Friedrich-Alexander-Universität
Erlangen-Nürnberg

Module description

for the degree programme

Master of Science

Molecular Science

(Version of examination regulation: 20202)

Table of contents

1	**Module name** 1999	**Masterarbeit (M.Sc. Molecular Science 20202)** Master's thesis	**30 ECTS**
2	Courses / lectures	No courses / lectures available for this module! Please note: • The master's thesis will be written at the student's choice normally in one of the research groups of the Department of Chemistry and Pharmacy or the Department of Biology! • Students must independently apply for a master's thesis in one of the department's research groups!	
3	Lecturers	No lecturers available since there are no courses / lectures for this module!	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	Written elaboration in form of a scientific manuscript with a length of approx. 20,000 words. It describes the scientific findings as well as the way leading to these findings. It contains justifications for decisions regarding chosen methods for the thesis and discarded alternatives. The student’s own substantial contribution to the achieved results has to be evident. In addition, the student presents his work in a seminar, in which the scientific quality and the scientific independence of his achievements are evaluated. Workload: 900h
6	**Learning objectives and skills**	Students • demonstrate their ability to perform independent scientific work focusing on an adequately challenging research topic. • rank their own research results in the context of current literature and research papers in the field and record their results in appropriate scientific writing and documentation style. • give oral and written presentations of the results and acquired knowledge in an appropriate scientific style in English language.
7	**Prerequisites**	Admission to the M. Sc. program Molecular Science, successfully passed core modules, mandatory elective, elective and research modules
8	**Integration in curriculum**	semester: 4
9	**Module compatibility**	Pflichtmodul Master of Science Molecular Science 20202
10	**Method of examination**	Written (6 Monate) • Thesis (3 hard copies in bound form + electronic version) with a length of approx. 20,000 words; • Referee report, 2 experts
11	**Grading procedure**	Written (100%) Averaged grade of the two reports
12	**Module frequency**	every semester
13	**Resit examinations**	The exams of this moduls can only be resit once.
14	**Workload in clock hours**	Contact hours: 675 h

		Independent study: 225 h
15	**Module duration**	1 semester
16	**Teaching and examination language**	english
17	**Bibliography**	no Bibliography information available!

Studienrichtung Drug Discovery

1	**Module name** 63066	**Biology-informed Drug Discovery** Concepts in biology	**10 ECTS**
2	Courses / lectures	Vorlesung: Biology-informed drug discovery (2 SWS)	-
3	Lecturers	Prof. Dr. Anja Lux Prof. Dr. Andreas Burkovski Prof. Dr. Lars Nitschke Prof. Dr. Thomas Winkler Prof. Dr. Christian Koch Prof. Dr. Steffen Backert Prof. Dr. Yves Muller Prof. Dr. Markus Albert	

4	**Module coordinator**	Prof. Dr. Yves Muller
5	**Contents**	Basic biology concepts of importance for the drug discovery process. The lectures cover three main topics, namely (i) selected experimental methods, (ii) the use of model organisms in drug discovery and (iii) the discussion of the biology of specific classes of drugs, namely antibodies and natural products. Part (i) focusses on omics methods (genomics, transcriptomics, proteomics, metabolomics) in drug target identification and drug validation as well as on the biological readout of high-throughput screening techniques. In addition, the question how to gain atomic insight into macromolecular drug targets is addressed by covering the topics of molecular modelling, nuclear magnetic resonance spectroscopy, X-ray crystallography and cryo-electron microscopy. In part (ii) basic methods in molecular biology are reviewed and the following model organisms are being addressed: Yeast as a not yet fully explored model organism for the identification of novel drug targets. The production of recombinant proteins and the synthesis of small molecule drugs by yeasts and aspergillus species are discussed. Plants as even less well characterized organisms for drug discovery, target screening and drug production as well as the third model organism mice and how the latter are exploited as disease model systems. Topics are: xenograft tumour models in mice and genetic mouse models for inherited diseases and tumour diseases. In part (iii) the isolation, production and use of monoclonal antibodies are being discussed together with natural products. A particular focus of the latter are novel antibiotic drugs and their role in the fight against increasingly prevalent bacterial infections. In addition, several concepts to enhance the targeted delivery of natural products are evaluated, using model dispositions, such as coeliac disease.
6	**Learning objectives and skills**	Learning objectives are the acquaintance of novel insights, concepts, and methods in biology-informed drug discovery. To be able to understand state-of-the-art methods/concepts in drug discovery and to critically assess the potential and limitations of the individual methods/ concepts. To be able to independently develop working hypotheses and to design experimental approaches to further the drug discovery process.

		As an integral part of the module, each student will have to present the content of a primary research article in a seminar presentation of approximately 20 minutes. Each student acquires the skill to understand, present, and critically discuss primary research reports in the field of drug discovery and to defend the findings before an audience. Attendance of the student presentations is mandatory. Only regular attendance of these student presentations will lead to a successful completion of the module. Justification: The learning objectives of this part can only be reached if the students actively discuss their literature findings with fellow students.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Drug Discovery Master of Science Molecular Science 20202
10	**Method of examination**	Written examination (90 minutes) PL: Written examination, 90 minutes
11	**Grading procedure**	Written examination (100%) (**Please note:** The grade of module "Biology-informed Drug Discovery"*, former: Concepts in Biology,* is only a part of the total grade of module package "Drug Discovery"!) Grading procedure of **"Drug Discovery"**: Medicinal Chemistry 25% + Biology-informed Drug Discovery *(former: Concepts in Biology)* 25% + Molecular Modeling 25% + Drug Discovery-Lab (Graded lab protocol) 25%
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 60 h Independent study: 240 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english
16	**Bibliography**	Course material is provided via the StudOn platform

1	**Module name** 63068	**Drug Discovery - Lab** Drug discovery - Lab	**10 ECTS**
2	Courses / lectures	Praktikum: Drug Discovery - LAB (15 SWS) 1) Lab course Biomolecular simulations (5 SWS) 2) Lab course Pharmacopeia-based drug analysis (5 SWS) 3) Lab course Instrumental and Bioanalytics (5 SWS) (Please note: Attendance in all lab courses and safety instructions is compulsory!)	10 ECTS
3	Lecturers	Prof. Dr. Jutta Eichler Prof. Dr. Monika Pischetsrieder Prof. Dr. Petra Imhof Prof. Dr. Simon Hammann	

4	**Module coordinator**	Prof. Dr. Monika Pischetsrieder
5	**Contents**	3 independent practical courses focusing on biomolecular simulations (block, 5 SWS), Pharmacopoeia-based drug analysis (block, 5 SWS) and instrumental analytical techniques (block, 5 SWS)
6	**Learning objectives and skills**	The students are able • to understand the basic and advanced principles of Pharmacopoeia-based drug analysis, instrumental and bioanalytics as well as computer chemistry-based applications in the field of modern drug research • to utilize modern instrumental analytical techniques for characterisation of samples and quantification of target analytes • to apply modern simulation techniques for the modeling of biomolecules • to interpret and to critically summarize experimental results in written form (lab report)
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Drug Discovery Master of Science Molecular Science 20202
10	**Method of examination**	Practical achievement pÜL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)
11	**Grading procedure**	Practical achievement (100%) (**Please note:** The grade of module "Drug Discovery - Lab" is only a part of the total grade of module package "Drug Discovery"!) Grading procedure of **"Drug Discovery"**: Medicinal Chemistry 25% + Concepts in Biology 25% + Molecular Modeling 25% + Drug Discovery-Lab (Graded lab protocol) 25%
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 225 h Independent study: 75 h

14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	Manuscripts are available on StudON

1	**Module name** 63065	**Medicinal Chemistry** Medicinal chemistry	**10 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Medicinal Chemistry (3 SWS)	-
3	Lecturers	Dr. Dorothée Weikert Prof. Dr. Peter Gmeiner Prof. Dr. Andriy Mokhir Prof. Dr. Nicolai Burzlaff Prof. Dr. Jutta Eichler Prof. Dr. Monika Pischetsrieder Prof. Dr. Markus Heinrich Dr. Jürgen Einsiedel Dr. Stefan Löber Prof. Dr. Susanne Mühlich	

4	**Module coordinator**	Prof. Dr. Peter Gmeiner
5	**Contents**	Genomics, transcriptomics, proteomics; in-vitro assay systems, assay technology; target screening and drug production in plants, drug screening and production in yeast; experimental structural biology; chemoinformatics; molecular modeling: molecular dynamics simulation, force-fields, modeling of proteins, proteinligand docking; drug synthesis and combinatorial chemistry; redox-active metal complexes, metalloenzyme inhibitors; stereochemistry in drug design; organic reactions in medicinal chemistry; drug metabolism; peptidomimetics;
6	**Learning objectives and skills**	The students are able • to understand the basic and advanced principles of medicinal chemical, molecular biological and Computer chemistry based applications in the field of modern drug design research
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Drug Discovery Master of Science Molecular Science 20202
10	**Method of examination**	Written examination (90 minutes)
11	**Grading procedure**	Written examination (100%) (**Please note:** The grade of module "Medicinal Chemistry" is only a part of the total grade of module package "Drug Discovery"!) Grading procedure of **"Drug Discovery":** Medicinal Chemistry 25% + Concepts in Biology 25% + Molecular Modeling 25% + Drug Discovery-Lab (Graded lab protocol) 25%
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 90 h Independent study: 210 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english

16	**Bibliography**	G. Klebe, Drug Design: Methodology, Concepts, and Mode-of-Action, Springer 2013

1	**Module name** 63067	**Molecular Modelling** Molecular modelling	**10 ECTS**
2	Courses / lectures	Seminar: Modelling of Complex Systems (2V/1UE) (3 SWS)	-
3	Lecturers	Prof. Dr. Dirk Zahn Prof. Dr. Petra Imhof	

4	**Module coordinator**	Prof. Dr. Petra Imhof
5	**Contents**	*WS:* • Rationalizing Complex Systems from Statistics: Probability distributi-ons, Concepts of Information and Entropy; • Thermodynamics of Monte-Carlo simulation and state-of-the art ana-lyses of transition pathways; • Molecular dynamics simulations of complex systems: data evaluation and reduction to key information. *SS:* • Model building and setup of first-guess configurations; • Enhanced sampling techniques to tackle manifolds of configurations and to find reaction paths; • Machine-learning and prediction of real-world properties from molecular data.
6	**Learning objectives and skills**	Students • master the basics of molecular modelling, • are able to select and apply from a wide range of different simulation techniques the one that is relevant and suitable for different problems, • can analyse, evaluate and present data and results, • monitor and control their own progress.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Drug Discovery Master of Science Molecular Science 20202
10	**Method of examination**	Written examination (90 minutes)
11	**Grading procedure**	Written examination (100%) (**Please note:** The grade of module "Molecular Modelling" is only a part of the total grade of module package "Drug Discovery"!) Grading procedure of "**Drug Discovery"**: Medicinal Chemistry 25% + Concepts in Biology 25% + Molecular Modeling 25% + Drug Discovery-Lab (Graded lab protocol) 25%
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 90 h Independent study: 210 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english

16	**Bibliography**	• B. Smit, D. Frenkel: Understanding Molecular Simulation: From Algo-rithms to Applications • A. Leach: Molecular Modelling: Principles and Applications

Studienrichtung Molecular Nanoscience

1	**Module name** 63071	**Molecular Nanoscience I** Molecular nanoscience I	**15 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Self-Assembly: Molecular, Particulate and Hybrid Nanostructures (3 SWS) Seminar: Seminar Self-Assembly: Molecular, Particulate and Hybrid Nanostructures (1 SWS) Seminar: Supramolecular Chemistry and Molecular Materials (2 SWS) Seminar: Nanoprobes (2 SWS) Seminar: From 2D assemblies to bulk (2 SWS) Seminar: Molecular Nano Science (winter semester) (2 SWS)	- - - - - -
3	Lecturers	Prof. Dr. Franziska Gröhn Prof. Dr. Andreas Hirsch Prof. Dr. Henry Dube Prof. Dr. Rainer Fink Prof. Dr. Julien Bachmann	

4	**Module coordinator**	Prof. Dr. Rainer Fink Prof. Dr. Andreas Hirsch
5	**Contents**	• Concepts in supramolecular chemistry; host-guest chemistry; energetics of supramolecular complexes: experimental methods; templates and self-assembly. Molecular devices. Supramolecular catalysis: principles of supramolecular catalysis, supramolecular metal catalysis, self-assembled catalysts, metal-free catalysis, enzyme mimics, antibodies, imprinted polymers. • Nanoscaled systems, general issues of microscopic techniques; experimental techniques with nanometer resolution: resolution determination; image processing techniques, light microscopic techniques with light in the visible and IR range, confocal techniques, scanning probes (STM,AFM and related scanning probes). • Specific topics in synthesis and analysis of specific molecule-based nanoscale objects • 2D film fabrication techniques (PVD, ALD, etc.)
6	**Learning objectives and skills**	The students are capable ... • to explain the fundamental chemical and physical properties of nano-scale materials • to distinguish and to compare some properties, structure and applications of different nanomaterials • to describe and to evaluate the major concepts in supramolecular chemistry, molecular self-assembly and nano-scaled 2D materials and transfer knowledge to related topics • to judge on potential nano-analytical tools with optimized image contrast

7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Molecular Nanoscience Master of Science Molecular Science 20202
10	**Method of examination**	Oral O30 (PL): Oral Examination, 30 Minutes
11	**Grading procedure**	Oral (100%) (Please note: The grade of module "Molecular Nanoscience I" is only a part of the total grade of module package "Molecular Nanoscience"!)
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 150 h Independent study: 300 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 63072	**Molecular Nanoscience II** Molecular nanoscience II	**15 ECTS**
2	Courses / lectures	Vorlesung: Molecular Switches and Molecular Machines (2 SWS) Vorlesung: Carbon allotropes: from characterization to applications (2 SWS) Seminar: Nanoprobes (2 SWS) Vorlesung: Modelling & Simulations (2 SWS) Vorlesung: Inorganic Nanoparticles & Supraparticles (2 SWS) Seminar: Molecular Nano Science (summer semester) (2 SWS)	- - - - - -
3	Lecturers	Prof. Dr. Henry Dube Prof. Dr. Dirk Michael Guldi Prof. Dr. Rainer Fink Prof. Dr. Dirk Zahn Prof. Dr. Bernd Meyer Prof. Dr. Karl Mandel Prof. Dr. Andreas Hirsch Prof. Dr. Franziska Gröhn	

4	**Module coordinator**	Prof. Dr. Andreas Hirsch
5	**Contents**	• Concepts in supramolecular chemistry; molecular switches, molecular machines; • Nanoanalytical tools with charged particle: ion microscopy (FIM, HeIM, Nano-SIMS), electron microscopy (PEEM, LEEM, SEM, (S)TEM), aberration correction, x-ray tools, hybrid type microscopies; coherent imaging; 3D imaging (tomography, laminography) • Carbon allotropes: from molecules to carbon nanodots, fullerenes, carbon nanotubes and nanohorns; synthesis, properties and applications. • Inorganic nanoparticles and industrial applications, synthesis methods, sol-gel science and technology, concept of inorganic supraparticles & practical assembly techniques; characterization methods for supraparticulate systems; applications of supraparticles. • Modelling of molecular materials, molecular assembly, molecular dynamics • Specific topics in molecular nanoscience
6	**Learning objectives and skills**	The students are capable ... • to explain the fundamental chemical and physical properties of nano-scale materials • to distinguish and to compare some properties, structure and applications of different nanomaterials

		• to describe and to evaluate the major concepts in supramolecular chemistry, molecular machines, self-assembly and supraparticules, or carbon allotropes and transfer this knowledge to related topics • to judge on potential nano-analytical tools with optimized image contrast
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Molecular Nanoscience Master of Science Molecular Science 20202
10	**Method of examination**	Oral O30 (PL): Oral examination, 30 Minutes
11	**Grading procedure**	Oral (100%) (Please note: The grade of module "Molecular Nanoscience II" is only a part of the total grade of module package "Molecular Nanoscience"!)
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 180 h Independent study: 270 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• E. Katz: Molecular and Supramolecular Information Processing", Wiley-VCH • D. Attwood: Soft x-rays and extreme ultraviolet radiation" (Cambridge); C. Jacobsen: X-ray microscopy" (Cambridge) • L. Reimer: Scanning electron Microscopy (Springer, 2020) and others

1	**Module name** 63073	**Molecular Nanoscience - Lab** Molecular nanoscience - Lab	**10 ECTS**
2	Courses / lectures	Praktikum: Molecular Nanoscience - Lab (7 SWS) • Attendance in lab course is compulsory! • Attendance at safety instruction is compulsory! • Attendance in winter or summer term possible! • A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de	-
3	Lecturers	Prof. Dr. Andreas Hirsch Prof. Dr. Julien Bachmann Prof. Dr. Rainer Fink	

4	**Module coordinator**	Prof. Dr. Rainer Fink
5	**Contents**	Research practicals in selected modern fields of molecular nanoscience: Topics according to an annually updated list of experiments, which includes molecule or nanoparticle synthesis, spectroscopic and microscopic analysis, thin-film and device preparation, characterization
6	**Learning objectives and skills**	The students are capable ... • to use their theoretical and practical background to plan and perform advanced research experiments under supervision of experienced scientists • to synthesize nanoscaled materials • to interprete spectroscopic or microscopic data taking advantage of modern research tools • to provide a state-of-the-art documentation and discussion of their experimental results • to present, communicate and discuss scientific results in scientific english.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Studienrichtung Molecular Nanoscience Master of Science Molecular Science 20202
10	**Method of examination**	Practical achievement
11	**Grading procedure**	Practical achievement (100%) (Please note: The grade of module "Molecular Nanoscience - Lab" is only a part of the total grade of module package "Molecular Nanoscience"!)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 225 h Independent study: 75 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english

16	**Bibliography**	Lecture notes from the various course lectures in Molecular Nanoscience" (see module descriptions "Molecular Nanoscience-I" and "Molecular Nanoscience-II")

Advances in bioorganic and bio-inorganic chemistry

1	**Module name** 46511	**Advanced Bio-Organic and Bio-Inorganic Chemistry** Advanced bio-organic and bio-inorganic chemistry	**5 ECTS**
2	Courses / lectures	Seminar: Seminar Advanced Bioinorganic Chemistry, Metalloenzymes and Metals in Medicine (1 SWS)	-
3	Lecturers	Prof. Dr. Nicolai Burzlaff Prof. Dr. Norbert Jux	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • are introduced into recent activities and achievements in the fields • of bioorganic and bioinorganic chemistry and metals in medicine: • porphyrins and heme enzymes • PDT • electron transfer (cofactors, ferredoxins, inner sphere mechanism, outer sphere mechanism, Marcus theory) • photosynthesis • copper containing proteins and enzymes • nitrogenases and other Mo containing enzymes • drugs based on Pt, Ru, Au and As • biominerals • implant materials and technology
6	**Learning objectives and skills**	The students • are introduced into recent activities and achievements in the fields of bioorganic and bioinorganic chemistry and metals in medicine
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as part of the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester

15	**Teaching and examination language**	english
16	**Bibliography**	• W. Kaim, B. Schwederski, A. Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, 2. Edition, John Wiley & Sons, Ltd, 2013

1	**Module name** 46514	**Bio-Organic and Bio-Inorganic Chemistry - Lab** Laboratory course: Bio-organic and bio-inorganic chemistry	**5 ECTS**
2	Courses / lectures	Praktikum: Bio-Organic & Bio-Inorganic LAB (7 SWS) Please note: Attendance at lab course is compulsory!	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Nicolai Burzlaff Prof. Dr. Norbert Jux Prof. Dr. Carola Kryschi Prof. Dr. Petra Imhof	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • deepen their knowledge in special topics of bioorganic and bioinorganic chemistry and nanomedicine that are in the research focus of the involved research groups of the department depending on their own choice • perform practical studies and small research projects regarding topics of the preparative, mechanistic or more biological bioorganic and bioinorganic chemistry and nanomedicine in an advanced level
6	**Learning objectives and skills**	The students • can characterise and evaluate bioinorganic models • manage the preparation of bioorganic compounds and bioinorganic models as well as synthesis of functionalized nanoparticles, their characterization as well as their application in mechanistic studies • carry out bioorganic and bioinorganic research projects largely independently using a wide range of bioorganic and bioinorganic theories and are able to reflect upon the gained results
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 • Lab module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total!)
10	**Method of examination**	Practical achievement Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)
11	**Grading procedure**	Practical achievement (100%)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 105 h Independent study: 45 h
14	**Module duration**	1 semester

15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46513	**Metallic nanoparticles in Medicine** Metallic nanoparticles in medicine	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Metallic Nanoparticles in Medicine (3 SWS)	-
3	Lecturers	PD Dr. Christina Janko PD Dr. Rainer Tietze Prof. Dr. Carola Kryschi Prof. Dr. Olaf Prante Prof. Dr. Ingrid Span Dr. Stefanie Klein	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • are introduced into recent research activities and achievements in the fields of nanomedicine • evaluate and assess the basic theories, principles and concepts of bioorganic and bioinorganic che- mistry and nanomedicine (in compliance with a research-orientated master course)
6	**Learning objectives and skills**	The students • can explain and reflect upon the bioorganic and bioinorganic nanochemistry aspects in medicinal chemistry and toxicology
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46512	**Special Aspects in Bio-Organic Chemistry** Special aspects in bio-organic chemistry	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Special Aspects in Bio-Organic Chemistry (3 SWS) Please note: • Seminar: time and place by agreement!	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Petra Imhof	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • learn about: nucleic acid structure, synthesis, and reactivity; nucleic acid modifications; nucleic acid-protein interactions, nucleic acid-based drugs, nucleic acid biochemistry, modelling of nucleic acids
6	**Learning objectives and skills**	The students • can explain, apply and reflect upon the theories, terminology, specialities, boundaries and different school of bioorganic and bioinorganic chemistry critically and in depth
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • As Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• A. Bloomfield, D.M. Crothers, I. Tinoco, Jr. „Nucleic Acids: structures, properties, and functions“, University Science Books, Sausalito, CA, USA 1999 • D. L. van Vranken, G. A. Weiss, Introduction to Bioorganic Chemistry and Chemical Biology, 1. Aufl., Garland Publishers 2012, ISBN: 978-0815342144

		• W. Saenger„Principles of Nucleic Acid Structure“,Springer-Verlag New York Inc. 1984 • T. Schlick: "Molecular modelling and simulation: An interdisciplinary guide", Springer New York Dordrecht Heidelberg London 2nd ed. 2010 • A. Vologodskii: “Biophysics of DNA”, Cambridge University press, 2015, DOI 10.1017/CBO9781139542371

Advances in homogeneous catalysts

1	**Module name** 46524	**Homogeneous Catalysis - Lab** Laboratory course: Homogeneous catalysis	**5 ECTS**
2	Courses / lectures	Praktikum: Homogenous Catalysis - Lab (7 SWS) • Attendance in lab course is compulsory! • Attendance at safety instructions is compulsory! • A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de	5 ECTS
3	Lecturers	Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta Prof. Dr. Andriy Mokhir Prof. Dr. Karsten Meyer Prof. Dr. Svetlana Tsogoeva	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	Students • Students get in touch with modern research topics in the field of homogenous catalysis & research tools or advanced spectroscopic tools (Practical work in one of the involved research groups!) • deepens her/his knowledge in special topics of homogeneous catalysis that are in the research focus of the involved research groups • will be trained in the practical aspects of advanced homogeneous catalysis
6	**Learning objectives and skills**	Students • get in touch with modern research topics in the field of homogenous catalysis & research tools or advanced spectroscopic tools • manage the preparation and full characterization of catalysts • learn methods to evaluate catalyst performance in a series of catalytic reactions and are able to discuss scope and relevance
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 • Lab module within the Compulsory Elective Module (20 ECTS)! • Lab module as part of the elective module (5 ECTS, not graded)!
10	**Method of examination**	Practical achievement Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)
11	**Grading procedure**	Practical achievement (100%)
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 105 h Independent study: 45 h

14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46521	**Organometallic Catalysis** Metal-organic catalysis	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Organometallic Catalysis (3 SWS) Seminar: Organometallic Catalysis - Seminar (1 SWS)	- -
3	Lecturers	Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	• Harder: Introduction and basic principles of advanced catalysis, homogeneous vs. heterogeneous catalysis, mechanisms of substrate activation (C=C, C=O), control by ligand and metal choice, classical catalytic cycles: Wilkinson catalyst, C-C cross coupling, hydroformylation, polymerization catalysis, catalysis with main group metals. • Dorta: Review of basic organometallic mechanisms & reactivity (elementary reactions, isolobality); Hydrogenation of alkenes and aromatics; CC cross coupling; Atom-economical CC formation (alkene hydroformylation & hydrocyanation, alkene oligomerization, methanol carbonylation); Synthetic fuels form CO (methanol, MTG, Fischer-Tropsch); Alkene metathesis; Selective CO bond formation (epoxidations and Wacker-type oxidations)
6	**Learning objectives and skills**	The student • understands basic principles and underlying reaction mechanisms in organometallic catalysis • is able to outline reaction mechanisms and catalytic cycles • knows the tools for the characterization of catalysts and how to evaluate catalyst performance • acquires knowledge on topics of current interest and recent breakthroughs in organometallic catalysis
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective module "Advances in Homogenous Catalysis" in M. Sc. Chemistry or Molecular Science (20 ECTS in total, graded) • As Elective Module in M. Sc. Chemistry or Molecular Science (5 ECTS, ungraded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail

12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Fundamentals of Organometallic Catalysis, Dirk Steinborn, Wiley-VCH, 2012 • Early Main Group Metal Catalysis – Concepts and Reactions, Sjoerd Harder, Wiley-VCH, 2020 • Metal-catalysis in Industrial Organic Processes, Gian Paolo Chiusoli & Peter Maitlis, Royal Society of Chemistry, 2019 • Fundamentals of Organometallic Catalysis, Dirk Steinborn, Wiley-VCH, 2012 • Homogeneous Catalysis, Parshall & Ittel, 2nd ed., Wiley Interscience 1992

1	**Module name** 46522	**Organocatalysis and Catalytic Reactions in Water** Organocatalysis and catalytic reactions in water	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Organocatalysis and Catalytic Reactions in Water (3 SWS)	-
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	• History and basic principles of organocatalysis, • Different types of organocatalysts, • Enantioselective organocatalysis, • Domino reactions and important examples. • Catalytic reactions in water: Important reactions in biological chemistry, Metabolism of biomolecules and artificial bioorthogonal reactions.
6	**Learning objectives and skills**	The student • can explain basic principles and underlying reaction mechanisms in organo- and organometallic catalysis and biological chemistry • deepens her/his knowledge in special topics of homogeneous catalysis that are in the research focus of the involved research groups • is able to construct important reaction mechanisms and catalytic cycles and can critically discuss each step.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 Organocatalysis and Catalytic Reactions in Water can be taken • within the Compulsory Elective Module "Advances in Homogenous Catalysis" (20 ECTS in total) • as Elective Module (5 ECTS, not graded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46523	**Small Molecule Activation** Small molecule activation	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Small Molecule Activation (3 SWS)	-
3	Lecturers	Prof. Dr. Karsten Meyer Prof. Dr. Ingrid Span	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	**Lecture:** • Inorganic coordination chemistry, catalytic and electrocatalytic transformation of abundant small molecules N2, O2, CO or CO2, H2O and NH3, into value-added commodities, fine-chemicals, ac-tive pharmaceutical ingredients and polymers. • Selective oxidation reactions. • CO2 reduction to CO and subsequent Fischer-Tropsch catalysis for the production of carbon-based fuels. • Reductive activation of atmospheric N2 to NH3 and the production of H2 from H2O splitting catalysis. Applications, e.g. fuel-cell technologies for carbon-free energy production.
6	**Learning objectives and skills**	The student • can explain basic principles and underlying reaction mechanisms in small molecule activation • is able to construct important reaction mechanisms and catalytic cycles • can critically discuss small-molecule activation
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective Module (20 ECTS in total!) • Lecture module as part of the Elective Module (5 ECTS, not graded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

Advances in Interface Research and Catalysis A

1	**Module name** 46533	**Heterogenous Catalysis and Kinetics** Heterogeneous catalysis and kinetics	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Heterogeneous Catalysis and Kinetics (3 SWS)	-
3	Lecturers	Prof. Dr. Jörg Libuda	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	Syllabus: • Concepts in heterogeneous catalysis: definition of terms, industrial processes • Characterization methods for real catalysts (in-situ and operando methods, TEM, SEM, XRD, EXAFS, XANES, XPS, SIMS, DRIFTS, Raman, TPR, etc.) • Surface Reaction Dynamics: dynamics of adsorption, reaction, desorption, molecular beam experiments, laser spectroscopies • Elementary Kinetics: microkinetics, transition-state theory, relaxation kinetics, rate-determining step; microkinetic experiments, TAP, SSITKA, etc. • Model Catalysis: growth processes, preparation and characterization of model catalysts; kinetics on nanostructured surfaces • Energy-related model catalysis (incl. examples from current research)
6	**Learning objectives and skills**	Students ... • acquire the professional competence in heterogeneous catalysis and respective topics • obtain advanced knowledge in different experimental or theoretical models, their application to current problems, the corresponding data evaluation and interpretation using current research examples • get familiar with various modern experimental techniques and are able to apply them in a targeted manner
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective Module “Advances in Interface Science & Catalysis" in M. Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • As part of the Elective Module in M.Sc. Chemistry/MSc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester

13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	see lecture notes

1	**Module name** 46534	**Interfaces and Catalysis - Lab** Laboratory course: Interfaces and catalysis	**5 ECTS**
2	Courses / lectures	Praktikum: Interface & Catalysis LAB (7 SWS) • Attendance in lab course is compulsory! • Please check lab instructions (contact lab supervisor) • Laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de	5 ECTS
3	Lecturers	Prof. Dr. Julien Bachmann PD Dr. Christian Papp Prof. Dr. Bernd Meyer Prof. Dr. Jörg Libuda	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	Practical introduction to state-of-the-art research in the fields of surface science, interface science, heterogeneous catalysis, electrocatalysis or materials characterization. Guided work on a current research project in a research group. Research topics may cover spectroscopy at surfaces, microscopy at surfaces, in-situ or operando spectroscopy, characterization of catalytic materials, in-situ methods in electrocatalysis, preparation and characterization of nanomaterials, modelling and simulation of interfaces and nanomaterials or similar. Practical laboratory experience to introduce state-of-the-art experimental tools in surface and catalysis research, among them: • Electron spectroscopies • Vibrational spectroscopies • Microscopy at interfaces • Other characterization methods for surfaces / interfaces • In-situ and operando spectroscopy and microscopy • Characterization of nanomaterials • Electrochemical in-situ characterization • Photochemical / photoelectrochemical in-situ characterization • Modelling on processes at interfaces
6	**Learning objectives and skills**	The students ... • get familiar with the current state-of-knowledge for a specific research topic. • apply fundamental knowledge of physical chemistry to a specific research topic. • understand and test model-like descriptions for complex physicochemical problems. • operate complex state-of-the-art instrumentation. • get in contact with development of new methodologies to answer open questions in interface science and catalysis. • analyze data with state-of-the-art methodologies. • record, document, and analyze research data in in appropriate form. • present and discuss experimental results and develop interpretations.

		• present own results in written form and scientific style English language.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 • Obligatory lab course module (5 ECTS) within the Compulsory elective module Interfaces and Catalysis within the degree programmes M.Sc. Chemistry or M.Sc. Molecular Science
10	**Method of examination**	Practical achievement PL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation) Please note: Module examination organized by supervising group!
11	**Grading procedure**	Practical achievement (100%)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 105 h Independent study: 45 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	Will be provided by the supervising research group

1	**Module name** 46532	**Surface and Interface Science** Surfaces and interface science	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Surfaces and Interface Science (3 SWS)	-
3	Lecturers	Prof. Dr.-Ing. Marcus Bär	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	• Vacuum and pressure measurement (pumps, pressure and flow ranges) • Lab-based and synchrotron-based light sources (principles, optics, insertion devices, etc.) • Theory of photoemission and electronic structure • XPS (elemental / chemical sensitivity, cross sections, quantification, examples) • UPS (gas phase, adsorbates, 2D band structures, 3D band structures, orbital tomography) • IPES (probing of unoccupied states, energy level alignment determination) • HAXPES (depth-resolved photoemission measurements, examples) • PEEM (spatially-resolved photoemission measurements, examples) • NEXAFS (principle and examples) • XES & RIXS (principle and examples) • Structure of surfaces/ diffraction at surfaces (LEED, definitions and examples) • X-ray spectroscopy based materials research on energy conversion devices (examples from current research)
6	**Learning objectives and skills**	Students ... • understand the principles of photoemission variants and their applications • can judge the quality of data evaluation and its pitfalls • can deliberately select an X-ray spectroscopic analysis method to address given scientific question and are able to evaluate the collected data
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Interfaces and Catalysis" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as part of the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%)

		As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Hüfner: Photoelectron Spectroscopy: Principles and Applications" Springer-Verlag Berlin Heidelberg • Ertl, Küppers: Low Energy Electrons and Surface Chemistry" VCH Weinheim • D. Attwood, Soft X-rays and Extreme Ultraviolett Radiation, Cambridge University Press, 1999 • D. Briggs, M.P. Seah: PracticalSurface Analysis: AugerandX-Ray PhotoelectronSpectroscopy, Wiley, 1996 • M. Bär, L. Weinhardt, and C. Heske: Advanced Characterization Techniques for Thin Film Solar Cells, edited by D. Abou-Ras, T. Kirchartz, and U. Rau (Wiley VCH Verlag GmbH & Co KGaA, ISBN: 978-3-527-33992-1), 2nd Extended Edition, Volume 2, Chap. 18. • A. Meisel, G. Leonhardt, R. Szargan: X-ray Spectra and Chemical Binding, Springer, 1989

1	**Module name** 46531	**Theory of Catalytic Processes** Theory of catalytical processes	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Theory of Catalytic Processes (3 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Bernd Meyer	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	The module focuses on physical, chemical or technological aspects of modification, manipulation and characterization of interfaces. These aspects relate to the research of ideal model systems (surfaces and adsorbates on single crystal surfaces) or real systems, in which the interface plays a crucial role for the respective properties. In all cases, the local electronic and chemical interactions at the interface affect the geometric structure (e.g. adsorption geometry) and consequently the chemical and physical properties.
6	**Learning objectives and skills**	Students • deepen their knowledge in experimental methods and theoretical aspects to describe and characterize interface phenomena • are able to perform experiments independently and to analyse the data • are familiar with the model-type description of experimental data
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module Advances in Interfaces and Catalysis A (IntCat-3A) (20 ECTS in total)! • Module can also be taken as part of the elective module (5 ECTS, not graded)! <u>Please note:</u> **MSc Molecular NANO Science students** have to attend the module **"Advances in Interfaces and Catalysis A (IntCat-3A)**" / **MSc Chemistry students** can **choose** between the module "**Advances in Interfaces and Catalysis A (IntCat-3A)"** and the module "**Nanostructured Materials and Interfaces B (IntCat-3B)"** of Prof. Bachmann!
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h

		Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

Advances in energy materials

1	**Module name** 46542	**Advanced Electrochemistry** Advanced electrochemistry	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Advanced Electrochemistry (3 SWS)	-
3	Lecturers	Dr. Christian Ehli	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Comprehensive survey of the fundamentals for electrode processes (thermodynamics and kinetics) • Introduction to electrochemical techniques (e.g. cyclic voltammetry, rotating disk voltammetry, differential pulse voltammetry, spectroelectrochemistry, electrochemical impedance spectroscopy) • Applications of electrochemistry (e.g. corrosion prevention, batteries) • Seminars will be based on the discussion of practical aspects and electrochemical exercises
6	**Learning objectives and skills**	Students • plan and perform own electrochemical experiments • characterize electroactive materials by common electrochemical methods • analyze, interpret and discuss electrochemical experimental results • discuss and evaluate current electrochemical publications
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module "Advances in Energy Materials" in M.Sc. Chemistry or M.Sc. Molecular Science (20 ECTS in total)! • as part of the Elective Module in M.Sc. Chemistry or M.Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english

16	**Bibliography**	• Allen J. Bard, Larry R. Faulkner: "Electrochemical Methods: Fundamentals and Applications", John Wiley & Sons, New York, NY • Carl H. Hamann, Andrew Hamnett, Wolf Vielstich: "Electrochemistry", Wiley-VCH, Weinheim For further literature, please see the current list on studon.

1	**Module name** 46544	**Energy Materials - Lab** Laboratory course: Energy materials	**5 ECTS**
2	Courses / lectures	Praktikum: Energy Materials - LAB (7 SWS) • Attendance at lab course is compulsory! • Attendance at safety instructions is compulsory! • A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de	5 ECTS
3	Lecturers	Dr. Christian Ehli Prof. Dr. Dirk Michael Guldi	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Practical introduction to electrochemical techniques • Guided work on the characterization of electroactive materials • Attempts to solve independently a scientific problem • Documentation of experimental results
6	**Learning objectives and skills**	Students • plan and perform own electrochemical experiments • characterize electroactive materials by common electrochemical methods • analyze, interpret, and discuss electrochemical experimental results • discuss and evaluate current electrochemical publications.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 • Within the Compulsory Elective Module "Advances in Energy Materials" in M.Sc. Chemistry or M.Sc. Molecular Science (20 ECTS in total)! • The module can be taken as part of the Elective Module (5 ECTS, not graded)!
10	**Method of examination**	Practical achievement pÜL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)
11	**Grading procedure**	Practical achievement (100%)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 105 h Independent study: 45 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46541	**Semiconductor Materials for Energy Applications** Semiconductor materials for energy applications	**5 ECTS**
2	Courses / lectures	Seminar: Semiconductor Materials for Energy Applications - Seminar (1 SWS) Vorlesung: Semiconductor Materials for Energy Applications - Lecture (2 SWS)	- -
3	Lecturers	Dr. Ryan Crisp	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Fundamentals of semiconductors: Crystal structure, Electronic structure, Electrical transport, Interaction with light • Semiconductor devices: Tunnelling, The pn junction, The transistor • Photovoltaics: Principles, Types of solar cells • The interface to a solution: Charged electrolytic interfaces, Electrocatalysis and photoelectrocatalysis
6	**Learning objectives and skills**	The students • are familiar with the fundamentals and modern developments in semiconductor science and applications • understand theoretical and practical aspects in state-of-the-art semiconductor devices • can present, communicate and discuss scientific results with experts in English.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • within the Compulsory Elective Module "Advances in Energy Materials" in M. Sc. Chemistry or M.Sc. Molecular Science (20 ECTS in total) • part of the Elective Module in M. Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination, 20 minutes
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46543	**Solar Energy Conversion** Solar energy conversion	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Solar Energy Conversion (3 SWS)	-
3	Lecturers	Prof. Dr. Dirk Michael Guldi	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Demand and supply of energy • Solar cells: Silicon solar cells, dye-sensitized solar cells, organic solar cells, perovskite solar cells, singlet fission • Fundamentals of Electron Transfer • Photosynthesis: natural photosynthesis, artificial photosynthesis
6	**Learning objectives and skills**	The students • are familiar with the fundamentals and modern applications in solar energy research and applications • understand design principles in solar energy devices and can transfer this knowledge to related topics • can present, communicate and discuss scientific results with experts in English.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module "Advances in Energy Materials" MSc Chemistry and Molecular Science (20 ECTS in total!) • Module can be taken as part of the Elective Module, too (5 ECTS, not graded)!
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

Quantum chemistry

1	**Module name** 46508	**Quantum Chemistry laboratory** Laboratory course: Quantum chemistry	**10 ECTS**
2	Courses / lectures	Praktikum: Training in Applied Computational Chemistry (5 SWS) Praktikum: Quantum Chemistry - Lab / Scientific Programming (10 SWS) • Attendance in lab course is compulsory! • Internship in one of the Theoretical Chemistry groups (Profs Görling, Imhof, B. Meyer, Zahn), time and place by agreement! • Training has to be taken only once: in winter or in summer term (time and place by agreement)! • Module starts only in winter term (Duration: 2 semester)!	- -
3	Lecturers	Prof. Dr. Dirk Zahn Prof. Dr. Andreas Görling Prof. Dr. Bernd Meyer Prof. Dr. Petra Imhof Dr. Christian Neiß	

4	**Module coordinator**	Prof. Dr. Andreas Görling
5	**Contents**	• Operating system Linux for high-performance computing (HPC) • Scientific programming in Fortran and Python • Using numerical and mathematical libraries/modules • Introduction to parallel computing • Exercises • Programming project • Training in applied computational chemistry
6	**Learning objectives and skills**	Students .... • get familiar with Linux as operating system for HPC • are able to create computer programs for scientific purposes • can use numerical and mathematical libraries/modules in home-made programs • obtain knowledge about basic parallelization paradigms • apply quantum chemical methods to scientific questions under guidance
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Quantum Chemistry Master of Science Molecular Science 20202 • Lab module within the Core module „Quantum Chemistry“ in M. Sc. Chemistry • Lab module within the Compulsory Elective Module in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science
10	**Method of examination**	Practical achievement Graded Lab Protocol: Successful implementation of the programming project (working program) including Lab report (ca. 5 pages)

11	**Grading procedure**	Practical achievement (100%) 100% Graded Computer Program
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 225 h Independent study: 75 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Stephen J. Chapman: Fortran for Scientists and Engineers, McGraw Hill 2017 (4th ed.) • Bernd Klein: Einführung in Python 3, Hanser 2017 (3rd ed.) • Stefan Gerlach: Computerphysik, Springer Spektrum 2019 (2nd ed.)

1	**Module name** 46507	**Quantum Chemistry** Quantum chemistry	**10 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Quantum Chemistry 2 (3 SWS) Vorlesung mit Übung: Quantum Chemistry 1 (3 SWS) Please note: • The core module "Quantum Chemistry" starts only in winter term!	- -
3	Lecturers	Prof. Dr. Andreas Görling	

4	**Module coordinator**	Prof. Dr. Andreas Görling
5	**Contents**	• Introduction to modern methods and current research issues in the field of quantum and computer chemistry • Hartree-Fock, DFT, Many Body Perturbation Theory • Configuration Interaction, Second Quantization, Coupled Cluster • TD-HF, TD-DFT, RPA
6	**Learning objectives and skills**	Students ... • obtain sound knowledge in basic and advanced methods of quantum chemistry • are able to solve mathematical problems occurring in quantum chemistry • are able to understand and assess scientific reports in the field of quantum chemistry
7	**Prerequisites**	Required Qualifications: • good knowledge of basic quantum mechanics: axioms of QM, application to simple systems (particle in a box, harmonic oscillator, rigid rotator) • good knowledge in mathematics: differential calculus of functions of several variables, basic linear algebra
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Quantum Chemistry Master of Science Molecular Science 20202 • Lecture module within the Core module „Quantum Chemistry“ in M. Sc. Chemistry • Lecture module within the Compulsory Elective Module in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science
10	**Method of examination**	Oral (30 minutes) O30 (PL): Oral Examination (30 minutes)
11	**Grading procedure**	Oral (100%)
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 90 h Independent study: 210 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english

16	**Bibliography**	• Attila Szabo, Neil S. Ostlund: Modern Quantum Chemistry, Dover 1996 • Frank Jensen: Introduction to Computational Chemistry, Wiley 2017 (3rd ed.) • Ira N. Levine: Quantum Chemistry, Pearson 2016 (7th ed.)

Research module

1	**Module name** 63069	**Research Lab - Drug Discovery** Research lab - Drug discovery	**15 ECTS**
2	Courses / lectures	Praktikum: Research Module - Drug Discovery (23 SWS)	15 ECTS
3	Lecturers	Prof. Dr. Andreas Burkovski Prof. Dr. Peter Gmeiner Prof. Dr. Christian Koch Prof. Dr. Jutta Eichler Prof. Dr. Monika Pischetsrieder Prof. Dr. Markus Heinrich Prof. Dr. Andrea Büttner Prof. Dr. Dagmar Fischer	

4	**Module coordinator**	Prof. Dr. Peter Gmeiner
5	**Contents**	Research lab project full time (about 6 weeks: 21SWS LAB/2SWS Seminar) in a work group of the students choice at a research group in Medicinal Chemistry, Food Chemistry, or the disciplines of Biology involved in teaching at the Department of Chemistry and Pharmacy
6	**Learning objectives and skills**	Students ... • are provided with the up-to-date practical and operative know-how suitable for future scientific and/or applied work in research institutes, pharmaceutical/food industry, medical care laboratories, bio-technological, bio-analytical and environmental branches • get an advanced theoretical background and an overview of emerging trends in life sciences (chemistry, biology and medicine) • look at living systems through the lens of basic chemical principles • are prepared to work in interdisciplinary environment and participate in national and international development of forefront fields such as translational medicine.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 3
9	**Module compatibility**	Research module Master of Science Molecular Science 20202
10	**Method of examination**	Practical achievement pÜL: Graded Lab Protocol (approx. 20 pages plus raw data documentation)
11	**Grading procedure**	Practical achievement (100%)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 345 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english

16	**Bibliography**	no Bibliography information available!

1	**Module name** 63074	**Research Lab - Molecular Nanoscience** Research lab - Molecular nanoscience	**15 ECTS**
2	Courses / lectures	Praktikum: Research Module - Molecular Nanoscience (23 SWS)	15 ECTS
3	Lecturers	Prof. Dr. Dirk Zahn Prof. Dr. Julien Bachmann Prof. Dr. Rainer Fink Prof. Dr. Bernd Meyer Prof. Dr. Franziska Gröhn Prof. Dr. Karl Mandel Prof. Dr. Henry Dube Dr. Ryan Crisp	

4	**Module coordinator**	Prof. Dr. Rainer Fink
5	**Contents**	research lab project (23 SWS) fulltime in one of the research groups of Molecular Nanoscience
6	**Learning objectives and skills**	Students ... • are provided with the up-to-date practical and operative know-how suitable for future scientific and/or applied work in research institutes and nanoscience-labs • get an advanced theoretical background and an overview of emerging trends in nano sciences • look at living systems through the lens of basic chemical principles • are prepared to work in interdisciplinary environment and participate in national and international development of forefront fields.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 3
9	**Module compatibility**	Research module Master of Science Molecular Science 20202
10	**Method of examination**	Practical achievement
11	**Grading procedure**	Practical achievement (100%) pÜL: Graded Lab Protocol (approx. 20 pages plus raw data documentation)
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 345 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

Elective modules

1	**Module name** 46511	**Advanced Bio-Organic and Bio-Inorganic Chemistry** Advanced bio-organic and bio-inorganic chemistry	**5 ECTS**
2	Courses / lectures	Seminar: Seminar Advanced Bioinorganic Chemistry, Metalloenzymes and Metals in Medicine (1 SWS)	-
3	Lecturers	Prof. Dr. Nicolai Burzlaff Prof. Dr. Norbert Jux	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • are introduced into recent activities and achievements in the fields • of bioorganic and bioinorganic chemistry and metals in medicine: • porphyrins and heme enzymes • PDT • electron transfer (cofactors, ferredoxins, inner sphere mechanism, outer sphere mechanism, Marcus theory) • photosynthesis • copper containing proteins and enzymes • nitrogenases and other Mo containing enzymes • drugs based on Pt, Ru, Au and As • biominerals • implant materials and technology
6	**Learning objectives and skills**	The students • are introduced into recent activities and achievements in the fields of bioorganic and bioinorganic chemistry and metals in medicine
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as part of the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester

15	**Teaching and examination language**	english
16	**Bibliography**	• W. Kaim, B. Schwederski, A. Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, 2. Edition, John Wiley & Sons, Ltd, 2013

1	**Module name** 46542	**Advanced Electrochemistry** Advanced electrochemistry	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Advanced Electrochemistry (3 SWS)	-
3	Lecturers	Dr. Christian Ehli	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Comprehensive survey of the fundamentals for electrode processes (thermodynamics and kinetics) • Introduction to electrochemical techniques (e.g. cyclic voltammetry, rotating disk voltammetry, differential pulse voltammetry, spectroelectrochemistry, electrochemical impedance spectroscopy) • Applications of electrochemistry (e.g. corrosion prevention, batteries) • Seminars will be based on the discussion of practical aspects and electrochemical exercises
6	**Learning objectives and skills**	Students • plan and perform own electrochemical experiments • characterize electroactive materials by common electrochemical methods • analyze, interpret and discuss electrochemical experimental results • discuss and evaluate current electrochemical publications
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module "Advances in Energy Materials" in M.Sc. Chemistry or M.Sc. Molecular Science (20 ECTS in total)! • as part of the Elective Module in M.Sc. Chemistry or M.Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english

16	**Bibliography**	• Allen J. Bard, Larry R. Faulkner: "Electrochemical Methods: Fundamentals and Applications", John Wiley & Sons, New York, NY • Carl H. Hamann, Andrew Hamnett, Wolf Vielstich: "Electrochemistry", Wiley-VCH, Weinheim For further literature, please see the current list on studon.

1	**Module name** 46563	**Advanced Spectroscopic Techniques** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Advanced Spectroscopy in Organic Chemistry (3 SWS)	5 ECTS
3	Lecturers	Dr. Alexander Scherer Prof. Dr. Henry Dube	

4	**Module coordinator**	Prof. Dr. Henry Dube
5	**Contents**	Fundamentals of spectroscopy in organic chemistry will be reviewed. More in-depth methods of molecular spectroscopy in organic chemistry are covered. Advanced methods of NMR-spectroscopy are also covered, such as NMR-spectroscopy of various nuclei (e.g., 1H, 13C, 19F, 31P). Two-dimensional methods of NMR-spectroscopy using scalar spin-spin couplings (e.g., HSQC, HMBC) are discussed. Furthermore, NMR-spectroscopic methods relying on interactions between coupling nuclear dipoles, which are transmitted directly through space are covered (e.g., NOESY). In addition, other optical spectroscopic methods will be reviewed and discussed in more depth (e.g., UV/Vis-, CD-, IR-spectroscopy and Mass spectrometry).
6	**Learning objectives and skills**	The students • master the reliable use and gain an understanding of spectroscopic methods in organic chemistry, which are used to elucidate organic molecules; • are able to characterize unknown molecules and to determine their structure as well as their dynamics and interactions (the correlations between the spectroscopic results and the characteristics of the molecules should become understandable and comprehensible); • discuss practical examples of spectroscopic results and the related correlations in the exercises and practice the structure elucidation on examples.
7	**Prerequisites**	Basic knowledge of spectroscopy is recommended.
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • Elective Module within the degree programmes MSc Chemistry and Molecular Science, 5 ECTS/not graded
10	**Method of examination**	Tutorial achievement SL: practical exercise performance (15- 20 minutes), non-graded
11	**Grading procedure**	Tutorial achievement (0%) pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester

15	**Teaching and examination language**	english
16	**Bibliography**	• "Basic one- and two-dimensional NMR spectroscopy, edited by H. Friebolin, Wiley-VCH • "NMR From spectra to structures edited by T. N. Mitchell, B. Costisella, Springer • "Spectroscopic methods in organic chemistry, Edited by D. H. Williams, I. Flemming, McGraw Hill • "Modern NMR spectroscopy, Edited by J. K. M. Sanders, E. C. Constable, B. K. Hunter, C. M. Pearce, Oxford

1	**Module name** 46562	**Biological and Synthetic Molecular Switches and Machines** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung: Molecular Switches and Molecular Machines (2 SWS)	-
3	Lecturers	Prof. Dr. Henry Dube	

4	**Module coordinator**	Prof. Dr. Henry Dube
5	**Contents**	Examination of molecular triggers, switches and machines in biology and in synthetic systems as foundation of nanotechnology; working mechanisms; types of systems; design principles; seminal contributions; historical backgrounds are given. The material is ordered in introduction and context, basic principles, triggers, switches, machines, integrated systems, future prospective. The course will be updated to implement the newest developments yearly
6	**Learning objectives and skills**	The Students ... • acquire a fundamental understanding in the working mechanisms and design principles of molecular triggers, switches, and machines. • will be able to develop strategies for implementing responsiveness into nanostructured biological or synthetic systems and will be equipped with an exhaustive overview of historical developments and current state of the art in the field by discussing representative examples in depth. • will therefore be educated in one of the most prominent fields of modern (bio)chemistry and nanosciences. Compulsory attendance will be necessary. The skills will be appropriate for Masters level and will partially repeat and build on knowhow from supramolecular, biological, and photochemistry as well as on fundamental physical organic chemistry, biochemistry, nanotechnology, and spectroscopy.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 Module compatibility: • as Elective Module in MSc Molecular Life Science (not applicable for Molecular Nanoscience), 5 ECTS/not graded • as Elective Module in MSc Chemistry, 5 ECTS/not graded
10	**Method of examination**	Tutorial achievement O20 (SL): 20 min oral examination in the form of a seminar talk presenting the content of a seminal original publication (Non-graded seminar presentation)
11	**Grading procedure**	Tutorial achievement (0%) pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h

		Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• "Molecular Switches, edited by Ben L. Feringa, Wiley-VCH • "From Non-Covalent Assemblies to Molecular Machines, Edited by Jean-Pierre Sauvage & Pierre Gaspard, Wiley-VCH • "Molecular Machines and Motors Recent Advances and Perspectives edited by Alberto Credi, Serena Silvi, Margherita Venturi, Springer

1	**Module name** 46549	**Biomolecules and metal ions - evolution, biological functions, and biomedicine** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung: Biomolecules and metal ions (3 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Ingrid Span	

4	**Module coordinator**	Prof. Dr. Ingrid Span
5	**Contents**	• Roles of metal ions in biology with focus on photosynthesis & oxygen transport • Metalloproteins • Metal ions in evolution, extremophile organisms • Metal ions in biomedicine (imaging and therapy) • Fundamentals of protein crystallography • Fundamentals of spectroscopic techniques for characterizing metalloproteins • Seminars in form of presenting scientific research articles on metallobiochemistry
6	**Learning objectives and skills**	Students ... • can explain the fundamental properties of biomolecules, the occurrence and the role of metals in biological systems, and the chemistry of life. • gain a better understanding of the relevance of metals in evolution and the application of metals in biomedicine. • get insight into different techniques that can be used to analyse metal-binding biomolecules. • are able to transfer the acquired knowledge to solve unrelated scientific problems.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 The module (5 ECTS, not graded) can be taken as part of the elective module (in total 15 ECTS) within the Master programme Chemistry or Molecular Science
10	**Method of examination**	PL: Written exam, 60 minutes, not graded
11	**Grading procedure**	PL: W60 (0%) pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Bioinorganic Chemistry - Inorganic Elements in the Chemistry of Life: An Introduction and Guide (Second Edition 2013) Wolfgang Kaim, Brigitte Schwederski, Axel Klein

		• Bioanorganische Chemie - Metalloproteine, Methoden und Konzepte (1. Auflage August 2017) Sonja Herres-Pawlis, Peter Klüfers

1	**Module name** 46548	**Economics**	**5 ECTS**
2	Courses / lectures	Seminar: Economics A: Betriebswirtschaftslehre I (0 SWS) Seminar: Economics C: Strategische Planung & Projektmanagement (0 SWS) Seminar: Economics B: Betriebswirtschaftslehre II (0 SWS) Seminar: Economics - BWL und Projektmanagement (SWS) Seminar: Blockseminar Economics - Chemistry (SWS) Seminar: Economics für Chemie und Molecular Science: BWL und Projektmanagement (SWS)	1,5 ECTS 2 ECTS 1,5 ECTS 5 ECTS 5 ECTS 5 ECTS
3	Lecturers	Andreas Späth Prof. Dr. Rainer Fink Prof. Dr. Nicolai Burzlaff Prof. Dr. Rainer Fink	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	**Economics A: Betriebswirtschaftslehre I (BWL-I):** Einführung in ... • Funktionsbereiche • Unternehmensformen • Bilanz/GuV/Kostenrechnung **Economics B: Betriebswirtschaftslehre II (BWL-II):** • Bilanzanalyse • Kennzahlen • Kostenrechnung **Economics C: Strategische Planung & Projektmanagement (BWL-III):** Einführung in ... • Methoden der strategischen Analyse • Innovationsstrategien • F&E Projektmanagement • Agiles Projektmanagement und Lean
6	**Learning objectives and skills**	Die Studierenden ... • erwerben Kenntnisse über Grundfragen der allgemeinen Betriebswirtschaftslehre • kontrollieren ihr Wissen durch online Follow-Up Self-Assessments • arbeiten erfolgreich mit gängigen Analysetools • beherrschen grundlegende Techniken des Projektmanagements • erarbeiten selbständig eine Unternehmensanalyse • präsentieren die Ergebnisse
7	**Prerequisites**	None

8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • Economics ist ein Wahlmodul im MSc Chemistry oder MSc Molecular Science / 5 ECTS, unbenotet • Für die Anrechnung des Wahlmoduls müssen alle Lehrveranstaltungen (Economics 1-3) besucht werden!
10	**Method of examination**	Variable SL: Erstellung und Präsentation einer Projektstudie (Vortrag ca. 15 - 20 min)
11	**Grading procedure**	Variable (0%) pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	german
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46533	**Heterogenous Catalysis and Kinetics** Heterogeneous catalysis and kinetics	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Heterogeneous Catalysis and Kinetics (3 SWS)	-
3	Lecturers	Prof. Dr. Jörg Libuda	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	Syllabus: • Concepts in heterogeneous catalysis: definition of terms, industrial processes • Characterization methods for real catalysts (in-situ and operando methods, TEM, SEM, XRD, EXAFS, XANES, XPS, SIMS, DRIFTS, Raman, TPR, etc.) • Surface Reaction Dynamics: dynamics of adsorption, reaction, desorption, molecular beam experiments, laser spectroscopies • Elementary Kinetics: microkinetics, transition-state theory, relaxation kinetics, rate-determining step; microkinetic experiments, TAP, SSITKA, etc. • Model Catalysis: growth processes, preparation and characterization of model catalysts; kinetics on nanostructured surfaces • Energy-related model catalysis (incl. examples from current research)
6	**Learning objectives and skills**	Students ... • acquire the professional competence in heterogeneous catalysis and respective topics • obtain advanced knowledge in different experimental or theoretical models, their application to current problems, the corresponding data evaluation and interpretation using current research examples • get familiar with various modern experimental techniques and are able to apply them in a targeted manner
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective Module “Advances in Interface Science & Catalysis" in M. Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • As part of the Elective Module in M.Sc. Chemistry/MSc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester

13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	see lecture notes

1	**Module name** 46536	**Lebensmittelchemie** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung: Chemie und Technologie der Lebensmittel, Teil 2, 5, 6 oder 9 (1 SWS) Vorlesung: Chemie und Technologie der Lebensmittel, Teil 1, 4, 7 oder 8 (1 SWS) Vorlesung: Chemie und Technologie der Lebensmittel, Teil 2, 5, 6 oder 9 (1 SWS) Seminar: Seminare Bioanalytik oder Instrumentelle Analytik für Lebensmittelchemie und Molecular Science (1 SWS) Bitte beachten: • Die Vorlesung Lebensmittelchemie hat je nach Semester unterschiedliche inhaltliche Schwerpunkte (Lebensmittelchemie I-XI)! • Die Studierenden müssen 2 Vorlesungen (im Umfang von 2 SWS) und das Seminar (1 SWS) besuchen!	- - - -
3	Lecturers	Prof. Dr. Monika Pischetsrieder Prof. Dr. Simon Hammann	

4	**Module coordinator**	Prof. Dr. Monika Pischetsrieder
5	**Contents**	• Es werden toxikologisch, technologisch und physiologisch relevante Inhaltsstoffe von Lebensmitteln ausführlich vorgestellt und diskutiert. • Ausgehend von den grundlegenden Kenntnissen der organischen Chemie werden Reaktionsmechanismen, die während der Prozessierung oder Entstehung von Lebensmitteln ablaufen, erläutert. • Ausgehend von grundlegenden Kenntnissen der analytischen Chemie werden die wichtigsten weiterführenden und aktuellen instrumentellanalytischen und bioanalytischen Analysenmethoden besprochen.
6	**Learning objectives and skills**	Die Studierenden • erarbeiten sich die Sachkompetenz zur theoretischen Beurteilung und praktischen Handhabung wichtiger Fragestellungen der Lebensmittelchemie • sind in der Lage, die wichtigsten relevanten Arbeitstechniken aus dem Gebiet der Lebensmittelchemie und analytik und eines anderen Gebiets der Lebensmittelwissenschaften selbständig anzuwenden • können die wesentlichen Prinzipien der Lebensmittelanalytik auf praktische Probleme anwenden und kritisch reflektieren.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202

		• kann als Teil des Wahlmoduls/Elective module belegt werden (5 ECTS/unbenotet)
10	**Method of examination**	(SL): Seminarvortrag, 30 Minuten, unbenotet
11	**Grading procedure**	SL (0%): unbenotet bestanden/nicht bestanden
12	**Module frequency**	every semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	german
16	**Bibliography**	Wird von den Dozenten aktualisiert zur Verfügung gestellt.

1	**Module name** 46513	**Metallic nanoparticles in Medicine** Metallic nanoparticles in medicine	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Metallic Nanoparticles in Medicine (3 SWS)	-
3	Lecturers	PD Dr. Christina Janko PD Dr. Rainer Tietze Prof. Dr. Carola Kryschi Prof. Dr. Olaf Prante Prof. Dr. Ingrid Span Dr. Stefanie Klein	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • are introduced into recent research activities and achievements in the fields of nanomedicine • evaluate and assess the basic theories, principles and concepts of bioorganic and bioinorganic che- mistry and nanomedicine (in compliance with a research-orientated master course)
6	**Learning objectives and skills**	The students • can explain and reflect upon the bioorganic and bioinorganic nanochemistry aspects in medicinal chemistry and toxicology
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46521	**Organometallic Catalysis** Metal-organic catalysis	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Organometallic Catalysis (3 SWS) Seminar: Organometallic Catalysis - Seminar (1 SWS)	- -
3	Lecturers	Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	• Harder: Introduction and basic principles of advanced catalysis, homogeneous vs. heterogeneous catalysis, mechanisms of substrate activation (C=C, C=O), control by ligand and metal choice, classical catalytic cycles: Wilkinson catalyst, C-C cross coupling, hydroformylation, polymerization catalysis, catalysis with main group metals. • Dorta: Review of basic organometallic mechanisms & reactivity (elementary reactions, isolobality); Hydrogenation of alkenes and aromatics; CC cross coupling; Atom-economical CC formation (alkene hydroformylation & hydrocyanation, alkene oligomerization, methanol carbonylation); Synthetic fuels form CO (methanol, MTG, Fischer-Tropsch); Alkene metathesis; Selective CO bond formation (epoxidations and Wacker-type oxidations)
6	**Learning objectives and skills**	The student • understands basic principles and underlying reaction mechanisms in organometallic catalysis • is able to outline reaction mechanisms and catalytic cycles • knows the tools for the characterization of catalysts and how to evaluate catalyst performance • acquires knowledge on topics of current interest and recent breakthroughs in organometallic catalysis
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective module "Advances in Homogenous Catalysis" in M. Sc. Chemistry or Molecular Science (20 ECTS in total, graded) • As Elective Module in M. Sc. Chemistry or Molecular Science (5 ECTS, ungraded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail

12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Fundamentals of Organometallic Catalysis, Dirk Steinborn, Wiley-VCH, 2012 • Early Main Group Metal Catalysis – Concepts and Reactions, Sjoerd Harder, Wiley-VCH, 2020 • Metal-catalysis in Industrial Organic Processes, Gian Paolo Chiusoli & Peter Maitlis, Royal Society of Chemistry, 2019 • Fundamentals of Organometallic Catalysis, Dirk Steinborn, Wiley-VCH, 2012 • Homogeneous Catalysis, Parshall & Ittel, 2nd ed., Wiley Interscience 1992

1	**Module name** 46564	**Modern Methods in Mass Spectrometry** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Modern Methods in Mass Spectrometry (3 SWS)	-
3	Lecturers	Prof. Dr. Thomas Drewello	

4	**Module coordinator**	Prof. Dr. Thomas Drewello
5	**Contents**	• Advanced aspects of Soft Ionization methods (MALDI, ESI, related Atmospheric Pressure Ionization methods) • Advanced aspects of mass analyzers (FT-ICR, orbitrap, hybrids: multi sector, BEqQ, QToF, QIT-ToF) • Ion Activation (CID, BIRD, IRMPD, SID, ECID) • Applications (thermochemistry, kinetic method, equilibrium methods, ion/molecule-reactions) • "Omics (proteomics, petroleomics, metabolomics) • Further applications: 14C dating, accelerator MS, stable isotope MS, MS in space, ICP-MS. • Seminars in form of problem solving classes
6	**Learning objectives and skills**	Students ... • gain insight into the different ion formation processes • are able to decide on an ionization method for a given compound class • are able to evaluate the use of different mass spectrometers • gain understanding of ion activation processes in the gas phase
7	**Prerequisites**	The course builds on the master module "Applied Spectroscopy (Compulsory Module Physical Chemistry)
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • Lecture module as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (0%) pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Jürgen H. Groß: "Mass Spectrometry, a textbook Springer, Heidelberg • Edmond De Hoffmann: "Mass Spectrometry, principles and applications, Wiley

1	**Module name** 46558	**Modern X-ray Structure Determination** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Modern X-ray structure determination of single crystals (3 SWS)	5 ECTS
3	Lecturers	Dr. Frank Heinemann	

4	**Module coordinator**	Dr. Frank Heinemann
5	**Contents**	• Fundamentals of crystallization and polymorphism • Structural description of single crystals, crystal systems, unit cell, symmetry and symmetry elements, space groups • Diffraction power of crystals, diffraction conditions, structure factor • Generation of X-rays, single crystal diffractometers, detection techniques • Structure solution techniques and refinement procedures, software, problems and pitfalls, interpretation of results • Anomalous dispersion and absolute structure • Graphical representations, use of data bases
6	**Learning objectives and skills**	Students ... • get insight into thermodynamics of crystallization and crystallization techniques • get fundamentals of the theory behind crystal structure determination • get practice in crystal selection, mounting and measurement set-up • get hands-on training in structure solution and refinement using up-to-date software • are enabled to interpret and compare results of a single crystal structure determination
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Tutorial achievement (PL): Lab report in manuscript style (max. 2000 words plus raw data), not graded
11	**Grading procedure**	Tutorial achievement (0%) not graded: pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english

16	**Bibliography**	• Werner Massa: Kristallstrukturbestimmung. Teubner Studienbücher Chemie, Vieweg und Teubner, 6. Auflage, 2009, ISBN: 3834806498 • William Clegg: Crystal Structure Determination. Oxford Chemistry Primers. Oxford University Press, 1998, ISBN: 0198559011 • Further literature will be recommended in the course

1	**Module name** 46535	**Neurotech: Physics and Chemistry of Neuromodulation Technologies** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Neurotech: Physics and Chemistry of Neuromodulation Technologies (3 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Danijela Gregurec	

4	**Module coordinator**	Prof. Dr. Danijela Gregurec
5	**Contents**	• Introduction to neuromodulation technologies (definition, history, nervous anatomy, stimulation targets-ion channels, action potential) • Imaging and spectroscopic concepts (MRI, EEG, Calcium imaging, electrophysiology) • Current tech and principles (Invasive and noninvasive approaches, Deep brain stimulation, Transcranial magnetic stimulation, Pain management, BMI summary) • Organic materials and approaches (viral vectors, optogenetics, Chemogenetics (DREED) • Micro- and macroscale materials (Mechanical properties and compatibility of neural implants, Electrodes (Utah arrays, Neuralink), Flexible electrodes, Optical fibers) • Nanomaterials (Nanomaterial properties leveraged for neuromodulation (Importance of surface chemistry in bio(nano)materials, Quantum confinement and quantum dots, Plasmons and photothermal neuromodulation, Magnetism, Magnetoelectric particles for electric stimulation, Magnetic nanoparticles for magnetothermal and magnetomechanical stimulation
6	**Learning objectives and skills**	Students will gain the knowledge, skills, and competences to be able to ... • understand biophysical aspects of neuronal signaling and its correlation to cognition and behavior. • learn physical foundations, biological concepts, and chemical approaches crucial for materials used in neuromodulation and neurotechnology. • apply acquired knowledge to realize design criteria of technology that governs the modulation of neuronal signaling.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 Module compatibility: • Lecture module within the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral examination (20 minutes, ungraded)
11	**Grading procedure**	not graded - pass/fail
12	**Module frequency**	only in summer semester

13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Knotkova, Rasche; Springer-Verlag New York (2015) | Textbook of Neuromodulation: Principles, Methods and Clinical Applications| • Luan et al, Front Neuroeng 7 (2014) |Neuromodulation: present and emerging methods| • Frank, et al, Nat Biotech 37 (2019) |Next-generation interfaces for studying neural function| • Chen et al, Nat Rev Mat 2 (2017) |Neural recording and modulation technologies| |**Literature will be updated with leading peer-reviewed papers during lectures|

1	**Module name** 46545	**Organic thin films**	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Organic Thin Films (3 SWS) Seminar: Seminar Organic thin films (1 SWS)	5 ECTS -
3	Lecturers	Prof. Dr. Rainer Fink	

4	**Module coordinator**	Prof. Dr. Rainer Fink
5	**Contents**	• Molecular interactions and molecular self-organization • Influence of molecualr geometry and functionalization • Thin film preparation techniques: Langmuir-Blodgett, Self-Assembled Monolaers (SAMs), other solvent-based techniques (e.g. spin-casting, doctor blading, etc.), vacuum sublimation • Analytical techniques, in-situ analysis • Effect of templates • Organic thin film applications • Seminars will be based on recent literature
6	**Learning objectives and skills**	Students • get insight into the major preparation techniques of organic thin films • are able to evaluate to prepare organic thin film specimens • know to analyse thin film specimens with respect to structural and electronic properties • are aware of recent studies and modern applications of organic thin films
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • lecture module can be taken as part of the Elective Module!
10	**Method of examination**	Variable O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Variable (0%) pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46522	**Organocatalysis and Catalytic Reactions in Water** Organocatalysis and catalytic reactions in water	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Organocatalysis and Catalytic Reactions in Water (3 SWS)	-
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	• History and basic principles of organocatalysis, • Different types of organocatalysts, • Enantioselective organocatalysis, • Domino reactions and important examples. • Catalytic reactions in water: Important reactions in biological chemistry, Metabolism of biomolecules and artificial bioorthogonal reactions.
6	**Learning objectives and skills**	The student • can explain basic principles and underlying reaction mechanisms in organo- and organometallic catalysis and biological chemistry • deepens her/his knowledge in special topics of homogeneous catalysis that are in the research focus of the involved research groups • is able to construct important reaction mechanisms and catalytic cycles and can critically discuss each step.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 Organocatalysis and Catalytic Reactions in Water can be taken • within the Compulsory Elective Module "Advances in Homogenous Catalysis" (20 ECTS in total) • as Elective Module (5 ECTS, not graded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46559	**Quantum Chemistry 1** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Quantum Chemistry 1 (3 SWS)	-
3	Lecturers	Dr. Christian Neiß Prof. Dr. Andreas Görling	

4	**Module coordinator**	Prof. Dr. Andreas Görling
5	**Contents**	• Mathematical concepts and current research issues in the field of quantum and computer chemistry • Hartree-Fock, DFT
6	**Learning objectives and skills**	Students ... • obtain sound knowledge in basic methods of quantum chemistry • are able to solve mathematical problems occurring in quantum chemistry • are able to understand and assess scientific reports in the field of quantum chemistry
7	**Prerequisites**	Strongly recommended Qualifications: • good knowledge of basic quantum mechanics: axioms of QM, application to simple systems (particle in a box, harmonic oscillator, rigid rotator) • good knowledge in mathematics: differential calculus of functions of several variables, linear algebra
8	**Integration in curriculum**	semester: 1;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes) O20 (PL): Oral Examination (20 minutes, not graded: pass/fail)
11	**Grading procedure**	Oral (0%) not graded: pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Attila Szabo, Neil S. Ostlund: Modern Quantum Chemistry, Dover 1996 • Frank Jensen: Introduction to Computational Chemistry, Wiley 2017 (3rd ed.) • Ira N. Levine: Quantum Chemistry, Pearson 2016 (7th ed.)

1	**Module name** 46561	**Quantum Chemistry 2** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Quantum Chemistry 2 (3 SWS)	-
3	Lecturers	Prof. Dr. Andreas Görling	

4	**Module coordinator**	Prof. Dr. Andreas Görling
5	**Contents**	• Many-Body Perturbation Theory • Configuration Interaction, Second Quantization, Coupled Cluster • TD-HF, TD-DFT, RPA
6	**Learning objectives and skills**	Students ... • obtain sound knowledge in advanced methods of quantum chemistry • are able to solve mathematical problems occurring in quantum chemistry • are able to understand and assess scientific reports in the field of quantum chemistry
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;4
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded) if Quantum Chemistry I was already chosen as Elective Module!
10	**Method of examination**	Oral (20 minutes) O20 (PL): Oral Examination (20 minutes, not graded: pass/fail)
11	**Grading procedure**	Oral (0%) not graded: pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Attila Szabo, Neil S. Ostlund: Modern Quantum Chemistry, Dover 1996 • Frank Jensen: Introduction to Computational Chemistry, Wiley 2017 (3rd ed.) • Ira N. Levine: Quantum Chemistry, Pearson 2016 (7th ed.)

1	**Module name** 46556	**Scientific Programming** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Praktikum: Quantum Chemistry - Lab / Scientific Programming (10 SWS) Please note: • Attendance in the lab course is mandatory! • Module starts only in winter term (duration: 2 semesters)	-
3	Lecturers	Dr. Christian Neiß Prof. Dr. Andreas Görling	

4	**Module coordinator**	Prof. Dr. Andreas Görling
5	**Contents**	• Operating system Linux for high-performance computing (HPC) • Scientific programming in Fortran and Python • Using numerical and mathematical libraries/modules • Introduction to parallel computing • Exercises • Programming project
6	**Learning objectives and skills**	Students .... • get familiar with Linux as operating system for HPC • are able to create computer programs for scientific purposes • can use numerical and mathematical libraries/modules in home-made programs • obtain knowledge about basic parallelization paradigms
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 1;2
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded) - please note: the module cannot be combined with the module Quantum Chemistry - Lab
10	**Method of examination**	Practical achievement PL: Successful implementation of the programming project (working program), ungraded - module has to be passed
11	**Grading procedure**	Practical achievement (0%) not graded: pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 150 h Independent study: 0 h
14	**Module duration**	2 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Stephen J. Chapman: Fortran for Scientists and Engineers, McGraw Hill 2017 (4th ed.) • Bernd Klein: Einführung in Python 3, Hanser 2017 (3rd ed.)

		• Stefan Gerlach: Computerphysik, Springer Spektrum 2019 (2nd ed.)

1	**Module name** 46541	**Semiconductor Materials for Energy Applications** Semiconductor materials for energy applications	**5 ECTS**
2	Courses / lectures	Seminar: Semiconductor Materials for Energy Applications - Seminar (1 SWS) Vorlesung: Semiconductor Materials for Energy Applications - Lecture (2 SWS)	- -
3	Lecturers	Dr. Ryan Crisp	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Fundamentals of semiconductors: Crystal structure, Electronic structure, Electrical transport, Interaction with light • Semiconductor devices: Tunnelling, The pn junction, The transistor • Photovoltaics: Principles, Types of solar cells • The interface to a solution: Charged electrolytic interfaces, Electrocatalysis and photoelectrocatalysis
6	**Learning objectives and skills**	The students • are familiar with the fundamentals and modern developments in semiconductor science and applications • understand theoretical and practical aspects in state-of-the-art semiconductor devices • can present, communicate and discuss scientific results with experts in English.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • within the Compulsory Elective Module "Advances in Energy Materials" in M. Sc. Chemistry or M.Sc. Molecular Science (20 ECTS in total) • part of the Elective Module in M. Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination, 20 minutes
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46523	**Small Molecule Activation** Small molecule activation	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Small Molecule Activation (3 SWS)	-
3	Lecturers	Prof. Dr. Karsten Meyer Prof. Dr. Ingrid Span	

4	**Module coordinator**	Prof. Dr. Sjoerd Harder
5	**Contents**	**Lecture:** • Inorganic coordination chemistry, catalytic and electrocatalytic transformation of abundant small molecules N2, O2, CO or CO2, H2O and NH3, into value-added commodities, fine-chemicals, ac-tive pharmaceutical ingredients and polymers. • Selective oxidation reactions. • CO2 reduction to CO and subsequent Fischer-Tropsch catalysis for the production of carbon-based fuels. • Reductive activation of atmospheric N2 to NH3 and the production of H2 from H2O splitting catalysis. Applications, e.g. fuel-cell technologies for carbon-free energy production.
6	**Learning objectives and skills**	The student • can explain basic principles and underlying reaction mechanisms in small molecule activation • is able to construct important reaction mechanisms and catalytic cycles • can critically discuss small-molecule activation
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Homogenous Catalysis Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory Elective Module (20 ECTS in total!) • Lecture module as part of the Elective Module (5 ECTS, not graded)
10	**Method of examination**	Oral O20(PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46543	**Solar Energy Conversion** Solar energy conversion	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Solar Energy Conversion (3 SWS)	-
3	Lecturers	Prof. Dr. Dirk Michael Guldi	

4	**Module coordinator**	Prof. Dr. Dirk Michael Guldi
5	**Contents**	• Demand and supply of energy • Solar cells: Silicon solar cells, dye-sensitized solar cells, organic solar cells, perovskite solar cells, singlet fission • Fundamentals of Electron Transfer • Photosynthesis: natural photosynthesis, artificial photosynthesis
6	**Learning objectives and skills**	The students • are familiar with the fundamentals and modern applications in solar energy research and applications • understand design principles in solar energy devices and can transfer this knowledge to related topics • can present, communicate and discuss scientific results with experts in English.
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Energy Materials Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module "Advances in Energy Materials" MSc Chemistry and Molecular Science (20 ECTS in total!) • Module can be taken as part of the Elective Module, too (5 ECTS, not graded)!
10	**Method of examination**	Written examination (60 minutes)
11	**Grading procedure**	Written examination (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46512	**Special Aspects in Bio-Organic Chemistry** Special aspects in bio-organic chemistry	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Special Aspects in Bio-Organic Chemistry (3 SWS) Please note: • Seminar: time and place by agreement!	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Petra Imhof	

4	**Module coordinator**	Prof. Dr. Nicolai Burzlaff
5	**Contents**	The students • learn about: nucleic acid structure, synthesis, and reactivity; nucleic acid modifications; nucleic acid-protein interactions, nucleic acid-based drugs, nucleic acid biochemistry, modelling of nucleic acids
6	**Learning objectives and skills**	The students • can explain, apply and reflect upon the theories, terminology, specialities, boundaries and different school of bioorganic and bioinorganic chemistry critically and in depth
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • As Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral O20 (PL): Oral examination (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• A. Bloomfield, D.M. Crothers, I. Tinoco, Jr. „Nucleic Acids: structures, properties, and functions“, University Science Books, Sausalito, CA, USA 1999 • D. L. van Vranken, G. A. Weiss, Introduction to Bioorganic Chemistry and Chemical Biology, 1. Aufl., Garland Publishers 2012, ISBN: 978-0815342144

		• W. Saenger„Principles of Nucleic Acid Structure“,Springer-Verlag New York Inc. 1984 • T. Schlick: "Molecular modelling and simulation: An interdisciplinary guide", Springer New York Dordrecht Heidelberg London 2nd ed. 2010 • A. Vologodskii: “Biophysics of DNA”, Cambridge University press, 2015, DOI 10.1017/CBO9781139542371

1	**Module name** 46532	**Surface and Interface Science** Surfaces and interface science	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Surfaces and Interface Science (3 SWS)	-
3	Lecturers	Prof. Dr.-Ing. Marcus Bär	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	• Vacuum and pressure measurement (pumps, pressure and flow ranges) • Lab-based and synchrotron-based light sources (principles, optics, insertion devices, etc.) • Theory of photoemission and electronic structure • XPS (elemental / chemical sensitivity, cross sections, quantification, examples) • UPS (gas phase, adsorbates, 2D band structures, 3D band structures, orbital tomography) • IPES (probing of unoccupied states, energy level alignment determination) • HAXPES (depth-resolved photoemission measurements, examples) • PEEM (spatially-resolved photoemission measurements, examples) • NEXAFS (principle and examples) • XES & RIXS (principle and examples) • Structure of surfaces/ diffraction at surfaces (LEED, definitions and examples) • X-ray spectroscopy based materials research on energy conversion devices (examples from current research)
6	**Learning objectives and skills**	Students ... • understand the principles of photoemission variants and their applications • can judge the quality of data evaluation and its pitfalls • can deliberately select an X-ray spectroscopic analysis method to address given scientific question and are able to evaluate the collected data
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Lecture module within the Compulsory elective module "Advances in Interfaces and Catalysis" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total) • Lecture module as part of the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%)

		As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	• Hüfner: Photoelectron Spectroscopy: Principles and Applications" Springer-Verlag Berlin Heidelberg • Ertl, Küppers: Low Energy Electrons and Surface Chemistry" VCH Weinheim • D. Attwood, Soft X-rays and Extreme Ultraviolett Radiation, Cambridge University Press, 1999 • D. Briggs, M.P. Seah: PracticalSurface Analysis: AugerandX-Ray PhotoelectronSpectroscopy, Wiley, 1996 • M. Bär, L. Weinhardt, and C. Heske: Advanced Characterization Techniques for Thin Film Solar Cells, edited by D. Abou-Ras, T. Kirchartz, and U. Rau (Wiley VCH Verlag GmbH & Co KGaA, ISBN: 978-3-527-33992-1), 2nd Extended Edition, Volume 2, Chap. 18. • A. Meisel, G. Leonhardt, R. Szargan: X-ray Spectra and Chemical Binding, Springer, 1989

1	**Module name** 46546	**Symmetry and Group Theory** Symmetry and group theory	**5 ECTS**
2	Courses / lectures	Seminar: Seminar Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (1 SWS) Vorlesung mit Übung: Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (3 SWS)	- -
3	Lecturers	Prof. Dr. Jörg Libuda	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	• Symmetry of Molecules (symmetry elements, operations, point groups, notations) • Symmetry of Crystals, Surfaces and Interfaces (symmetry in 1, 2 and 3 dimensional periodic strutures, lattices, crystal classes, space groups) • Compact Course Group Theory (elements group theory, definitions, reducible and irreducible representations, orthogonality theorem, character tables) • Group Theory and Quantum Mechanics (representations, operators and symmetry, matrix elements, direct product functions, projection operators) • Symmetry of Organic Molecules: From Electronic Structure to Reactivity (symmetry adaption, cyclic groups, many electron systems, electronic transitions, configuration interaction, symmetry controlled reactions • Symmetry in Anorganic Chemistry: From Atoms to Complexes (MO models, transition metal complexes, direct product groups, rotation inversion group, angular momentum coupling, crystal field splitting, vibronically allowed transitions) • Symmetry and Spectroscopy: Vibrational Spectroscopies (analysis of vibrational modes, normal coordinate analysis, symmetry of vibrational wave functions, vibrational spectroscopy, selection rules) • Symmetry in Crystal Physics: Tensor Description of Physical Properties (tensors, axial, polar, representations, transformation properties, intrinsic symmetry, Neumann's principle, Curie's principle) • Symmetry and Electronic Structure of Solids: Band Structures (translation group and irreps, reciprocal lattice, k-space, Bloch functions, Brillouin zones, symmetry of bands)
6	**Learning objectives and skills**	Students • acquire detailed understanding how to use symmetry properties and the mathematical tools of group theory in a broad range of application fields in chemistry, physics and materials science.
7	**Prerequisites**	None

8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • Lecture module can be taken as part of the Elective module (5 ECTS, not graded)
10	**Method of examination**	Variable O20(PL): Oral Examination (20 minutes)
11	**Grading procedure**	Variable (0%) pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46531	**Theory of Catalytic Processes** Theory of catalytical processes	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Theory of Catalytic Processes (3 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Bernd Meyer	

4	**Module coordinator**	Prof. Dr. Jörg Libuda
5	**Contents**	The module focuses on physical, chemical or technological aspects of modification, manipulation and characterization of interfaces. These aspects relate to the research of ideal model systems (surfaces and adsorbates on single crystal surfaces) or real systems, in which the interface plays a crucial role for the respective properties. In all cases, the local electronic and chemical interactions at the interface affect the geometric structure (e.g. adsorption geometry) and consequently the chemical and physical properties.
6	**Learning objectives and skills**	Students • deepen their knowledge in experimental methods and theoretical aspects to describe and characterize interface phenomena • are able to perform experiments independently and to analyse the data • are familiar with the model-type description of experimental data
7	**Prerequisites**	None
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Advances in Interface Research and Catalysis A Master of Science Molecular Science 20202 Elective modules Master of Science Molecular Science 20202 • Within the Compulsory Elective Module Advances in Interfaces and Catalysis A (IntCat-3A) (20 ECTS in total)! • Module can also be taken as part of the elective module (5 ECTS, not graded)! Please note: **MSc Molecular NANO Science students** have to attend the module **"Advances in Interfaces and Catalysis A (IntCat-3A)**" / **MSc Chemistry students** can **choose** between the module "**Advances in Interfaces and Catalysis A (IntCat-3A)"** and the module "**Nanostructured Materials and Interfaces B (IntCat-3B)"** of Prof. Bachmann!
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (100%) As part of the elective module: 0% - pass/fail
12	**Module frequency**	only in winter semester
13	**Workload in clock hours**	Contact hours: 45 h

		Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!

1	**Module name** 46557	**Theory of Surface Phenomena** no english module name available for this module	**5 ECTS**
2	Courses / lectures	Vorlesung mit Übung: Theory of Surface Phenomena / Theorie der Oberflächenphänomene (3 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Bernd Meyer	

4	**Module coordinator**	Prof. Dr. Bernd Meyer
5	**Contents**	• Brief introduction into quantum-chemical methods for surface science studies • Introduction of basic nomenclature of how to describe the atomic and electronic structure of surfaces • Basic concepts on how to understand the electronic properties of metal, semiconductor and insulator surfaces, such as surface states, dangling bonds, passivation, charge neutralization with respect to polar and nonpolar surfaces • Thermodynamic analysis of the stability of surface structures; surface phase diagrams • Methods for calculating STM and AFM data to support the analysis of experimental data from local probe measurements
6	**Learning objectives and skills**	The students ... • are familiar with the most common theoretical and experimental techniques for surface science studies • have a sound knowledge in basic principles governing surface structure and reactivity • can perform first quantum chemical calculations on their own and interprete the data
7	**Prerequisites**	Basic knowledge of quantum mechanics and quantum chemical calculations is strongly recommended
8	**Integration in curriculum**	semester: 2;3
9	**Module compatibility**	Elective modules Master of Science Molecular Science 20202 • Elective module (5 ECTS, ungraded) within the M.Sc. degree programme Chemistry or M.Sc. Molecular Science (especially Molecular NANO science)
10	**Method of examination**	Oral (20 minutes)
11	**Grading procedure**	Oral (0%) pass/fail
12	**Module frequency**	only in summer semester
13	**Workload in clock hours**	Contact hours: 45 h Independent study: 105 h
14	**Module duration**	1 semester
15	**Teaching and examination language**	english
16	**Bibliography**	no Bibliography information available!