Theoretical Spectroscopy

<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 9</td>
<td>150 h</td>
<td>5 CP</td>
<td>2</td>
<td>each SuS</td>
<td>1 semester</td>
</tr>
</tbody>
</table>

1. **Teaching Methods**
   - a) Lectures
   - b) Exercises

2. **Hours per week**
   - a) 2 h
   - b) 1 h

3. **Contact time**
   - 45 h

4. **Self-study**
   - 105 h

2. **Learning objectives**

   Students understand and are able to explain theoretical approaches relying on time-dependent methods to compute observables which are obtained experimentally using spectroscopic, scattering, and diffraction techniques. They are able to assess the scope and limitations of such methods in the context of Solvation Science with a focus on (bio)molecular condensed phase systems, in particular aqueous solutions and soft matter.

3. **Soft skills: methodological, self, social competences**

   - Structure, summarize, and revise principal lecture contents, identify and consult relevant literature; interactively present in front of an audience
   - Develop study strategies, independently assess their effectiveness, and adapt/optimize them as needed
   - Learn and work cooperatively, effectively communicate scientific contents to peers

4. **Prerequisite(s)**

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

5. **Evaluation of the learning process**

   Active participation during lectures, weekly homework corrected by teaching assistant and/or interactive presentation of homework during exercises

6. **Mode of examination**

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

7. **Requirements for acquiring credit points**

   Passing the oral or written examination

8. **Significance for overall grade**

   Weighted according to CPs

9. **Module contents**

   Review of standard molecular spectroscopy: approximate decoupling of time-independent Schrödinger equation in terms of translational, rotational, vibrational and electronic contributions, ro-vibrational spectroscopy of diatomics based on rigid rotor/harmonic oscillator approximation, selection rules, vibronic effects in the Frank-Condon approximation, Frank-Condon principle applied to the solvation of chromophores, normal mode analysis of vibrations of polyatomic molecules

   Time-dependence in quantum mechanics: time-dependent Schrödinger equation and its wavepacket solutions, properties of free particle and Gaussian wavepackets, quantum/classical correspondence and Ehrenfest Theorem, time-evolution operator formalism and Dyson equation, Schrödinger versus Heisenberg versus Dirac pictures of quantum dynamics, time-dependent variational principle (Dirac-Frenkel TDVP), linear TDVP, essentials of the time-dependent Hartree (TDH) method and its multiconfiguration (MCTDH) extension, Gaussian wavepacket propagation methods (Heller, Singer)

   Time-dependent perturbation theory for spectroscopy: formalism and applications to important schematic models, linear TDVP in Dirac picture, first- and second-order diagrams, virtual states and transitions, Fermi’s Golden Rule
Molecular systems in the radiation field for spectroscopy: transition probability, absorption cross section, dipole approximation, transition dipole, semiclassical approach to molecule-radiation field coupling, basics of the quantization of the radiation/electromagnetic field for spontaneous emission, multi-photon processes and non-linear spectroscopy, Raman scattering process, transformation of spectroscopy formulated in the static Schrödinger picture to the dynamic Heisenberg picture (Kubo-Gordon formalism to compute spectra), time-autocorrelation functions and spectral line shape function, time-domain versus frequency-domain spectroscopy

Neutron scattering and x-ray diffraction: van Hove formalism, Born approximation, Fermi contact potential, dynamic and static structure factor, scattering length and form factors, coherent and incoherent scattering, van Hove correlation function and the structural dynamics of liquids, pair correlation functions, radial distribution functions

<table>
<thead>
<tr>
<th>10</th>
<th><strong>Person in charge / Lecturer(s)</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Prof. Dr. D. Marx</td>
</tr>
</tbody>
</table>