Biomolecular Simulation (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
6 EC	5 CP	150 h	1. Sem.	Each WiS	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
a) Lectures b) Exercises			a) 2 SWS b) 1 SWS	105 h	10 – 20 Students

Prerequisites

Admission to the Master Course Program

Learning outcomes

Students acquire advanced knowledge of both experimental techniques as well as molecular simulation methods for studying biomolecular systems, ranging from the solvation of small solutes to proteins to biological interfaces. The focus will be on structure-dynamics-function relationships and the underlying thermodynamic properties and principles. A number of selected techniques will be introduced and it will be discussed how simulations can be used to interpret the experiments at the molecular or even atomic level. A particular objective is to provide insights into the merits and limitations of the respective methods.

Content

Fundamentals: Energy landscape, Boltzmann ensemble, hierarchy of timescales (Frauenfelder), energy density, thermal energy, soft vs. hard degrees of freedom, fluctuations, entropy.

Biological (macro)molecules: Structure and relevant interactions, H-bonds, electrostatics, van-der-Waals, hydrophobic effect. Dielectric properties of water, polarizability.

Molecular models: Degrees of freedom, sampling (Molecular Dynamics, Monte Carlo), spatial boundary conditions, ingredients and parameterization of force fields. Water models.

Förster resonance energy transfer: Basic principles of fluorescence (Einstein coefficients, spontaneous vs. induced emission, transition dipole moments, radiative lifetimes, Jablonsky diagrams, quantum yields), FRET (energy transfer efficiency, Förster radius, distance measurements), orientation of transition dipoles, FRET from MD simulations.

Binding: Isothermal titration calorimetry (basic principle, description of the apparatus, binding isotherm), statistical mechanics (canonical/grand-canonical/isobaric-isothermal ensemble, partition function, free energy, phase space integrals), potential of mean force, thermodynamic integration. Applications to ligand-receptor binding, protein folding. Enthalpy-entropy compensation.

Protein dynamics: Dimensionality reduction, principal component analysis, normal mode analysis, harmonic vs. quasiharmonic approximation, entropy estimation.

Teaching methods

Lectures and exercises with active participation during lectures, interactive presentation of homework during exercises

Mode of assessment

30-45 min end-of-term oral exam or 2-hour end-of-term written exam

Requirement for the award of credit points

Passing the end-of-term exam

Module applicability

M.Sc iMOS Elective Course; cross-posted M.Sc. Chemistry as Biomolecular Simulation: Understanding Experiments at the Molecular Level

Weight of the mark for the final score According to CPs
Module coordinator and lecturer(s) L. Schäfer
Further information