RUHR-UNIVERSITÄT BOCHUM

RUB

Faculty of Chemistry and Biochemistry

Module Manual

iMOS

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

Curriculum

Sem.	No.	Module	L	E/S	P	Type	CP	Responsible
1	E	Scientific English for non-native speakers	2	2	-	optional		Language Center (ZFA)
1	1	Concepts of Quantum Mechanics [a]	2	1	-	EC	5	Physics
	2	Statistical Physics and Thermodynamics [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**
		22-25 wch	8-10	4-5	10		28-33	
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**
	12	**Fundamentals of Magnetic Resonance [a]**	**2**	**1**	**-**	**EC**	**5**	**RESOLV**
	13	**Scientific Programming Methods for Chemists [a]**	**2**	**1**	**-**	**EC**	**5**	**PC**
		22-25 wch	8-10	4-5	10		28-33	
3	14	International Course	-	-	14	RC	14	International Partners
	15	Focal Point Practical	-	-	15	RC	15	Participating groups
		29 wch	-	-	29		29	
4	16	Master's Thesis				RC	30	Participating groups
Total			18	9	49		120	

a) three out of the seven elective courses must be taken.

Notes:

L: lecture; E: exercise session; P: practical; CP: credit points; EC: elective course (Wahlpflichtveranstaltung); RC: required course (Pflichtveranstaltung); wch: weekly contact hours (Semesterwochenstunden); SuS: summer semester, WiS: winter semester.

New or substantially modified courses in bold face.

The lecture period comprises 15 weeks in the winter semester, 13 weeks in the summer semester.

Lecturers:

AC (Inorganic Chemistry): Däschlein-Gessner, Devi, Schmid, Metzler-Nolte
OC (Organic Chemistry): Sander
PC (Physical Chemistry): Havenith-Newen, Herrmann, Nürnberger, Ebbinghaus, Morgenstern
RESOLV Cluster of Excellence: Bordignon
TeC (Technical Chemistry): Muhler
ThC (Theoretical Chemistry): Marx, Hättig, Schäfer
Physics: Drautz, Czarnetzki, Polyakov
ICAMS (Interdisciplinary Centre for Advanced Materials Simulation): Steinbach, Varnik, Darvishi Kamachali
PTT (Faculty for Electrical Engineering: Photonics and Terahertz technology): Hofmann
ZFA (Zentrum für Fremdsprachenausbildung, language center): various

Scientific English for Non-Native Speakers					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module E	75 h	0 CP	1	each WiS	1 semester

1	**Teaching methods**	**Hours per week**	**Contact time**	**Self-study**
	Face-to-face lessons incl. feedback sessions	2 h	30 h	45 h

2	**Learning objectives** Students will consolidate their English knowledge, improve their language skills with an emphasis on technical terms required for the master course program, and gain confidence in applying spoken and written English to situations common in science, such as oral presentations and written reports.
3	**Soft skills** identification and recording of principal lecture contents, independent revision of module contents, active communication in a foreign language
4	**Prerequisite(s)** Admission to the Master Course Program; recommended for all students
5	**Evaluation of the learning process** active participation during weekly sessions, interactive correction of homework, oral and written contributions
6	**Mode of examination** none (not necessary, optional pre-course)
7	**Requirements for acquiring credit points** n/a
8	**Significance for overall grade** n/a
9	**Module contents** 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)
10	**Person in charge / Lecturer(s)** Dr. Heimann-Bernoussi M. Mariano, *Zentrum für Fremdsprachenausbildung (ZFA)*

Concepts of Quantum Mechanics						
Code No.	**Workload**	**Credit points**	**Available in semester**		**Frequency**	**Course duration**
Module 1	150 h	5 CP	1		each WiS	1 semester
1	**Teaching methods**		**Hours per week**	**Contact time**		**Self-study**
	a) Lectures b) Exercises		a) 2 h b) 1 h	45 h		105 h
2	**Learning objectives** Students acquire advanced knowledge of selected topics of concepts and techniques of quantum mechanics and quantum statistical mechanics as needed in the realm of (bio)molecular systems such as molecules, clusters, liquids, solids and surfaces. This knowledge will be necessary to better understand dynamics and simulation, electronic and molecular structure, and theoretical spectroscopy of the aforementioned systems.					
3	**Soft skills** identification and recording of principal lecture contents, independent revision of module contents and reading of relevant literature; interactive presentation in front of an audience					
4	**Prerequisite(s)** Admission to the Master Course Program					
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** introduction to/motivation of quantum mechanics (2h) review of basic quantum mechanics: real-space and momentum-space representation, Hilbert space concept and bra/ket notation (2h) harmonic oscillator: algebraic solution, ladder operators (2h) Pauli principle and antisymmetrization of wavefunction, spin/orbital angular momenta and their coupling (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, propagator/Green function concept (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, restricted summation for identical particles, classical limit, interpretation of canonical partition function as path integral, basic ideas of path integral formalism of quantum mechanics and quantum-statistical mechanics: time-dependent propagator, free particle solution, thermal propagator (Feynman-Kac) and connection to statistical mechanics (6h)
10	**Person in charge / Lecturer(s)** Prof. Dr. Polyakov M. Polyakov, lecturers from the *Institute of Theoretical Physics* at RUB

Statistical Physics and Thermodynamics						
Code No.	**Workload**	**Credit points**	**Available in semester**		**Frequency**	**Course duration**
Module 2	150 h	5 CP	1		each WiS	1 semester
1	**Teaching methods**		**Hours per week**	**Contact time**		**Self-study**
	a) Lectures b) Seminar & group work		a) 2 h b) 1 h	45 h		105 h
2	**Learning objectives** Students gain knowledge of the fundamental concepts of equilibrium thermodynamics and statistical mechanics, enabling students with engineering backgrounds to understand the basic physical concepts and develop skills in applying these concepts to materials modelling and solid state physics.					
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents, independent consultation of the relevant literature					
4	**Prerequisite(s)** Admission to the Master Course Program					
5	**Evaluation of the learning process** active participation during lectures, weekly homework corrected by teaching assistant, interactive presentation of homework during exercises					
6	**Mode of examination** end-of-term written examination					
7	**Requirements for acquiring credit points** Passing the written examination					
8	**Significance for overall grade** Weighted according to CPs					
9	**Module contents** • Introduction to key concepts of probability theory: probability distributions, expectation values, central limit theorem • Physical concepts in classical mechanics required for the understanding of statistical mechanics • Basic concepts in classical thermodynamics: state variables, thermodynamic functionals, entropy, extremal principles, Legendre transformations, Maxwell relations, phase equilibria, Clausius-Clapeyron equation, ideal gas, reversibility and irreversibility, adiabatic processes • Linking classical mechanics to statistical mechanics: microcanonical, canonical and grand canonical ensemble, equipartition theorem, Maxwell distribution • Basic aspects of quantum statistics					
10	**Person in charge / Lecturer(s)** Prof. Dr. I. Steinbach, Prof. Dr. F. Varnik, Dr. R. Darvishi Kamachali; lecturers from the *Interdisciplinary Centre for Advanced Materials Simulation (ICAMS)*					

Dynamics and Simulation					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 3	270 h	9 CP	1	each WiS	1 semester

1	**Teaching methods**	**Hours per week**	**Contact time**	**Self-study**
	a) Lectures b) Exercises c) integrated practical	a) 2 h b) 1 h c) 5 h	120 h	150 h

2	**Learning objectives** Students acquire advanced knowledge of the theory and techniques of statistical mechanics and (bio)molecular dynamics 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 Solvation Science.
3	**Soft skills** identification and recording of principal lecture contents, independent revision of module contents and reading the relevant literature, interactive presentation in front of an audience
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation in lecture and practical, presentation of homework during exercises, feedback during and on virtual experiments, written homework and lab reports
6	**Mode of examination** 30 - 45 min end-of-term oral exam or 2-hour end-of-term written exam on the content of the lectures, and graded lab reports handed in during the term on the integrated practicals
7	**Requirements for acquiring credit points** Passing the oral or written examination and acceptance of lab reports
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** 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.
10	**Person in charge / Lecturer(s)** Prof. Dr. D. Marx

Concepts of Spectroscopy 1

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 4	240 h	9 CP	1	each WiS	1 semester

	Teaching methods	Hours per week	Contact time	Self-study
1	a) Lectures b) Exercises c) integrated practical	a) 2 h b) 1 h c) 5 h	120 h	120 h

2	**Learning objectives** The course aims to provide 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. The course material covers the application of laser spectroscopic techniques from the THz to the VUV wavelength region to the study of molecules and their interactions in molecular beams, Helium nanodroplets, rare gas matrices, the liquid phase and at interfaces. The accompanying lab course is intended to foster the practical understanding of the laser spectroscopic techniques and their application in ongoing research projects through a hands-on approach.
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents and reading the relevant literature
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation during lectures, weekly written short tests (15min), homework corrected by teaching assistant, interactive presentation of homework during exercises
6	**Mode of examination** 2-hour end-of-term written exam on the content of the lectures, and graded lab reports handed in during the term on the integrated practicals
7	**Requirements for acquiring credit points** Passing the written examination and acceptance of lab reports
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** 1. The electromagnetic spectrum, theory of generation and properties of ns, ps, and fs laser pulses, tunable pulsed and cw lasers, pulse duration, spectral bandwidth, Fourier transformation. 2. Line broadening mechanisms and their removal: rare gas matrix, supersonic jet expansion, molecular beam, Helium nanodroplet. 3. Molecular symmetry, point groups, molecular symmetry groups. 4. Rotational spectroscopy: linear, symmetric, spherical, and asymmetric rigid rotor molecules, rotational infrared, millimeter, microwave spectra, structure determination from rotational constants, determination of conformational geometries. 5. Vibrational spectroscopy: diatomic and polyatomic molecules, infrared and Raman spectra, vibrational selection rules, normal mode analysis (Wilson FG matrix method), effective and exact

	molecular Hamiltonians, double resonance techniques, intramolecular vibrational redistribution (IVR). 6. Electronic spectroscopy: diatomic and polyatomic molecules, electronic and vibronic selection rules, one- and multi-dimensional Franck-Condon analysis, intramolecular nonradiative processes (internal conversion, intersystem crossing), curve crossings and conical intersections. Frequency domain methods (e.g. LIF), Transition State spectroscopy (negative ion photodetachment), velocity map ion imaging. 7. Photoelectron spectroscopy: ionization process and Koopmans' theorem, molecular UV photoelectron spectra in the frequency-domain, Franck-Condon analysis, ZEKE spectroscopy.
10	**Person in charge / Lecturer(s)** Prof. Dr. Havenith-Newen M. Havenith-Newen, K. Morgenstern, P. Nürnberger, C. Herrmann

Concepts of Molecular Chemistry 1					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 5	150 h	5 CP	1	each WiS	1 semester

1	**Teaching methods**	**Hours per week**	**Contact time**	**Self-study**
	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h	105 h

2	**Learning objectives** Students acquire basic knowledge of molecular reactivity and the concepts of physical organic chemistry such as properties related to electron density and potential energy surfaces. They learn to estimate the thermodynamics and kinetics of chemical reactions from simple concepts such as additivity rules, and to evaluate the experimental basis of such rules.
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents and reading the relevant literature
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation during lectures, homework corrected by teaching assistant and/or interactive presentation of homework during exercises
6	**Mode of examination** 30-min. end-of-term oral exam
7	**Requirements for acquiring credit points** Passing the oral examination
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** Concepts of covalent and non-covalent bonds, thermodynamics and kinetics of chemical reactions, potential energy surfaces, the basis of force field calculations, Benson additivity rules, linear free energy relationships
10	**Person in charge / Lecturer(s)** Prof. Dr. W. Sander

Biomolecular Simulation: Understanding Experiments at the Molecular Level						
Code No.	**Workload**	**Credit points**	**Available in semester**		**Frequency**	**Course duration**
Module 6	150 h	5 CP	1		each WiS	1 semester
1	**Teaching methods**	**Hours per week**	**Contact time**		**Self-study**	
	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h		105 h	
2	**Learning objectives** 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.					
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents, independent consultation of the relevant literature					
4	**Prerequisite(s)** Admission to the Master Course Program					
5	**Evaluation of the learning process** active participation during lectures, 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** **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, effect of mutations. Enthalpy-entropy compensation. **NMR**: Basic principles (nuclei in B-field, chemical shifts, spin coupling, Karplus-equation), pulse techniques in NMR (spin relaxation, longitudinal and transverse relaxation, inversion recovery, Hahn echo, Bloch equations), line broadening, chemical/conformational exchange, nuclear Overhauser effect. 2D NMR. MD simulations and NMR.
10	**Person in charge / Lecturer(s)** Prof. Dr. L. Schäfer

Electronic and Molecular Structure Theory					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 7	240 h	9 CP	2	each SuS	1 semester

1	**Teaching Methods**	**Hours per week**	**Contact time**	**Self-study**
	a) Lectures b) Exercises c) Practical	a) 2 h b) 1 h c) 5 h	120 h	120 h

2	**Learning objectives** Students acquire advanced knowledge of electronic and molecular structure theory and quantum chemical methods and how these methods can be applied to solve typical problems e.g. in thermochemistry, spectroscopy, or structure determination. Furthermore they will learn how to judge the accuracy and reliability of methods and how to analyze and present results of electronic and molecular structure calculations.
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents, consultation of the relevant literature
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation, homework corrected by teaching assistant, presentation and discussion of homework and results from practicals in exercise session
6	**Mode of examination** 30 - 45 min end-of-term oral exam on the content of the lectures, and graded lab reports handed in during the term on the integrated practicals
7	**Requirements for acquiring credit points** Passing the oral examination and acceptance of lab reports
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** Many-electron wavefunctions: quantum mechanical description of many-particle systems, Pauli principle, Slater determinants, matrix elements for Slater determinants and many-electron wavefunctions Second quantization (particle number representation): Fock space and occupation number vectors, creation and annihilation operators, representation of one- and two-electron interactions in second quantization, representation of excited determinants, spin free operators Self-consistent field (SCF) and multi-configurational self-consistent field (MCSCF) methods: Hartree-Fock and coupled perturbed Hartree-Fock equations in second quantization, solution of HF equations, exponential parameterization of unitary transformations, MCSCF methods as e.g. CASSCF and RASSCF, choice and validation of active spaces Multi-reference correlation methods: multi-reference perturbation theory, CASPT(2), multireference CI, internally and externally contracted variants, construction of the many-particle basis functions

	Coupled-Cluster methods: the coupled-cluster wavefunction ansatz and its properties, the projected Schrödinger equation, size-consistency, the standard coupled-cluster models, perturbative triples corrections, CCSD(T) Explicitly-correlated F12 methods: static and dynamic correlation, explicitly correlated wavefunctions, R12 ansatz of Kutzelnigg, modern F12 methods, MP-F12 and CCSD-F12 Efficient methods for large systems: direct methods, integral screening and approximations Application of quantum chemical methods to typical problems, e.g. structure optimization, ionization energies, electron affinities, UV and CD spectra, IR and Raman spectra, reaction and activation energies, entropies, enthalpies and free enthalpies. Basis set convergence and accuracy of quantum chemical methods, additive correction schemes.
10	**Person in charge / Lecturer(s)** Prof. Dr. C. Hättig

Concepts of Spectroscopy 2

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 8	240 h	9 CP	2	each SuS	1 semester

	Teaching Methods	Hours per week	Contact time	Self-study
1	a) Lectures b) Exercises c) Practical	a) 2 h b) 1 h c) 5 h	120 h	120 h

2	**Learning objectives** Students learn the basics of nonlinear optics important for non-linear spectroscopic and microscopic techniques to investigate structure, dynamics and interactions of chemical and biochemical samples. The accompanying lab course is intended to foster the practical understanding of spectroscopic methods using model systems. Students are integrated in ongoing research projects through a hands-on approach.
3	**Soft skills** interactive presentation in front of an audience, identification and recording of principal lecture contents, unsolicited revision of module contents, unsolicited consultation of the relevant literature
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation during lectures and exercises, interactive presentation of exercises
6	**Mode of examination** 30 - 45 min end-of-term oral exam or 2-hour end-of-term written exam on the content of the lectures, and graded lab reports handed in during the term on the integrated practicals
7	**Requirements for acquiring credit points** Passing the oral or written examination and acceptance of lab reports
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** 1. Principles of non-linearity Electromagnetic waves in vacuum and in matter, Non-linear responses, Anharmonic oscillator model, Phase matching, Higher order processes 2. Non-linear spectroscopy techniques Raman spectroscopy, SERS, Ellipsometry, SFG, SHG, Time-resolved spectroscopy 3. Non-linear microscopy techniques Confocal microscopy, Fluorescence microscopy, Super-resolution microscopy, Multi-photon microscopy methods, Scanning methods
10	**Person in charge / Lecturer(s)** Prof. Dr. Havenith-Newen K. Morgenstern, M. Havenith-Newen, P. Nürnberger, C. Herrmann

Theoretical Spectroscopy

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 9	150 h	5 CP	2	each SuS	1 semester

	Teaching Methods	Hours per week	Contact time	Self-study
1	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h	105 h

2 Learning objectives

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

3 Soft skills

identification and recording of principal lecture contents, independent revision of module contents and reading of the relevant literature; interactive presentation in front of an audience

4 Prerequisite(s)

Admission to the Master Course Program

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
10	**Person in charge / Lecturer(s)** Prof. Dr. D. Marx

Concepts of Molecular Chemistry 2						
Code No.	**Workload**	**Credit points**	**Available in semester**		**Frequency**	**Course duration**
Module 10	150 h	5 CP	2		each SuS	1 semester
1	**Teaching Methods**	**Hours per week**	**Contact time**		**Self-study**	
	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h		105 h	
2	**Learning objectives** Students acquire 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.					
3	**Soft skills** Interactive presentation in front of an audience, identification and recording of principal lecture contents, independent revision of module contents and reading of the relevant literature					
4	**Prerequisite(s)** 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					
5	**Evaluation of the learning process** Active participation during lectures, homework corrected by teaching assistant and/or interactive presentation of homework during exercises					
6	**Mode of examination** 2-hour end-of-term written exam					
7	**Requirements for acquiring credit points** Passing the written examination					
8	**Significance for overall grade** Weighted according to CPs					
9	**Module contents** Reactivity, properties and electronic structure of organometallic, inorganic and bioinorganic compounds. Content may include one or several of the following topics: – 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					

10	**Person in charge / Lecturer(s)** Prof. Dr. Däschlein-Gessner V. Däschlein-Gessner, N. Metzler-Nolte, A. Devi

Methods of Structural Analysis

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 11	150 h	5 CP	2	each SuS	1 semester

	Teaching Methods	Hours per week	Contact time	Self-study
1	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h	105 h

2	**Learning objectives** Students acquire 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.
3	**Soft skills** Note-taking and scientific discussions during lectures, independent revision of module contents and reading of the relevant literature, revision of exercises by an online peer-review process.
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation during lectures and exercises, homework corrected by fellow students within a peer-review process, hands-on sessions during exercises
6	**Mode of examination** 2-hour end-of-term written exam
7	**Requirements for acquiring credit points** Passing the written examination
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** Foundations of crystallography: crystal lattices, Bravais-lattices, lattice planes, symmetry elements (Schoenflies-symbols), space groups (Hermann-Mauguin-symbols). 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.
10	**Person in charge / Lecturer(s)** Prof. Dr. Schmid B. Mallick, E. Hofmann, R. Schmid

Fundamentals of Magnetic Resonance

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 12	150 h	5 CP	2	each SuS	1 semester

	Teaching Methods	Hours per week	Contact time	Self-study
1	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h	105 h

2 Learning objectives

This course provides a theoretical introduction to nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) spectroscopy. It starts from a general classical description of the magnetic resonance phenomena with Bloch equations. It continues with the quantum description of the spin system, spin Hamiltonian, time-dependent Schroedinger equation, spin density operators, Liouville von Neumann equation, product operator formalism, calculation of the effects of different pulsed NMR and EPR sequences on the initial density operator.

3 Soft skills

Interactive presentation in front of an audience, identification and recording of principal lecture contents, unsolicited consultation of the relevant literature

4 Prerequisite(s)

Admission to the Master Course Program

5 Evaluation of the learning process

Active participation during lectures, exercises corrected by teaching assistants, hands-on lab experience during exercise hours.

6 Mode of examination

45 minutes end-of-term oral examination

7 Requirements for acquiring credit points

Passing the oral examination

8 Significance for overall grade

Weighted according to CPs

9 Module contents

- Classic description of the magnetization, Bloch equations in the lab and rotating frames.
- ON-OFF resonance pulses. NMR spectra, classical experiments.
- Steady state solution of Bloch equations. Continuous wave (CW) techniques. Scheme of a CW spectrometer.
- Chemical exchange: McConnell equations.
- Quantum description of the spin system. Density matrix formalism. Liouville von Neumann equation.
- Spin Hamiltonian. Zeeman term.
- Interaction frame representation.
- Hyperfine interaction.
- J coupling. Dipolar coupling.
- Product operator formalism. Application to some EPR/NMR sequences.

10 Person in charge / Lecturer(s)

Prof. Dr. Bordignon

Scientific Programming Methods for Chemists					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 13	150 h	5 CP	2	each SuS	1 semester

1	**Teaching Methods**	**Hours per week**	**Contact time**	**Self-study**
	a) Lectures b) Exercises	a) 2 h b) 1 h	45 h	105 h

2	**Learning objectives** Students will get a basic knowledge of numerical methods and algorithms for solving typical problems in natural sciences, the implementation of such algorithms in a computer language and how to judge the accuracy and reliability of numerical methods.
3	**Soft skills** identification and recording of principal lecture contents, presentation of results to an audience, writing, compiling and testing computer programs
4	**Prerequisite(s)** Admission to the Master Course Program
5	**Evaluation of the learning process** active participation during lectures, homework corrected by teaching assistant, presentation of solutions 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** The module is designed as a first course in applied mathematics and scientific computing. Therefore the course will cover a selection a numerical methods for typical problems in natural sciences as e.g.: Solution of systems of linear equations (LR decomposition, Cholesky decomposition, numerical errors of solutions, condition of a matrix, iterative methods) Interpolation: Lagrange interpolation, spline interpolation Numerical Integration: Newton-Cotes methods, composite schemes, errors of numerical integration schemes, Gauss formulas, multidimensional integration schemes Fast Fourier Transformation Finite element methods for Differential equations: basics of variation methods, Euler DE, nodal basis sets Systems of non-linear equations: Newton method, damped Newton method, convergence Ordinary differential equations: one-step and multi-step procedures, trapezoidal rule, Euler methods, stability

	Computation of eigenvalues and eigenvectors: power iteration, Rayleigh quotient iteration, inverse iteration, QR algorithm
10	**Person in charge / Lecturer(s)** Prof. Dr. C. Hättig C. Hättig, R. Schmid

International Course					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 14	420 h	14 CP	3	each WiS	6 weeks full-time or equivalent

1	**Teaching Methods**	**Hours per week**	**Contact time**	**Self-study**
	research oriented lab project in one of the international research groups	Compact course	typically 300 h	n/a

2	**Learning objectives** Students acquire advanced knowledge of the application of computational and/or experimental methods employed in state-of-the-art research in order to understand the properties of (bio)molecular systems. They learn to critically assess the scope and limitations of various approaches/approximations, to visualize and present results.
3	**Soft skills** international team-working and collaboration, graphical presentation of practical results, general knowledge of experimental and computational methods, acquaintance with alternative work flow organization
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 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.
10	**Person in charge / Supervisor(s)** Prof. Dr. Havenith-Newen Faculty of the partner universities of the international Master Molecular Sciences

Focal Point Practical

Code No.	Workload	Credit points	Available in semester	Frequency	Course duration
Module 15	450 h	15 CP	3	each WiS	6 weeks full-time or equivalent

	Teaching Methods	Hours per week	Contact time	Self-study
1	research oriented lab project in one of the research groups	Compact course	typically 250 h	n/a

2 Learning objectives

Students obtain advanced knowledge of how to apply computational and/or experimental methods employed in state-of-the-art research in order to understand the properties of (bio)molecular systems. They learn to critically assess the scope and limitations of various approaches/approximations, to visualize and present results.

3 Soft skills

team-working and collaboration while carrying out a project, graphical presentation of practical results, general knowledge of experimental and computational methods

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-grained force fields as well as QM/MM methods. Free energy simulations, incl. enthalpy/entropy decomposition. Enhanced sampling methods. Simulation of NMR relaxation. 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 Nürnberger 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).
10	**Person in charge / Supervisor(s)** Prof. Dr. Havenith-Newen Faculty of the international Master Molecular Sciences

Master Thesis					
Code No.	**Workload**	**Credit points**	**Available in semester**	**Frequency**	**Course duration**
Module 16	900 h	30 CP	4	each SuS	6 months full-time or equivalent

1	**Teaching Methods**	**Hours per week**	**Contact time**	**Self-study**
	active supervision: regular progress meetings, supervised presentation of project and results.	Compact course	typically 700 h	n/a

2	**Learning objectives** Students acquire the ability to plan, organize, develop, operate and present complex problems in Molecular Sciences and Simulation (MOS). The master thesis qualifies students to work independently in a MOS subject under the supervision of an advisor. The students' are able to deal with subject-specific problems and to present them in an appropriate and comprehensible manner and according to scientific standards. They have acquired the profound specialized knowledge, which is required to take the step from their studies to professional life.
3	**Soft skills** Interdisciplinary team-working and collaboration while carrying out project, graphical presentation of complex topics, detailed knowledge of experimental and computational methods.
4	**Prerequisite(s)** Proof of 14 credit points in to Module 11 (International Course) and of 15 credit points in Module 12 (Focal Point Practical)
5	**Evaluation of the learning process** Feedback on progress meeting reports, feedback during and on (computer) experiments.
6	**Mode of examination** Required is a written report (typically 50-100 pages) describing the project and its results in detail.
7	**Requirements for acquiring credit points** Passing of the master thesis (grade "adequate", 4,0 or better)
8	**Significance for overall grade** Weighted according to CPs
9	**Module contents** The master thesis can be theoretically and/or practically oriented. Its topic is determined by the respective supervisor.
10	**Person in charge / Supervisor(s)** Prof. Dr. Havenith-Newen Faculty of the international Master Molecular Sciences