Dynamics and Simulation (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
3 RC	9 CP	270 h	1. Sem.	Each WiS	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
a) Lectures b) Exercises c) Integrated computer practical			a)+b) 2+1 SWS c) 5 SWS	150 h	10 – 20 Students

Prerequisites

Undergraduate level knowledge in classical mechanics, statistical mechanics and time-independent non-relativistic quantum mechanics

Learning outcomes

a**)+b)** Students acquire advanced knowledge of the theory and computational techniques of statistical mechanics and (bio)molecular dynamics simulations in the realm of (bio)molecular systems such as (bio)molecules, clusters, liquids, solids and surfaces. In addition, analysis methods to extract observables of experimental interest, such as various spectroscopic, scattering, and diffraction techniques, are presented such that the students can judge both their strengths and weaknesses with the focus on topical problems in Theoretical Chemistry with a focus on Solvation Science.

c) Students will be familiar with software for molecular dynamics simulations, know how to apply modern molecular simulation techniques to practical problems with a focus on Solvation Science and how to analyze, visualize and present results obtained from such molecular simulations.

Content

a**)+b) Essentials of classical and statistical mechanics**: formulations according to Newton, Lagrange and Hamilton, corresponding equations of motion, conservation laws/conserved quantities, Liouville theorem, ensembles, distribution functions, first and second moments of distributions, connection to averages and fluctuations of observables, correlation functions in space and time, pair and radial correlation function, van Hove correlation function.

Potential energy surfaces: valence force fields, pair potentials, many-body effects, empirical versus ab initio parameterizations, characterization of stationary points, connection between properties of hypersurfaces and chemical concepts, adiabatic chemical reactions.

Molecular dynamics: basic idea of classical molecular dynamics, deriving integrators via "pedestrian approach" and via Liouville formalism, ergodicity, extended phase space/Lagrangian methods, finite-size effects, boundary conditions, convergence criteria for dynamical computer simulations, realizing various ensembles in terms of simulation algorithms, holonomic constraints, ab initio molecular dynamics, equations of motion according to Ehrenfest, Born-Oppenheimer and Car-Parrinello, nuclear quantum effects via path integral simulations.

Integrated practical work in the computer lab will closely follow the theoretical discussion during the lecture and will supplement the analytical exercises (homework). In particular, structure, dynamics and properties of selected (bio)molecular condensed phase systems at finite temperatures and subject to periodic boundary conditions, such as molecular liquids, solutions, and solvated biomolecules, will be in the focus of the virtual experiments.

c) Integrated practical work in the computer lab will closely follow the theoretical and methodological presentation and discussion in a) and b) and will supplement the analytical exercises (homework). In particular, structure, dynamics and properties of selected (bio)molecular condensed phase systems at finite temperatures and subject to periodic boundary conditions, such as molecular liquids, solutions, and solvated biomolecules, will be in the focus of the virtual experiments.

Teaching methods a)+b) Lectures and exercises with problems for self-studying, Q&A and discussion sessions with presentations given by the participants, digital material provided via TheoChem Cloud. c) Computational hands-on problems to be solved in the iMOS computer lab using state-of-the-art scientific software packages done partially in supervised sessions and partially as self-study
Mode of assessment a+b) Written or oral end-of-semester exam and homework b) Grading of the lab reports on the computational hand-on problems
Requirement for the award of credit points a+b) Passing the end-of-semester exam b) Acceptance of the lab reports on the computational hand-on problems
Module applicability a+b+c) M.Sc. iMOS; a+b) M.Sc. Chemistry; a+b) M.Sc. Biochemistry (Focal Point Program "Biomolecular Chemistry")
Weight of the mark for the final score iMOS: CP-weighted average of the exam (5 CP) and the lab report (4 CP) grades according to the examination regulations
Module coordinator and lecturer(s) D. Marx
Further information Module components a+b) can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program "Biomolecular Chemistry"