Focal Point Practical (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
15 RC	15 CP	450 h	3. Semester	Each WiS	10 weeks full-time or equivalent
Courses research oriented lab project in one of the research groups			**Contact hours** Full-time 250 h	**Self-Study** 200 h	**Group size** individual

Prerequisites

Proof of at least 46 credit points obtained in courses attributed to the first and second semester.

Learning outcomes

After successful completion of the module/course, students will be able to:

- Obtain advanced knowledge of how to apply computational and/or experimental methods employed in state-of-the-art research to understand the properties of (bio)molecular systems
- Learn to critically assess the scope and limitations of various approaches and approximations
- Visualize and present results
- Write reports with theories, experiments, and discussion of results
- Utilize digital techniques to analyze and evaluate the data
- Develop teamwork skills

Content

The practical is carried out in one or several groups participating in the Master of Molecular Sciences and Simulation program.

Examples of elective project topics:

Marx group portfolio: force field simulation of peptides in water: hydrophilic vs. hydrophobic solvation, Car-Parrinello simulation of de/protonation reactions in explicit solvent computation, decomposition and assignment of infrared spectra of molecules in solution

Sander/Schmid portfolio: The students will learn to characterize reactive molecules by low temperature (matrix isolation) and time resolved spectroscopy in combination with quantum chemical (DFT and ab initio) calculations.

Hättig portfolio: computation of UV and CD spectra and investigation of excited states, energetics and structure of weakly interacting complexes, computation of reaction and activation enthalpies, computer implementation of quantum chemical methods

Schäfer portfolio: MD simulations of large biomolecular systems on long time- and length-scales, using all-atom and coarse-grained force fields as well as QM/MM methods. Free energy simulations, incl. enthalpy/entropy decomposition. Enhanced sampling methods. Simulation of NMR relaxation.

Havenith portfolio: study the interaction of small molecules by helium droplet spectroscopy, investigate solute-solvent interactions for aqueous solutions of molecular compounds in the THz and other spectral ranges, use different microscopic techniques to study and chemically map surfaces at nanoscale

Däschlein-Gessner portfolio: The students will learn to synthesize and characterize reactive molecules and organometallic compounds (inert gas techniques) and apply them in further transformations (synthetic chemistry) or they will learn to study organometallic compounds by

computational methods, e.g. their electronic structure, reaction mechanisms etc. (DFT methods).
Teaching methods Research oriented lab project in one of the research groups
Mode of assessment Positive assessment of the lab report
Requirement for the award of credit points Successful project completion and satisfactory written-up lab report
Module applicability M.Sc. iMOS
Weight of the mark for the final score Weighted according to CPs
Module coordinator and lecturer(s) M. Havenith-Newen Faculty of M.Sc. iMOS
Further information