<table>
<thead>
<tr>
<th>Code No.</th>
<th>Workload</th>
<th>Credit points</th>
<th>Available in semester</th>
<th>Frequency</th>
<th>Course duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Module 15</td>
<td>450 h</td>
<td>15 CP</td>
<td>3</td>
<td>each WiS</td>
<td>10 weeks full-time or equivalent</td>
</tr>
</tbody>
</table>

1. **Teaching Methods**
   - Research oriented lab project in one of the research groups

2. **Learning objectives**
   - Students are competent in applying computational and/or experimental methods within the context of state-of-the-art research, and in using the results to understand the properties of (bio)molecular systems. They are able to critically assess the scope and limitations of various approaches/approximations, to visualize and to present results.

3. **Soft skills: methodological, self, social competences**
   - Present research results graphically; understand and apply state-of-the-art experimental and/or computational methods, become familiar with alternative work-flow organization
   - Assess personal strengths and weaknesses, deal with challenges and set-backs; enhance self-motivation skills
   - Work collaboratively within an international team; communicate effectively

4. **Prerequisite(s)**
   - Proof of at least 46 credit points obtained in courses attributed to the first and second semester

5. **Evaluation of the learning process**
   - Active participation in practical, feedback during and on the experiment, feedback on written lab report by teaching assistants

6. **Mode of examination**
   - Successful project completion and satisfactory written-up lab report

7. **Requirements for acquiring credit points**
   - Positive assessment of the lab report

8. **Significance for overall grade**
   - Weighted according to CPs

9. **Module contents**
   - 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-

Havenith/Ebbinghaus 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

Nümberger portfolio:
Time-resolved exploration of photochemical reactions and solvent influences by various ultrafast techniques, e.g. transient absorption in the visible and mid-infrared, fluorescence upconversion, or time-correlated single photon counting. Photochemical reactions may comprise molecular switching, charge- or energy-transfer processes, isomerization, rearrangement, and photolysis.

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).

Person in charge / Supervisor(s)
Prof. Dr. Havenith-Newen

Faculty of the international Master Molecular Sciences