title of module	Modular Advanced Practical in Theoretical Chemistry

credit points	4	***available in semester(s)***	1, 2
hours per week	5	***compact course***	☒

lecturer(s)	J. Behler, C. Hättig, D. Marx
teaching methods	computer lab course (8 hours per week per module), these compact courses take place during the first or second half of a semester
evaluation of learning progress	active participation in practical, feedback during and on the virtual experiments, feedback on written lab reports by teaching assistants
mode of examination	all virtual experiments are completed successfully and written up satisfactorily in lab reports
learning objectives	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 and presentation of results, gaining first insights into simple programming
soft skills	teamworking and collaboration while carrying out virtual experiments, graphical presentation of practical results, general knowledge of operating systems, software and computing

contents of module	This computer practical is composed of several independent compact courses which are devoted to specific topics as follows: Module on 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 generation of interatomic potentials Module on electronic structure and spectroscopy: computing electronic properties and sprectra of selected molecules, clusters, and complexes using wavefunction-based methods or density functional theory (DFT). Module on 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