RUHR-UNIVERSITÄT BOCHUM

RUB

Fakultät für Chemie und Biochemie

Master of Science (MSc) in **Molecular Sciences** – Spectroscopy and Simulation

Module Handbook

Module Handbook Index

The Master's programme Molecular Sciences – Spectroscopy and Simulation (iMOS) is modularised according to the curriculum in Table 1, which lists all available Modules 1 – 16 detailed in this Module Handbook. This document highlights and expands on curriculum content as prescribed by the programme's Examination Regulations / Prüfungsordnung.

Sem.	No.	Module (interactive PDF - click to page)	L	E/S	P	Type	ECTS	Department
1	E	Scientific English	2	2	-	option		Language Center (ZFA)
1	1	Concepts of Quantum Mechanics [a]	2	1	-	EC	5	Physics / RESOLV
	2	Statistical Mechanics and Fundamental Materials Physics [a]	2	1	-	EC	5	ICAMS
	3	Dynamics and Simulation	2	1	5	RC	9	ThC
	4	Concepts of Spectroscopy 1	2	1	5	RC	9	PC / PTT
	5	Concepts of Molecular Chemistry 1	2	1	-	RC	5	OC
	6	Biomolecular Simulation [a]	2	1	-	EC	5	ThC
	12	Biophysical Chemistry 2 [a]	2	1	-	EC	5	PC
		22-25 weekly contact hours	8-10	4-5	10		28-33[a]	
2	7	Electronic and Molecular Structure Theory	2	1	5	RC	9	ThC
	8	Concepts of Spectroscopy 2	2	1	5	RC	9	PC / TeC
	9	Theoretical Spectroscopy	2	1	-	RC	5	ThC
	10	Concepts of Molecular Chemistry 2 [a]	2	1	-	EC	5	AC
	11	Methods of Structural Analysis [a]	2	1	-	EC	5	AC
	13	Scientific Programming Methods for Chemists [a]	2	1	-	EC	5	AC / ThC
		22-25 weekly contact hours	8-10	4-5	10		28-33[a]	
3	14	International Course	-	-	14	RC	14	International Partners
	15	Focal Point Practical	-	-	15	RC	15	Participating groups
		29 weekly contact hours	-	-	29		29	
4	16	Master's Thesis				RC	30	Participating groups
Total			18	9	49		120	

Table 1 a) Only three (3) out of the seven (7) elective courses must be taken. E.g. required credit points 23 plus 1 or 2 EC per semester. See Course of Study below.

Legend L: lecture; E: exercise session; P: practical; ECTS: European Credit Transfer System points; EC: elective course / Wahlpflichtveranstaltung; RC: required course / Pflichtveranstaltung

Semester 1 includes all the Modules available in the winter semester (WiSe), and for Semester 2, those available in the summer semester (SuSe). Modules are based on lectures (L) with associated exercises (E), seminars (S), and laboratory practicals (P) as well as on coursework in internships (P). The programme is completed with a one-semester Master's thesis in the fourth semester. The modules can be composed of various partial performances. All coursework and examinations are taken during the course of study. The extent of the respective performance is expressed in credit points (CP) and ECTS.

Principle and participating Module Lecturers

of the following departments / Lehrstühle of the Faculty of Chemistry and Biochemistry.

AC / Inorganic Chemistry	Däschlein-Gessner, Devi, Schmid, Metzler-Nolte
OC / Organic Chemistry	Sander
PC / Physical Chemistry	Havenith-Newen, Herrmann, Petersen, Kruss, Morgenstern
TeC / Technical Chemistry	Muhler
ThC / Theoretical Chemistry	Marx, Hättig, Schäfer

Physics Faculty and — Sulpizi
RESOLV (Ruhr Explores Solvation Cluster of Excellence)

ICAMS — Varnik, Hartmaier
(Interdisciplinary Centre for Advanced Materials Simulation)

PTT — Saraceno
(Faculty for Electrical Engineering: Photonics and Teraherz Technology)

ZFA — Various
(Zentrum für Fremdsprachenausbildung, language center)

Participating Groups – Home Research Groups

Please refer to the iMOS Home Research Groups website. Additional faculty members may be considered by the examination committee.

Current for 2023 at RUB are Prof. Drs. Christof Hättig, Martina Havenith-Newen, Christian Herrmann, Sebastian Kruss, Dominik Marx, Marialore Sulpizi, Karina Morgenstern, Martin Muhler, Poul Petersen, Wolfram Sander, Lars Schäfer, and Rochus Schmid.

International Partners

Please inquire with the iMOS Office for the current list of international university departments. Students may also arrange an internship outside of the partner list upon equivalency approval of the faculty.

Course of Study

Semester		
1 Optional	Scientific English for Non-native Speakers	
1	3 Required Modules 23 CP	3 Elective Modules 15 CP (5 + 5 + 5 CP)
2	3 Required Modules 23 CP	
3	Focal Point Practical 15 CP	International Course 14 CP
4	Master's Thesis 30 CP	

The ideal **course of study** is presented above, culminating in 120 CP. Within the first year of studies, students must select three out of the seven electives to complete, as available in the winter (1st semester) or summer semester (2nd semester) in the Curriculum – Module Handbook Index, alongside 3 required modules per semester. For example, students may take two elective modules and associated examinations for credit in the first semester (23 RC + 5 + 5 = 33 CP) and one elective in the second semester (23 RC + 5 = 28 CP) or vice versa, for a total of 61 CP in the first year of studies. When selecting which elective courses to take, only those listed in the Curriculum – Module Handbook Index may be taken for credit and a total of 3 may be included in the cumulative grade point average of this master's degree.*

The Focal Point Practical (15 CP) and the International Course (14 CP) may be scheduled when the prerequisites, listed in the module description, are met. The Master's Thesis work may begin when the first 3 semesters of coursework is completed and grades are recorded with the Examination Office / Prüfungsamt. Students must submit the proper forms to the Examination Office / Prüfungsamt on time. Note that the Master's Thesis must take precisely 5 plus an optional 1 month to complete.

* Please review the iMOS Examination Regulations for further details, particularly on grading, examination sign-ups and attempts, course substitution, and in case of failed Modules or Module components. *Students are required to sign-up for examinations on time.* Also note, the legally binding Examination Regulations are the German language version of the iMOS "Prüfungsordnung".

Module Descriptions

Individual module descriptions are presented in this handbook with the total workload for all module components, which includes weekly lectures and exercises, conducted over the specified contact hours per week (SWS). For example, a 2 SWS lecture would meet for 2 hours per week over the 13-15 week-long semester lecture-period. Total hours for reference may be listed, e.g. 30 h for the entire module duration. Self-Study hours are listed for the complete duration of the module. The term lists the prescribed semester a student should take the module based on the Examination Regulations curriculum plan, and the Frequency is which university semester season the module is scheduled for.

The Moodle course – Molecular Sciences – Spectroscopy and Simulation is a point of reference for student support and course programming and is updated regularly.

The **eCampus Course Catalogue** VVZ (Vorlesungsverzeichnis), is updated ahead of each semester and includes module scheduling information.

Scientific English for Non-Native Speakers (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
E optional	2.5 CP	75 h	1. Semester	WiSe	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
Face-to-face lessons with active feedback			2 SWS	45 h	10-20 Students

Prerequisites

Admission to the iMOS Programme

Learning outcomes

After completion of this course, students will be able to
- understand and express both everyday and scientific concepts in English.
- use technical terms accurately in their field of study
- be more confident in applying spoken and written English to situations common in science, such as oral presentations and written reports.
- plan, prepare, and deliver presentations in English
- structure, phrase, and finalize written scientific documents such as reports and papers

Content

Language skills: consolidation of English skills based on IELTS level 6.0 or better, improvement of active and passive vocabulary, broadening of technical vocabulary and terminology relevant for the master course program and application to everyday scientific situations

Presentation techniques: basic concepts and practical application to realistic scenario (conference presentation)

Scientific Writing: basic concepts and practical examples (e.g. lab report, scientific paper)

Teaching methods

Lectures with active participation during weekly sessions, revision of assignments based on individual feedback provided in a variety of formats, oral and written contributions

Mode of assessment

Grading (pass/fail) of deliverables (1 presentation, 1 written text)

Requirement for the award of credit points

Achieve a 'pass' grade for the two examined deliverables, attend at least 75% of face-to-face sessions

Module applicability

M.Sc. iMOS

Weight of the mark for the final score

N/A – Module mark is not included in the final cumulative GPA for the M.Sc. degree

Module coordinator and lecturer(s)

Dr. Heimann-Bernoussi
Various instructors from the *Zentrum für Fremdsprachenausbildung (ZFA)*

Further information

Please coordinate attendance in July with the iMOS Office prior to the start of the programme. A comparable course may be available with other Chemistry and Biochemistry programme students during the summer session. Attendance in either module does not fulfill a prerequisite and may not qualify the student for early / pre-enrollment in the iMOS programme.

Concepts of Quantum Mechanics (iMOS)

Module	**Credits**	**Workload**	**Term**	**Frequency**	**Duration**
1 EC	5 CP	150 h	1 Semester	Each WiS	1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) 2 SWS b) 2 SWS	**Self-Study** 90 h	**Group size** 10-20 Students

Prerequisites

Knowledge of the following principles: Mathematics (Differential calculus, Integral calculus and Calculus of variations, Real and complex functions)
Basic principles of probability theory
Elementary quantum mechanics (harmonic oscillator, spin)

Learning outcomes

After completion of this course, students will know selected concepts and techniques of quantum mechanics and quantum statistical mechanics suitable to describe (bio)molecular systems such as molecules, clusters, liquids, solids and surfaces at an advanced level. They will be skilled in assessing which tool is suited to address a given question concerning dynamics and simulation, electronic and molecular structure, and theoretical spectroscopy of the aforementioned systems, and able to select relevant techniques and apply them to the quantum mechanical assessment of (bio)molecular systems.

Content

Introduction to quantum mechanics: postulates of quantum mechanics, Schrödinger equation, uncertainty principle (2h)

Review of basic quantum mechanics: real-space and momentum-space representation, bra/ket formalism and connection to the vector space and completeness relation (2h)

Free particle, particle in a box (1D and 2D) (2h)

Harmonic oscillator: algebraic solution, ladder operators (2h)

Central potentials: the Hydrogen atom (2h)

Pauli principle and antisymmetrization of wavefunction, spin and orbital angular momenta (4h)

Non-degenerate time-independent perturbation theory, variational principle (Rayleigh-Ritz), Hartree Fock (4h)

Time-dependent quantum mechanics: Schrödinger, Heisenberg and Dirac picture, time-dependent Schrödinger equation, Heisenberg equation of motion, time evolution operator (4h)

Time-dependent perturbation theory: intermediate/interaction picture, transition probabilities, constant and periodic perturbations, sudden approximation (4h)

Introduction to quantum-statistical mechanics: statistical/density operator, thermal density matrices, quantum-statistical expectation values, statistical mixtures and pure states, thermal Boltzmann operator (2h)

Teaching methods

Lectures and exercises with active participation during lectures, weekly homework corrected by teaching assistant and/or 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 oral or written examination
Module applicability M.Sc. iMOS
Weight of the mark for the final score According to CP
Module coordinator and lecturer(s) Prof. Dr. Sulpizi lecturers from the *Institute of Theoretical Physics* at RUB
Further information These course components may also be in the RUB Module Handbook for M.Sc. Physics as Module 2b, Advanced Quantum Mechanics

Statistical Mechanics and Fundamental Materials Physics (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
2 EC	5 CP	150 h	1. Sem.	Each WiS	1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) 3 SWS b) 1 SWS	**Self-Study** 90 h	**Group size** 20 Students

Prerequisites

Admission to M.Sc. iMOS

Learning outcomes

Students are able to describe the basic concepts of mechanical behaviour of materials. They gain an overview on the different mechanical properties and their assessment methods, including the microstructural strengthening mechanisms of materials. They understand the definition of mechanical equilibrium and are able to apply it to solve simple problems. They also memorize basic thermodynamic concepts for phase stability and liquid-solid or solid-solid phase transformations, as Maxwell relations and phase diagrams.

The students can apply statistical methods to connect physical quantities such as temperature, hydrostatic pressure and stress tensor to atomic and molecular features. They memorize approximate microscopic models and can apply them to describe heat capacity, electric conductivity, mechanical properties and magnetism. On the mesoscopic side, they can employ variational approaches to examine phase separation and domain growth.

Content

- Introduction to mechanical properties of materials and their assessment methods
- Microscopic origin of plastic deformation and fracture
- Thermodynamical concepts to describe phase equilibria and phase transformations in
- liquid and solid states
- Introduction to functional (electrical, magnetic, optical) properties of materials
- Introduction to probability theory and statistical ensembles
- Classical and quantum statistics (Boltzmann, Fermi and Bose-Einstein)
- Heat capacity of crystalline solids (Debye theory)
- Magnetism (para-magnetism and mean field theory of ferro-magnetism)

Teaching methods

Lecture and group work in exercises.

Mode of assessment

Written examination (2 hours), bonus points can be gained by providing solutions to the problem sheet in class.

Requirement for the award of credit points

Passing the examination

Module applicability

M.Sc. iMOS

Weight of the mark for the final score

According to CP

Module coordinator and lecturer(s)

Prof. Dr. Alexander Hartmaier, Prof. Dr. Fathollah Varnik
lecturers from the *Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)*

Further information

These course components are also in the RUB M.Sc. Module Handbook Material Science and Simulation as Required Course Module 2c.

Literature: McQuarrie: Statistical Mechanics, C. Garrod: Statistical mechanics and thermodynamics, D.R. Gaskell; Introduction to the thermodynamics of materials, D.A. Porter & K.E. Easterling; Phase transformation in metals and alloys.

Dynamics and Simulation (iMOS)

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

Concepts of Spectroscopy 1 (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
4 RC	9 CP	270 h	1. Semester	Each WiS	1 Semester
Courses a) Lectures b) Exercises c) Integrated laboratory practical			**Contact hours** a) 2 SWS b) 1 SWS c) 5 SWS	**Self-Study** 120 h	**Group size** a+b) 20 - 50 c) 5-20 Students

Prerequisites

a, b, c) Basic knowledge in quantum chemistry, quantum mechanics, spectroscopic techniques and the necessary mathematical formalism
c) Admission to M.Sc. iMOS

Learning outcomes

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

- Obtain theoretical and practical knowledge of modern linear and nonlinear spectroscopic methods (time- and frequency-domain) which allow for the elucidation of molecular structure and dynamics in different environments
- Understand applications of laser spectroscopic techniques from the THz to the VUV wavelength region to the study of molecules and their interactions
- Understand practical laser spectroscopic techniques in the lab course and their application in ongoing research projects through a hands-on approach
- Write reports with theories, experiments, and discussion of results

Content

- Electromagnetic radiation, molecular structure, light-matter interaction
- Optical and spectroscopic elements
- Line broadening mechanisms, spectral bandwidth, Fourier transformation
- Molecular symmetry, point groups, molecular symmetry groups
- Rotational spectroscopy: linear, symmetric, spherical, and asymmetric rigid rotor molecules, rotational infrared, millimeter, microwave and Raman spectra
- Vibrational spectroscopy: diatomic and polyatomic molecules, infrared and Raman spectra, vibrational selection rules, normal mode analysis
- Electronic spectroscopy: diatomic and polyatomic molecules, electronic and vibronic selection rules, Franck-Condon transitions, intramolecular nonradiative processes (internal conversion, intersystem crossing), curve crossings and conical intersections
- Laser basics, population inversion and gain mediums, cavity modes, properties of coherent radiation, specific laser systems
- Introduction to nonlinear spectroscopy

Teaching methods

a+b) Active participation during lectures and exercises with problems for self-studying, Q&A and discussion sessions with presentations given by the participants, Moodle course with online material
c) Hands-on laboratory projects to be done in supervised sessions

Mode of assessment

a+b) 2-hour end-of-term written exam on the content of the lectures
c) graded lab reports handed in during the term on the integrated practical

Requirement for the award of credit points

a+b) Passing the written examination and
c) successful acceptance of lab reports

Module applicability a+b+c) M.Sc. iMOS; a+b) M.Sc. Chemistry, M.Sc. Lasers and Photonics
Weight of the mark for the final score Weighted according to CPs 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) P. Petersen Lecturers from Physical Chemistry departments
Further information

Concepts of Molecular Chemistry I (iMOS)

Module	**Credits**	**Workload**	**Term**	**Frequency**	**Duration**
5 RC	5 CP	150 h	1. Sem.	WS	1 Semester
Courses a) Lecture b) Exercises			**Contact hours** a) 2 SWS / 30 h b) 1 SWS / 14 h	**Self-Study** 105 h	**Group size** 30 Students

Prerequisites

Learning outcomes

Students acquire advanced knowledge on the theory and techniques of the basic concepts of physical organic chemistry such as bond models, thermochemistry, and the theoretical evaluation of properties of experimental interest, in particular the theory of potential energy reaction surfaces. The main focus lies on the interplay between theoretical and experimental methods.

Students learn to read and understand advanced selected scientific publications in the topic of physical organic chemistry, how to summarize the publication in an abstract, and to present the essentials of the publication in an oral presentation using presentation software (15 min + 5 min discussion).

Content

- The covalent chemical bond (properties, experimental methods)
- The non-covalent chemical bond (van der Waals complexes, hydrogen bonds, supramolecular chemistry, peptides)
- Thermochemistry (properties, Benson's additivity rules)
- Potential energy surfaces (internal coordinates, Born Oppenheimer approximation, stationary points, reaction coordinates, Marcus theory, Curtin Hammett principle, More O'Ferral-Jencks diagrams, reactivity and selectivity, tunneling)
- Force field calculations (MM2)
- Linear free energy relations
- Experimental techniques (matrix isolation)

Teaching methods

Lecture, seminar based teaching with active participation of the student

Mode of assessment

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

Requirement for the award of credit points

Successful oral presentation, passing the exam

Module applicability

M.Sc iMOS Required Course; cross-posted M.Sc. Chemistry as Concepts of Molecular Chemistry I: Physical Organic Chemistry

Weight of the mark for the final score

According to CPs

Module coordinator and lecturer(s): W. Sander

Further information

Biomolecular Simulation (iMOS)

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

Electronic and Molecular Structure Theory (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
7 RC	9 CP	270 h	2. Semester	Each SuS	1 Semester
Courses a) Lectures b) Exercises c) Integrated computer practical			**Contact hours** a+b) 3 SWS c) 5 SWS	**Self-Study** a) 30 h b) 75 h c) 75 h	**Group size** 10-20 Students

Prerequisites

Learning outcomes

a+b) After completing this course students will have basic knowledge of modern wavefunction-based computational electronic and molecular structure methods and how these methods can be applied to solve typical problems in structure determination, spectroscopy, and the investigation of mechanisms and energetics of chemical reactions. Furthermore, they will know how to judge the accuracy and reliability of such methods.

c) They will be familiar with software for electronic structure calculations, know how apply modern electronic structure methods to practical problems and how to analyze, visualize and present results of electronic and molecular structure calculations.

Content

a+b) The course starts with basic principles for quantum mechanical many-particle systems and how their wavefunctions can be described in compact ways and then discusses a variety of modern wavefunction methods and their application:

- Pauli principle and Slater determinants
- Particle number representation (second quantization)
- Hartree-Fock and Multiconfigurational Self-Consistent Field methods
- Single- and Multiconfigurational Configuration Interaction methods
- Single- and Multireference Perturbation Theory
- Coupled-Cluster Methods
- Explicitly Correlated F12 Methods
- Response Theory approach to excitation energies and spectra
- Basis set convergence and basis set extrapolation
- Thermochemistry protocols

c) Application of electronic structure methods to determine molecular structures, energy differences between conformers, barriers for interconversion, vibrational spectra (IR and Raman), characterization of electronically excited states, optical spectra (UV-Vis), accurate reaction energies and intermolecular binding energies.

Teaching methods

a+b) Lectures and exercises with problems for self-studying, Q&A and discussion sessions with presentations given by the participants, Moodle course with online material.
c) Computational hands-on projects to be solved on own laptops and/or a computer lab with different software packages, done partially in supervised sessions and partially as self-study.

Mode of assessment

a+b) submission and grading of the solution sheets for the exercises and a final oral end-of-semester exam
c) submission and grading of reports of the computational hands-on projects

Requirements for the award of credit points

c) successful acceptance of the reports for the computational hands-on projects and

a+b) passing the oral end-of-semester exam
Module applicability M.Sc. iMOS and M.Sc. Chemistry
Weight of the mark for the final score According to CP
Module coordinator and lecturer(s) C. Haettig
Further information

Concepts of Spectroscopy 2 (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
8 RC	9 CP	270 h	2. Semester	Each SuS	1 Semester
Courses a) Lectures b) Exercises c) Integrated laboratory practical			**Contact hours** a) 2 SWS b) 1 SWS c) 5 SWS	**Self-Study** 120 h	**Group size** a+b) 20 - 50 c) 5-20 Students

Prerequisites

a, b, c) Advanced knowledge in quantum chemistry, quantum mechanics and spectroscopic techniques, such as provided by the modules Concepts of Spectroscopy 1 and Dynamics and Simulation.
c) Admission to M.Sc. iMOS

Learning outcomes

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

- Obtain theoretical and practical knowledge of nonlinear optics important for non-linear spectroscopic and microscopic techniques to investigate structure, dynamics and interactions of chemical and biochemical samples
- Understand practical laser spectroscopic techniques in the lab course and their application in ongoing research projects through a hands-on approach
- Write reports with theories, experiments, and discussion of results
- Develop presentation skills in front of an audience
- Utilize digital techniques to prepare and conduct a presentation

Content

- Principles of non-linearity: Electromagnetic waves in vacuum and in matter, Non-linear responses, Anharmonic oscillator model, Phase matching, Higher order processes
- Non-linear spectroscopy techniques: SFG, SHG, Time-resolved spectroscopy
- Non-linear microscopy techniques: Confocal microscopy, Fluorescence microscopy, Super-resolution microscopy, Multi-photon microscopy methods, Scanning methods.

Teaching methods

a+b) Active participation during lectures and exercises with problems for self-studying, Q&A and discussion sessions with presentations given by the participants, Moodle course with online material.
c) Hands-on laboratory projects to be done in supervised sessions

Mode of assessment

a + b) 20 - 40 min end-of-term oral exam or 2-hour end-of-term written exam on the content of the lectures
c) graded lab reports handed in during the term on the integrated practical

Requirement for the award of credit points

a+b) Passing the written examination
c) successful acceptance of lab reports

Module applicability

a+b+c) M.Sc. iMOS; a+b) M.Sc. Chemistry, M.Sc. Lasers and Photonics

Weight of the mark for the final score

Weighted according to CPs
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) P. Petersen Lecturers from Physical Chemistry departments
Further information

Theoretical Spectroscopy (iMOS)

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

Prerequisites

Undergraduate level knowledge in classical mechanics, statistical mechanics and time-independent non-relativistic quantum mechanics and advanced knowledge at the level of the Dynamics and Simulation M.Sc. course

Learning outcomes

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.

Content

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, first Born approximation, 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

Teaching methods

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.

Mode of assessment Written or oral end-of-semester exam and homework
Requirement for the award of credit points Passing the end-of-semester exam
Module applicability M.Sc. iMOS; M.Sc. Chemistry; M.Sc. Biochemistry (Focal Point Program “Biomolecular Chemistry”)
Weight of the mark for the final score According to CP
Module coordinator and lecturer(s) D. Marx
Further information Module can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program “Biomolecular Chemistry”

Concepts of Molecular Chemistry 2 (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
10 EC	5 CP	150 h	2. Sem.	Each SuS	1 Semester
Courses a) Lecture b) Exercise			**Contact hours** a) 2 SWS/30 h b) 1 SWS/15 h	**Self-Study** 105 h	**Group size** About 50

Prerequisites

Admission to the Master Course Program; basic knowledge general in synthetic chemistry (organic and inorganic chemistry) and the structure of molecular compounds, complexes (molecular orbitals, Lewis structures) is recommended

Learning outcomes

After the successful completion of the module

- Students have acquired advanced knowledge of the interpretation of the electronic structure, properties and reactivities of organometallic, inorganic molecular and solid state compounds and systems of higher and lower dimensionality.
- Students will be able to apply their knowledge independently on current, and intellectually demanding research problems in modern inorganic chemistry
- Students will be able to analyze research questions and develop solutions and solution strategies.

Content

The module focuses on the reactivity, properties and electronic structure of organometallic, inorganic and bioinorganic compounds. These topics may include:

- Concepts of organometallic chemistry: Stabilization of reactive intermediates, control of electronic and steric properties of ligands, applications in homogenous catalysis, trends in the periodic table
- Concepts of bioinorganic chemistry and medicinal chemistry
- Concepts in inorganic solid state and materials chemistry
- Application of spectroscopic methods for the characterization of inorganic solid state materials, molecular compounds and complexes and the elucidation of reaction mechanisms; computational methods in structure elucidation and mechanistic studies
- Modern trends in organometallic, inorganic and/or bioinorganic chemistry

Teaching methods

Lecture with exercises und accompanying e-learning modules

Mode of assessment

end-of-term written exam

Requirement for the award of credit points

Passing the written examination

Module applicability

M.Sc. iMOS; cross-posted for M.Sc. Chemistry as Inorganic Chemistry IV

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

Prof. Dr. Däschlein-Gessner

V. Däschlein-Gessner, N. Metzler-Nolte, A. Devi and lecturers from inorganic chemistry

Further information

Methods of Structural Analysis (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
11 EC	5 CP	150 h	2. Sem.	Each SuS	1 Semester
Courses c) Lecture d) Exercise			**Contact hours** c) 2 SWS/30 h d) 1 SWS/15 h	**Self-Study** 105 h	**Group size** 10-20 students

Prerequisites

Basic knowledge of general, inorganic and organic chemistry (chemical structure and bonding)

Learning outcomes

After the successful completion of the module, students have acquired advanced knowledge of symmetry in crystalline materials and the techniques to resolve the molecular structure from X-ray diffraction experiments, ranging from small molecules to large proteins. In addition, they are able to interpret and analyze the topology of the electron density in terms of the "Atoms in Molecules" concept. Students will be able to independently revise module contents and readd of the relevant literature, revision of exercises by an online peer-review process.

Content

The module presents the foundations of crystallography: crystal lattices, Bravais-lattices, lattice planes, symmetry elements (Schoenflies-symbols), space groups (Hermann-Mauguin-symbols). Detailed topics may include:
X-ray diffraction: Generation of X-rays, diffraction at the crystal lattice, Bragg law, Laue classes, reciprocal lattice, Ewald-construction, systematic extinction, symmetry equivalent reflexes, internal R-value, atomic form factors, structure factors, setup of a diffractometer and a detector, data collection.
X-ray structure analysis: crystal growth, structure solution (direct methods, Patterson, charge flipping), structure refinement (difference Fourier-analysis), quality factors, critical evaluation of results, problems with the determination of space groups, determination of absolute structure, disorder, twining, database search (ICSD, CCDC).
Powder X-ray: X-ray diffraction of powders, identifications of compounds with the MATCH database.
Protein crystallography: Crystal growth, synchrotron radiation, methods to solve the phase problem, refinement of protein structures, evaluation and interpretation of protein structures.
Topology of the electron density: Connection between molecular structure and electron density, topological analysis by the „Atoms in Molecules" concept, interpretation of the analysis (bond critical points, ellipticity, Laplacian of the density etc.), charge analysis by AIM and other methods, exercises with applications to practical examples with freely available computer programs.

Teaching methods
Lectures and exercises, homework corrected by fellow students within a peer-review process, hands-on sessions during exercises

Mode of assessment
End-of-term 2-hour written exam

Requirement for the award of credit points
Passing the written examination

Module applicability
M.Sc. iMOS; cross-posted as Methoden der Strukturanalyse II for BSc. Chemistry

Weight of the mark for the final score
Weighted according to CPs

Module coordinator and lecturer(s)

Prof. Dr. Schmid; and lecturers from inorganic chemistry

Further information

Biophysical Chemistry II (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
12 EC	5 CP	150 h	1. Sem.	WiSe	1 Semester

Courses	Contact hours	Self-Study	Group size
a) Lectures b) Exercises c) Seminar	a) 2 SWS b) 1 SWS c) 1 SWS	90 h	30 Students

Prerequisites

Knowledge in basic Physical Chemistry.

Learning outcomes

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

- Acquire advanced knowledge in experimental methods in the investigation of dynamics and thermodynamics of proteins and membranes, and on protein reaction and function based on selected examples
- Understand their applications, advantages, and disadvantages of the methods
- Analyze and screen relevant literatures independently
- Develop presentation skills in front of an audience
- Utilize digital techniques to prepare and conduct a presentation

Content

Advanced Biophysical techniques:

- Microcalorimetry in protein characterization
- Fluorescence-based methods in protein interactions
- Advanced fluorescence microscopy
- Fourier transform spectroscopy
- Attenuated total reflection (ATR) spectroscopy
- Vibrational spectroscopy in biomolecular solvation
- Scanning probe microscopy (SPM) in biochemistry

Teaching methods

Lecture (2 SWS, 30 h), Exercise (1 SWS, 15 h), Seminar (1 SWS, 15 h).

Mode of assessment

Participation in all seminars and presentation about an assigned publication.
Written exam of 60 mins.

Requirement for the award of credit points

Pass both parts: presentation (50%) and written exam (50%).

Module applicability

M.Sc. iMOS, cross-posted to M.Sc. Chemistry, M.Sc. Biochemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

Lecturers from Physical Chemistry departments.

Further information

Scientific Programming Methods for Chemists

Module	Credits	Workload	Term	Frequency	Duration
13 EC	5 CP	150 h	2. Sem.	SuSe	1 Semester

Courses	Contact hours	Self-Study	Group size
a) Lecture b) Exercises	a) 2 SWS b) 1 SWS	a) 30 h b) 75 h	10-20 Students

Prerequisites

None

Learning outcomes

After successful completion of the module students will:

- have basic knowledge programming concepts of modern programming languages
- know how to structure code and how to test and validate source code
- be able to turn scientific modelling problems into programmable algorithms
- have some experience on how to use code libraries to solve standard mathematical problems and to visualize scientific data

Content

The lecture uses Python as an example of a modern object-oriented programming language to introduce students to:

- elementary data types (integers, floats, strings, etc.) and their representation in computers
- control structures (loops, conditions, functions, etc.)
- basics of object orientation (classes, inheritance, etc.)
- complex data types (lists, tuples, dictionaries, etc.)
- reading and writing data from/to files
- math libraries (numpy, scipy, blas, lapack)
- visualization of data with matplotlib
- solving differential equations numerically on grids
- solving algebraic problems (linear equations, SVD, eigenvalue problems)

Teaching methods

Lecture, Hands-on coding projects for self-studying on own laptops with online support by teaching assistants via a chat work space, Q&A and discussion sessions, Moodle course with online material.

Mode of assessment

submission and grading of the solution sheets for the hands-on problems and a final written or oral end-of-semester exam

Requirements for the award of credit points

successful written or oral end-of-semester exam

Module applicability

M.Sc. iMOS; M.Sc. Chemistry

Weight of the mark for the final score

by CP

Module coordinator and lecturer(s)

R. Schmid, C. Haettig

Further information

International Course (iMOS)					
Module 14 RC	**Credits** 14 CP	**Workload** 420 h	**Term** 3. Semester	**Frequency** WiSe	**Duration** 8 weeks full-time or equivalent
Courses Research oriented lab project in one of the international research groups			**Contact hours** Full-time 300 h	**Self-Study** 120 h	**Group size** individual

Prerequisites

Proof of at least 46 credit points and full or partial completion (with approval) of all required courses attributed to the first and second semester as outlined in the Examination Regulations (§8, clause 6)

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
- Get acquaintance with alternative workflow organization
- Develop International teamwork and collaboration

Content

The practical is carried out in a research group located at one of our international partner universities/scientific institutions. Students will learn methods complementary to those available at Ruhr University Bochum.

Students are expected to extend their experimental/theoretical skills to techniques not available in Bochum or to apply skills gained in Bochum to research topics in the hosting group.

A wide variety of topics are possible. Examples of completed projects:

- AIMD simulations and theoretical assignment of coupled solute-solvent modes (Université d'Evry val d'Essonne)
- Assignment of Tunneling motions in small water cluster (UC Berkeley)
- Messenger spectroscopy of ionic liquids in the IR; gas phase IR spectroscopy (Yale University)
- Simulation of Hv1 to investigate the opening mechanism of the proton channel (UC Irvine)
- Single-point analysis on selected frames of a CPMD trajectory file; developing Ab-initio based potentials for ions using dipoles and force fitting procedure (ENS Paris)

Students will give an oral presentation of results on their return to RUB.

Teaching methods

Research oriented lab project in one of the international research groups

Mode of assessment

Active participation in practical, feedback during and on the experiment, feedback on written lab

report by teaching assistants
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 According to CPs
Module coordinator and lecturer(s) M. Havenith-Newen Faculty of the partner universities of the international Master Molecular Sciences – Spectroscopy and Simulation

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	Contact hours	Self-Study	Group size
research oriented lab project in one of the research groups	Full-time 250 h	200 h	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

Master's Thesis (iMOS)

Module	Credits	Workload	Term	Frequency	Duration
16 RC	30 CP	900 h	4. Semester	Each SuS	5 to 6 months full-time
Courses			**Contact hours**	**Self-Study**	**Group size**
Master Thesis (iMOS) practical work			Full-time 700 h	200 h	individual

Prerequisites

Proof of 14 credit points for Module 14 (International Course) and of 15 credit points in Module 15 (Focal Point Practical)

Learning outcomes

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

- Acquire ability to plan, organize, develop, operate, and present complex problems in Molecular Sciences: Spectroscopy and Simulation (iMOS)
- Work independently in an iMOS subject under the supervision of an advisor
- Deal with subject-specific problems and to present them in an appropriate and comprehensible manner and according to scientific standards
- Acquire profound specialized knowledge, which is required to take the step from their studies to professional life
- Obtain detailed knowledge of experimental and computational methods
- Develop interdisciplinary teamwork and collaboration while carrying out projects
- Utilize digital techniques for graphical presentation of complex topics

Content

The master thesis can be theoretically and/or practically oriented. Its topic is determined by the respective supervisor.

Teaching methods

Active supervision: regular progress meetings, supervised presentation of project and results

Mode of assessment

Required is a written report (typically 50-100 pages) describing the project and its results in detail

Requirement for the award of credit points

Passing of the master thesis (grade "adequate", 4,0 or better)

Module applicability

M.Sc. iMOS

Weight of the mark for the final score

According to CPs

Module coordinator and lecturer(s)

M. Havenith-Newen

Faculty of the M.Sc. iMOS

Further information