Modulhandbuch für den Master-Studiengang Chemie

Studienplan für den Master-Studiengang Chemie

Der folgende Studienplan gilt in Verbindung mit der Prüfungsordnung des Master-Studiengangs der Fakultät für Chemie und Biochemie.

(1) Die Gliederung des Studienplans beruht auf dem Studienjahr mit Studienbeginn im Wintersemester.

(2) Es wird empfohlen, die Lehrveranstaltungen in der angegebenen Reihenfolge zu besuchen. Für einzelne Praktika ist die erfolgreiche Teilnahme an vorhergehenden Lehrveranstaltungen entsprechend Abs. 3 erforderlich.

(3) Die Zulassung zu den nachstehend genannten Lehrveranstaltungen ist abhängig von dem Vorliegen eines Leistungsnachweises für die im Ausbildungsgang vorhergehenden Lehrveranstaltungen (Vorleistungen) gemäß folgender Zusammenstellung:

Lehrveranstaltung	Vorleistung
Spezialisierungspraktikum	"Practical Science and Communication" und Vertiefungspraktika I - III
Master-Arbeit	Spezialisierungspraktikum

(4) Kennzeichnung der Lehrveranstaltungen

Com = Compulsory Module
Elec = Elective Module
CP = Credit Points für den jeweiligen Leistungsnachweis

(5) Die Vertiefungspraktika I bis III müssen jeweils aus unterschiedlichen Lehrveranstaltungen stammen.

(6) Wahlfreiheit. Wahlpflichtmodule und Vertiefungspraktika können frei aus dem gesamten Lehrangebot der Fakultät für Chemie und Biochemie für den Master-Studiengang gewählt werden. Die Wahl vergleichbarer Module aus anderen Fakultäten kann gegebenenfalls auf Antrag durch den Prüfungsausschuss genehmigt werden.

Sem.	Module	L	E/S	Pr	Type	CP
1. (WS)	Physical Chemistry V	2	1	-	Com	5
	Practical Science and Communication	-	2	6	Com	6
	Elective Lecture I	2	1	-	Elec	5
	Elective Lecture II	2	1	-	Elec	5
	In-Depth Practical I	-	-	9	Elec	8
26 HpW	Total: 1st Semester	6	5	15		29
2.(SS)	Elective Lecture III	2	1	-	Elec	5
	Organic Chemistry IV	2	1	-	Com	5
	Inorganic Chemistry IV	2	1	-	Com	5
	In-Depth Practical II	-	-	9	Elec	8
	In-Depth Practical III	-	-	9	Elec	8
30 HpW	Total: 2nd Semester	8	4	18		31
3.(WS)	Elective Lecture IV	2	1	-	Elec	5
	Elective Lecture V	2	1	-	Elec	5
	Elective Lecture VI	2	1	-	Elec	5
	Focal Point Practical	-	-	15	Com	15
21 HpW	Total: 3rd Semester	6	3	15		30
4. (SS)	Master Thesis				Com	30
77 HpW	**Total: 1. – 4. Sem.**	**18**	**11**	**48**		**120**

Modulliste Masterstudiengang Chemie

Pflichtveranstaltungen

Inorganic Chemistry IV

Module	Credits	Workload	Term	Frequency	Duration
1.1	5 CP	150 h	2. Sem.	Each SuS	1 Semester

Courses	Contact hours	Self-Study	Group size
Inorganic Chemistry IV a) Lecture b) Exercise	a) 2SWS/30 h b) 1 SWS/15 h	105 h	All students of the respective semester, ca. 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 focusses on the 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

Teaching methods
Lecture with exercises und accompanying e-learning moduls

Mode of assessment
end-of-term written exam

Requirement for the award of credit points
Passing the written examination

Module applicability
Chemistry (Master), IMOS

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

Organic Chemistry IV					
Module 1.2	**Credits** 5 CP	**Workload** 150 h	**Term** 2. Sem.	**Frequency** nur SS	**Duration** 1 Semester
Courses a) lecture b) exercise			**Contact hours** 3+1 SWS	**Self-Study** 100 h	**Group size** 60 Studierende
Prerequisites -General knowledge of thermodynamics, statistical mechanics, and quantum mechanics.					
Learning outcomes • students aquire knowledge on the theory of advanced topics and concepts of organic chemistry such as pericyclic reactions, heterocycles and supramolecular chemistry. In addition links are drawn to theoretical, physical and spectroscopical aspects of these concepts.					
Content • The concept of aromaticity; pericyclic reactions: Molecular orbitals and theoretical background, electrocyclic reactions, sitmatropic reactions, cycloadditions, cheletropic reactions. • heterocycles: nomenclature, saturated heterocycles, aromatic heterocycles, natural heterocycles and their role in biochemistry, synthesis of heterocycles • fundamentals of supramolecular chemistry and molecular recognition • organocatalysis • natural compounds: sugars and carbohydrates					
Teaching methods *a) lecture b) exercise*					
Mode of assessment Written exam (120 min) at the end of the module					
Requirement for the award of credit points *Passing the written exam*					
Module applicability *M. Sc. Chemistry*					
Weight of the mark for the final score					
Module coordinator and lecturer(s) Prof. Dr. Lukas Gooßen, Prof. Dr. Stefan Huber, Dr. Wolf Matthias Pankau, Dr. Dirk Grote					
Further information					

Physical Chemistry V: Molecular Reaction Dynamics

Module	Credits	Workload	Term	Frequency	Duration
1.3	5 CP	120 h	1. or 3. . Sem.	nur WS	1 Semester
Courses a) lecture b) exercise			**Contact hours** 3 SWS	**Self-Study** 75 h	**Group size** 20 Studierende

Prerequisites
-

Learning outcomes
- Students acquire a broad overview over experimental techniques and theoretical approaches aiming at the determination and prediction of reaction rate coefficients in the gas phase and in solution.

Content
- Reaction rate coefficients of uni- and bimolecular reactions in the gas phase and in solution; Pressure dependence: Collisions, Lindemann-Hinshelwood mechanism, Master equation approach; Temperature dependence: Arrhenius equation, Transition State Theory; Energy dependence: RRK and RRKM theories, other Transition State Theory derivatives; Viscosity dependence: Kramers theory; Time- and frequency-domain spectroscopic experiments: molecular beam methods; femtosecond pump-probe laser spectroscopy.

Teaching methods
Lecture, exercise

Mode of assessment
Written exam (120 min) at the end of the module

Requirement for the award of credit points
Passing the written exam

Module applicability
M. Sc. Chemistry

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

Module coordinator and lecturer(s)
lecturers Physical Chemistry

Further information
The lectures are recorded to video and audio, and posted on the electronic Blackboard with password protection as an e-learning module. The screencasts can also be used for inverted classroom sessions.

Practical Science and Communication					
Module 1.4	**Credits** 6 CP	**Workload** 180 h	**Term** 1. Sem.	**Frequency** WiSe	**Duration** 2 Semester
Course offered as *Data Literacy and Scientific Communication (DLSC)*			**Contact hours** 1 SWS	**Self-Study** 120 h	**Group size** 60 students

Prerequisites
General knowledge in chemistry

Learning outcomes
The students gain skills in common scientific presentation formats using their own research results from Bachelor theses and in-depth practicals

Content
Data Literacy. In an eLearning environment (Moodle course), the students learn about scientific journals, the publishing process (editorial office, peer-reviews), practical aspects of using scientific databases such as Scifinder for data research.
Short communications. Students write two short communications (2 pages) on their own work, which is peer-reviewed by other students of the course and subsequently revised. After the first round of reviews, a seminar on common mistakes during reviewing stages further teaches good reviewing practices.
Oral presentations. Using own research results as topics, each student gives a 15 minutes oral presentation which is reviewed by means of an evaluation sheet that the audience fills out. Thereby, the students get feedback on their presentation style.
Poster presentations. In a poster symposium, all students present posters on the research done during their in-depth practicals, thus generating a first feeling for poster sessions.

Teaching methods
a) *Seminars* b) *Peer-review assisted writing*

Mode of assessment
Peer-review by students of the course

Requirement for the award of credit points
Passing abstract and short communications reviewing phases, active participation

Module applicability
M.Sc. Chemistry

Weight of the mark for the final score
--

Module coordinator and lecturer(s)
C. Merten, R. Schmid, K. Merz

Further information

Master Wahlvorlesungen

Analytical Chemistry

Advanced Electrochemistry: From Fundamentals to Applications I					
Module 2.1	**Credits** 5 CP	**Workload** 150 h	**Term** 1.,3. Sem.	**Frequency** WS	**Duration** 1 Semester
Courses a) Elective Course b) Elective Lecture I-VI			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 108 h	**Group size** 30 Students
Prerequisites Knowledge of basic electrochemistry					
Learning outcomes The students should gain an advanced understanding of theory and practice of modern electrochemical techniques, applications, and possible combinations with other methods like e.g. spectroscopic methods.					
Content General Principles in Electrochemistry (Electrochemical Thermodynamics; Mass Transport in Solution (Fundamentals) ; The Electrochemical Double Layer) Kinetics of Electrochemical Reactions (Activation Energies and Their Consequences for Electrochemistry, Tafel analysis; CV Shapes as Means to Identify Reaction Mechanisms; The Marcus Theory in Electrochemistry and Beyond) Electrocatalysis (Mass Transport and its Effect on Voltammetry; Fundamentals of Rotating Disc Electrodes and Rotating Ring Disc electrodes; Electrocatalysis: Fundamentals and Wording) Electrochemical Impedance Spectroscopy (Introduction to Electrochemical Impedance Spectroscopy; Revision on Impedance Characteristics of Electrical Circuits; Equivalent Circuit Models in Electrochemistry and Data Acquisition)					
Teaching methods a)Lecture; b) Exercise					
Mode of assessment 30 - 45 min end-of-term oral exam					
Requirement for the award of credit points Passing the oral exam					
Module applicability Master of Science Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) K. Tschulik, C. J. Bondue, H. Amin, J. Linnemann					
Further information					

Advanced Electrochemistry: From Fundamentals to Applications II					
Module 2.2	**Credits** 5 CP	**Workload** 150 h	**Term** 2. Sem.	**Frequency** SoSe	**Duration** 1 Semester
Courses a) Elective Course b) Elective Lecture I-VI			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 108 h	**Group size** 30 Students

Prerequisites
Knowledge of basic electrochemistry; attending Advanced Electrochemistry I beforehand is recommended

Learning outcomes
The students should gain an advanced understanding of theory and practice of modern electroanalytical techniques, applications, and possible combinations with other methods like e.g. spectroscopic methods.

Content
Local and Nanoscale Electrochemistry (Mass transport at microelectrodes; Mass transport at heterogeneous and nanoparticle modified electrodes; Electrochemical scanning probe techniques)
Electrochemical Adsorption Processes (Adsorption Isotherms and competitive adsorption; Exploiting electrochemical adsorption to determine surface areas, underpotential deposition; Mechanisms of hydrogen evolution, Langmuir-Hinshelwood and Eley-Ridal mechanism)
Electrocatalysis II (Factors controlling electrocatalysis; Molecular electrocatalsis)
Advanced Electrochemical Impedance Spectroscopy (Electrochemical impedance characteristics for different modes of mass transport; Electrochemical impedance characteristics for adsorption processes and porous electrodes)

Teaching methods
Lecture and Seminar

Mode of assessment
30 - 45 min end-of-term oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Master of Science Chemistry

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

Module coordinator and lecturer(s)
K. Tschulik, C. J. Bondue, H. Amin, J. Linnemann

Further information

<table>
<tr><td colspan="6">Research practical in the focal point programme</td></tr>
<tr><td>Module
2.3</td><td>Credits
15 CP</td><td>Workload
450 h</td><td>Term
3. Sem.</td><td>Frequency
Every semester</td><td>Duration
1 Semester</td></tr>
<tr><td colspan="3">Courses
Practical lab course (15 hours per week) within research projects.</td><td>Contact hours
15 h per week</td><td>Self-Study
240 h</td><td>Group size
1</td></tr>
<tr><td colspan="6">Prerequisites
Knowledge of analytical and/or electrochemical methods</td></tr>
<tr><td colspan="6">Learning outcomes
The students should gain an advanced theoretical and practical understanding of surface analytical techniques, electrochemical methodology including micro- and nanoelectrochemistry, and electrocatalysis for energy conversion embedded within actual research projects in the research groups of the chairs of analytical chemistry. They gain insight into modern research methods and topics in the actual research projects. The students should develop skills to self-reliantly plan, set up, work up and analyze experiments.</td></tr>
<tr><td colspan="6">Contents:
• Surface functionalization and characterization of biointerfaces
• Bioelectrochemistry with applications in biosensors and biofuel cells
• Electrocatalysis for energy conversion in fuel cells and electrolyzers
• High-throughput electrochemical materials screening
• Synthesis and characterization of electrocatalysts for energy conversion reactions
• Microelectrochemistry and single-entity electrochemistry
• Battery research
• Electrodeposition, magneto-electrochemistry,
• Scanning electrochemical microscopy; scanning electrochemical cell microscopy</td></tr>
<tr><td colspan="6">Teaching methods
Practical lab course</td></tr>
<tr><td colspan="6">Mode of assessment
Lab report</td></tr>
<tr><td colspan="6">Requirement for the award of credit points
All experiments are completed successfully and available in the electronic lab book. The results are summarized in a written report.</td></tr>
<tr><td colspan="6">Module applicability
Master of Science Chemistry</td></tr>
<tr><td colspan="6">Weight of the mark for the final score
Weighted according to CPs</td></tr>
<tr><td colspan="6">Module coordinator and lecturer(s)
Research group leaders of the chair of analytical chemistry</td></tr>
<tr><td colspan="6">Further information</td></tr>
</table>

In-depth Practical "Biointerfaces"					
Module 2.4	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses Lab course with a) 30 hours per week for 5 to 6 weeks lab work b) 2 weeks for writing of the report and preparation of the oral presentation			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size** Individuals or small teams (<5 students)
Prerequisites Fundamental knowledge about spectroscopy					
Learning outcomes The in-depth course is a practical introduction to the preparation and characterization of (bio-) functional interfaces. Functional coatings will be prepared by self-assembly, grafting and surface initiated synthesis. A training in different optical, infrared and imaging techniques is provided. Besides surface characterization, specific and nonspecific adsorption as well as biological attachment experiments are part of the training.					
Content Self assembly, chemical grafting, surface initiated polymerization reactions, spectral ellipsometry, contact angle goniometry, ATR-FTIR, SPR, Fluorescence microscopy, microfluidics.					
Teaching methods Lab course and Seminar					
Mode of assessment Lab report and oral presentation					
Requirement for the award of credit points The course is successfully completed with the approved written report and oral presentation (20 min)					
Module applicability Master of Science Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) A. Rosenhahn					
Further information					

In-depth Practical "Advanced Electrochemistry – From Fundamental to Applications"

Module	Credits	Workload	Term	Frequency	Duration
2.5	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester
Courses lab course a) Elective Course b) Elective Lecture I-VI			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size** 1 Student

Prerequisites
Knowledge of basic electrochemistry

Learning outcomes
The students will gain a high-level understanding and practical expertise in advanced methods in electrochemistry. This includes electrode preparation, modification and characterization, performing of electrochemical measurements, data analysis and interpretation of data. Students will learn to plan, perform and interpret experiments as a means to solve analytical and physical-chemistry problems.

Content
Individual research projects are offered, covering one or more topics.
Topics: Activity testing of electrocatalysts and single entities; Surface characterization; Electrosynthesis for the sustainable production of value-added chemical and renewable fuels; Electrodeposition of metals, alloys and conducting polymers; Magnetic field enhanced electrochemistry; Electrochemical energy conversion and storage: batteries, superconductors, redox-flow batteries; Development of electrochemical sensors.
In these projects one or more of the following techniques will be employed:
Standard Techniques of Electrochemistry: potential step experiments, impedance spectroscopy, voltammetry at catalyst-modified electrodes including rotating (ring) disk electrode (R(R)DE) measurements; Single particle electrochemistry, Electrochemical quartz crystal microbalance measurements.
Electrochemistry Combined with Advanced Analysis Techniques: Electrochemistry coupled to Raman, IR, Hyperspectral imaging dark field microscopy; Electrochemical atomic force microscopy; Differential electrochemical mass spectrometry (DEMS); Scanning electrochemical techniques
Numerical Simulations: Besides these experimental courses, theory practicals are offered on numerical simulation of mass transport in electrochemical systems

Teaching methods
lab course a) 30 hours per week for 5-6 weeks b) 2-3 weeks for writing and preparation of the oral presentation

Mode of assessment
Lab report and oral presentation

Requirement for the award of credit points
All experiments are completed successfully and written up in a lab report, oral presentation (15 minutes)

Module applicability
Master of Science Chemistry

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

Module coordinator and lecturer(s)
K. Tschulik, J. Linnemann, C. Bondue

Further information

In-depth Practical "Scanning Electrochemical Microscopy and Microelectrochemistry"					
Module 2.6	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses Elective Course Elective Lecture I-VI			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size**
Prerequisites Basics in electrochemistry					
Learning outcomes The students should gain an advanced theroretical and practical understanding on the preparation and application of ultra-microelectrodes and electrolyte-filled capillaries and their positioning in scanning electrochemical microscopes (SECM), scanning electrochemical cell microscopes (SECCM). And scanning droplet cells (SDC). This contains knowledge of the control software, different operation modi of the SECM, SDC and SECCM. The students should learn to plan, perform and interpret SECM, SECCM and SDC experiments to solve analytical problems.					
Content Microelectrodes, preparation of micro- and nanoelectrodes (Pt, carbon fibers), SECM, SECCM, SDC, operation modi, control software, application of SECM, SDC and SECCM.					
Teaching methods Lab course with a) 30 hours per week for 5 to 6 weeks lab work b) 2 weeks for writing of the report and preparation of the oral presentation					
Mode of assessment Lab report and oral presentation					
Requirement for the award of credit points Passing the oral exam All experiments are completed successfully and available in the electronic lab book. The results are summarized in a written report. Oral presentation (20 min)					
Module applicability Master of Science Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) K. Tschulik; W. Schuhmann					
Further information					

In-depth Practical "Sensors and Bioanalytics"					
Module 2.7	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses Elective Course Elective Lecture I-VI			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size** 1

Prerequisites
Basics in electrochemistry

Learning outcomes
The students should gain an advanced theoretical and practical understanding of the preparation and application of biosensors. This contains the synthesis and use of redox polymers in amperometric biosensors, as well as the immobilisation of enzymes on electrode surfaces. The students should learn to plan, perform and interpret measurements for the solution of analytical problems by means of amperometric biosensors.

Content
Amperometric biosensors, electron transfer between redox enzymes and electrodes, redox mediators, redox polymers, electrodeposition paints, immobilization of enzymes in polymer layers and on self-assembled monolayers, chronoamperometry, flow injection analytics, sequential injection analytics

Teaching methods
Lab course with
a) 30 hours per week for 5 to 6 weeks lab work
b) 2 weeks for writing of the report and preparation of the oral presentation

Mode of assessment
Lab report and oral presentation

Requirement for the award of credit points
All experiments are completed successfully and available in the electronic lab book. The results are summarized in a written report. Oral presentation (20 min)

Module applicability
Master of Science Chemistry

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

Module coordinator and lecturer(s)
W. Schuhmann

Further information

In-depth Practical "Nanomaterials – Synthesis, Characterization and Application"					
Module 2.8	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses Elective Course Elective Lecture I-VI			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size** 1 Student
Prerequisites Knowledge of basic electrochemistry					
Learning outcomes Students will gain an advanced practical experience and understanding of the synthesis and characterization of functional nanoparticles and nanostructured materials. Methods in nanoparticle synthesis, modification of nanomaterials and surface-immobilization will be complemented with different physical and chemical characterization methods of nanomaterials. Applications will range from electrocatalysis and electrosynthesis to sensing of molecules, nanoparticles and micro-organisms in real-world sample.					
Content (1) Wet-chemical nanoparticle synthesis of: core/shell nanoparticles, alloys, nanowires, and nanocubes; (2) surface immobilization of nanoparticles including electrodeposition of nanowires; (3) Nanoparticle modification by: ligand exchange, underpotential deposition and electrochemical dealloying; (4) Single nanoparticle electrochemistry; (5) Combined electrochemical and microscopy analysis of nanoparticles includingidentical location electron microscopy and atomic force microscopy. (6) electrocatalytic activity testing also in the context of electrosynthesis. (6) Nanoparticle corrosion and aggregation studies, (7) Spectroscopic nanomaterial characterization to deterimine size- and shape-depend reactivity in(electro)catalysis					
Teaching methods lab course a) 30 hours per week for 5-6 weeks b) 2-3 weeks for writing and preparation of the oral presentation					
Mode of assessment Lab report and oral presentation					
Requirement for the award of credit points All experiments are completed successfully and written up in a lab report, oral presentation (15 min)					
Module applicability Master of Science Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) K. Tschulik, W. Schuhmann					
Further information					

In-depth Practical "Electrocatalysis and Energy Conversion"					
Module 2.9	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses Elective Course Elective Lecture I-VI			**Contact hours** a) 30 h	**Self-Study** b) 60 h	**Group size** 1
Prerequisites Basics in electrochemistry					
Learning outcomes The students should gain an advanced theoretical and practical understanding of the characterization and optimization of materials for energy conversion and electrocatalysis. This contains knowledge of the preparation procedures as well as of the practical performance of electrochemical measurements. The students should learn to plan, perform and interpret electrochemical experiments including cyclic voltammetry, impedance spectroscopy, rotating disc and rotating ring-disk measurements, operation of model electrolyzers etc.					
Content Electrocatalysis: optimization of the activity of electrocatalysts; catalyst ink preparation, gas diffusion electrodes fabrication, electrocatalyst synthesis and characterization					
Teaching methods Lab course with a) 30 hours per week for 5 to 6 weeks lab work b) 2 weeks for writing of the report and preparation of the oral presentation					
Mode of assessment Lab report and oral presentation					
Requirement for the award of credit points All experiments are completed successfully and available in the electronic lab book. The results are summarized in a written report. Oral presentation (20 min)					
Module applicability Master of Science Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) K. Tschulik; W. Schuhmann					
Further information					

Inorganic Chemistry

Bioinorganic Chemistry I					
Module 3.1	**Credits** 5 CP	**Workload** 150 h	**Term** 1^{st} or 3^{rd} Sem.	**Frequency** Only WS	**Duration** 1 Semester
Courses a) Bioinorganic Chemistry I (Lecture and Seminar)			**Contact hours** 3 SWS	**Self-Study** 105 h	**Group size**
Prerequisites Basic Understanding of general chemistry, coordination chemistry and biochemistry					
Learning outcomes After successful completion of this module, the students have - A basic understanding of the role of metals in a biological environment - Knowledge about the structure, function and properties of metalloenzymes The students are able to - Identify, solve, and discuss problems related to the role of metal centers in biomolecules - Find, read, and critically comment on pertinent literature in the field of Bioinorganic Chemistry					
Content The lecture covers classical bioinorganic chemistry topics, including but not restricted to the following: Occurrence of metal ions and compounds in the environment, metal ion uptake and homeostasis, metals as active sites in metalloenzymes, spectroscopic characterization of metal centers in biomolecules, reaction mechanisms of metalloenzymes, model compounds for metalloenzymes, activation and metabolism of small molecules by metal centers and metalloenzymes (e.g. H_2, O_2, N_2, CH_4, etc.).					
Teaching methods Lecture and Seminar with student contributions (e.g. presentation, video, written contribution such as project draft or grant application)					
Mode of assessment Written exam and grading of student contributions					
Requirement for the award of credit points Active participation in student contribution, successful completion of written exam					
Module applicability Master Chemistry, Master Biochemistry, Master Biology					
Weight of the mark for the final score Weighted according to CP					
Module coordinator and lecturer(s) Nils Metzler-Nolte, Ulf-Peter Apfel and Members of Inorganic Chemistry I					
Further information					

Crystal Engineering – Chemistry beyond the molecule

Module	Credits	Workload	Term	Frequency	Duration
3.2	5 CP	150 h	2. Sem.	Each SuS	1 Semester

Courses	Contact hours	Self-Study	Group size
c) Lecture d) Exercise	c) 2SWS/30 h d) 1 SWS/15 h	 105 h	Students of the respective semester, ca. 25

Prerequisites
After successful completion of the module, students have a basic knowledge of the aggregation behavior of small organic molecules in crystal structures.

Learning outcomes
After the successful completion of the module
- Students will have advanced knowledge of supramolecular synthons, intermolecular interactions, and the design of crystal structures with small organic molecules
- Students will be able to specifically design polymorphic forms as well as multi-component crystals based on crystal structure predictions.

Content
- Aggregation phenomena of organic molecules in solid state (crystal packing)
- Crystal Design Strategies with organic molecules
- Strong and weak intermolecular Interactions (focusing most of lectures series)
- Supramolecular Synthons
- Crystal Structure prediction (CSP)
- Polymorphism
- Multi-component crystals
- Applications
- Special crystallization techniques

Teaching methods
Lecture with exercises

Mode of assessment
end-of-term written exam and talks on selected topics

Requirement for the award of credit points
Passing the written examination and talks on selected topics

Module applicability
Chemistry (Master), IMOS

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

Module coordinator and lecturer(s)
Dr. Klaus Merz

Further information

Medicinal Inorganic Chemistry					
Module 3.3	**Credits** 5 CP	**Workload** 150 h	**Term** 2^{nd} or 4^{th} Sem.	**Frequency** Only SoS	**Duration** 1 Semester
Courses b) Medicinal Inorganic Chemistry (Lecture and Seminar)			**Contact hours** 3 SWS	**Self-Study** 105 h	**Group size**
Prerequisites Basic Understanding of general chemistry, coordination chemistry and biochemistry					
Learning outcomes After successful completion of this module, the students have - An advanced understanding of the role of metal ions in health and disease - Knowledge about the most important metallodrugs and their mode of action The students are able to - Identify, solve, and discuss problems related to the role of metal compounds in health and disease - Find, read, and critically comment on pertinent literature in the field of Medicinal Inorganic Chemistry					
Content The lecture covers medicinal inorganic chemistry topics, including but not restricted to the following: Concepts of drug discovery and development; Health and diseases in metal ion homeostasis; Toxicity of metals and metal compounds; Synthesis, properties and mode of action of metallodrugs (e.g. metal complexes as anti-cancer drugs, as anti-infectives, in neurodegenerative diseases, etc.).					
Teaching methods Lecture and Seminar with student contributions (e.g. presentation, video, written contribution such as project draft or grant application)					
Mode of assessment Written exam and grading of student contributions					
Requirement for the award of credit points Active participation in student contribution, successful completion of written exam					
Module applicability Master Chemistry, Master Biochemistry, Master Biology					
Weight of the mark for the final score Weighted according to CP					
Module coordinator and lecturer(s) Nils Metzler-Nolte and Members of Inorganic Chemistry I					
Further information					

Main Group Chemistry: From Curiosities to Catalysis					
Module 3.4	**Credits** 5 CP	**Workload** 150 h	**Term** 1st or 3rd Sem.	**Frequency** Only WS	**Duration** 1 Semester
Courses Main Group Chemistry: From Curiosities to Catalysis (Lecture and Seminar)			**Contact hours** 3 SWS	**Self-Study** 105 h	**Group size**

Prerequisites
Basic Understanding of general chemistry, organometallic chemistry and catalysis.

Learning outcomes
After successful completion of this module, the students have a basic understanding

- of the reactivity of organometallic compounds of the s- and p-block elements
- of structure reactivity relationships and applications in the activation of small molecules (H_2, N_2, CO, CO_2) and strong bonds as well as in homogeneous catalysis.

The students are able to

- Identify, solve, and discuss problems related to the bonding situation, properties and reactivity of s- and p-block element compounds
- Find, read, and critically comment on pertinent literature in the field of main group chemistry

Content
The lecture covers recent developments in molecular main group chemistry with focus on the stabilization of reactive species with unusual bonding situations and applications in catalysis.
The following topics may be covered:

- Synthesis, properties and reactivities of low-valent p-block element compounds and compounds including formal element multiple bonds.
- Synthesis, properties and reactivities of s-block metal organyls and hydrides
- Activation of strong bonds and small molecules with main group compounds, including different concepts such as Frustrated Lewis pairs and cooperative effects as well different mechanisms (e.g. oxidative addition, metathesis)
- Applications in homogeneous catalysis

The lecture will particularly focus on underlying concepts (Structure-activity relationships, acidity and basicity, trends in the periodic table etc.) and molecular design strategies.

Teaching methods
Lecture and seminar with student contributions (e.g. presentation, video, computational studies, written contribution such as project draft or grant application)

Mode of assessment
Written exam and grading of student contributions

Requirement for the award of credit points
Active participation in student contribution, successful completion of written exam

Module applicability
Master Chemistry

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

Module coordinator and lecturer(s)
Viktoria Däschlein-Gessner and Members of Inorganic Chemistry II

Further information

Green and Sustainable Chemistry					
Module 3.5	**Credits** 5 CP	**Workload** 150 h	**Term** 1st or 3rd Sem.	**Frequency** Only WS	**Duration** 1 Semester
Courses Green and Sustainable Chemistry (Lecture)			**Contact hours** 2 SWS	**Self-Study** 105 h	**Group size**

Prerequisites
Basic Understanding of general chemistry

Learning outcomes
After successful completion of this module, the students have

- A basic understanding of the principles of green and sustainable chemistry
- Concepts for mechanochemistry as well as technical electrochemistry
- Implementation of new technologies in an industrial context

The students are able to

- Identify, solve, and discuss problems related to sustainable processes
- Find, read, and critically comment on pertinent literature in the field of green and sustainable chemistry

Content
The lecture covers chemistry topics, including but not restricted to the following: The 12 principles of green chemistry, the development and necessity to create green and sustainable processes, the utilization of solvent reduced or free chemical processes, the electrification of chemical processes (including Power-to-X processes, batteries/redox-flow batteries, fuel cells etc.).

Teaching methods
Lecture

Mode of assessment
Written or oral exam

Requirement for the award of credit points
Successful completion of written exam

Module applicability
Master Chemistry, Master Biochemistry, Master Biology, Master Engineering

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

Module coordinator and lecturer(s)
Lars Borchardt, Ulf-Peter Apfel

Further information

In-depth practical: Green and Sustainable Chemistry					
Module 3.6	**Credits** 8 CP	**Workload** 240 h	**Term** 1^{st} to 3^{rd} Sem.	**Frequency** WS and SoS	**Duration** 6 Weeks
Courses Green and Sustainable Chemistry (Lab practical)			**Contact hours** 160 h	**Self-Study** 80 h	**Group size** Individual

Prerequisites
Basic Understanding of general chemistry, inorganic chemistry and analytical methods

Learning outcomes
After successful completion of this practical, the students have
- Hands-on experience in performing selected analytical methods frequently used and running the respective instruments
- A practical understanding of parameters defining green and sustainable processes

The students are able to
- Apply suitable methods to solve problems or answer questions in the field
- Analyse and professionally report / document analytical data
- Correlate the principles of green chemistry to individual problem sets and from experimental data, and critically comment on those

Content
In this lab practical, the students will identify and then perform suitable experiments to answer research questions related to a scientific project under the supervision of their mentor. Typically, the lab practical will involve first the synthesis of a new or known compound or material or reaction implementing the principles of green chemistry, and then comprise running the necessary experiments. The research topic will be in the scientific (PhD or postdoc) project of the supervisor, including but not limited to areas such as mechanochemistry, catalysis and electrochemistry.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a scientific publication

Requirement for the award of credit points
Active participation in lab work, successful completion of written report

Module applicability
Master Chemistry, Master Biochemistry, Master Physics, Master Engineering

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

Module coordinator and lecturer(s)
All professors and Independent Group Leaders in Inorganic Chemistry

Further information

In-depth Practical: Computational Chemistry in Inorganic Chemistry					
Module 3.7	**Credits** 8 CP	**Workload** 240 h	**Term** 1st to 3rd Sem.	**Frequency** WS and SoS	**Duration** 6 Weeks
Courses Computational Chemistry (Lab/office practical)			**Contact hours** 160 h	**Self-Study** 80 h	**Group size** Individual

Prerequisites
Basic Knowledge of Theoretical Methods and computer skills

Learning outcomes
After successful completion of this practical, the students have
- Hands-on experience in performing the current state-of-the-art computational methods used to theoretically model molecular and/or solid systems.
- A basic practical understanding of computational chemistry and the application of computational methods and programs

The students are able to
- apply state-of-the-art computational methods used to theoretically model molecular and/or solid systems.
- analyse, interpret and document computational results to answer a given research question.
- search the literature, related to the given research question, and relate their research results to the state-of-the-art.

Content
In this practical, the students will perform theoretical calculations to deduce structure-activity relationships and understand chemical properties and reactivities. They will learn how to use a UNIX type environment, edit input files and visualize chemical systems. Furthermore, they will be trained in applying different computational methods. Topics my include for example the use of
- density functional theory approaches to elucidate reaction profiles and bonding situations
- force field calculations of inorganic systems including structural optimizations and molecular dynamics, first principles calculations with DFT or wave function based methods for molecular systems and extended solids (structural analysis and/or spectroscopic properties like normal modes).
- Machine learning methods to quantitatively describe structure activity relationships

These computational methods are applied within a scientific context, connected to the current research projects of the supervisor, including but not limited to materials chemistry, organometallic and main group chemistry as well as catalysis.

Teaching methods
Computational practical

Mode of assessment
Written report, typically in the form of a scientific publication

Requirement for the award of credit points
Active participation in computational work, successful completion of written report

Module applicability
Master Chemistry

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

Module coordinator and lecturer(s)
Prof. Dr. Rochus Schmid, Prof. Dr. Viktoria Däschlein-Gessner

Further information

In-depth practical: Analytical Methods in Inorganic Chemistry					
Module 3.8	**Credits** 8 CP	**Workload** 225 h	**Term** 1st to 3rd Sem.	**Frequency** WS and SoS	**Duration** 6 Weeks
Courses Analytical Methods in Inorganic Chemistry (Lab practical)			**Contact hours** 160 h	**Self-Study** 80 h	**Group size** Individual
Prerequisites Basic Understanding of general chemistry, inorganic chemistry and analytical methods					
Learning outcomes After successful completion of this practical, the students have - Hands-on experience in performing selected analytical methods frequently used in inorganic chemistry, and running the respective instruments - A practical understanding of analytical methods in inorganic chemistry The students are able to - Apply suitable analytical methods to solve problems or answer questions in inorganic chemistry - Analyse and professionally report / document analytical data - Deduce structure and properties from analytical data, and critically comment on those					
Content In this lab practical, the students will identify and then perform suitable analytical experiments to answer research questions related to a scientific project under the supervision of their mentor. Typically, the lab practical will involve first the synthesis of a new or known compound or material or reaction, and then comprise running the necessary analytical experiments on advanced spectrometers or other equipment. The research topic will be in the scientific (PhD or postdoc) project of the supervisor, including but not limited to areas such as main group chemistry, organometallic or coordination chemistry, catalysis, or materials, green and medicinal inorganic chemistry.					
Teaching methods Lab practical					
Mode of assessment Written report, typically in the form of a scientific publication					
Requirement for the award of credit points Active participation in lab work, successful completion of written report					
Module applicability Master Chemistry, Master Biochemistry					
Weight of the mark for the final score Weighted according to CP					
Module coordinator and lecturer(s) All professors and Independent Group Leaders in Inorganic Chemistry					
Further information					

In-depth Practical: Bioinorganic Chemistry					
Module 3.9	**Credits** 8 CP	**Workload** 225 h	**Term** 1st to 3rd Sem.	**Frequency** WS and SoS	**Duration** 6 Weeks
Courses Bioinorganic Chemistry (Lab practical)			**Contact hours** 160 h	**Self-Study** 80 h	**Group size** Individual

Prerequisites
Basic Understanding of general chemistry, inorganic chemistry and biochemistry

Learning outcomes
After successful completion of this practical, the students have
- Hands-on experience in performing chemical synthesis and analytical methods typically used in bioinorganic or medicinal inorganic chemistry
- A basic practical understanding of bioinorganic chemistry

The students are able to
- Synthesize compounds of bioinorganic interest and analyze their properties (including biological), or otherwise study a biological system of interest to bioinorganic chemistry
- Analyse and document analytical data to deduce the answers to a given research question in bioinorganic chemistry
- Search the literature related to the given research question, and critically comment on the results

Content
In this lab practical, the students will perform chemical synthesis, analytical measurements, or otherwise lab experiments (e.g. including cell biology or microbiology work) as part of an ongoing research project in the broad area of bioinorganic chemistry. Data will be analyzed to deduce structure-activity relationship, and compared to published scholarly information. The research topic will be in the scientific (PhD or postdoc) project of the supervisor, including but not limited to areas such as organometallic or coordination chemistry, catalysis, enzyme or medicinal inorganic chemistry.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a scientific publication

Requirement for the award of credit points
Active participation in lab work, successful completion of written report

Module applicability
Master Chemistry, Master Biochemistry

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

Module coordinator and lecturer(s)
All professors and Independent Group Leaders in Inorganic Chemistry

Further information

In-depth Practical: Bioinorganic Chemistry					
Module 3.10	**Credits** 8 CP	**Workload** 225 h	**Term** 1st to 3rd Sem.	**Frequency** WS and SoS	**Duration** 6 Weeks
Courses Molecular Chemistry and Synthesis (Lab practical)			**Contact hours** 160 h	**Self-Study** 80 h	**Group size** Individual

Prerequisites
Basic Understanding of general chemistry, inorganic chemistry and synthesis methods

Learning outcomes
After successful completion of this practical, the students have
- Hands-on experience in performing chemical synthesis by methods frequently used in inorganic chemistry, and suitable methods of characterization of the new compound or material
- A practical understanding of synthesis methods in inorganic chemistry

The students are able to
- Synthesize new inorganic chemistry
- Analyse and document analytical data to establish identity and purity of inorganic compounds and materials
- Search the chemical literature for suitable synthesis methods, and critically comment on those

Content
In this lab practical, the students will perform chemical synthesis of known or new compounds or materials as part of an ongoing research project. Identity and purity of the product will be established by suitable methods, and the properties of the new compound / material will be analyzed. The research topic will be in the scientific (PhD or postdoc) project of the supervisor, including but not limited to areas such as main group chemistry, organometallic or coordination chemistry, catalysis, or materials, green and medicinal inorganic chemistry.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a scientific publication

Requirement for the award of credit points
Active participation in lab work, successful completion of written report

Module applicability
Master Chemistry, Master Biochemistry

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

Module coordinator and lecturer(s)
All professors and Independent Group Leaders in Inorganic Chemistry

Further information

Research Practical: Inorganic Chemistry					
Module 3.11	**Credits** 15 CP	**Workload** 450 h	**Term** 3rd Sem.	**Frequency** WS and SoS	**Duration** 3 Months
Courses Inorganic Chemistry (Lab practical)			**Contact hours** 320 h	**Self-Study** 130 h	**Group size** Individual

Prerequisites
Advanced Understanding of Inorganic Chemistry, including synthesis and analytical methods

Learning outcomes
After successful completion of this practical, the students have
- Advanced expertise in inorganic chemistry, including synthesis, analytical or computational methods as applicable to the project
- A good practical understanding of inorganic chemistry

The students are able to
- Search the chemical literature for suitable methods to address a given problem
- Select suitable methods and plan their research to solve the given problem
- Execute their research independently, but under supervision of a mentor
- Professionally analyse and document their data according to the established scholarly standards in inorganic chemistry

Content
The research practical will be performed as part of an ongoing research project, forming by itself a small independent project. Content will include a literature search, identification and application of suitable methods (e.g. synthesis, analytical, computational), and independent execution of the work, in close interaction with the supervisor / mentor. The research topic will be in the scientific project of the supervisor, including but not limited to areas such as main group chemistry, organometallic or coordination chemistry, catalysis, or materials, green and medicinal inorganic chemistry.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a project proposal

Requirement for the award of credit points
Active participation in lab work, successful completion of written report

Module applicability
Master Chemistry, Master Biochemistry

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

Module coordinator and lecturer(s)
All professors and Independent Group Leaders in Inorganic Chemistry

Further information

Biochemistry

Introduction to Bioinformatics					
Module 4.1	**Credits** 5 CP	**Workload** 150 h	**Term** 1st semester	**Frequency** only winter term	**Duration** 1 semester
Course a) Lecture: Introduction to Bioinformatics b) Computer Practical: Introduction to Bioinformatics			**Contact hours** 28 h	**Self-study** 122 h	**Group size** a) unlimited b) maximum 40 students in parallel sessions
Prerequisites: Knowledge of basic concepts of Biochemistry, Genetics and Molecular Biology lectures					
Learning outcomes In this combined lecture/practical module the students are introducted to the basic concepts of Bioinformatics. The topics covered range from basic sequence analysis to the visualization and interpretation of 3D structures of proteins. Strong emphasis is given to classical structure prediction methods for RNA and proteins, being also complemented to novel artifical intelligence techniques. The algorithmic principles are teached as necessary for a basic understanding. A strong focus lies on the extension of theoretical knowledge to development of practical skills, enabling the student to become familiar with tools available free of charge from the internet, and to make use of them for the theoretical planning and experimental interpretation of their own laboratory work. These subjects are further engrossed by the exercises and computer practicals.					
Content a) Lecture • Introduction and Overview of Bioinformatics • Genomes and Genome Analysis – Next Generation Sequencing • Databases I – Literature Search - Virtual Cloning • Binary Sequence Comparison • Local AlignmentsLocal and Global Alignments - Motifs and Profiles • Global Multiple Sequence Alignments • Molecular Dynamics Simulation I - Visualization of proteins • Molecular Dynamics Simulation II – Structure Prediction of Proteins using AI • Databases II - Protein Structure Base - Visualization of Biomolecules • Validation of ProteinStructures • Phylogeny • Structure Prediction and Gene Finding • RNA analysis -Transcriptome Analysis • Machine Learning in Bioinformatics b) Exercise and Computer Practical • Databases • Virtual Cloning • Phylogenetic Analysis • Transcriptome Analysis • Validation of Protein Structures • Structure Prediction • Molecular Dynamics Simulation					
Teaching methods a) Lecture					

b) Exercises and Computer Practical. Home work on selected assignments and supervision of script-based practical work at the computer pool of the university
Mode of assessment Written exam
Requirement for the award of credit points Passing the exam
Module applicability Master of Science Biochemistry, also open to M. Sc. students of Stem Cell Biology, Applied Informatics, Physics, Medical Physics, and to B. Sc. students of Biology
Weight of the mark for the final score Weighted by CP
Module coordinator and lecturer(s) M. Lübben, R. Stoll, T. Rudack, A. Mosig
Further information

Biochemistry III					
Module 4.2	**Credits** 5 CP	**Workload** 120 h	**Term** 5. Sem.	**Frequency** nur WS	**Duration** 1 Semester
Courses Biochemistry III (184500)			**Contact hours** 32 h	**Self-Study** 88 h	**Group size** ca. 55 students

Prerequisites

none

Learning outcomes

The lecture imparts knowledge about the complex regulatory processes specific to eukaryotic cells that play a role in the expression of genetic information from the chromosome to the mRNA. Furthermore, the regulatory mechanisms of the targeting of proteins transported within the cell, cell cycle regulation and the molecular basis of the immune system are taught. In addition, the participants are introduced to the scientific language English by using the English language while simultaneously showing German-language slides. After completing the lecture, the participants have an overview of the regulatory mechanisms in eukaryotes and an understanding of the basic English-language terms of biochemistry.

Content

The lecture deals with the complex regulatory mechanisms in eukaryotes:

- Structure of eukaryotic cells: differences to prokaryotes, organelles
- Chromosome structure: polyteny, nucleosomes, chromatin structure
- Replication in eukaryotes: mechanism, DNA polymerases, DNA topology, topoisomerases, telomerase
- Recombination mechanisms: DNA repair, heteroduplex, Holliday structure, recA protein, gene conversion, transgenic animals
- Transposable elements: pseudogene and processed genes, transposons, retroposons, yeast TY, *Drosophila* FB elements
- Reassociation of nucleic acids: stability of double-stranded nucleic acids, Tm value, repetitive DNA
- Transcription in eukaryotes: nuclear structure, transport through nuclear pores, capping, RNA classes
- RNA polymerase I: ribosomal RNA, promoter, processing, nucleolus
- RNA polymerase III: gene structure, tRNA structure, promoter structure, DNA binding proteins, zinc finger proteins, leucine zipper, regulation of transcription factors
- RNA polymerase II: promoter structure, RNA capping, polyadenylation, spliceosome, splice variants
- Ribozymes: self-splicing introns, ribozymes, tetrahymena, RNase, editing of RNA
- Regulation of gene expression: transcription initiation, enhancer/silencer, modular transcription factors, 2-hybrid system, steroid receptors
- Translocation of proteins: signaling hypothesis, SRP, docking proteins, integration of membrane proteins, import into organelles
- Cell cycle: phases of the cell cycle, cyclins, CDKs, regulation
- Immune system: immune cells, antibody structure, antibody diversity, T cell receptor, MHC molecules
- Complement system: complement activation, amplification cascade, MAC

Teaching methods

Lecture

Mode of assessment

Written exam

Requirement for the award of credit points

Passing the exam
Module applicability (in other studies courses) Master studies course Chemistry
Weight of the mark for the final score weighted according to the CP (5 CP)
Module coordinator and lecturer(s) M. Hollmann, D. Tapken
Further information

Biochemistry IV - Biochemistry of Membrane Receptors

Module	Credits	Workload	Term	Frequency	Duration
4.3	7 CP	210 h	2nd semester	only summer term	1 semester
Courses			**Contact hours**	**Self-Study**	**Group size**
Biochemistry IV – Biochemistry of Membrane Receptors (185820)			28 h	182 h	45 students

Prerequisites
Familiarity with the contents of the Bachelor studies course lectures Biochemistry 0, I, II, and III.

Learning outcomes
Students will gain an overview of the various membrane receptors and ion channels, their structure-function relationships, and the intracellular signal transduction pathways these receptors are connected to. A further focus will be on understanding the interplay between different signal transduction pathways as well as the regulatory principles governing them. Students are supposed to grasp the wide-ranging implications that signal transduction pathways have for cell physiology and the organism as a whole. Furthermore, students are expected to learn and understand basic concepts in biochemistry. In the context of the specific topics listed below, reference will be made to those basic concepts of previous lectures (Biochemistry I-III) that are considered crucial for an in-depth understanding of the principles of biochemistry.

Content

- **Cell-cell contacts:** Structure of tight junctions, anchoring junctions, gap junctions; function of gap junctions.
- **Cell-cell adhesion:** Cell migration, N-CAMs, cadherins, selectins, integrins, activation of endothelial cells, extracellular matrix proteins: FGF, chondroitin sulfate, laminin, fibronectin, tenascin. Integrin receptors: MIDAS motif, I-domain, signal transduction; integrin regulation from within the cell, regulation of the cytoskeleton, focal adhesion kinase, function during fertilization.
- **Voltage-activated ion channels:** Resting membrane potential, signal propagation, sodium currents, potassium currents, action potential; single channel conductivity, patch clamp technique.
- **Presynaptic function and vesicle release:** Life cycle of a vesicle, vesicular proteins, SNARE complex formation, fusion pore formation, NSF and SNARE complex dissolution.
- **Ligand-activated ion channels:** Glutamate receptors (NMDA, kainate, AMPA receptors), post-transcriptional modifications, structure-function relationship, ligand binding site, receptor modulation, molecular correlates of memory formation, LTP. Acetylcholine receptors: structure, acetylcholine release, pore opening. GABA and glycine receptors: structure and function.
- **Structure of the synapse:** Presynaptic terminal, vesicle release, postsynaptic organization, structure of the nerve-muscle synapse, chemical vs. electrical synapses, EPSPs, miniature postsynaptic potentials
- **Signal transduction pathways:** Introduction, protein kinase A, structure-function relationship in the catalytic center.
- **Receptor protein tyrosine kinases**: Subclasses. Insulin receptor and FGF receptor: extra- and intracellular domains, heparin, EGF-receptor, PDGF receptor. Signaling modules SH2 domain, SH3 domain, TRK and GDNF receptors. Protein-protein interaction domains: SHC-GRB2, IRS-1, protein tyrosine phosphate binding domain (PTB), pleckstrin homology domain (PH), phospholipase C-g.
- **Signal transduction of cellular survival:** PI-3 kinase: P85 subunits, a, b, g, d subunits, catalytic subunits; Bcl-2 protein family: Bcl-xl, Bak; Ras protein, MAP kinase; serine-threonine kinases: TGF-b receptors, structure of the cytoplasmic domain, comparison to PKA, SMAD.
- **Phosphotyrosine phosphatases:** Mechanism, PTP-BL,PDZ domains, catalytic center

• **Non-receptor tyrosine kinases**: Src kinase family, structure-function relationship. • **Cytokines:** Families I through IV of cytokine receptors. Class I: growth hormone, erythropoietin, and prolactin receptors, janus kinases (JAKs), STATs, IL-6 receptor family: signal transduction, Il-2 receptor family, gene therapy. Class II: Interferon alpha (ligand), signal transduction of the interferon alpha receptor. Class III: Tumor necrosis factor receptor family (p55), TRAFs, TRADD, FAAD, RIP, death domain (Fas, TNFR1, p75NTR), caspases (9.3.1), and their inhibition. Class IV: Interleukin-1 receptor, IRAP. • **Seven-transmembrane receptors/G proteins:** (GPCRs): Classification, GTP-ase cycle, transducin, regulation of GDP/GTP exchange activity, rhodopsin, regulation of guanylate cyclase, calcium-dependent proteins, Ca/calmodulin, arrestin, photo transduction, G proteins
Teaching methods Lecture
Mode of assessment Written exam
Requirement for the award of credit points Passing the exam
Module applicability (in other studies courses)
Weight of the mark for the final score Weighted by CP
Module coordinator and lecturer(s) M. Hollmann, T. Günther-Pomorski, S. Neumann
Further information The PowerPoint slides shown are available on disc and/or deposited in the corresponding Moodle course. Note-taking during lectures is encouraged. Independent post-preparation of module contents as well as independent consultation of course material is recommended to prepare for the exam.

<table>
<tr><td colspan="6">Modular Advanced Practicals in the Focal Point Programme</td></tr>
<tr><td>Module
4.4</td><td>Credits
15 CP</td><td>Workload
450 h</td><td>Term
1st semester</td><td>Frequency
only WS</td><td>Duration
1 semester</td></tr>
<tr><td colspan="3">Courses
Four modular practicals from four different focal points. The individual courses offered are listed on the following pages.</td><td>Contact hours
256 h</td><td>Self-Study
194 h</td><td>Group size
1–4 students</td></tr>
<tr><td colspan="6">Prerequisites
none</td></tr>
<tr><td colspan="6">Learning outcomes
Students learn advanced techniques applied in research labs of the different focal points involved in the studies course as well as theoretical aspects of the topics investigated in these labs.
Details on the learning outcomes of the individual courses can be found on the following pages.</td></tr>
<tr><td colspan="6">Content
See individual course descriptions.</td></tr>
<tr><td colspan="6">Teaching methods
Practical</td></tr>
<tr><td colspan="6">Mode of assessment
Varies between courses, usually active and successful participation in the practical and either a written project report, a presentation or a poster to present the results of the practical. Details for each individual course can be found on the following pages.</td></tr>
<tr><td colspan="6">Requirement for the award of credit points
See individual course descriptions.</td></tr>
<tr><td colspan="6">Module applicability (in other studies courses)</td></tr>
<tr><td colspan="6">Weight of the mark for the final score
Each of the four courses weighted by its CPs (4 CP for each course)</td></tr>
<tr><td colspan="6">Module coordinator and lecturer(s)
Module coordinator: I. Dietzel-Meyer
Lecturers: See individual course descriptions.</td></tr>
<tr><td colspan="6">Further information</td></tr>
</table>

Research Practical in the Focal Point Programme					
Module 4.5	**Credits** 15 CP	**Workload** 450 h	**Term** 3. Sem.	**Frequency** WS	**Duration** 1 Semester
Courses a) Lab course b) Seminar			**Contact hours** 256 h	**Self-Study** 194 h	**Group size** Individual training

Prerequisites
Both Advanced Practicals of Master semester 2 have to be passed

Learning outcomes
Students, coached by their chosen supervisor, are expected to learn how to plan a research project related to a topic that is linked, in the widest sense, to the biochemistry and molecular neurobiology of the nervous system. Students then proceed to carry out the experiments independently over the course of one semester, thus practicing experimentation in a research lab, and how to properly evaluate and document experimental data. Finally they practive how to write a protocol that contains all necessary information. Finally, they show their data in the lab seminar of their supervisor in an oral or poster presentation, thereby practicing how to present experimental data to an audience. They also write a Master exposé detailing how they will develop their Research Practical topic into a Master thesis project. This Master exposé is to be written in the style of a regular DFG grant proposal, with the work done during the Research Practical described as preliminary work. The work programme should comprise at least one third of the total exposé volume, which should be around 10 pages (half the size of a regular DFG grant proposal). The Master exposé is graded by the supervisor to provide the grade for the Research Practical.

Content
Research projects are provided by the members of the Focal Point Programme "Biochemistry of the Nervous System". Topicwise, any current research question within the wide area of the biochemistry of the nervous system, neurobiochemistry, or molecular neuroscience can be offered as a project
Seminar:
Students participate in the seminars of the research group of their practical supervisor, and at the end of their practical present their results in the form of a seminar or poster contribution.

Teaching methods
Lab course and Seminar

Mode of assessment
A protocol, and a Master exposé in the style of a DFG grant application, which is limited to 10 pages

Requirement for the award of credit points
The protocol and the Master exposé have to be submitted and accepted

Module applicability
Master of Science Biochemistry; Master of Science Chemistry

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

Module coordinator and lecturer(s)
All members of the Focal Point Programme "Biochemistry of the Nervous System"

Further information

Biophysical Chemistry

Biophysical Chemistry I					
Module 7.1	**Credits** 5 CP	**Workload** 150 h	**Term** 2. Semester	**Frequency** SS	**Duration** 1 Semester
Courses a) Biophysical Chemistry I			**Contact hours** 4 SWS, 60 h	**Self-Study** 90 h	**Group size** 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 techniques in biophysical chemistry with a focus on structure determining methods.
- 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:

- Protein structures
- Molecular interactions
- Computational approaches
- X-ray diffraction
- Calorimetry techniques
- Fluorescence theory, FRET
- Super-resolution microscopy

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. 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

Biophysical Chemistry II					
Module 7.2	Credits 5 CP	Workload 150 h	Term 3. Semester	Frequency WS	Duration 1 Semester
Courses a) Biophysical Chemistry II			**Contact hours** 4 SWS, 60 h	**Self-Study** 90 h	**Group size** 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. 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

In-depth Practical: Biopolymers in vivo					
Module number	**Credits** 8 CP	**Workload** 240 h	**Term** 1. to 3. Sem.	**Frequency** every semester,	**Duration** 6 weeks
Courses In-depth practical: Biopolymers in vivo			**Contact hours** 8 SWS	**Self-Study** 120 h	**Group size** 1 student

Prerequisites
Basic knowledge in cell biology and polymer chemistry

Learning outcomes
After the successful completion:

- Students will know about different cell-based methods to study (bio-) molecules
- Students will know about the theoretical background of cell culture-based techniques
- Students will have learned the handling and treatment of experimental data
- Students will know how to scientifically document results in a report format and discuss the results in the context of the latest research / state-of-the-art
- Students had the opportunity of sharing and discussing scientific questions also with other group members during the regular group seminars

Content
Laboratory safety, Principles of cell culture-based techniques, preparation and handling of experimental samples, scientific analysis of results,

Teaching methods
Hands-on internship with experimental and theoretical parts

Mode of assessment
Written laboratory report

Requirement for the award of credit points
Active participation in the experiments and following analysis and writing of scientific report

Module applicability
M.Sc. Chemistry

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

Module coordinator and lecturer(s)
Prof. Dr. Simon Ebbinghaus

Further information

In-depth Practical: Biophotonics					
Module number	**Credits** 8 CP	**Workload** 240 h	**Term** 1. to 3. Sem.	**Frequency** every semester,	**Duration** 6 weeks
Courses In-depth practical: Biophotonics			**Contact hours** 8 SWS	**Self-Study** 120 h	**Group size** 1 student
Prerequisites Basic knowledge in cell biology and on spectroscopic techniques					
Learning outcomes After the successful completion: • Students will know about different spectroscopic methods to study (bio-) molecules • Students will know about the theoretical background of spectroscopy and fluorescence-based techniques • Students will have learned the handling and treatment of experimental data • Students will know how to scientifically document results in a report format and discuss the results in the context of the latest research / state-of-the-art • Students had the opportunity of sharing and discussing scientific questions also with other group members during the regular group seminars					
Content Lasersafety, Principles of spectroscopic and fluorescence-based techniques, preparation and handling of experimental samples, scientific analysis of results,					
Teaching methods Hands-on internship with experimental and theoretical parts					
Mode of assessment Written laboratory report					
Requirement for the award of credit points Active participation in the experiments and following analysis and writing of scientific report					
Module applicability M.Sc. Chemistry					
Weight of the mark for the final score Weighted according to CP					
Module coordinator and lecturer(s) Prof. Dr. Simon Ebbinghaus					
Further information					

Organic and Bioorganic Chemistry

<table>
<tr><td colspan="6">Enzyme Catalysis In Organic Chemistry: White Biotechnology</td></tr>
<tr><td>Module
6.1</td><td>Credits
5 CP</td><td>Workload
120 h</td><td>Term
semester 1-3</td><td>Frequency
Every 2nd summer semester</td><td>Duration
1 semester</td></tr>
<tr><td colspan="3">Courses
Enzyme Catalysis In Organic Chemistry: White Biotechnology</td><td>Contact hours
3 SWS</td><td>Self-Study
100 h</td><td>Group size
20 students</td></tr>
<tr><td colspan="6">Prerequisites
Knowledge of basic organic chemistry and biochemistry</td></tr>
<tr><td colspan="6">Learning outcomes
Students will gain a broad overview of biotechnology in chemical synthesis, with particular emphasis on enzyme engineering methods and strategies.</td></tr>
<tr><td colspan="6">Teaching methods
Offered as hybrid lecture (lecture hall / Zoom) with supporting materials provided via moodle.</td></tr>
<tr><td colspan="6">Mode of assessment
Oral exam</td></tr>
<tr><td colspan="6">Requirement for the award of credit points
Passing the oral exam</td></tr>
<tr><td colspan="6">Module applicability
Elective Lecture I-VI</td></tr>
<tr><td colspan="6">Weight of the mark for the final score
Weighted according to CPs</td></tr>
<tr><td colspan="6">Module coordinator and lecturer(s)
Frank Schulz</td></tr>
<tr><td colspan="6">Further information
Textbooks: K. Faber, Biotransformations in Organic Chemistry, M. T. Reetz: Directed Evolution of Selective Enzymes: Catalysts for Organic Chemistry and Biotechnology</td></tr>
</table>

Metabolomics for the discovery of new natural products and biomarkers					
Module 6.2	**Credits** 5 CP	**Workload** 120 h	**Term** semester 1-3	**Frequency** 1/year	**Duration** 1 semester
Courses Metabolomics for the discovery of new natural products and biomarkers			**Contact hours** 3 SWS	**Self-Study** 100 h	**Group size** 20 students
Prerequisites Knowledge of basic analytical and organic chemistry, basic biochemistry					
Learning outcomes Students acquire a broad overview upon instrumental analytics for the identification of natural products and biomarkers for various diseases.					
Teaching methods Offered as hybrid lecture (lecture hall / Zoom) with supporting materials provided via moodle.					
Mode of assessment Oral exam					
Requirement for the award of credit points Passing the oral exam					
Module applicability Elective Lecture I-VI					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) Frank Schulz					
Further information The lecture will be based on review articles, selected book chapter and current primary research publications.					

Organofluorine Chemistry					
Module 6.3	**Credits** 5 CP	**Workload** 120 h	**Term** 2. Sem.	**Frequency** each SoS	**Duration** 1 Semester
Courses a) Lecture b) Exercises	**Contact hours** 2 + 1 SWS			**Self-Study** 75 h	**Group size** 20 Students

Prerequisites
None. Ideally: knowledge of basic methods for organic transformations.

Learning outcomes
Students will acquire a broad overview of organofluorine chemistry. After completion of the course, students will know all fundamental approches toward the synthesis of organofluorine compounds and will be able to independently devise synthetic routes and solve corresponding problems. Students will also be able to interpret the sometimes unusual reactivity of organofluorine components and to analyze the influence of fluorine substituents in organic molecules. In addition to textbook knowledge, current publications in the field will also repeatedly be included in the lecture.

Content	
Synthesis of organofluorine compounds	History of organofluorine chemistry, Sources of fluorine - fundamental fluorine reagents - direct (per)fluorination, electrochemical fluorination - nucleophilic and "electrophilic" fluorination - synthesis of fluoroarenes - conversion of functional groups
Properties and structures of organofluorine compounds	- C-F bond: fundamentals - steric effects - physic-chemical properties - Bent's rule and special fluorine effect - dipol interactions, intramolecular interactions - analytics: 19F-NMR - acidities - fluorine substituents as pi-donors
Reactivity of organofluorine compounds	- fundamental considerations - perfluorocarbons and substituted perfluorocarbons, fluorinated alkanes - per- and polyfluoroolefins - fluoroarenes: SNAr and ortho metalation - C-F activation and polyfluoroarenes in cross-coupling reactions (C-H activation) - fluorinated enol ethers and analogues
Applications	- fluorous biphase catalysis - pharmaceuticals

Teaching methods
Blackboard and Powerpoint, online videos, discussion of recent research papers

Mode of assessment
Written exam (90 min)

Requirement for the award of credit points
Passing of final written examination

Module applicability
Master of Science Chemistry

Weight of the mark for the final score
according to credit points

Module coordinator and lecturer(s)
S. Huber

Further information

Supramolecular Chemistry

Module	Credits	Workload	Term	Frequency	Duration
6.4	5 CP	120 h	1./3. Sem.	each WS	1 Semester
Courses a) Lecture b) Exercises			**Contact hours** 2 + 1 SWS	**Self-Study** 75 h	**Group size** 20 Students

Prerequisites
None. Ideally: knowledge of basic methods for organic transformations.

Learning outcomes
Students will acquire a broad overview of supramolecular chemistry. After completion of the course, students will be aware of all relevant concepts in supramolecular chemistry and will be able to identify them independently. Participants will also study all relevant noncovalent interactions, including their electronic origin, their manipulation and their limitations. On the basis of the most common structural motifs, cation binders, anion binders and neutral molecule binders will be discussed. Students will be aware of the fundamentals of self-assembly as well as of its most important applications. Finally, participants will be able to interpret the use of non-covalent interactions in organocatalysis. In addition to textbook knowledge, current publications in the field will also repeatedly be included in the lecture.

Content	Definition, history
Concepts	- Lock & key, induced fit - binding constants - cooperativity / chelate effect - preorganization / complementarity, selectivity
Noncovalent Interactions	- ion pairing, ion-dipole, dipole-dipole - hydrogen bonding, halogen bonding, further closed-shell interactions - cation-□, □□/□□ , anion-□□ interactions - van-der-Waals interactions, solvation and hydrophobic effect, entropy
Fundamental Techniques	- high-dilution synthesis - template synthesis
Cation Binding	- crown ethers, lariat ethers - cryptands, Spherands - calixarenes
Anion Binding	- recognition by electrostatics - recognition by electrostatics and hydrogen bonding - recognition by hydrogen bonding - recognition by Lewis acids, core motifs
Neutral Guest Binding	- recognition by hydrogen bonding - recognition by hydrophobic effect
Self-Assembly	- rotaxanes - catenanes, knots - capsules
Applications in Catalysis	- reactions in confined space (capsules) - noncovalent organocatalysis - self-replication, noncovalent catalyst assembly, “classical” supramolecular catalysis

Teaching methods
Blackboard and Powerpoint, online videos, discussion of recent research papers

Mode of assessment
Written exam (90 min)

Requirement for the award of credit points
Passing of final written examination

Module applicability
Master of Science Chemistry

Weight of the mark for the final score
according to credit points

Module coordinator and lecturer(s)
S. Huber

Further information

Organic Synthesis I: Stoechiometric Organometallics					
Module 6.5	**Credits** 5 CP	**Workload** 120 h	**Term** semester 1-3	**Frequency** every semester	**Duration** 1 semester
Courses Organic Synthesis II: Stoechiometric Organometallics			**Contact hours** 3 SWS	**Self-Study** 100 h	**Group size** 20 students

Prerequisites
Knowledge of basic organic reactions.

Learning outcomes
Students acquire a broad overview upon applications of stoechiometric organometallic reagents, focussing on selectivities connected with various metals.

Content
HSAB-concept in organometallic synthesis; endocyclic restriction test; DOM reactions, organometallic reagents based on lithium, magnesium, zink, titanium, boron and copper; stereoselective reactions with organometallic reagents.

Teaching methods
Offered as e-learning module; Link: http://www.ruhr-uni-bochum.de/oc2/dyker/Vorlesungen.html

Mode of assessment
Oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Elective Lecture I-VI

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

Module coordinator and lecturer(s)
Gerald Dyker

Further information

Organic Synthesis II: Catalytic Organometallics					
Module 6.6	**Credits** 5 CP	**Workload** 120 h	**Term** semester 1-3	**Frequency** every semester	**Duration** 1 semester
Courses Organic Synthesis II: Catalytic Organometallics			**Contact hours** 3 SWS	**Self-Study** 100 h	**Group size** 20 students
Prerequisites Knowledge of basic organic reactions.					
Learning outcomes Students acquire a broad overview upon applications for homogeneous transition metal catalysis.					
Content Key steps in catalytic cycles; Heckreaction and other Pd-catalyzed domino processes, catalytic activities of Au-, Co-, Cu-, Fe-, Mn-, Ni-, Rh-, Ru- and Lanthanoid-complexes.					
Teaching methods Offered as e-learning module; Link: http://www.ruhr-uni-bochum.de/oc2/dyker/Vorlesungen.html					
Mode of assessment Oral exam					
Requirement for the award of credit points Passing the oral exam					
Module applicability Elective Lecture I-VI					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) Gerald Dyker					
Further information					

Organic Synthesis III: Designing Organic Syntheses					
Module 6.7	**Credits** 5 CP	**Workload** 150 h	**Term** semester 1-3	**Frequency** every semester	**Duration** 1 semester
Courses Organic Synthesis III: Designing Organic Syntheses			**Contact hours** 3 SWS	**Self-Study** 100 h	**Group size** 20 students

Prerequisites
Knowledge of basic organic reactions.

Learning outcomes
- Knowledge of the retron concept
- Ability to identify strategic bonds
- Ability to develop a synthesis plan for target molecules with medium complexity.

Content
Key expressions of retrosynthesis: strategic bonds, synthon, synthetic equivalent, retron, bidirectional synthesis, linear and konvergent synthesis plan. Typical structural units in retrosynthetic analysis such as 1,n-dicarbonyl compounds and hetarenes; exercises in developing strategies for synthesis of target molecules.

Teaching methods
Offered as e-learning module; Link: http://www.ruhr-uni-bochum.de/oc2/dyker/Vorlesungen.html

Mode of assessment
Oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Elective Lecture I-VI

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

Module coordinator and lecturer(s)
Gerald Dyker

Further information

Concepts of Molecular Chemistry I: Physical Organic Chemistry

Module 6.8	**Credits** 5 CP	**Workload** 150 h	**Term** 1., 3. Sem.	**Frequency** WS	**Duration** 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

Weight of the mark for the final score

Module coordinator and lecturer(s): W. Sander

Further information

Modern Organotransition metal catalysis					
Module 6.9	**Credits** 5 CP	**Workload** 150 h	**Term** 2./4. Sem.	**Frequency** nur SS	**Duration** 1 Semester
Courses a) lecture b) exercise			**Contact hours** 2+1 SWS	**Self-Study** 100 h	**Group size** 10 students
Prerequisites -					
Learning outcomes • students aquire knowledge on the theory of transition metal catalysed coupling reactions and their mechanistic principles					
Content • Cross-coupling reactions and their elementary catalytic steps • Catalytic activation of C-O bonds, C-C bonds and C-H bonds: mechanistic approaches, selected examples, synthetic applications. • Catalytic functionalization of alkenes.					
Teaching methods *b) lecture b) exercise*					
Mode of assessment Oral exam (30 min) after the module					
Requirement for the award of credit points *Passing the exam*					
Module applicability *M. Sc. Chemistry*					
Weight of the mark for the final score					
Module coordinator and lecturer(s) Prof. Dr. Lukas Gooßen					
Further information					

In-depth Practical: Organocatalysis					
Module 6.10	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem.	**Frequency** Every semester	**Duration** 1 Semester
Courses In-depth Practical: Organocatalysis			**Contact hours** 9 SWS	**Self-Study** 105 h	**Group size** Max 3 students
Prerequisites					
Learning outcomes • Students acquire advanced knowledge on the theory and techniques of the basic concepts of Supramolecular Chemistry • Students learn to write a detailed lab report on the topic and experimental results of the practical • Students learn scientific work under the guidance of teaching assistants, teamworking in collaboration while carrying out experiments, general knowledge of software and of necessary lab equipment.					
Content - Students will mostly perform various organic syntheses, including ones under inert-gas conditions. This comprises literature-known protocols and unpublished methods developed within the group. They will also test new approaches to synthetic problems. Compounds will be characterized by the usual means, including NMR and mass spectroscopy. Binding constants will be obtained via NMR and ITC titrations, and catalyst performance will be judged by obtaining reaction kinetics on model reactions.					
Teaching methods Practical under guidance of research assistent					
Mode of assessment Active participation in practical, feedback during the experiments, feedback on written lab reports by teaching assistant.					
Requirement for the award of credit points All experimets are completed successfully and written up satisfactorily in a lab report					
Module applicability					
Weight of the mark for the final score					
Module coordinator and lecturer(s) S. Huber					
Further information					

<table>
<tr><td colspan="6">In-depth Practical: Supramolecular Chemistry</td></tr>
<tr><td>Module
6.11</td><td>Credits
8 CP</td><td>Workload
240 h</td><td>Term
1., 2. Sem.</td><td>Frequency
Every semester</td><td>Duration
1 Semester</td></tr>
<tr><td colspan="3">Courses
In-depth Practical: Supramolecular Chemistry</td><td>Contact hours
9 SWS</td><td>Self-Study
105 h</td><td>Group size
Max 3 Studierende</td></tr>
<tr><td colspan="6">Prerequisites</td></tr>
<tr><td colspan="6">Learning outcomes
• Students acquire advanced knowledge on the theory and techniques of the basic concepts of Supramolecular Chemistry
• Students learn to write a detailed lab report on the topic and experimental results of the practical
• Students learn scientific work under the guidance of teaching assistants, teamworking in collaboration while carrying out experiments, general knowledge of software and of necessary lab equipment.</td></tr>
<tr><td colspan="6">Content
- Students will mostly perform various organic syntheses, including ones under inert-gas conditions. This comprises literature-known protocols and unpublished methods developed within the group. They will also test new approaches to synthetic problems. Compounds will be characterized by the usual means, including NMR and mass spectroscopy. Binding constants will be obtained via NMR and ITC titrations, and catalyst performance will be judged by obtaining reaction kinetics on model reactions.</td></tr>
<tr><td colspan="6">Teaching methods
Practical under guidance of research assistant</td></tr>
<tr><td colspan="6">Mode of assessment
Active participation in practical, feedback during the experiments, feedback on written lab reports by teaching assistant.</td></tr>
<tr><td colspan="6">Requirement for the award of credit points
All experiments are completed successfully and written up satisfactorily in a lab report</td></tr>
<tr><td colspan="6">Module applicability</td></tr>
<tr><td colspan="6">Weight of the mark for the final score</td></tr>
<tr><td colspan="6">Module coordinator and lecturer(s)
S. Huber</td></tr>
<tr><td colspan="6">Further information</td></tr>
</table>

In-depth Practical: Metal-Organic Chemical Synthesis					
Module 6.12	Credits 8 CP	Workload 240 h	Term semester 1-3	Frequency every semester	Duration 8 weeks
Courses In-depth Practical: Metal-Organic Chemical Synthesis			**Contact hours** 25 SWS	**Self-Study** 40 h	**Group size** 2 students

Prerequisites

Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics

Learning outcomes

- Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography
- Interpreting observations and results
- Writing presentations of own scientific results

Content

Synthesis of target molecules within the context of a current research project.

Teaching methods

Practical lab course within research projects

Mode of assessment

Rating of the protocol and of the performance in the lab

Requirement for the award of credit points

Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol

Module applicability

In-depth Practical I-III

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

Gerald Dyker

Further information

In-Depth Practical: "Semi-Synthesis Of Natural Products"					
Module 6.13	**Credits** 8 CP	**Workload** 240 h	**Term** semester 1-3	**Frequency** 1/year	**Duration** 8 weeks
Courses In-Depth Practical: "Semi-Synthesis Of Natural Products"			**Contact hours** 25 SWS	**Self-Study** 40 h	**Group size** 2 students
Prerequisites Knowledge of basic methods for organic transformations. Recommendation: successful participation in practicals: OC F.					
Learning outcomes • Performing preparative experiments towards the synthesis of natural products derivatives or related synthesis targets • Interpreting observations and results • Writing presentations of own scientific results					
Content Synthesis of target molecules within the context of a current research project.					
Teaching methods Practical lab course within research projects					
Mode of assessment Rating of the protocol and of the performance in the lab					
Requirement for the award of credit points Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol					
Module applicability In-depth Practical I-III					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) Frank Schulz					
Further information					

In-Depth Practical: "Natural Products Chemistry and Biochemistry"					
Module 6.14	**Credits** 8 CP	**Workload** 240 h	**Term** semester 1-3	**Frequency** 1/year	**Duration** 8 weeks
Courses In-Depth Practical: "Natural Products Chemistry and Biochemistry "			**Contact hours** 25 SWS	**Self-Study** 40 h	**Group size** 2 students
Prerequisites Knowledge of basic methods from organic chemistry or biochemistry and analytical chemistry					
Learning outcomes • HPLC and mass spectrometry for the identification of natural products • Statistical data interpretation in the framework of metabolomics • Interpreting observations and results • Writing presentations of own scientific results					
Content Biosynthesis, isolation and characterization of target molecules within the context of a current research project.					
Teaching methods Practical lab course within research projects					
Mode of assessment Rating of the protocol and of the performance in the lab					
Requirement for the award of credit points Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol					
Module applicability In-depth Practical I-III					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer(s) Frank Schulz					
Further information					

In-Depth Practical: "Fermentation of Natural Products"

Module	Credits	Workload	Term	Frequency	Duration
6.15	8 CP	240 h	semester 1-3	1/year	8 weeks

Courses	Contact hours	Self-Study	Group size
In-Depth Practical: "Fermentation of Natural Products"	25 SWS	40 h	2 students

Prerequisites
Knowledge of basic methods from organic chemistry or biochemistry

Learning outcomes

- Fermentation of microorganisms
- Isolation of natural products from fermentation broths or harvested cells
- Interpreting observations and results
- Writing presentations of own scientific results

Content
Biosynthesis, isolation and characterization of target molecules within the context of a current research project.

Teaching methods
Practical lab course within research projects

Mode of assessment
Rating of the protocol and of the performance in the lab

Requirement for the award of credit points
Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol

Module applicability
In-depth Practical I-III

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

Module coordinator and lecturer(s)
Frank Schulz

Further information

In depth practical „Organotransition metal catalysis“

Module 6.16	**Credits** 8 CP	**Workload** 240 h	**Term** 2./4. Sem.	**Frequency** By appoitment	**Duration** 1 Semester
Courses a) practical			**Contact hours** 9 SWS	**Self-Study** 100 h	**Group size** 3 students

Prerequisites

Learning outcomes

- students acquire experience in practical organic and metal-organic labwork and associated techniques of analysis and spectroscopical methods

Content

- Syntheses in the field of organometallic chemistry;
- Handling of air sensitive compounds
- Hands-on work with analytical methods such as GC, GC-MS, NMR
- Mechanism evaluation by e. g. deuteration experiments
- study of catalytic processes

Teaching methods

c) Practical lab course

Mode of assessment

active participation in practical, feedback during and on the experiments, feedback on written lab reports

Requirement for the award of credit points

successful performance of experiments in the lab and satisfactorily written lab reports

Module applicability

M. Sc. Chemistry

Weight of the mark for the final score

Module coordinator and lecturer(s) Prof. Dr. Lukas Gooßen

Further information

Physical Chemistry

Concepts of Spectroscopy 1					
Module 7.3	**Credits** 5 CP	**Workload** 150 h	**Term** 1. Semester	**Frequency** Each WS	**Duration** 1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 105 h	**Group size** a+b) 20 - 50

Prerequisites
Basic knowledge in quantum chemistry, quantum mechanics, spectroscopic techniques and the necessary mathematical formalism

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

Content
1. Electromagnetic radiation, molecular structure, light-matter interaction
2. Optical and spectroscopic elements
3. Line broadening mechanisms, spectral bandwidth, Fourier transformation
4. Molecular symmetry, point groups, molecular symmetry groups
5. Rotational spectroscopy: linear, symmetric, spherical, and asymmetric rigid rotor molecules, rotational infrared, millimeter, microwave and Raman spectra
6. Vibrational spectroscopy: diatomic and polyatomic molecules, infrared and Raman spectra, vibrational selection rules, normal mode analysis
7. 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
8. Laser basics, population inversion and gain mediums, cavity modes, properties of coherent radiation, specific laser systems
9. Introduction to nonlinear spectroscopy

Teaching methods
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

Mode of assessment
2-hour end-of-term written exam on the content of the lectures

Requirement for the award of credit points
Passing the written examination

Module applicability
M.Sc. Chemistry; M.Sc. iMOS; M.Sc. Lasers and Photonics

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

Module coordinator and lecturer(s)
P. Petersen
Lecturers from Physical Chemistry departments

Further information

Concepts of Spectroscopy 2					
Module 7.4	Credits 5 CP	Workload 150 h	Term 2. Semester	Frequency Each SuSe	Duration 1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 105 h	**Group size** a+b) 20 - 50

Prerequisites

Advanced knowledge in quantum chemistry, quantum mechanics and spectroscopic techniques, such as provided by the modules Concepts of Spectroscopy 1 and Dynamics and Simulation.

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
- Develop presentation skills in front of an audience
- Utilize digital techniques to prepare and conduct a presentation

Content

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

Teaching methods

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.

Mode of assessment

20 - 40 min end-of-term oral exam or 2-hour end-of-term written exam on the content of the lectures

Requirement for the award of credit points

Passing the written examination

Module applicability

M.Sc. Chemistry; M.Sc. iMOS; 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

Compact Course "Scanning Probe Microscopy"					
Module 7.6	**Credits** 5 CP	**Workload** 150 h	**Term** 1., 3. Sem	**Frequency** WS	**Duration** 3 weeks
Courses Compact Course "Scanning Probe Microscopy"			**Contact hours** a) 18 h b) 32 h c) 5 h	**Self-Study** 65 h	**Group size** 15 Students

Prerequisites

Knowledge in basic Physical Chemistry.

Learning outcomes

After participating in the scanning probe microscopy (SPM) compact course the students
- are familiar with the basics of scanning probe microscopy.
- are familiar with the functionality of different SPM techniques.
- have an overview of applications of scanning probe microscopy.

After participating in the SPM compact course the students are able to
- process and analyze SPM data in a proper way.
- perform AFM and STM measurements with commercial microscope systems.
- recognize imaging artifacts in SPM images.
- present results of an individual experimental SPM project (12 hours) in a short talk.

Content

Quantum mechanical tunneling effect; basics of scanning tunneling microscopy (STM) and atomic force microscopy (AFM); functionality of different SPM imaging techniques; image processing and imaging artifacts; preparation of STM tips; spectroscopic measurements with an STM; STM and AFM measurements of oxides and biological samples; sample preparation in ultra high vacuum; digression scanning electron microscopy (SEM); combined SEM/STM measurements; manipulation with an SPM

Teaching methods

(a) lecture (b) practical exercises (c) seminar

Mode of assessment

Oral exam

Requirement for the award of credit points

Passing the oral exam

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

Lecturers from Physical Chemistry departments.

Further information

The registration for the SPM compact course is necessary.

In-depth practical: Laser spectroscopy in clusters, liquids and interfaces

Module	Credits	Workload	Term	Frequency	Duration
7.7	8 CP	240 h	1. & 2. Sem.	WS, SS	1 Semester
Courses a) In-depth practical: Laser spectroscopy in clusters, liquids and interfaces			**Contact hours** 8 SWS, 120 h	**Self-Study** 120 h	**Group size**

Prerequisites
Knowledge in basic Physical Chemistry.

Learning outcomes
After successful completion of the module/course, students will be able to:
- Acquire advanced knowledge in laser safety issues and laser spectroscopic techniques
- Carry out supervised laser experiments on molecular clusters, on liquids, or on interfaces
- Obtain general knowledge of necessary lab equipment
- Visualize and present results orally and in written form
- Write reports with theories, experiments, and discussion of results in adequate manner
- Utilize digital techniques to analyze and evaluate the data and for graphical presentation
- Develop teamwork skills and collaboration while carrying out hands on experiments

Content
In this practical, an experiment chosen from the research fields available in the Havenith's group will be carried out. The student summarizes his findings independently in a written report.
Included topics:
1. Laser safety: laser classes, risks, and protection measures
2. Selection of experimental methods:
   - Spectroscopy in helium nanodroplets
   - THz spectroscopy of liquid and solid phases using a Fourier transform spectrometer
   - THz time-domain spectroscopy

3. Selection of topics
   - Vacuum techniques
   - Dealing with ultracold gases (e.g. liquid helium and nitrogen)
   - Leak detection
   - Mass spectrometry
   - Laser technology: OPO, diode laser, or femto second laser
   - Generation of THz radiation
   - Wavelength dependent: appropriate detector elements
   - Phase sensitive signal detection (lock-in techniques, modulation techniques)

Teaching methods
Hands-on lab course (8 hours per week per module).

Mode of assessment
Active participation in practical, feedback during and on the experiments, feedback on written lab reports by teaching assistants.

Requirement for the award of credit points
All experiments are completed successfully and written up satisfactorily in a lab report.

Module applicability
M.Sc. Chemistry.

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

Module coordinator and lecturer(s)
M. Havenith-Newen, G. Schwaab.

Further information

In-depth Practical: Nanoscale surface characterization					
Module 7.8	**Credits** 8 CP	**Workload** 240 h	**Term** 1.to 3. Sem	**Frequency** Every semester	**Duration** 5 weeks
Courses In-depth Practical: Nanoscale surface characterization			**Contact hours** up to 40 h per week	**Self-Study** 40 h	**Group size** 1 Student
Prerequisites Physical Chemistry I to IV.					
Learning outcomes Students acquire a knowledge about different methods used in physical chemistry and their applications					
Content scanning probe methods, photoelectron spectroscopy, low energy electron diffraction, electron energy loss spectroscopy					
Teaching methods practical					
Mode of assessment Report					
Requirement for the award of credit points Performing experiments and the report					
Module applicability M.Sc. Chemistry					
Weight of the mark for the final score Weighted according to CPs.					
Module coordinator and lecturer(s) Lecturers from Physical Chemistry departments.					
Further information possible start independent of lecture schedule; length in weeks depends on availability of student during week					

In-depth Practical: Fluorescence microscopy and spectroscopy					
Module 7.9	**Credits** 8 CP	**Workload** 240 h	**Term** 1.to 3. Sem	**Frequency** Every semester	**Duration** 6 weeks half time or equivalent
Courses In depth practical Fluorescence microscopy and spectroscopy			**Contact hours** 8 h	**Self-Study** 120 h	**Group size** 1 Student

Prerequisites

Knowledge of basic spectroscopy principles

Learning outcomes

After successful completion of the module/course, students will have:

- Acquired advanced knowledge in fluorescence-based methods
- Carried out supervised microscopy and spectroscopy experiments of fluorescent samples
- Obtained general knowledge on different types of fluorophores and spectral ranges (visible, near infrared)
- Analyzed data (spectra/images) with standard software and Python-based scripts
- Written reports and interpreted data with respect to the current literature

Learned to discuss with group members and assess the scientific advance or limitations of experimental approaches and results

Content

Laser safety; Principles of fluorescence spectroscopy and microscopy; preparation of fluorescent samples; chemical modification of fluorophores; image and spectral image processing techniques.

Teaching methods

Hands on lab course of current research topics

Mode of assessment

Written lab report

Requirement for the award of credit points

Active participation in lab course and successful summary of the lab course results.

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

S. Kruss

Further information

In-depth Practical: Nanomaterials and Biointerfaces					
Module 7.10	**Credits** 8 CP	**Workload** 240 h	**Term** 1.to 3. Sem	**Frequency** Every semester	**Duration** 6 weeks half time or equivalent
Courses In depth practical Nanomaterials and Biointerfaces			**Contact hours** 8 h	**Self-Study** 120 h	**Group size** 1 Student

Prerequisites

Knowledge of chemical conjugation techniques and basic spectroscopy

Learning outcomes

After successful completion of the module/course, students will have:

- Acquired advanced knowledge in synthesis and assembly of fluorescent nanomaterials
- Prepared nanomaterials and modified their surface using biofunctionalization techniques
- Carried out microscopy or spectroscopy experiments with these samples
- Obtained general knowledge on the interplay between surface chemistry and photophysics
- Analyzed data (spectra/images) with standard software and Python-based scripts
- Written reports and interpreted data with respect to the current literature

Learned to discuss with group members and assess the scientific advance or limitations of experimental approaches and results

Content

Preparation of fluorescent nanomaterials; optical characterization techniques (absorption spectroscopy, fluorescence spectroscopy, Raman spectroscopy); surface chemistry approaches; biofunctionalization techniques; spectral data processing techniques.

Teaching methods

Hands on lab course of current research topics

Mode of assessment

Written lab report

Requirement for the award of credit points

Active participation in lab course and successful summary of the lab course results.

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

S. Kruss

Further information

In-depth practical: Chemical Microscopy of Surfaces and Biomaterials					
Module 7.11	**Credits** 8 CP	**Workload** 240 h	**Term** 1., 2. Sem	**Frequency** Every semester	**Duration** 6 weeks half time or equivalent
Courses In-depth Practical: I - III			**Contact hours** 8 h	**Self-Study** 120 h	**Group size** ~ 1-3 Students

Prerequisites

Knowledge of basic spectroscopic and data evaluation techniques.

Learning outcomes

Students acquire knowledge on how to prepare samples, how to investigate them with Raman microscopic techniques and how to analyse the image and spectral data acquired.

Content

Laser safety; Principles of confocal Raman microscopy; preparation of chemical and/or biological samples; data acquisition techniques; estimates of data quality; image and spectral image processing techniques.

Teaching methods

hands on lab course

Mode of assessment

Written lab report

Requirement for the award of credit points

Active participation in lab course and successful summary of the lab course results.

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

Lecturers from Physical Chemistry departments.

Further information

Research Practical in the Focal Point Programme "Physical Chemistry"					
Module 7.12	**Credits** 15 CP	**Workload** 450 h	**Term** 3. Sem	**Frequency** Every semester	**Duration** 1 semester
Courses Research Practical in the Focal Point Programme			**Contact hours** 15 h	**Self-Study** 120 h	**Group size** 1 Student

Prerequisites

"Practical Science and Communication", In-depth practical I–III, basic knowledge of physical chemistry

Learning outcomes

The student will be introduced to and trained in the scientific methods applied in one of the Physical Chemistry research groups. Initially under the guidance of experienced research staff, the student will acquire advanced scientific knowledge and will learn the skills necessary in order to design, implement, perform, and analyze a research project related to the current research of the groups. The student will become acquainted with the experimental techniques and/or the software needed for analysis and simulation, learn how to search the scientific literature for previous work relevant for the project, and acquire the ability to summarize and discuss the results in the context of current research.

Content

The student will participate in an experiment from the research areas of the Physical Chemistry groups. These comprise spectroscopy, microscopy, biophysical chemistry, photochemistry, processes at surfaces and interfaces, calorimetric methods, solvation, nanoclusters, mass spectrometry, vacuum techniques, structural properties and dynamics, development of scientific apparatus, signal demodulation, advanced data evaluation techniques, lab safety, laser safety, and more specialized physicochemical topics.
The student will also take part in the meetings of the research group on a regular basis and actively contribute to the discussion of the project.
The student summarizes the findings independently in a written report and/or will present the results in a seminar talk.

Teaching methods

Hands-on lab course, active participation in experimental data acquisition and/or analysis & simulation

Mode of assessment

written lab report and/or seminar talk

Requirement for the award of credit points

all experiments and/or simulations are completed successfully; they are written up satisfactorily in a lab report and/or presented in an adequate manner in a seminar talk.

Module applicability

Master of Science Chemistry

Weight of the mark for the final score

Weighted according to CPs.

Module coordinator and lecturer(s)

Lecturers from Physical Chemistry departments.

Further information

possible start independent of lecture schedule; length in weeks depends on availability of student during week

Industrial Chemistry

Heterogeneous Catalysis

Module	Credits	Workload	Term	Frequency	Duration
8.1	5 CP	150 h	1. Sem.	only WS	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
Heterogeneous Catalysis			a) 2 SWS b) 1 SWS	105 h	All students choosing Industrial Chemistry

Prerequisites
Solid knowledge of basics in Industrial Chemistry, Physical Chemistry, Inorganic Chemistry, and Organic Chemistry

Learning outcomes

- Students get insight into the scientific basis of heterogeneous catalysis, with emphasis on the elementary steps of catalytic reactions, on relations between catalyst structure and reactive properties, between preparation routes and obtained structures, and on the interdisciplinary approaches in catalyst research. They are introduced to the most important characterization methods for heterogeneous catalysts and get an overview over the most important technical applications of heterogeneous catalysis. The course enables students to orient themselves in the multifaceted field of industrial heterogeneous catalysis and creates the basis for own scientific activities in catalysis research.
- Soft skills: interactive presentation to an experienced audience, taking notes during lectures, unsolicited follow-up of module contents, unsolicited consultation of relevant literature

Content

1. Elementary steps of heterogeneous catalysis - chemisorption: energetics, adsorption sites and surface phases; surface reaction, surface reaction dynamics
2. Relations between structure and reactivity of catalytic surfaces - spatial structure: anisotropy of surface structures and properties in metal and non-metal catalysts, ensemble effects and their use, electronic structure - volcano relations and their basis, ligand effects
3. Promotors and poisons in catalysis - chemical and structure promoters and mechanisms of their function, promoting selectivity and stability, basics of poisoning effects
4. Supported catalysts - introduction to texture properties, structure and properties of important supports, surface chemistry of typical supports, interactions between supported components and supports
5. Preparation and activation of catalysts - basis steps in the preparation of solid materials from the viewpoint of catalysis, addition of active components to supports, shaping of catalyst pellets, thermal aftertreatment, activation of catalyst precursors
6. Important catalyst types and their application - metal catalysts (including bifunctional catalysis), catalysis with redox oxides, industrial acid catalysis, environmental catalysis
7. Characterization of heterogeneous catalysts - laboratory reactors for reactivity characterization, texture characterization by physisorption and chemisorption techniques, thermoanalytical (temperature-programmed) methods, structural analysis by XRD, by X-ray absorption, surface analysis by XPS, ISS, vibrational spectroscopy, optical and scanning probe microscopy, miscellaneous techniques (incl. Mößbauer-, EPR-, NMR- and UV-vis spectroscopy)

Teaching methods
a) Lecture; b) Exercises

Mode of assessment
30 min end-of-term oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Master of Chemistry, focal point Industrial Chemistry

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

Module coordinator and lecturer(s) B. Mei, M. Muhler

Further information
All lectures, additional contents of exercises, summaries of student lectures are distributed via *moodle*.

Industrial Chemistry II: Chemical Reaction Engineering

Module	Credits	Workload	Term	Frequency	Duration
8.2	5 CP	180 h	1. Sem.	only WS	1 Semester

Courses	Contact hours	Self-Study	Group size
Industrial Chemistry II: Chemical Reaction Engineering	a) 2 SWS b) 1 SWS	105 h	All students choosing Industrial Chemistry

Prerequisites
Solid knowledge of basics in Industrial Chemistry and Physical Chemistry

Learning outcomes

- Students acquire advanced knowledge about reactors used in chemical industry. They can apply mathematical models to describe ideal reactors und will know reasons of deviations from ideal behavior and know basic models for description of non-ideal reactors. In addition, students can apply thermodynamic and kinetic tools in the analysis of reactions and are able to evaluate consequences of transport limitations on overall reaction rates and are able to select appropriate counteractive measures.
- Soft skills: interactive presentation to an experienced audience, taking notes during lectures, unsolicited follow-up of module contents, unsolicited consultation of relevant literature

Content

1. Basics of chemical reaction engineering: terms and definitions
2. Stoichiometry and thermodynamics: stoichiometric balance and chemical conversion, calculation of reaction enthalpy under reaction conditions, chemical equilibrium, definition of equilibrium constants in diluted and concentrated systems, Michaelis-Menten-Kinetik
3. Kinetics of chemical reactions: volume-constant reactions in ideal reactors, kinetics of multiple homogeneous reactions (first Damköhler number, polymerization, Michaelis-Menten-kinetics), kinetics of heterogeneous reactions (catalysis, steps, Langmuir isotherm, competitive adsorption, monomolecular and bimolecular reactions, Langmuir-Hinshelwood-, Eley-Rideal-, Hougen-Watson rate laws, Bodenstein principle, rate-limiting step, most abundant surface intermediate, mass transport in heterogeneous reactions
4. Combination of mass and heat transfer: kinetics of heterogeneous reactions limited by surface reaction or transfer processes, reaction through liquid/liquid interface, effectiveness factors, consecutive model in heterogeneous catalysis (second Damköhler number) and in reaction through liquid/liquid interface, parallel approach in heterogeneous reactions (Thiele modulus) and in reactions through liquid/liquid interface (Hatta number), especially for catalytic reactions (generalized Thiele modulus, criteria for limitation of mass transfer - Weisz modulus, mass transfer and overall kinetics, combining of reaction and heat transfer - Prater number)
5. Reactors in chemical industry (overview): ideal reactors (types, calculation of conversion, residence time distribution, cascade of CSTRs, complex reactions in CSTR, PFR, selectivity, non-isothermal reactions, instability), non-ideal reactors (residence time distribution, dispersion model, CSTRs-in-series model, segregation, time of mixing, influence of segregation on kinetics)
6. Modelling of real reactors, selectivity in parallel and consecutive reaction networks
7. Non-steady state reactor operation: transition behavior of a CSTR, transient experiments

Teaching methods	a) Lecture; b) Exercises
Mode of assessment	30 min end-of-term oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Master of Chemistry, focal point Industrial Chemistry

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

Module coordinator and lecturer(s)
M. Muhler, B. Mei

Further information
All documents are provided via *moodle*

Modern Microkinetics

Module	Credits	Workload	Term	Frequency	Duration
8.3	5 CP	150 h	2. Sem.	only SoS	1 Semester
Courses Modern Microkinetics			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 105 h	**Group size** All students choosing Industrial Chemistry

Prerequisites
Solid knowledge of basics in *Chemical Reaction Engineering*, Industrial Chemistry and Physical Chemistry

Learning outcomes

- By means of examples students acquire advanced knowledge on basics and application of modern simulation tools used in chemical engineering. The kinetics of a reaction is described based on elementary steps. After the course students are able to solve basic problems of chemical reaction engineering using MATLAB.
- Soft skills: interactive presentation to an experienced audience, taking notes during lectures, unsolicited follow-up of module contents, unsolicited consultation of relevant literature

Content

8. Modeling a chemical reaction using elementary steps: introduction of microkinetic modeling, description of adsorption, desorption and reaction on a molecular basis, statistical thermodynamics, estimation of kinetic parameters, modeling of temperature-programmed experiments, simulation of SSITKA experiments
9. Microkinetic models: determination of kinetic parameters, Levenberg-Marquardt algorithm, examples
10. Reactor models: adiabatic packed-bed reactors, heterogeneous and pseudo-homogeneous models, consideration of non-steady reactor states, model selection, programs of estimation of kinetic constants
11. numerical tools for solution of non-linear algebraic equations and non-linear differential equations: boundary and initial value problems, one- and multiple-step procedure
12. overview of commercial software and routines in numerical/statistical libraries, introduction to MATLAB

Teaching methods
a) Lecture; b) Exercises using MATLAB

Mode of assessment
30 min end-of-term oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Master of Chemistry, focal point Industrial Chemistry

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

Module coordinator and lecturer(s)
M. Muhler, B. Mei

Further information
All documents are provided via *moodle*

Processes in Chemical Production - Past, Present and Future

Module	Credits	Workload	Term	Frequency	Duration
8.4	5 CP	150 h	2. Sem.	only SoS	1 Semester
Courses Processes in Chemical Production - Past, Present and Future			**Contact hours** a) 2 SWS b) 1 SWS	**Self-Study** 105 h	**Group size** All students choosing Industrial Chemistry

Prerequisites
Solid knowledge of basics in Industrial Chemistry, Inorganic Chemistry, Organic Chemistry, and Physical Chemistry

Learning/Course Objectives:
Students will acquire knowledge on important processes in chemical production and on the network of raw materials and product flows in a national economy into which these are integrated. They are to appreciate the influences of access to raw materials including renewables, technological standard and regional conditions on the structure of the chemical industry and to know important final products of chemical production and typical quality characteristics targeted in the production process. They get insight in important management aspects in the chemical industry, in particular related to the assessment and innovation of production processes.

Content
1. Raw materials for industrial organic chemistry in past, present and future
2. Oil refining, processes and actual trends
3. Production and use of synthesis gas and of hydrogen; production and use of olefins; oxidation processes in chemical industry; synthesis, properties and technology of polymer materials
4. Basic processes of inorganic chemical technology (incl. fertilizers)
5. Industrial use of renewables, presence and perspective
6. Business-management aspects of a chemists' job in industry
7. Criteria for the evaluation of chemical production processes, methodology for the design of new chemical production processes

Teaching methods
a) Lecture; b) Exercises

Mode of assessment
30 min end-of-term oral exam

Requirement for the award of credit points
Passing the oral exam

Module applicability
Master of Chemistry, focal point Industrial Chemistry

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

Module coordinator and lecturer(s)
B. Mei, H. Zanthoff, A. Wolf, M. Muhler

Further information
All lectures and additional contents of exercises are distributed via *moodle*.

In-depth Practical: Characterization of Heterogeneous Catalysts

Module	Credits	Workload	Term	Frequency	Duration
8.5	8 CP	240 h	1. Sem.	only WS	1 Semester
Courses Characterization of Heterogeneous Catalysts			**Contact hours** a) 8 SWS b) 1 SWS	**Self-Study** 105 h	**Group size** Max. 12 participants

Prerequisites

Solid knowledge of basics in *Heterogeneous Catalysis*, *Chemical Reaction Engineering*, Physical Chemistry, and in Industrial Chemistry

Learning/Course Objectives:

Practical experience with important characterization techniques for heterogeneous catalysts, the related data treatment methods and approaches to data interpretation,

critical assessment of the potential of the techniques, the accuracy of the data and the significance of the results for catalyst research,

training in reporting, presentation and public discussion of the results.

Content

Practical experiments using

- nitrogen physisorption,
- thermogravimetry,
- X-ray photoelectron spectroscopy,
- FTIR spectroscopy,
- Raman spectroscopy,
- UV-Vis spectroscopy,
- X-ray diffraction,

and virtual experiments (treatment of measured data only) in

- X-ray absorption spectroscopy
- and other methods

are offered. 4 selected experiments are performed by groups of 2 students.

Teaching methods

a) Practical; b) Seminar

Mode of assessment

50 min end-of-term presentation of the results including discussion

Requirement for the award of credit points

Successful experimental performance, 4 accepted protocols, and successful oral presentation

Module applicability

Master of Chemistry, focal point Industrial Chemistry

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

B. Mei, M. Muhler

Further information

All required documents incl. safety instructions are distributed via *moodle*.

<table>
<tr><td colspan="6">In-depth Practical: Industrial Catalysis</td></tr>
<tr><td>Module
8.6</td><td>Credits
8 CP</td><td>Workload
240 h</td><td>Term
1.-2. Sem.</td><td>Frequency
WS and SoS</td><td>Duration
1 Semester</td></tr>
<tr><td colspan="3">Courses
Industrial Catalysis</td><td>Contact hours
a) 8 SWS
b) 1 SWS</td><td>Self-Study
105 h</td><td>Group size
Max. 4 participants</td></tr>
<tr><td colspan="6">Prerequisites
Solid knowledge of basics in Chemical Reaction Engineering, Heterogeneous Catalysis and in Industrial Chemistry</td></tr>
<tr><td colspan="6">Learning/Course Objectives:
Students plan, perform and evaluate experiments in the field of fundamental research under the supervision of an experienced scientist. They receive a detailed introduction into selected scientific methods used in modern research in the field of heterogeneous catalysis.
Soft skills: teamwork and collaboration while carrying out experiments, graphical presentation of practical results, general knowledge about operating systems, software and computing, scientific writing skills</td></tr>
<tr><td colspan="6">Content
Scientific collaboration in a team working on a selected problem of heterogeneous catalysis
Detailed introduction to the scientific methods applied in fundamental research
Literature search and evaluation of the scientific tasks
Planning, performing and evaluating of the experiments under the supervision of an experienced scientist
Written report and oral presentation of the theoretical basics and obtained results</td></tr>
<tr><td colspan="6">Teaching methods
a) Practical; b) Seminar</td></tr>
<tr><td colspan="6">Mode of assessment
50 min end-of-term presentation of the results including discussion</td></tr>
<tr><td colspan="6">Requirement for the award of credit points
Successful experimental performance, accepted protocol, and successful oral presentation</td></tr>
<tr><td colspan="6">Module applicability
Master of Chemistry, focal point Industrial Chemistry</td></tr>
<tr><td colspan="6">Weight of the mark for the final score
Weighted according to CPs</td></tr>
<tr><td colspan="6">Module coordinator and lecturer(s)
M. Muhler, B. Mei</td></tr>
<tr><td colspan="6">Further information
All required documents incl. safety instructions are distributed via moodle.</td></tr>
</table>

In-depth Practical: Reaction Engineering of Heterogeneously Catalyzed Reactions

Module	Credits	Workload	Term	Frequency	Duration
8.7	8 CP	240 h	1. Sem.	only WS	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
Reaction Engineering of Heterogeneously Catalyzed Reactions			a) 8 SWS b) 1 SWS	105 h	Max. 8 participants

Prerequisites
Solid knowledge of basics in *Chemical Reaction Engineering*, *Heterogeneous Catalysis*, Physical Chemistry, and in Industrial Chemistry

Learning/Course Objectives:
Advanced knowledge in basic fields of chemical reaction engineering, which are important for heterogeneously catalyzed reactions: ignition/quenching behavior and stability, reaction limitation by external and internal mass transfer, influence of mixing on conversion. After the course students are familiar with procedures used for the analysis of kinetics of heterogeneously catalyzed reactions (operation of a challenging flow set-up with on-line analysis, test for transfer limitations, collection of kinetic data, data processing).
Soft skills: teamwork and collaboration while carrying out experiments, graphical presentation of practical results, general knowledge about operating flow systems, software and computing

Content
In-depth kinetic experiment (one experiment per group of two students):
- steam reforming of methane
- photocatalytic degradation of methylene blue
- isothermal and transient biochar oxidation
- further experiments depending on availability

Investigation of the kinetics of a complex heterogeneously catalyzed reaction (calibration of the experimental set-up, testing the analytical detection of reaction products, standard tests of external and internal mass transfer limitations, measurement of concentration/time dependences, evaluation of practical results concerning the reaction mechanism, calculation of kinetic parameters)

Basic experiments (for each group of two students):
- nitrite reduction
- polytropic tank reactor
- residence time distribution and conversion calculation

Studying ignition/quenching behavior and instabilities (oscillations) exemplified with an exothermic reaction (decomposition of hydrogen peroxide); influence of internal mass transfer (pore diffusion, Thiele modulus) on the overall reaction rate in a three-phase system (nitrite reduction); experimental determination of residence time behavior and conversion of different reactors (CSTR, PFR, CSTRs-in-series) depending on mixing; data evaluation using different models for ideal and non-ideal reactors (dispersion, CSTRs-in-series and segregation model, calculation of Bodenstein and Damköhler number).

Teaching methods
a) Practical; b) Seminar

Mode of assessment
50 min end-of-term presentation of the results including discussion

Requirement for the award of credit points
Successful experimental performance, accepted protocols (1+3), and successful oral presentation

Module applicability
Master of Chemistry, focal point Industrial Chemistry

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

Module coordinator and lecturer(s)
M. Muhler, B. Mei

Further information
All required documents incl. safety instructions are distributed via *moodle*.

Theoretical Chemistry

Computational Chemistry I: Structure and Dynamics of Molecules					
Module 9.1	**Credits** 5 CP	**Workload** 150 h	**Term** 1., 3. Sem	**Frequency** WS	**Duration** 1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) (2 SWS) b) (1 SWS)	**Self-Study** 75 h	**Group size** ~ 10 students
Prerequisites Admission to the Master Course Program					
Learning outcomes Students acquire a broad overview upon computational techniques applied in drug design					
Content Forcefields, Quantum chemical methods (semiempiric, ab initio, DFT, TDDFT), Protein structures, Molecular dynamics, Monte Carlo, Free Energy Calculations					
Teaching methods a) Lecture (2 hours per week) b) Computer exercises (1 hour per week or block course)					
Mode of assessment Oral examination					
Requirement for the award of credit points Passing the oral examination					
Module applicability M.Sc. Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer M. Schindler					
Further information					

Computational Chemistry II: Quantitative Structure-Activity Relations in Drug Design					
Module 9.2	**Credits** 5 CP	**Workload** 150 h	**Term** 2., 4. Sem	**Frequency** SS	**Duration** 1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) (2 SWS) b) (1 SWS)	**Self-Study** 75 h	**Group size** ~ 10 students
Prerequisites Knowledge acquired in Computational Chemistry I					
Learning outcomes Students acquire a broad overview upon computational techniques applied in drug design					
Content Classical QSARs in rational drug design: MLR, PCR (Hansch, Free-Wilson, LFER), Partial least squares, Advances methods: 3D-QSAR(CoMFA, WAVE3D), ANN, SVM, Fuzzy Logic, Protein modeling, Design of experiments					
Teaching methods a) Lecture (2 hours per week) b) Computer exercises (1 hour per week or block course)					
Mode of assessment Oral examination					
Requirement for the award of credit points Passing the oral examination					
Module applicability M.Sc. Chemistry					
Weight of the mark for the final score Weighted according to CPs					
Module coordinator and lecturer M. Schindler					
Further information					

Theoretical Chemistry II: Dynamics and Simulation (Chemistry)

Module	**Credits**	**Workload**	**Term**	**Frequency**	**Duration**
9.3	5 CP	150 h	1. or 3. Sem.	Each WiSe	1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a)+b) 2+1 SWS	**Self-Study** a) 30 h b) 75 h	**Group size** 10 – 20 Students

Prerequisites
Undergraduate level knowledge in classical mechanics, statistical mechanics and time-independent non-relativistic quantum mechanics

Learning outcomes
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.

Content
Essentials of classical and statistical mechanics: Formulations according to Newton, Lagrange and Hamilton, corresponding equations of motion, conservation laws/conserved quantities, Noether theorem, Liouville theorem, ensembles, distribution functions, first and second moments of distributions, connection to averages and fluctuations of observables, correlation functions in space and time, van Hove correlation function, pair and radial correlation function with connection to x-ray diffraction and neutron scattering experiments, dynamic and static structure factors.
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 for thermostatting and barostatting, finite system size effects, boundary conditions, convergence criteria for dynamical computer simulations, realizing various ensembles in terms of simulation algorithms, holonomic constraints, deriving molecular dynamics from the time-dependent Schroedinger equation, time-dependent self-consistent field dynamics, ab initio molecular dynamics equations of motion according to Ehrenfest, Born-Oppenheimer and Car-Parrinello, including nuclear quantum effects via path integral simulations.

Teaching methods
Lecture 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

Requirement for the award of credit points
Passing the end-of-semester exam

Module applicability
M.Sc. Chemistry and 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”

Biomolecular Simulation: Understanding Experiments at the Molecular Level						
Module 9.4		**Workload** 150 h	**Credit points** 5 CP	**Available in semester** 1	**Frequency** Each WiSe	**Course duration** 1 Semester
1	**Teaching methods** a) Lecture b) Exercises		**Hours per week** a) 2 h b) 1 h		**Contact time** 45 h	**Self-study** 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 end-of-term exam					
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. Enthalpy-entropy compensation. **Protein dynamics**: Dimensionality reduction, principal component analysis, normal mode analysis, harmonic vs. quasiharmonic approximation, entropy estimation.					
10	Person in charge / Lecturer(s) L. Schäfer					

)

Theoretical Chemistry III: Electronic and Molecular Structure Theory (Chemistry)

Module	Credits	Workload	Term	Frequency	Duration
9.5	5 CP	150 h	2. or 4. Sem.	Each SoSe	1 Semester

Courses	**Contact hours**	**Self-Study**	**Group size**
a) Lectures b) Exercises	a+b) 3 SWS	a) 30 h b) 75 h	10-20 Students

Prerequisites

Learning outcomes

After completing this course students will 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. Futhermore they will know how to judge the accuracy and reliability of such methods.

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 princple 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

Teaching methods

Lecture and exercises with problems for self-studying,Q&A and discussion sessions with presentations given by the participants, Moodle course with online material.

Mode of assessment

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

Requirements for the award of credit points

Passing the oral end-of-semester exam

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

According to CP

Module coordinator and lecturer(s)

C. Haettig

Further information

Atomistic Simulations with Machine Learning

Module 9.6	**Credits** 5 CP	**Workload** 150 h	**Term** 1-4 (tba)	**Frequency** annually	**Duration** 1 Semester
Courses a) Lectures (2 SWS) b) Exercises (1 SWS)			**Contact hours** a) 30 hours b) 15 hours	**Self-Study** 105 h	**Group size** 10-20 students

Prerequisites Admission to the Master Course Program

Learning outcomes
After the successful participation in the module
a) the students will have obtained knowledge about
- different machine learning algorithms
- suitable input descriptors/feature vectors for machine learning
- different generations of machine learning potentials
- the construction of machine learning interatomic potentials
- the combination of machine learning potentials with simulation tools of theoretical chemistry

b) the students will have obtained practical skills in
- training and validating neural network potentials
- choosing reference structures by active learning
- applying neural network potentials in molecular dynamics
- managing workflows for machine learning potentials with python and jupyter notebooks

Content
a) The lecture will focus on the use of machine learning for atomistic simulations in chemistry and materials science
- machine learning algorithms like neural networks, Gaussian processes, support vector machines and others
- mandatory properties of input descriptors, various forms of atom-centered symmetry functions, Coulomb matrix, smooth overlap of atomic positions, atomic cluster expansion, etc.
- different forms of representing the potential energy using atomic energy contributions, electrostatics, dispersion interactions, long-range charge transfer, magnetism
- training algorithms for parameter optimization
- validation methods for machine learning potentials, extrapolation, interpolation errors, uncertainty quantification
- combination of machine learning potentials with molecular dynamics and Monte Carlo

b) In the computer exercises practical experience in the construction, validation and use of neural network potentials will be gained
- setting up working environments and computational frameworks
- selection of suitable training structures
- training different generations of high-dimensional neural network potentials
- validation and applicability of machine learning potentials
- running molecular dynamics simulations using neural network potentials

Teaching methods
a) Lecture (2 hours per week) b) Computer exercises (1 hour per week or block course)

Mode of assessment
a) 30-45 min end-of-term oral exam or 2-hour end-of-term written exam b) computer exercises

Requirement for the award of credit points
a) passing the end-of-term exam b) active participation in the exercises and reports

Module applicability M.Sc. Chemistry and M.Sc. Biochemistry

Weight of the mark for the final score
The final score corresponds to the score of the exam

Module coordinator and lecturer J. Behler

Further information
Some knowledge in Python, electronic structure calculations and/or molecular dynamics is recommended

Machine Learning for Chemists

Module 9.6b	**Credits** 5 CP	**Workload** 150 h	**Term** 1-4 (tba)	**Frequency** yearly	**Duration** 1 Semester
Courses a) Lectures (2 SWS) b) Exercises (1 SWS)			**Contact hours** a) 30 hours b) 15 hours	**Self-Study** 105 h	**Group size** 14 students

Prerequisites
Admission to the Master Course Program

Learning outcomes
After the successful participation in the module
a) the students will have obtained knowledge about

- fundamentals of statistics and data handling
- concepts of machine learning and relevance in chemistry
- machine learning techniques
- case studies in chemistry

b) the students will have obtained practical skills in

- construction of machine learning models
- uncertainty quantification and active learning
- dimensionality reduction and data visualization
- managing workflows for machine learning with python and jupyter notebooks

Content
The lecture will focus on machine learning in chemistry and materials science

- machine learning methods like neural networks, Gaussian processes and support vector machines
- setting up working environments and computational frameworks
- handling and learning of data sets
- training different types of machine learning models
- data visualization

Teaching methods
a) Lecture (2 hours per week)
b) Computer exercises (1 hour per week or block course)

Mode of assessment
a) 30-45 min end-of-term oral exam or 2-hour end-of-term written exam
b) computer exercises

Requirement for the award of credit points
a) passing the exam
b) active participation in the exercises

Module applicability
Master Chemistry and Master Biochemistry

Weight of the mark for the final score
The final score corresponds to the score of the exam

Module coordinator and lecturer
Prof. Dr. J. Behler

Further information
knowledge in Python is recommended

Theoretical Spectroscopy (Chemistry)

Module	**Credits**	**Workload**	**Term**	**Frequency**	**Duration**
9.7	5 CP	150 h	2. or 4. Sem.	Each SoSe	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
a) Lectures b) Exercises			a+b) 2+1 SWS	105 h	10 – 20 Students

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

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
Lecture 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

Requirement for the award of credit points
Passing the end-of-semester exam

Module applicability
M.Sc. Chemistry and 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"

Industrial Computational Chemistry I: Fundamentals

Module	Credits	Workload	Term	Frequency	Duration
9.8	5 CP	150 h	3. Sem	WS	1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) (2 SWS) b) (1 SWS)	**Self-Study** 100 h	**Group size** ~ 10 students

Prerequisites

Learning outcomes
Students acquire working knowledge on the techniques of computational chemistry in the realm of (bio)molecular systems such as small drug-like molecules and proteins. Besides calculated and experimentally determined molecular properties of small molecules, valuable sources of information are published X-ray stuctures of enzyme-substrate complexes or transition metal complexes, the critical evaluation of which is mandatory before they can be uses in rational drug and catalysis design.

Content
Essentials of classical and statistical mechanics: formulations according to Newton, Lagrange and Hamilton, corresponding equations of motion, conservation laws/conserved quantities, ensembles
Born-Oppenheimer approximation, potential energy surfaces
Computational methods for molecular geometries and properties: valence force fields, semi-empirical, ab initio (Hartree-Fock and beyond) and density functional methods, incorporation of solvent effects by continuum approaches, conceptual DFT derived properties like electronegativity, hardness, Fukui functions and reactivity descriptors
Experimental protein-substrate complexes, X-ray structures from the protein database. Basics of protein strucure prediction: bioinformatics tools necessary for constructing 3D-structure models of relevant but unknown proteins from experimentally know ones by homology modelling.
Monte Carlo and molecular dynamics approaches:
basic ideas and techniques of MC and MD, introduction of different ensembles, long-range forces and boundary conditions. Applications in protein homology modelling and thermodynamic cycles for Free Energy calculations.

Teaching methods
a) Lecture (2 hours per week)
b) Computer exercises (1 hour per week or block course)

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 exam

Module applicability
M.Sc. Chemistry

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

Module coordinator and lecturer
R. Franke

Further information

Industrial Computational Chemistry II: Applications in Process Development					
Module 9.9	**Credits** 5 CP	**Workload** 150 h	**Term** 3. Sem	**Frequency** WS	**Duration** 1 Semester
Courses a) Lectures b) Exercises			**Contact hours** a) (2 SWS) b) (1 SWS)	**Self-Study** 100 h	**Group size** ~ 20 students

Prerequisites

Learning outcomes
Students become aquainted with various theoretical tools used within projects for process development.
Essential contributions of computational chemistry are in the field of chemical and physical properties of complex systems, in development and understanding of reaction mechanism, and in microkinetic modelling.
Important issues in industrial research are the timelines of projects. These and the inherent limitations of methods determine the milestone plans of industrial computational chemistry projects.

Content
- Short overview of the chemical business.
- Introduction into innovation management and new product development in chemical industry.
- Short overview of project management.
- A recapitulation of mixed phase thermodynamics with focus on gases and liquids is given.
- Group contribution methods commonly used in process sythesis are briefly introduced.
- The semiempirical COSMO-RS approach is derived and its use and limitations are illustrated.
- Gibbs ensemble Monte Carlo and molecular dynamics methods using empirical force fields for calculation of industrial relevant phase diagrams are illustrated.
- Calculations of thermodynamical properties of gas-phase reactions with emphasis of highly accurate ab initio methods are reviewed.
- Generic aspects of catalysis are recapitulated.
- Short overview of important homogeneously catalysed reactions in chemical industry is given.
- The formulation of the system of differential equations describing the microkinetics of a catalytic cycle based on the Christiansen formalism is introduced.
- Selected examples of computational chemistry research projects on homogeneous catalysis are discussed.

Teaching methods
a) Lecture (2 hours per week)
b) Computer exercises (1 hour per week or block course)

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 exam

Module applicability
M.Sc. Chemistry

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

Module coordinator and lecturer
R. Franke

Further information

Scientific Programming Methods for Chemists					
Module 9.10	**Credits** 5 CP	**Workload** 150 h	**Term** 2. or 4. Sem.	**Frequency** only in SoS	**Duration** 1 Semester
Courses a) Lecture "Scientific Programming Methods for Chemists" b) Exercises for Scientific Programming Methods for Chemists			**Contact hours** 3 SWS	**Self-Study** a) 30 h b) 75 h	**Group size** 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
Master of Science in Chemistry and Master‘s program Molecular Sciences – Spectroscopy and Simulation (iMOS)

Weight of the mark for the final score
by CP

Module coordinator and lecturer(s)
R. Schmid, C. Haettig

Further information

Electronic and Molecular Structure Theory

Module	Credits	Workload	Term	Frequency	Duration
9.11	9 CP	270 h	2. Semester	Each SuS	1 Semester

Courses	Contact hours	Self-Study	Group size
a) Lectures b) Exercises c) Integrated computer practical	a+b) 3 SWS c) 5 SWS	a) 30 h b) 75 h c) 75 h	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

In-depth Practical in Theoretical Chemistry

(up to three such modules in Theoretical Chemistry during winter semester 1 and summer semester 2)

Module	**Credits**	**Workload**	Term	Frequency	Duration
9.12	8 CP	240 h	1.+2. Sem.	Every semester	1 Semester
Courses			**Contact hours**	**Self-Study**	**Group size**
Computer lab course			9 SWS	105 h	5-10 students

Prerequisites

Methodological and computational working knowledge in Theoretical Chemistry at the level of the B.Sc. Chemistry degree at RUB subject to specialization in Theoretical Chemistry

Learning outcomes

Advanced knowledge of the use of computational methods employed in state-of-the-art research in order to understand the properties of (bio)molecular systems in the broadest sense, critical assessment of the scope and limitations of various approaches/approximations in theoretical and computational (bio)chemistry, visualization and presentation of results, gaining first insights into simple programming. Team working and collaboration while carrying out virtual experiments, general knowledge of operating systems, software and computing close to the level of state-of-the-art research in Theoretical Chemistry, presentation of the research results close to the level of scientific publications in Theoretical Chemistry

Content

This computer practical is composed of several independent compact courses which are devoted to specific topics. Some examples are provided here, but the specific options are subject to the preferences of the students and adjustments depending on advances in Theoretical Chemistry:
Module on classical molecular dynamics and molecular modeling: Simulating structure and dynamics of selected (bio)molecular condensed phase systems at finite temperature and subject to periodic boundary conditions, such as molecular liquids and solutions, critical evaluation and/or generation of interatomic potentials.
Module on electronic structure and spectroscopy: Computing electronic properties, response properties and spectra of selected molecules, clusters, and complexes using wavefunction-based methods or density functional theory (DFT).
Module on molecular structure and reactions: Computing accurate equilibrium structure with various quantum chemistry methods, searching reaction pathways and transition states, accurate calculations of reaction and activation enthalpies.
Module of solid state and surface calculations: Computation of two and three-dimensional periodic structures including crystal surfaces with vacancies, adatoms, admolecules, thermodynamic description of condensed matter.

Teaching methods

Hands-on computer course with integrated seminar (9 hours per week per module): These blocked courses take place during either the first or second half of a given semester and might take place embedded within the research groups or in our Virtual Lab “Theoreticum” both subject to very intense supervision by experienced teaching assistants. The virtual experiments must be introduced (“motivation”), presented in terms of tables, graphs, text and critically discussed (“results and discussion”) as well as summarized (“abstract”) and concluded (“conclusions and outlook”) in a practical report that notably also includes an concise introduction into the corresponding methodological and computational underpinnings (“methods and computational details”) all with pertinent references, thus overall mimicking a short scientific publication.

Mode of assessment

The virtual experiments must be completed successfully and written up satisfactorily in terms of a practical report as outlined above.

Requirement for the award of credit points

Acceptance of the practical report based on the formal criteria outlined above.

Module applicability

M.Sc. Chemistry and M.Sc. Biochemistry (Focal Point Program “Biomolecular Chemistry”)

Weight of the mark for the final score

According to CP
Module coordinator and lecturer(s) J. Behler, C. Hättig, D. Marx, L. Schäfer
Further information Module can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program “Biomolecular Chemistry”

Focal-point Research Practical in Theoretical Chemistry					
Module 9.13	**Credits** 15 CP	**Workload** 450 h	**Term** 3. Sem.	**Frequency** Each WiSe	**Duration** 1 Semester
Courses Computational research practical			**Contact hours** 15 SWS	**Self-Study** 225 h	**Group size** 5 – 10 Students

Prerequisites
Methodological and computational working knowledge in Theoretical Chemistry at the level of the B.Sc. Chemistry degree at RUB subject to specialization in Theoretical Chemistry

Learning outcomes
Planning of a self-contained research project, advanced knowledge of the use of computational methods employed in state-of-the-art research in order to understand the properties of (bio)molecular systems in the most general sense, critical assessment of the scope and limitations of various approaches/approximations in theoretical and computational (bio)chemistry in the broadest sense, visualization, written and oral presentation of results, simple programming tasks, critical evaluation of the relevant scientific literature, writing of a practical report that mimicks state-of-the-art scientific publications. Team working and collaboration while carrying out virtual experiments, general knowledge of operating systems, software and computing close to the level of state-of-the-art research in Theoretical Chemistry, presentation of the research results close to the level of scientific publications in Theoretical Chemistry.

Content
This research computer practical can be devoted to a topic that is covered by one of the research groups in the field of Theoretical Chemistry at RUB. The specific topic can be in subjects such as computational inorganic chemistry, biochemistry, organic chemistry, physical chemistry, solvation science, surface science, or materials science. The corresponding research groups can be found on the homepage of the Fakultaet as well as the research fields that are currently covered by these groups in their contemporary scientific research. A critical component is the practical or lab report which should mimic a typical scientific publication.

Teaching methods
This research computer practical typically takes place within a specific research group where the student is hosted together with other group members. This will also involve teamwork and collaboration typically within the group but possibly also involving experimental groups depending on the topic. There will be close contact to the group members as well as with the group leader and/or an experienced coworker. The latter provide feedback during and on the virtual experiments as well as feedback on the written lab report supervised by teaching assistants. In The virtual experiments must be introduced (“motivation”), presented in terms of tables, graphs, text and critically discussed (“results and discussion”) as well as summarized (“abstract”) and concluded (“conclusions and outlook”) in a practical report that notably also includes an concise introduction into the corresponding methodological and computational underpinnings (“methods and computational details”) all with pertinent references, thus overall mimicking a short scientific publication.

Mode of assessment
The virtual experiments must be completed successfully and written up satisfactorily in terms of a practical report as outlined above.

Requirement for the award of credit points
Acceptance of the practical report based on the formal criteria outlined above.

Module applicability
M.Sc. Chemistry and M.Sc. Biochemistry (Focal Point Program “Biomolecular Chemistry”)

Weight of the mark for the final score
According to CP

Module coordinator and lecturer(s)
J. Behler, C. Hättig, D. Marx, L. Schäfer

Further information
Module can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program “Biomolecular Chemistry”

Crossdisciplinary Lectures and Practicals

Introduction to Computational Chemistry					
Module 10.1	**Credits** 4 CP	**Workload** 120 h	**Term** x. Sem.	**Frequency** Every WS	**Duration** 1 Semester
Courses a) Lecture (2h per week) b) Hands on exercises (HoE) with a 1h Q&A session per week (online)			**Contact hours** 3 SWS	**Self-Study** 5h per week (including HoE)	**Group size** about 10-15 students

Prerequisites
None

Learning outcomes
Students who have finished this course will ...

- have basic knowledge about modern computational chemistry methods, ranging from force field models over density functional theory to wave function based post-Hartree-Fock electronic structure methods.
- be able to apply such methods for routine applications in their future scientific work.
- are able to understand and assess the quality of computational chemistry applications in publications and other scientific studies.

Content
Within this module basic concepts in computational chemistry are discussed. The following methods to compute a potential energy surface of a chemical system are discussed:

- Force Field methods and parameterized models
- Density Functional Theory (DFT) based methods
- Post Hartree-Fock methods to include electron correlation

The following concepts and methods are treated in the module:

- Optimizing structures and transition states
- Basic concepts of Molecular Dynamics simulations
- Periodic Boundary Conditions for crystalline systems
- Exchange and Correlation Functional in DFT
- Basis sets for the representation of electronic wave functions (and densities)
- Frequency analysis, vibrational spectra and calculation of thermochemical data
- Working with computational chemistry codes (on LINUX environments)
- Using modern GUIs for performing computations

Teaching methods
Lecture, Hands on exercises on own laptop (BYOD) for different methods during the semester, Q&A sessions (online) by student assistants and support from student assistants by a specific messaging server to ask questions. Content is provide via a Moodle course.

Mode of assessment
Oral examination based on results from Hands on Exercises

Requirement for the award of credit points
Passing of oral exam

Module applicability
Master of Science in Chemistry, IMOS

Weight of the mark for the final score: by CP

Module coordinator and lecturer(s): Prof. Dr. Christof Hättig, Prof. Dr. Christian Merten, Prof. Dr. Rochus Schmid

Further information

From top-level science to top-level business

Module	Credits	Workload	Term	Frequency	Duration
10.2	5 CP	125 h	x. Sem.	Only WS	1 Semester

Courses	Contact hours	Self-Study	Group size
a) Seminar b) Lecture	3 SWS	90 h	30 Students

Prerequisites
The module is intended for students from the 5th semester onwards in the Bachelor's and Master's degree in addition to doctoral students, but without exclusion criteria. Previous knowledge, especially in business administration or corporate law, is explicitly not required.

Learning outcomes
After successful completion of the module

- students develop business ideas using different creativity techniques
- design their ideas using different prototyping methods
- understand how to define target groups
- select appropriate methods for customer interviews
- students master the presentation technique of pitching

Content
The module pursues the overarching goal of sensitising students and doctoral students of chemistry and related, similarly basic science degree programmes to a possible business start-up. To this end, the students are not only provided with basic knowledge on how to start a business, but also with tools to first develop an idea of a business model that suits their specific professional and/or methodological skills and to identify ways to master the transfer from science to practice. Personal experience reports by successful founders, who all have a strong background in basic research at the RUB, additionally provide vivid practical reports as "role models" in personal contributions. In addition to these practical reports, the participants benefit from the involvement of experts from different disciplines, such as customer interviews or pitching, who convey content in an application-oriented manner and enable the students to apply it independently. International external experts also help the participants to broaden their horizons.

Teaching methods
Seminar-based teaching, group work, digital teaching formats.

Mode of assessment
On the last day of the course, there is a 10-minute presentation of an individual business idea in group work using the creative techniques learned for business model generation. In addition, students are required to submit an individual guideline-based short reflection on the learned content one week later.

Requirement for the award of credit points
Successful final presentation as well as timely submission of the guideline-based reflection.

Module applicability

Weight of the mark for the final score
The decisive assessment criterion is the group presentation of the business idea. The guiding question-based reflection has an individual effect with tendencies of one mark level.

Module coordinator and lecturer(s)
K. Tschulik, A. Beyer, F. Lehmann

Further information

Introduction to Chemistry of Materials (lecture series)					
Module 5.2	**Credits** 5 CP	**Workload** 150 h	**Term** 1, 3	**Frequency** Each WS	**Duration** 1 Semester
Courses e) Lecture series f) Guest lectures, colloquia			**Contact hours** e) 150 h	**Self-Study** 75 h	**Group size** Students of the respective semester, ca. 40

Prerequisites

Admission to Master Course Program: Basic knowledge of general, inorganic, and analytical chemistry; fundamental knowledge on material synthesis and properties.

Learning outcomes

- The purpose of this module is to familiarize students with important but selected examples of advanced materials and issues relating to their advantages, disadvantages and limitations
- Guiding the students to get an overview of various interdisciplinary research topics ranging from materials synthesis to their properties and applications
- The module will provide a knowledge basis and orientation for the students to choose from the various elective courses offered within the Focal Point Functional Materials; students communicate and discuss with active scientists (e.g. "colloquia", guest lectures).

Content

- A series of topics in the field of Functional Materials are covered by this overarching module. The team teaching covers topics that bridge chemistry and processing of materials for technological applications with an emphasis on solid state materials. Examples are drawn from industrial practice in semiconductor manufacturing, protective coatings, energy generation and storage, to emerging technologies such as batteries, sensors, electronic devices, antifouling coatings etc.
- The detailed contents of this module will be composed from selected research areas currently including the following:
  - Semiconductor, electronic and optoelectronic materials: processing and application
  - Mesoporous materials for catalysis and sensors
  - Protective coatings
  - Materials for energy conversion and electrochemical sensing

Teaching methods

Lecture with seminars

Mode of assessment

End-of-term written exam

Requirement for the award of credit points

Passing the written examination

Module applicability

Chemistry (Master)

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

Anjana Devi, Axel Rosenhahn, Ferdi Schüth, Kristina Tschulik

Further information

In-depth practical: Solid State and Material Synthesis

Module	**Credits**	**Workload**	**Term**	**Frequency**	**Duration**
5.3	8 CP	225 h	1^{st} to 3^{rd} Sem.	WS and SoS	6 Weeks
Courses			**Contact hours**	**Self-Study**	**Group size**
Analytical Methods in Inorganic Chemistry (Lab practical)			160 h	80 h	Individual

Prerequisites
Basic Understanding of general chemistry, inorganic and materials chemistry and analytical methods

Learning outcomes
After successful completion of this practical, the students

- will be able to independently apply or transfer materials synthesis skills and methods to other scientific contexts which may be connected with or dependent on materials chemistry.
- Hands-on experience in performing selected material synthesis via solid state, vapor phase or wet chemical routes frequently used in inorganic materials chemistry
- A practical understanding of materials synthesis and material analysis
- Analyze and professionally report / document analytical data

Content
In this lab practical, the students will further develop the experimental skills at an advanced level and introduces modern materials processing techniques closely related to the various research areas of the scientific supervisor (guided by PhD or Postdoc). The student will be trained in critical thinking and evaluation of obtained data related to challenges in materials synthesis and characterisation. After completion of the module, the student will be able to independently apply or transfer these skills and methods to other scientific contexts which may be connected with or dependent on materials chemistry.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a scientific publication and oral presentation

Requirement for the award of credit points
Active participation in lab work, successful completion of written report and oral presentation

Module applicability
Master Chemistry

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

Module coordinator and lecturer(s)
Ulf-Peter Apfel, Lars Borchardt, Anjana Devi

Further information

Research Practical: Functional Materials

Module	Credits	Workload	Term	Frequency	Duration
5.4	15 CP	450 h	3rd Sem.	WS and SoS	3 Months
Courses Functional Materials (Lab practical)			**Contact hours** 320 h	**Self-Study** 130 h	**Group size** Individual

Prerequisites
Advanced Understanding of Materials Chemistry, including synthesis and analytical methods

Learning outcomes
After successful completion of this practical, the students have
- advanced expertise in materials chemistry, including synthesis, analytical or computational methods as applicable to the project
- a good practical understanding of materials chemistry

The students are able to
- select suitable material systems to address a given problem
- select suitable methods and plan their research to solve the given problem
- execute their research under supervision of a mentor
- professionally analyze and document their data according to the established scholarly standards in materials chemistry

Content
The research practical will be performed as part of an ongoing research project, forming by itself a small independent project. Content will include a literature search, identification, and application of suitable methods (e.g., materials synthesis, analytical techniques), and independent execution of the work, in close interaction with the supervisor / mentor. The research topic will be in the scientific project of the supervisor.

Teaching methods
Lab practical

Mode of assessment
Written report, typically in the form of a project proposal or manuscript and oral presentation

Requirement for the award of credit points
Active participation in lab work, successful completion of written report and oral presentation

Module applicability
Master Chemistry, master of engineering

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

Module coordinator and lecturer(s)
Ulf-Peter Apfel, Lars Borchardt, Anjana Devi

Further information

Master Thesis					
Module 11	**Credits** 30 CP	**Workload** 900 h	**Term** 4. Sem.	**Frequency** Any time	**Duration** 1 Semester
Courses Master Thesis			**Contact hours**	**Self-Study**	**Group size** 1

Prerequisites
"Practical Science and Communication" and Focal-Point Practical

Learning outcomes
The Master Thesis is the written presentation of an experimental study on a chemical subject, including the interpretation of the experimental data and the evaluation within the scientific context. Within 6 months of working time the participants should prove their ability to apply modern methods for solving or investigating a scientific problem self-reliently in the field of chemistry.

Content
Cooperation within a scientific research group
Literature survey for a scientific project
Introduction to spezialized scientific methods
Planing, performing, analyzing and evaluating scientific experiments
Presentation of scientific results

Teaching methods
Coaching

Mode of assessment

Requirement for the award of credit points
Master Thesis accepted as sufficient or better by two lecturers

Module applicability

Weight of the mark for the final score
According to CP

Module coordinator and lecturer(s)
All lecturers affiliated with the study program for M. Sc. Chemistry

Further information