and computational (bio)chemistry, visualization, written and oral presentation of results, simple programming tasks, critical evaluation of the relevant scientific literature
soft skills	teamworking and collaboration while carrying out virtual experiments, presentation of practical results, general knowledge of operating systems, software, and computing

contents of module	This computer practical can be devoted to a topic in a research group. This topic can be in the field of inorganic chemistry, biochemistry, organic chemistry, physical chemistry, surface science, and materials science. Examplary topics are: Classical simulation and molecular modeling: simulating structure and dynamics of selected (bio)molecular condensed phase systems at finite temperature and subject to periodic boundary conditions, such as molecular liquids and solutions, critical evaluation and/or construction of classical potentials Electronic structure and spectroscopy: computing electronic properties and sprectra of selected molecules, clusters, and complexes using wavefunction-based and density-based methods relying on the Hartree-Fock and Kohn-Sham equations Molecular structure and reactions: computing accurate equilibrium structure with various quantum chemistry methods, searching reaction pathways and transition states, accurate calculations of reaction and activation enthalpies