

Module description

for the degree programme

Master of Science Chemistry

(Version of examination regulation: 20202)

for the summer term 2024

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1	Module name 1999	Masterarbeit (M.Sc. Chemistry 20202) Master's thesis	30 ECTS
2	Courses / lectures	No courses / lectures available for this module! Please note: <ul style="list-style-type: none"> The master's thesis will be written at the student's choice in one of the research groups of the Department of Chemistry and Pharmacy! 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 <ul style="list-style-type: none"> 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	Before commencing work on the Master's thesis, students must have successfully completed the two subject-related compulsory elective modules, the supplementary compulsory elective module and the research module, coming to a total of 75 ECTS credits.	
8	Integration in curriculum	semester: 4	
9	Module compatibility	Pflichtmodul Master of Science Chemistry 20202	
10	Method of examination	Written (6 Monate) <ul style="list-style-type: none"> Thesis (2 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	Workload: 900 h
15	Module duration	1 semester
16	Teaching and examination language	english
17	Bibliography	

Inorganic chemistry

1	Module name 46501	Inorganic Chemistry	10 ECTS
2	Courses / lectures	Vorlesung mit Übung: Inorganic Chemistry (6.0 SWS)	10 ECTS
3	Lecturers	Prof. Dr. Nicolai Burzlaff Prof. Dr. Romano Dorta Prof. Dr. Karl Mandel	

4	Module coordinator	Prof. Dr. Karsten Meyer	
5	Contents	<ul style="list-style-type: none"> • Introduction to current research topics of Inorganic Chemistry • establishing fundamental knowledge required for appreciation of more specialized topics in Inorganic Chemistry; the expected standard is based on a research oriented masters program. 	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • acquire knowledge and expertise required for danger evaluation and practical handling of novel inorganic compounds 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 1;2	
9	Module compatibility	<p>Inorganic Chemistry Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Core module „Inorganic 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	<p>Oral (30 minutes) PL: Oral examination (30 minutes)</p>	
11	Grading procedure	Oral (100%)	
12	Module frequency	Every semester	
13	Workload in clock hours	<p>Contact hours: 90 h Independent study: 210 h</p>	
14	Module duration	2 semester	
15	Teaching and examination language	english	
16	Bibliography		

1	Module name 46502	Inorganic Chemistry laboratory	10 ECTS
2	Courses / lectures	Praktikum: Inorganic Chemistry - LAB (15.0 SWS) <ul style="list-style-type: none"> Attendance in lab course and at safety instruction is compulsory! A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de Registration: please contact Dr. Achim Zahl (achim.zahl@fau.de) 	10 ECTS
3	Lecturers	Prof. Dr. Karsten Meyer Prof. Dr. Julien Bachmann Prof. Dr. Nicolai Burzlaff Dr. Achim Zahl Prof. Dr. Romano Dorta PD Dr. Marat Khusniyarov Prof. Dr. Sjoerd Harder Prof. Dr. Ingrid Span Prof. Dr. Karl Mandel	

4	Module coordinator	Prof. Dr. Karsten Meyer	
5	Contents	<ul style="list-style-type: none"> practical laboratory experience aiming at introducing students to current and state of the art inorganic research topics work experience in a team of researchers establishing fundamental knowledge required for addressing individual molecular research problems at a state of the art level independent and self-driven approach to problem solving in an assigned research project 	
6	Learning objectives and skills	The students <ul style="list-style-type: none"> apply acquired fundamental knowledge and practical skills to an individual research problem that they work on independently manage and apply the fundamental safety regulations important to handling hazardous compounds and instruct other coworkers in relevant safety topics 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	None	
8	Integration in curriculum	semester: 1;2	
9	Module compatibility	Inorganic Chemistry Master of Science Chemistry 20202 <ul style="list-style-type: none"> Lab module within the Core module „Inorganic Chemistry“ in M. Sc. Chemistry 	

		<ul style="list-style-type: none"> 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 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: 225 h Independent study: 75 h
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	

Organic chemistry

1	Module name 46503	Organic Chemistry	10 ECTS
2	Courses / lectures	Vorlesung mit Übung: Organic Chemistry (3.0 SWS/WS) Vorlesung mit Übung: Organic Chemistry (3.0 SWS/SS)	10 ECTS
3	Lecturers	Prof. Dr. Svetlana Tsogoeva apl. Prof. Evgeny Kataev Prof. Dr. Henry Dube Norbert Jux Prof. Dr. Andreas Hirsch Prof. Dr. Andriy Mokhir	

4	Module coordinator	Prof. Dr. Henry Dube	
5	Contents	<ul style="list-style-type: none"> • Introduction to current research topics of Organic Chemistry • establishing fundamental knowledge required for appreciation of more specialized topics in Organic Chemistry; the expected standard is based on a research oriented Masters program 	
6	Learning objectives and skills	Students <ul style="list-style-type: none"> • acquire knowledge and expertise required for theoretical evaluation and practical handling of novel organic compounds 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 1;2	
9	Module compatibility	Organic Chemistry Master of Science Chemistry 20202 <ul style="list-style-type: none"> • Lecture module within the Core module „Organic 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	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		

1	Module name 46504	Organic Chemistry laboratory	10 ECTS
2	Courses / lectures	<p>No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.</p> <ul style="list-style-type: none"> Attendance at the preliminary briefing including 'safety instructions part 1': signature list serves as proof of attendance; Attendance at the briefing 'safety instructions part 2' in the lab; A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de 	
3	Lecturers		

4	Module coordinator	Prof. Dr. Svetlana Tsogoeva
5	Contents	<ul style="list-style-type: none"> Reactions / Synthesis: Oxidation reactions; Synthesis and application of Jacobsen Mn(III)-complex (Jacobsen epoxidation); Reductions; Reactions with lithium organic compounds; Cross-coupling reaction; Synthesis of the Evans-Auxiliary; Natural compounds; Heterocycles. Advanced practical lab work in organic chemistry, that includes molecular synthesis and use of state-of-the-art analytical tools. Instruction in laboratory safety regulations.
6	Learning objectives and skills	<p>The students are capable</p> <ul style="list-style-type: none"> to use their theoretical and practical background to make an individual contribution to an independent, actual and realistic research project; to organize a small research/synthesis project in theory and practise to plan experiments to prove or reject a given hypothesis to provide a state-of-the-art documentation and discussion of results obtained as a member of a research team to present, communicate and discuss scientific results with experts in English.
7	Prerequisites	Knowledge of the content of the lecture *Organic Chemistry* (CM-OC) is recommended.
8	Integration in curriculum	semester: 1;2
9	Module compatibility	<p>Organic Chemistry Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> Lab module within the Core module „Organic 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	<p>Practical achievement</p> <p>pÜL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)</p>
11	Grading procedure	Practical achievement (100%)
12	Module frequency	Only in winter 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	<ul style="list-style-type: none"> • L. F. Tietze, Th. Eicher, Reaktionen und Synthesen in organisch-chemischen Praktikum und Forschungslaboratorium • R. Brückner, et al., Praktikum Präparative Organische Chemie • Organikum, Wiley-VCH

Physical chemistry

1	Module name 46505	Physical Chemistry	10 ECTS
2	Courses / lectures	Vorlesung mit Übung: Advanced Physical Chemistry (Interfaces) (3.0 SWS,) Vorlesung mit Übung: Physical Chemistry (3.0 SWS,)	10 ECTS
3	Lecturers	Prof. Dr. Jörg Libuda Dr. Alejandro Cadranel Prof. Dr. Thomas Drewello	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi
5	Contents	<ul style="list-style-type: none"> • introduction to the current topics of research in the field of physical chemistry • developing the basics of physical chemistry at the level of a scientifically oriented Master's program • deepening of knowledge in the specialized field of the lecturers involved in this module to the limit of current knowledge
6	Learning objectives and skills	<p>Students</p> <ul style="list-style-type: none"> • apply fundamental knowledge of physical chemistry to particular topics in research • develop model-like descriptions for complex physicochemical systems and model experimental data
7	Prerequisites	None
8	Integration in curriculum	semester: 1;2
9	Module compatibility	<p>Physical Chemistry Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Core module „Physical 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 min)
11	Grading procedure	Oral (100%)
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	

1	Module name 46506	Physical Chemistry laboratory	10 ECTS
2	Courses / lectures	Praktikum: Physical Chemistry - Lab (15.0 SWS) Please note: <ul style="list-style-type: none"> • Attendance at safety instruction and lab-course 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 	10 ECTS
3	Lecturers	Prof. Dr. Dirk Michael Guldi Dr. Guido Sauer	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> • Practical introduction to current and state-of-the-art research topics in the field of physical chemistry • Advanced spectroscopic and image analysis • Guided work on current research projects using methods of physical chemistry • Documentation of experimental results <p>The practical part comprises 7 days in the physicochemical advanced practical course lab and, in addition, two 3-day practical projects in two different working groups of physical chemistry. The 3-day internships may be extended after consultation with the internship coordinator and the working group (in return the number of experiments in the practical lab course can be reduced).</p>	
6	Learning objectives and skills	<p>Students ...</p> <ul style="list-style-type: none"> • apply fundamental knowledge of physical chemistry to particular topics in research • develop model-like descriptions for complex systems and model experimental data • discover various modern experimental techniques and apply them systematically in practice • apply and transfer knowledge acquired during their studies to handle and solve open questions in research projects in physical chemistry • perform experiments/measurements, record and evaluate their results in appropriate scientific form and interpret results independently • present their own results and acquired knowledge in an appropriate scientific style in English language in oral and written form • evaluate the basic safety matters in handling hazardous materials and complex apparatus 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 1;2	
9	Module compatibility	Physical Chemistry Master of Science Chemistry 20202 <ul style="list-style-type: none"> • Lab module within the Core module „Physical Chemistry“ in M. Sc. Chemistry 	

		<ul style="list-style-type: none"> • 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 SeL: Poster presentation, 20 - 30 min
11	Grading procedure	Practical achievement (100%) Poster presentation (100%)
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	<ul style="list-style-type: none"> • P. Atkins, J. De Paula, Atkins Physical Chemistry, 10th edition, Oxford University Press, Oxford, 2014 • Literature references provided in the guidelines of each experiment

Quantum chemistry

1	Module name 46507	Quantum Chemistry	10 ECTS
2	Courses / lectures	<p>Vorlesung mit Übung: Quantum Chemistry 2 (3.0 SWS, SoSe 2024)</p> <p>Vorlesung mit Übung: Quantum Chemistry 1 (3.0 SWS, WiSe 2024)</p> <p>Please note:</p> <ul style="list-style-type: none"> The core module "Quantum Chemistry" starts only in winter term! 	10 ECTS
3	Lecturers	Prof. Dr. Andreas Görling	

4	Module coordinator	Prof. Dr. Andreas Görling	
5	Contents	<ul style="list-style-type: none"> 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	<p>Students ...</p> <ul style="list-style-type: none"> 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	<p>Required Qualifications:</p> <ul style="list-style-type: none"> 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	
9	Module compatibility	<p>Quantum Chemistry Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	<p>Oral (30 minutes)</p> <p>O30 (PL): Oral Examination (30 minutes)</p>	
11	Grading procedure	Oral (100%)	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 90 h</p> <p>Independent study: 210 h</p>	
14	Module duration	2 semester	

15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none">• 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 46508	Quantum Chemistry laboratory	10 ECTS
2	Courses / lectures	Praktikum: Training in Applied Computational Chemistry (5.0 SWS,) Praktikum: Quantum Chemistry - Lab / Scientific Programming (10.0 SWS,) <ul style="list-style-type: none"> • 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. Andreas Görling Prof. Dr. Dirk Zahn Prof. Dr. Petra Imhof Prof. Dr. Bernd Meyer Prof. Dr. Carolin Müller Dr. Christian Neiß	

4	Module coordinator	Prof. Dr. Andreas Görling
5	Contents	<ul style="list-style-type: none"> • 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 <ul style="list-style-type: none"> • 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 Chemistry 20202 <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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.)

Advances in bioorganic and bio-inorganic chemistry

Mandatory elective module (20 ECTS in total):

Please choose **3 lecture modules out of 4**:

- *Advanced Bio-Organic and Bio-Inorganic Chemistry*
- *Special Aspects in Bio-Organic Chemistry*
- *Sensory Sciences Lab*
- *Medical Life Sciences*

Please note:

- The lab module "*Bio-Organic and Bio-Inorganic Chemistry - Lab*" is **mandatory!**

1	Module name 46511	Advanced Bio-Organic and Bio-Inorganic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Nicolai Burzlaff	
5	Contents	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Oral O20 (PL): Oral examination (20 minutes)</p>	
11	Grading procedure	<p>Oral (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	

15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none">• 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 46512	Special Aspects in Bio-Organic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers. Please note: <ul style="list-style-type: none"> • Seminar: time and place by agreement! 	
3	Lecturers		

4	Module coordinator	Prof. Dr. Nicolai Burzlaff
5	Contents	The students <ul style="list-style-type: none"> • 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 <ul style="list-style-type: none"> • 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: 1;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 46514	Bio-Organic and Bio-Inorganic Chemistry - Lab	5 ECTS
2	Courses / lectures	Praktikum: Bio-Organic & Bio-Inorganic LAB (7.0 SWS) Please note: Attendance at lab course is compulsory!	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Nicolai Burzlaff Norbert Jux Prof. Dr. Petra Imhof Prof. Dr. Carola Kryschi	

4	Module coordinator	Prof. Dr. Nicolai Burzlaff
5	Contents	The students <ul style="list-style-type: none"> • 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 <ul style="list-style-type: none"> • 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 Chemistry 20202 <ul style="list-style-type: none"> • 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	

1	Module name 46515	Sensory Sciences Lab	5 ECTS
2	Courses / lectures	<p>No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.</p> <p><u>Please note:</u></p> <ul style="list-style-type: none"> The module "Sensory Sciences Lab" is an interdisciplinary module with a limited number of participants: only 10 students from MSc Chemistry or MSc Molecular Science will be admitted! Students from Molecular LIFE Science will be given priority! The module "Sensory Sciences Lab" can be taken as part of the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" (20 ECTS in total, all modules have to be graded) or as an elective module (5 ECTS, ungraded)! 	
3	Lecturers	-	

4	Module coordinator	Prof. Dr. Andrea Büttner
5	Contents	<p>The field of Sensory Sciences investigates how animals and humans sense, neurally process and perceive their environment. This research-oriented interdisciplinary course provides important concepts, theories, and methods of the Sensory Sciences to advanced students from three disciplines (Psychology, Medicine and Chemistry - Molecular Science). These topics comprise human auditory, visual and olfactory perception, chemocommunication, psychophysics, neuroimaging, molecular sensory receptors and technologies for neuromodulation (among others). The students apply these concepts in interdisciplinary teams to develop, conduct and analyse their own small research project. While engaging in an interdisciplinary collaboration and exchange, students can share and deepen their discipline-specific perspectives and competencies as well as learn about concepts and methods from other disciplines.</p>
6	Learning objectives and skills	<p>The students are able to</p> <ul style="list-style-type: none"> explain fundamental concepts and methods of the Sensory Sciences develop an own (limited) research question and design an empirical data collection to investigate the research question collect data in the laboratory and analyse the data present their findings in oral and written form communicate effectively in interdisciplinary teams understand and reflect the challenges and chances of interdisciplinary collaborations.
7	Prerequisites	None
8	Integration in curriculum	semester: 1;2;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202
10	Method of examination	Seminar achievement

		Written project report (20-30 pages)
11	Grading procedure	Seminar achievement (100%) 100% project report <ul style="list-style-type: none"> • Part of the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" in M.Sc. Molecular Science (5 ECTS, graded; PO 2020) • elective module (5 ECTS, ungraded; PO 2020)
12	Module frequency	Only in winter semester
13	Workload in clock hours	Contact hours: 30 h Independent study: 120 h
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • Literature will be announced in the first session • Scripts and materials will be provided via StudOn!

1	Module name 46516	Medical Life Sciences	5 ECTS
2	Courses / lectures	Vorlesung: Medical Life Sciences	5 ECTS
3	Lecturers	Prof. Dr. Stefan Lyer Dr. Stefanie Klein Prof. Dr. Ingrid Span Prof. Dr. Danijela Gregurec PD Dr. Christina Janko Prof. Dr. Olaf Prante PD Dr. Rainer Tietze	

4	Module coordinator	Prof. Dr. Ingrid Span
5	Contents	To lay the foundation for working in molecular disease research, the MedLife module provides knowledge in genetics, molecular biology, cell biology, nucleic acid and protein chemistry, enzymology, nuclear and nanomedicine.
6	Learning objectives and skills	The students <ul style="list-style-type: none"> • explain the basic principles and techniques of the various fields of research • engage with scientific texts • will be able to apply the essential principles to practical biological and chemical problems
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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) <p>*If students want to take the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" as a whole, they have to choose 3 out of the 4 lecture modules, the laboratory module "Bio-Organic and Bio-Inorganic Chemistry - Lab" (No.46514) must be taken compulsorily!</p>
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	

Advances in homogeneous catalysis

1	Module name 46521	Organometallic Catalysis	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Organometallic Catalysis (3.0 SWS) Seminar: Organometallic Catalysis - Seminar (1.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta	

4	Module coordinator	Prof. Dr. Sjoerd Harder
5	Contents	<p>Knowledge on homogeneous organometallic catalysis will be deepened by discussing the latest scientific breakthroughs and developments in modern areas of catalysis. The module consists of two parts.</p> <p>Harder-Part <i>Sustainable Main Group Metal Catalysis</i></p> <ul style="list-style-type: none"> • Activation of strong bonds and small molecules with main group metal complexes (who needs d-orbitals?). Replacing expensive rare transition metals with cheap and abundant main group metals. • Bond activation using the ball-mill method. • Catalysis with main group metal complexes (discussion of elementary steps and catalytic cycles). • Activation of metals and making metal catalysts using Metal-Vapor-Synthesis. The evaporation of metals under vacuum and co-condensation in an organic matrix is a great way to make highly active metal catalysts. <p>Dorta-Part <i>Asymmetric Catalysis by Chiral Metal Complexes – Applications in Industry</i></p> <ul style="list-style-type: none"> • Importance of chiral molecules in nature and life science • Chiral pharmaceutical drugs and agrochemicals • Asymmetric catalysis: Chiral catalysts acting as a chirality multiplier • Advantages in comparison with racemate separation or stoichiometric enantioselective syntheses. • Historical development of chiral technology and industrial applications. • Synthesis of enantiopure ligands (famous industrial examples will be discussed). • Mechanistic aspects (catalytic cycles).
6	Learning objectives and skills	<p>The student</p> <ul style="list-style-type: none"> • will learn the latest developments at the forefront of organometallic catalysis • will understand that the field of catalysis needs to become sustainable and that we move away from expensive rare metals to abundant main group metals

		<ul style="list-style-type: none"> • will be able to critically discuss catalytic cycles and understand reaction mechanisms • will be taught new methods (practical and theoretical) to study molecular properties • will be understand the need for new methods of catalyst preparation • will be up-to-date with asymmetric catalysis and industrial applications
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Homogenous Catalysis Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Oral</p> <p>O20(PL): Oral examination (20 minutes)</p>
11	Grading procedure	<p>Oral (100%)</p> <ul style="list-style-type: none"> • As part of the Compulsory Elective module "Advances in Homogenous Catalysis": O20, 100% • As part of the elective module: 0% - pass/fail
12	Module frequency	Only in summer semester
13	Workload in clock hours	<p>Contact hours: 45 h</p> <p>Independent study: 105 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • 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	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Organocatalysis and Catalytic Reactions in Water (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva	

4	Module coordinator	Prof. Dr. Sjoerd Harder	
5	Contents	<ul style="list-style-type: none"> 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	<p>The student</p> <ul style="list-style-type: none"> 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	<p>Advances in Homogenous Catalysis Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <p>Organocatalysis and Catalytic Reactions in Water can be taken</p> <ul style="list-style-type: none"> within the Compulsory Elective Module "Advances in Homogenous Catalysis" (20 ECTS in total) as Elective Module (5 ECTS, not graded) 	
10	Method of examination	<p>Oral</p> <p>O20(PL): Oral examination (20 minutes)</p>	
11	Grading procedure	<p>Oral (100%)</p> <p>As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h</p> <p>Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	
16	Bibliography		

1	Module name 46523	Small Molecule Activation	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Small Molecule Activation (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Karsten Meyer Prof. Dr. Ingrid Span	

4	Module coordinator	Prof. Dr. Sjoerd Harder	
5	Contents	Lecture: <ul style="list-style-type: none"> 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, active 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 <ul style="list-style-type: none"> 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 Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> 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		

1	Module name 46524	Homogeneous Catalysis - Lab	5 ECTS
2	Courses / lectures	Praktikum: Homogeneous Catalysis - Lab (7.0 SWS) <ul style="list-style-type: none"> • 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. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva Prof. Dr. Karsten Meyer Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta	

4	Module coordinator	Prof. Dr. Sjoerd Harder	
5	Contents	Students <ul style="list-style-type: none"> • 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 <ul style="list-style-type: none"> • 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 Chemistry 20202 <ul style="list-style-type: none"> • Lab module within the Compulsory Elective Module (20 ECTS)! 	
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	

Advances in Interface Research and Catalysis A

1	Module name 46531	Theory of Catalytic Processes	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Bernd Meyer	
5	Contents	<ul style="list-style-type: none"> • Introduction: catalysis as interdisciplinary multiscale problem • Atomic structure and thermodynamic stability of surfaces and adsorbates, surface phase diagrams, active surface sites • Reactivity concepts: d-band model, Newns-Anderson model of adsorption, trends in the periodic table • Microkinetic modelling, rate equations, steady-state limit, rate determining step, transition state theory, kinetic Monte Carlo • Descriptors for catalytic activity, scaling relations (Bronsted-Evans-Polanyi), volcano plots • Accelerated molecular dynamics for sampling rare events 	
6	Learning objectives and skills	<p>Students</p> <ul style="list-style-type: none"> • are familiar with the most common quantum-chemical methods for studies in heterogeneous catalysis • understand the principles of descriptor-based predictions of catalytic activity • can perform first quantum chemical calculations on their own and interpret the data 	
7	Prerequisites	Basic knowledge of quantum mechanics and quantum chemical calculations is strongly recommended!	
8	Integration in curriculum	semester: 1;2;3	
9	Module compatibility	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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)! <p>Please note:</p> <p>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!</p>	
10	Method of examination	<p>Oral (20 minutes) PL: O 20 - oral examination (20 minutes)</p>	
11	Grading procedure	Oral (100%)	

		<ul style="list-style-type: none"> • Within the Compulsory Elective Module "Advances in Interfaces and Catalysis A (IntCat-3A)": 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	<ul style="list-style-type: none"> • J.K. Norsov, T. Bligaard, J. Rossmeisl, C.H. Christensen, Towards the computational design of solid catalysts, Nature Chemistry, 2009, 1, 37

1	Module name 46532	Surface and Interface Science	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Surfaces and Interface Science (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr.-Ing. Marcus Bär	

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202</p> <p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 Ultraviolet Radiation, Cambridge University Press, 1999 • D. Briggs, M.P. Seah: Practical Surface Analysis: Auger and X-Ray Photoelectron Spectroscopy, 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 46533	Heterogeneous Catalysis and Kinetics	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Heterogeneous Catalysis and Kinetics (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Jörg Libuda	

4	Module coordinator	Prof. Dr. Jörg Libuda	
5	Contents	<p>Syllabus:</p> <ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202 Advances in Interface Research and Catalysis B Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	5 ECTS
2	Courses / lectures	Praktikum: Interface & Catalysis LAB (7.0 SWS) <ul style="list-style-type: none"> • 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. Bernd Meyer Prof. Dr. Jörg Libuda Prof. Dr. Julien Bachmann	

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	<p>Practical introduction to state-of-the-art research in the fields of surface science, interface science, heterogeneous catalysis, electrocatalysis or materials characterization.</p> <p>Guided work on a current research project in a research group.</p> <p>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.</p> <p>Practical laboratory experience to introduce state-of-the-art experimental tools in surface and catalysis research, among them:</p> <ul style="list-style-type: none"> • 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	<p>The students ...</p> <ul style="list-style-type: none"> • 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.

		<ul style="list-style-type: none"> present own results in written form and scientific style English language.
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202</p> <p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	<p>Practical achievement</p> <p>PL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)</p> <p>Please note: Module examination organized by supervising group!</p>
11	Grading procedure	Practical achievement (100%)
12	Module frequency	Every semester
13	Workload in clock hours	<p>Contact hours: 105 h</p> <p>Independent study: 45 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	Will be provided by the supervising research group

Advances in energy materials

1	Module name 46541	Semiconductor Materials for Energy Applications	5 ECTS
2	Courses / lectures	Seminar: Semiconductor Materials for Energy Applications - Seminar (1.0 SWS) Vorlesung: Semiconductor Materials for Energy Applications (2.0 SWS)	5 ECTS
3	Lecturers	Dr. Ryan Crisp	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi
5	Contents	<ul style="list-style-type: none"> 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	<p>The students</p> <ul style="list-style-type: none"> 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	

1	Module name 46542	Advanced Electrochemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> 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	<p>Students</p> <ul style="list-style-type: none"> 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	<p>Written examination (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	

16	Bibliography	<ul style="list-style-type: none">• 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 <p>For further literature, please see the current list on studon.</p>
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1	Module name 46543	Solar Energy Conversion	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers	-	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> • 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	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Written examination (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	
16	Bibliography		

1	Module name 46544	Energy Materials - Lab	5 ECTS
2	Courses / lectures	Praktikum: Energy Materials - LAB (7.0 SWS) <ul style="list-style-type: none"> • 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	Prof. Dr. Dirk Michael Guldi Dr. Christian Ehli	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students</p> <ul style="list-style-type: none"> • 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	<p>Advances in Energy Materials Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Practical achievement</p> <p>pÜL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)</p>
11	Grading procedure	Practical achievement (100%)
12	Module frequency	Every semester
13	Workload in clock hours	<p>Contact hours: 105 h</p> <p>Independent study: 45 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	

Advances in interface research and catalysis B

1	Module name 46532	Surface and Interface Science	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Surfaces and Interface Science (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr.-Ing. Marcus Bär	

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202</p> <p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 Ultraviolet Radiation, Cambridge University Press, 1999 • D. Briggs, M.P. Seah: Practical Surface Analysis: Auger and X-Ray Photoelectron Spectroscopy, 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 46533	Heterogeneous Catalysis and Kinetics	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Heterogeneous Catalysis and Kinetics (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Jörg Libuda	

4	Module coordinator	Prof. Dr. Jörg Libuda	
5	Contents	<p>Syllabus:</p> <ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202 Advances in Interface Research and Catalysis B Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	5 ECTS
2	Courses / lectures	Praktikum: Interface & Catalysis LAB (7.0 SWS) <ul style="list-style-type: none"> • 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. Bernd Meyer Prof. Dr. Jörg Libuda Prof. Dr. Julien Bachmann	

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	<p>Practical introduction to state-of-the-art research in the fields of surface science, interface science, heterogeneous catalysis, electrocatalysis or materials characterization.</p> <p>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.</p> <p>Practical laboratory experience to introduce state-of-the-art experimental tools in surface and catalysis research, among them:</p> <ul style="list-style-type: none"> • 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	<p>The students ...</p> <ul style="list-style-type: none"> • 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.

		<ul style="list-style-type: none"> present own results in written form and scientific style English language.
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202</p> <p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	<p>Practical achievement</p> <p>PL: Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)</p> <p>Please note: Module examination organized by supervising group!</p>
11	Grading procedure	Practical achievement (100%)
12	Module frequency	Every semester
13	Workload in clock hours	<p>Contact hours: 105 h</p> <p>Independent study: 45 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	Will be provided by the supervising research group

1	Module name 46537	Nanostructured Materials and Interfaces	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	no content description available!
6	Learning objectives and skills	no learning objectives and skills description available!
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 Module compability:</p> <ul style="list-style-type: none"> • within the Compulsory Elective Module Advances in Interfaces and Catalysis B (IntCat-3B) (20 ECTS)! • module can also be taken as part of the elective module (5 ECTS, not graded)! • MSc Chemistry student can choose between the compulsory elective module Advances in Interfaces and Catalysis A (IntCat-3A) and the compulsory elective module Advances in Interfaces and Catalysis B (IntCat-3B)
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	

Advances in Organic Chemistry

1	Module name 46568	Organic Chemistry Spectroscopy Lab	5 ECTS
2	Courses / lectures	Praktikum: Organic Chemistry Spectroscopy Lab (7.0 SWS) <ul style="list-style-type: none"> 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	apl. Prof. Evgeny Kataev Prof. Dr. Andreas Hirsch Norbert Jux Prof. Dr. Henry Dube Prof. Dr. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva	

4	Module coordinator	Norbert Jux
5	Contents	The students will analyse one (or two, depending on complexity) organic compound prepared in one of the research groups mentioned above by <ul style="list-style-type: none"> ¹H, ¹³C, and, if necessary, ¹⁹F, ³¹P NMR spectroscopies Advanced NMR techniques such as various 2D methods, HETCOR, etc. Mass spectrometries such as MALDI-TOF, ESI UV/Vis absorption and fluorescence spectroscopies IR and Raman spectroscopies ECD (electronic circular dichroism) spektroskopie
6	Learning objectives and skills	The students <ul style="list-style-type: none"> understand the preparation of samples in terms of purity and concentration are able to handle the spectrometers and analytical machinery are able to process spectra and information from raw data know how to properly store experimental data
7	Prerequisites	It is strongly recommended to have attended the lecture module "Advanced Spectroscopy in Organic Chemistry" as preparation!
8	Integration in curriculum	semester: 2;3
9	Module compatibility	Advances in Organic Chemistry Master of Science Chemistry 20202 Lab module within the Compulsory Elective Module "Advances in Organic Chemistry" (20 ECTS)!
10	Method of examination	Practical achievement pÜL: <ul style="list-style-type: none"> Analysis of one (or two, depending on complexity) organic molecule provided from the above-mentioned research groups Graded Lab protocol with processed spectra, 30-50 pages, including 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	<ul style="list-style-type: none"> • M. Hesse, H. Meier, B. Zeeh, Spektroskopische Methoden in der organischen Chemie, Thieme, 8. Edition, 2011, ISBN: 9783135761077. • H. Friebolin, Basic one- and two-dimensional NMR spectroscopy", Wiley-VCH, 5th ed., 2010, ISBN: 9783527327829. • T. N. Mitchell, B. Costisella, NMR – From spectra to structures, Springer, 2nd ed., 2007, ISBN: 9783540721956. • D. H. Williams, I. Fleming, McGraw Hill, Spectroscopic methods in organic chemistry", Springer, 7th ed., 2019, ISBN: 9783030182519. • K. M. Sanders, E. C. Constable, B. K. Hunter, C. M. Pearce, Modern NMR spectroscopy. A Workbook of Chemical Problems, Oxford University Press, 1989, ISBN: 9780198552871.

1	Module name 46569	Stereoselective Synthesis	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Stereoselective Synthesis (3.0 SWS)	5 ECTS
3	Lecturers	apl. Prof. Evgeny Kataev	

4	Module coordinator	apl. Prof. Evgeny Kataev	
5	Contents	<p>The students are introduced to advanced aspects of stereoselective synthesis:</p> <ul style="list-style-type: none"> • General/Fundamental principles of stereochemistry. • Determination of absolute configuration and enantiomeric composition. • Various types of stereoselective reactions, including alkylation, aldol-related reactions, asymmetric Diels-Alder, and cyclization reactions • Stereo- and enantioselective metal-catalyzed reactions, organocatalytic transformation, and enzymatic reactions. • Historical and recent developments in the field are given. • Exemplary stereoselective syntheses of essential drugs and other molecules. 	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • understand mechanisms in terms of selectivities, conditions, additives, • are able to offer synthetic pathways to various chiral drugs and other molecules. 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Compulsory elective module "Advances in Organic 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	<p>Written examination (60 minutes) W60 (PL): Written examination (60 minutes)</p>	
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> • Written examination: 100 % • As part of the elective module: 0% - pass/fail 	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	

16	Bibliography	<ul style="list-style-type: none">• Eliel, Wilen, Doyle, Basic Organic Stereochemistry, WileySons 2001;• Lin, Li, Chan, Principles and application of asymmetric synthesis, WileySons, 2001;• Carreira, Kvaerno, Classics in Stereoselective Synthesis, Wiley-VCH 2009;• Carey, F. A.; Sundberg, R. J.; Organic Chemistry Part A and B, Springer, Berlin 2007.
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1	Module name 46571	Heterocyclic Chemistry	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Heterocyclic Chemistry (3.0 SWS)	5 ECTS
3	Lecturers	Norbert Jux	

4	Module coordinator	Norbert Jux	
5	Contents	<p>The students are introduced to fundamental and advanced aspects of heterocyclic chemistry:</p> <ul style="list-style-type: none"> Nitrogen-, oxygen- and sulphur-containing heterocycles are discussed. Syntheses, characterization and properties of heterocycles with ring sizes from three to seven atoms are presented. Examples from pharmacy (drugs) and materials science underline the importance of heterocycles. Historical and recent developments in the field are given. Retrosynthetic analyses of heterocycles and drugs are described. Named reactions and important contributors to the field are presented. 	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> understand the formation reactions of heterocycles are able to analyse drugs and other molecules in terms of their components, in particular, heterocycles are able to offer synthetic pathways to various heterocycle-containing drugs and other molecules 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> Lecture module within the Compulsory elective module "Advances in Organic 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	<p>Written examination (60 minutes) W60 (PL): Written examination (60 minutes)</p>	
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> As part of the Compulsory Elective module "Advances in Organic Chemistry": W60, 100% As part of the elective module: 0% - pass/fail 	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	

14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • J. A. Joule, K. Mills, Heterocyclic Chemistry, Wiley-Blackwell, 5th Edition, 2010, ISBN-13: 978-1405133005. • T. L. Gilchrist, Heterocyclic Chemistry, Pearson Education Dorling Kindersley, 3rd Edition, 1997, ISBN: 978-8131707937. • Peter A. Jacobi, Introductory Heterocyclic Chemistry, Wiley, 1st Edition, 2018, ISBN: 978-1119417590. • T. Eicher, S. Hauptmann, A. Speicher, The Chemistry of Heterocycles, 3rd edition, Wiley 2013, ISBN: 978-3-527-66986-8.

1	Module name 46572	Advanced Spectroscopy in Organic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Henry Dube	
5	Contents	<p>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, ^{13}C, ^{19}F, ^{31}P). 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).</p> <p>In addition, other optical spectroscopic methods will be reviewed and discussed in more depth (e.g., UV/Vis-, CD-, IR-spectroscopy and Mass spectrometry).</p>	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • 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: 1;2;3	
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Compulsory Elective module "Advances in Organic Chemistry" in M. Sc. Chemistry or Molecular Science (20 ECTS in total, graded) • As Elective Module in M. Sc. Chemistry or Molecular Science (5 ECTS, not graded) 	
10	Method of examination	Written examination (60 minutes)	
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> • As part of the Compulsory Elective module "Advances in Organic Chemistry": W60, 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	<ul style="list-style-type: none"> • "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

Research module

Students are responsible for finding a place in one of the working groups of the Department of Chemistry according to their interests and the current availability. The Research Module is intended as preparation for the subsequent Master's thesis. Please choose one lab course (worth 15 ECTS) from the given 4 research areas:

1	Module name 46551	Forschungsmodul Inorganic Chemistry Research module: Inorganic chemistry	15 ECTS
2	Courses / lectures	Praktikum: Research module Inorganic Chemistry (23.0 SWS) Please note: <ul style="list-style-type: none"> • Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Inorganic Chemistry (time and place by appointment) • Attendance at safety instructions and in the lab course 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 	15 ECTS
3	Lecturers	Prof. Dr. Ingrid Span Prof. Dr. Karsten Meyer Prof. Dr. Karl Mandel Prof. Dr. Nicolai Burzlaff Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta Prof. Dr. Julien Bachmann	

4	Module coordinator	Prof. Dr. Karsten Meyer
5	Contents	<ul style="list-style-type: none"> • practical laboratory experience aiming at introducing students to current and state of the art inorganic research topics • work experience in a team of researchers • establishing fundamental knowledge required for addressing individual molecular research problems at a state of the art level • independent and self-driven approach to problem solving in an assigned research project
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • apply acquired fundamental knowledge and practical skills to an individual research problem that they work on independently • manage and apply the fundamental safety regulations important to handling hazardous compounds and instruct other coworkers in relevant safety topics • 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	None
8	Integration in curriculum	semester: 3
9	Module compatibility	Forschungsmodul Master of Science Chemistry 20202
10	Method of examination	Practical achievement

		Lab(PL): graded lab protocol of approx. 25 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	

1	Module name 46552	Forschungsmodul Organic Chemistry Research module: Organic chemistry	15 ECTS
2	Courses / lectures	Praktikum: Research module - Organic Chemistry (23.0 SWS) Please note: <ul style="list-style-type: none"> • Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Organic Chemistry (time and place by appointment) • Attendance at safety instructions and in the lab course 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 	15 ECTS
3	Lecturers	Norbert Jux apl. Prof. Evgeny Kataev Prof. Dr. Henry Dube Prof. Dr. Andreas Hirsch Prof. Dr. Svetlana Tsogoeva Prof. Dr. Andriy Mokhir	

4	Module coordinator	Prof. Dr. Andreas Hirsch
5	Contents	<ul style="list-style-type: none"> • Integration of students in an actual research group • self-organization of a research project both in theory and practice • planning of experiments in order to prove (or reject) a given hypothesis
6	Learning objectives and skills	The students are capable <ul style="list-style-type: none"> • to use their theoretical and practical background to make an individual contribution to an independent, actual and realistic research project • to provide a state-of-the-art documentation and discussion of results obtained as a member of a research team • to present, communicate and discuss scientific results with experts in English.
7	Prerequisites	None
8	Integration in curriculum	semester: 3
9	Module compatibility	Forschungsmodul Master of Science Chemistry 20202
10	Method of examination	Practical achievement Lab(PL): graded lab protocol of approx. 25 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	

1	Module name 46553	Forschungsmodul Physical Chemistry Research module: Physical chemistry	15 ECTS
2	Courses / lectures	Praktikum: Research Module - Physical Chemistry (23.0 SWS) Please note: <ul style="list-style-type: none"> • Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Physical Chemistry (time and place by appointment) • Attendance at safety instructions and in the lab course 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 	15 ECTS
3	Lecturers	Prof. Dr. Rainer Fink Prof. Dr. Franziska Gröhn Prof. Dr. Thomas Drewello Prof. Dr. Dirk Michael Guldi Prof. Dr. Hans-Peter Steinrück Prof. Dr. Jörg Libuda	

4	Module coordinator	Prof. Dr. Hans-Peter Steinrück	
5	Contents	<ul style="list-style-type: none"> • introduction to the current issues of research in the field of Physical Chemistry • integration in research group and instruction in scientific work • familiarisation in fundamental concepts within a special subject of Physical Chemistry to the limits of science • finding answers to open questions in research project by means of experimental work 	
6	Learning objectives and skills	Students <ul style="list-style-type: none"> • apply and transfer knowledge acquired during their studies to handle and solve open questions in research project • interpret experimental data independently • compare and evaluate results with literature data • illustrate data in meaningful graphs • present and discuss scientific results referring to literature in verbal and written form 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 3	
9	Module compatibility	Forschungsmodul Master of Science Chemistry 20202	
10	Method of examination	Practical achievement LAB (PL): graded lab protocol of approx. 25 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	

1	Module name 46554	Forschungsmodul Quantum Chemistry Research module: Quantum chemistry	15 ECTS
2	Courses / lectures	Praktikum: Research Module QC (23.0 SWS) <ul style="list-style-type: none"> • Research lab course (23 SWS) in one of the work groups of Quantum Chemistry • Attendance at lab course is compulsory! • Attendance at safety instructions 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 	15 ECTS
3	Lecturers	Prof. Dr. Dirk Zahn Prof. Dr. Bernd Meyer Prof. Dr. Petra Imhof Prof. Dr. Carolin Müller Prof. Dr. Andreas Görling	

4	Module coordinator	Prof. Dr. Andreas Görling
5	Contents	<ul style="list-style-type: none"> • Practical introduction to current and state- of- the- art research topics in the field of quantum and computer chemistry • Integration into a research group • Guided work on a current research project using the methods of quantum and computer chemistry • Attempts to solve independently a scientific problem
6	Learning objectives and skills	Students <ul style="list-style-type: none"> • apply and transfer knowledge acquired during their studies to handle and solve open questions in research projects in quantum and computer chemistry • put their own research results in relation to current literature and research papers in the field, and record their results in appropriate scientific writing and documentation style • present their own results and acquired knowledge in an appropriate scientific style in English language
7	Prerequisites	None
8	Integration in curriculum	semester: 3
9	Module compatibility	Forschungsmodul Master of Science Chemistry 20202
10	Method of examination	Practical achievement LAB (PL): graded lab protocol of approx. 25 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	

Elective modules

Elective modules (15 ECTS): specialist (please see below) or non-specialist modules have to be chosen, which may include, e.g., language courses, key skills, science courses, or others (list tba online in Campo)

1	Module name 46537	Nanostructured Materials and Interfaces	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	no content description available!
6	Learning objectives and skills	no learning objectives and skills description available!
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 Module compability:</p> <ul style="list-style-type: none"> • within the Compulsory Elective Module Advances in Interfaces and Catalysis B (IntCat-3B) (20 ECTS)! • module can also be taken as part of the elective module (5 ECTS, not graded)! • MSc Chemistry student can choose between the compulsory elective module Advances in Interfaces and Catalysis A (IntCat-3A) and the compulsory elective module Advances in Interfaces and Catalysis B (IntCat-3B)
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	

1	Module name 46511	Advanced Bio-Organic and Bio-Inorganic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Nicolai Burzlaff	
5	Contents	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Oral O20 (PL): Oral examination (20 minutes)</p>	
11	Grading procedure	<p>Oral (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	

15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none">• 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 46512	Special Aspects in Bio-Organic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers. Please note: <ul style="list-style-type: none"> • Seminar: time and place by agreement! 	
3	Lecturers		

4	Module coordinator	Prof. Dr. Nicolai Burzlaff
5	Contents	The students <ul style="list-style-type: none"> • 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 <ul style="list-style-type: none"> • 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: 1;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 46521	Organometallic Catalysis	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Organometallic Catalysis (3.0 SWS) Seminar: Organometallic Catalysis - Seminar (1.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Sjoerd Harder Prof. Dr. Romano Dorta	

4	Module coordinator	Prof. Dr. Sjoerd Harder
5	Contents	<p>Knowledge on homogeneous organometallic catalysis will be deepened by discussing the latest scientific breakthroughs and developments in modern areas of catalysis. The module consists of two parts.</p> <p>Harder-Part <i>Sustainable Main Group Metal Catalysis</i></p> <ul style="list-style-type: none"> • Activation of strong bonds and small molecules with main group metal complexes (who needs d-orbitals?). Replacing expensive rare transition metals with cheap and abundant main group metals. • Bond activation using the ball-mill method. • Catalysis with main group metal complexes (discussion of elementary steps and catalytic cycles). • Activation of metals and making metal catalysts using Metal-Vapor-Synthesis. The evaporation of metals under vacuum and co-condensation in an organic matrix is a great way to make highly active metal catalysts. <p>Dorta-Part <i>Asymmetric Catalysis by Chiral Metal Complexes – Applications in Industry</i></p> <ul style="list-style-type: none"> • Importance of chiral molecules in nature and life science • Chiral pharmaceutical drugs and agrochemicals • Asymmetric catalysis: Chiral catalysts acting as a chirality multiplier • Advantages in comparison with racemate separation or stoichiometric enantioselective syntheses. • Historical development of chiral technology and industrial applications. • Synthesis of enantiopure ligands (famous industrial examples will be discussed). • Mechanistic aspects (catalytic cycles).
6	Learning objectives and skills	<p>The student</p> <ul style="list-style-type: none"> • will learn the latest developments at the forefront of organometallic catalysis • will understand that the field of catalysis needs to become sustainable and that we move away from expensive rare metals to abundant main group metals

		<ul style="list-style-type: none"> • will be able to critically discuss catalytic cycles and understand reaction mechanisms • will be taught new methods (practical and theoretical) to study molecular properties • will be understand the need for new methods of catalyst preparation • will be up-to-date with asymmetric catalysis and industrial applications
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Homogenous Catalysis Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Oral</p> <p>O20(PL): Oral examination (20 minutes)</p>
11	Grading procedure	<p>Oral (100%)</p> <ul style="list-style-type: none"> • As part of the Compulsory Elective module "Advances in Homogenous Catalysis": O20, 100% • As part of the elective module: 0% - pass/fail
12	Module frequency	Only in summer semester
13	Workload in clock hours	<p>Contact hours: 45 h</p> <p>Independent study: 105 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • 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 (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Andriy Mokhir Prof. Dr. Svetlana Tsogoeva	

4	Module coordinator	Prof. Dr. Sjoerd Harder	
5	Contents	<ul style="list-style-type: none"> 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	<p>The student</p> <ul style="list-style-type: none"> 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	<p>Advances in Homogenous Catalysis Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <p>Organocatalysis and Catalytic Reactions in Water can be taken</p> <ul style="list-style-type: none"> within the Compulsory Elective Module "Advances in Homogenous Catalysis" (20 ECTS in total) as Elective Module (5 ECTS, not graded) 	
10	Method of examination	<p>Oral</p> <p>O20(PL): Oral examination (20 minutes)</p>	
11	Grading procedure	<p>Oral (100%)</p> <p>As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h</p> <p>Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	
16	Bibliography		

1	Module name 46523	Small Molecule Activation	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Small Molecule Activation (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Karsten Meyer Prof. Dr. Ingrid Span	

4	Module coordinator	Prof. Dr. Sjoerd Harder	
5	Contents	Lecture: <ul style="list-style-type: none"> 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, active 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 <ul style="list-style-type: none"> 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 Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> 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		

1	Module name 46531	Theory of Catalytic Processes Theory of catalytic processes	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Bernd Meyer	
5	Contents	<ul style="list-style-type: none"> • Introduction: catalysis as interdisciplinary multiscale problem • Atomic structure and thermodynamic stability of surfaces and adsorbates, surface phase diagrams, active surface sites • Reactivity concepts: d-band model, Newns-Anderson model of adsorption, trends in the periodic table • Microkinetic modelling, rate equations, steady-state limit, rate determining step, transition state theory, kinetic Monte Carlo • Descriptors for catalytic activity, scaling relations (Bronsted-Evans-Polanyi), volcano plots • Accelerated molecular dynamics for sampling rare events 	
6	Learning objectives and skills	<p>Students</p> <ul style="list-style-type: none"> • are familiar with the most common quantum-chemical methods for studies in heterogeneous catalysis • understand the principles of descriptor-based predictions of catalytic activity • can perform first quantum chemical calculations on their own and interpret the data 	
7	Prerequisites	Basic knowledge of quantum mechanics and quantum chemical calculations is strongly recommended!	
8	Integration in curriculum	semester: 1;2;3	
9	Module compatibility	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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)! <p>Please note:</p> <p>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!</p>	
10	Method of examination	<p>Oral (20 minutes) PL: O 20 - oral examination (20 minutes)</p>	
11	Grading procedure	Oral (100%)	

		<ul style="list-style-type: none"> • Within the Compulsory Elective Module "Advances in Interfaces and Catalysis A (IntCat-3A)": 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	<ul style="list-style-type: none"> • J.K. Norsov, T. Bligaard, J. Rossmeisl, C.H. Christensen, Towards the computational design of solid catalysts, Nature Chemistry, 2009, 1, 37

1	Module name 46532	Surface and Interface Science	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Surfaces and Interface Science (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr.-Ing. Marcus Bär	

4	Module coordinator	Prof. Dr. Jörg Libuda
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202</p> <p>Advances in Interface Research and Catalysis B Master of Science Chemistry 20202</p> <p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 Ultraviolet Radiation, Cambridge University Press, 1999 • D. Briggs, M.P. Seah: Practical Surface Analysis: Auger and X-Ray Photoelectron Spectroscopy, 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 46533	Heterogeneous Catalysis and Kinetics	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Heterogeneous Catalysis and Kinetics (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Jörg Libuda	

4	Module coordinator	Prof. Dr. Jörg Libuda	
5	Contents	<p>Syllabus:</p> <ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Advances in Interface Research and Catalysis A Master of Science Chemistry 20202 Advances in Interface Research and Catalysis B Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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 46535	Neurotech: Physics and Chemistry of Neuromodulation Technologies	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Neurotech: Physics and Chemistry of Neuromodulation Technologies (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Danijela Gregurec	

4	Module coordinator	Prof. Dr. Danijela Gregurec	
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students will gain the knowledge, skills, and competences to be able to ...</p> <ul style="list-style-type: none"> • 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	Wahlmodule Master of Science Chemistry 20202 Module compatibility: <ul style="list-style-type: none"> • Lecture module within the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded) 	
10	Method of examination	Oral (20 minutes) Oral examination (20 minutes, ungraded)	
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	<ul style="list-style-type: none"> • 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 <p> **Literature will be updated with leading peer-reviewed papers during lectures </p>

1	Module name 46536	Lebensmittelchemie Food chemistry	5 ECTS
2	Courses / lectures	<p>Vorlesung: Chemie und Technologie der Lebensmittel IV - Bioaktive pflanzl. Lebensmittel (1.0 SWS)</p> <p>Vorlesung: Lebensmittelchemie V - Proteine (1.0 SWS)</p> <p>Vorlesung: Chemie und Technologie der Lebensmittel, Teil 2, 5, 6 oder 9 (1.0 SWS)</p> <p>Seminar: Instrumentelle Analytik für Lebensmittelchemiker und das Wahlmodul Lebensmittelchemie /Master Molecular Science (1.0 SWS)</p> <p>Bitte beachten:</p> <ul style="list-style-type: none"> • 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	

4	Module coordinator	Prof. Dr. Monika Pischetsrieder
5	Contents	<ul style="list-style-type: none"> • 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 Analysemethoden besprochen.
6	Learning objectives and skills	<p>Die Studierenden</p> <ul style="list-style-type: none"> • 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: 1;2;3
9	Module compatibility	<p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • kann als Teil des Wahlmoduls/Elective module belegt werden (5 ECTS/unbenotet)

10	Method of examination	Seminar achievement (20 minutes) (SL): Seminarvortrag, 30 Minuten, unbenotet
11	Grading procedure	Seminar achievement (0%) 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 46541	Semiconductor Materials for Energy Applications	5 ECTS
2	Courses / lectures	Seminar: Semiconductor Materials for Energy Applications - Seminar (1.0 SWS) Vorlesung: Semiconductor Materials for Energy Applications (2.0 SWS)	5 ECTS
3	Lecturers	Dr. Ryan Crisp	

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> 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	<p>The students</p> <ul style="list-style-type: none"> 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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		

1	Module name 46542	Advanced Electrochemistry Advanced electrochemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> 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	<p>Students</p> <ul style="list-style-type: none"> 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> 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	<p>Written examination (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	

16	Bibliography	<ul style="list-style-type: none">• 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 <p>For further literature, please see the current list on studon.</p>
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1	Module name 46543	Solar Energy Conversion	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Dirk Michael Guldi	
5	Contents	<ul style="list-style-type: none"> • 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	<p>The students</p> <ul style="list-style-type: none"> • 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	<p>Advances in Energy Materials Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Written examination (100%) As part of the elective module: 0% - pass/fail</p>	
12	Module frequency	Only in winter semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	
16	Bibliography		

1	Module name 46545	Organic thin films	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Rainer Fink	
5	Contents	<ul style="list-style-type: none"> • Molecular interactions and molecular self-organization • Influence of molecular geometry and functionalization • Thin film preparation techniques: Langmuir-Blodgett, Self-Assembled Monolayers (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	<p>Students</p> <ul style="list-style-type: none"> • 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	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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		

1	Module name 46546	Symmetry and Group Theory	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Jörg Libuda	
5	Contents	<ul style="list-style-type: none"> • Symmetry of Molecules (symmetry elements, operations, point groups, notations) • Symmetry of Crystals, Surfaces and Interfaces (symmetry in 1, 2 and 3 dimensional periodic structures, 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	<p>Students</p> <ul style="list-style-type: none"> • 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	Wahlmodule Master of Science Chemistry 20202	

		<ul style="list-style-type: none"> 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	

1	Module name 46556	Scientific Programming	5 ECTS
2	Courses / lectures	Praktikum: Quantum Chemistry - Lab / Scientific Programming (10.0 SWS, WiSe 2024) Please note: <ul style="list-style-type: none"> • Attendance in the lab course is mandatory! • Module starts only in winter term (duration: 2 semesters) 	5 ECTS
3	Lecturers	Prof. Dr. Andreas Görling Dr. Christian Neiß	

4	Module coordinator	Prof. Dr. Andreas Görling
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students</p> <ul style="list-style-type: none"> • 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	<p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Practical achievement</p> <p>PL: Successful implementation of the programming project (working program), ungraded - module has to be passed</p>
11	Grading procedure	<p>Practical achievement (0%)</p> <p>not graded: pass/fail</p>
12	Module frequency	Only in winter semester
13	Workload in clock hours	<p>Contact hours: 150 h</p> <p>Independent study: 0 h</p>
14	Module duration	2 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • 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 46557	Theory of Surface Phenomena	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Theory of Surface Phenomena / Theorie der Oberflächenphänomene (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Bernd Meyer	

4	Module coordinator	Prof. Dr. Bernd Meyer
5	Contents	<ul style="list-style-type: none"> • 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	<p>The students ...</p> <ul style="list-style-type: none"> • 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 interpret 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	<p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	

1	Module name 46558	Modern X-ray Structure Determination	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Dr. Frank Wilhelm Heinemann	
5	Contents	<ul style="list-style-type: none"> • 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	<p>Students ...</p> <ul style="list-style-type: none"> • 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	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • 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 46559	Quantum Chemistry 1	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Andreas Görling	
5	Contents	<ul style="list-style-type: none"> Mathematical concepts and current research issues in the field of quantum and computer chemistry Hartree-Fock, DFT 	
6	Learning objectives and skills	Students ... <ul style="list-style-type: none"> 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: <ul style="list-style-type: none"> 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	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> 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	<ul style="list-style-type: none"> 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	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Quantum Chemistry 2 (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Andreas Görling	

4	Module coordinator	Prof. Dr. Andreas Görling	
5	Contents	<ul style="list-style-type: none"> • Many-Body Perturbation Theory • Configuration Interaction, Second Quantization, Coupled Cluster • TD-HF, TD-DFT, RPA 	
6	Learning objectives and skills	<p>Students ...</p> <ul style="list-style-type: none"> • 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	<p>Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • 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	<p>Oral (20 minutes) O20 (PL): Oral Examination (20 minutes, not graded: pass/fail)</p>	
11	Grading procedure	<p>Oral (0%) not graded: pass/fail</p>	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	
16	Bibliography	<ul style="list-style-type: none"> • 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 46562	Biological and Synthetic Molecular Switches and Machines	5 ECTS
2	Courses / lectures	Vorlesung: Molecular Switches and Molecular Machines (2.0 SWS)	5 ECTS
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	<p>The Students ...</p> <ul style="list-style-type: none"> • 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. <p>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.</p>	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	Wahlmodule Master of Science Chemistry 20202 Module compatibility: <ul style="list-style-type: none"> • 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	<ul style="list-style-type: none"> • "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 46564	Modern Methods in Mass Spectrometry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Thomas Drewello	
5	Contents	<ul style="list-style-type: none"> 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	<p>Students ...</p> <ul style="list-style-type: none"> 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	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> 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	<ul style="list-style-type: none"> Jürgen H. Groß: "Mass Spectrometry, a textbook Springer, Heidelberg Edmond De Hoffmann: "Mass Spectrometry, principles and applications, Wiley 	

1	Module name 46565	Self-assembly: molecular, particulate and hybrid nanostructures	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Franziska Gröhn	
5	Contents	<ul style="list-style-type: none"> • Inspired by Mother Nature: Designing Structures on the Nanoscale • Molecular Templates for Inorganic Nanostructures, Organic-Inorganic Hybrid Structures • Self-Assembly of Amphiphilic Molecules • Non-Covalent Interactions for Assembly and Particle Stabilization • Characterization Tools for Nanoparticles, Polymers and Assemblies in Solution • Dynamic Light Scattering • The Form Factor as Key to Particle Shape: SAXS, SANS and Static Light Scattering • Supramolecular Architectures through Combinations of Non-Covalent Interactions • Electrostatic Self-Assembly • Switchable Supramolecular Nanostructures: Light, pH- and Temperature Responsivity • Molecular and Hybrid Nano-Assemblies for Catalysis, Solar Energy Conversion and Drug Delivery 	
6	Learning objectives and skills	<p>Students ...</p> <ul style="list-style-type: none"> • gain insight into structural design concepts on the nanoscale • are able to evaluate the interplay of non-covalent interactions • know how to approach the analysis of complex nanostructures in solution • are aware of recent studies and applications of switchable and functional nano-assemblies 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • as Elective Module in MSc Chemistry, 5 ECTS/not graded 	
10	Method of examination	Oral (20 minutes)	
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	<ul style="list-style-type: none">• Recent literature• D. F. Evans, H. Wennerström: The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet, 2nd Edition, Wiley 1999• O. Glatter: Scattering Methods and their Application in Colloid and Interface Science, Elsevier 2018

1	Module name 46567	HZB Photon School	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr.-Ing. Marcus Bär	
5	Contents	<p>Students will be introduced to the</p> <ul style="list-style-type: none"> • functionality of a synchrotron (storage ring-based light sources, x-ray optics and beamlines for synchrotron radiation experiments), • fundamentals of the interaction of x-rays with matter, and • laboratory-based characterization methods that probe the molecular structure, function, and dynamics of complex material systems such as x-ray absorption spectroscopy, x-ray photoemission spectroscopy, magnetic spectroscopy and scattering, and x-ray microscopy. <p>The two-week program consists of basic and specialized lectures including exercises, given by experienced teachers who are HZB scientists or BESSY II super-users from HZB partner universities in the first week. The second week is dedicated to hands-on training at several BESSY II experimental stations and X-ray laboratories. Participants will get a vivid experience by joining up to two experiments to work in small groups. The second week's activities will teach participants how to collect, analyse, interpret, and present own data amongst peers and specialists.</p> <p>For further information, visit hz-b.de/photonschool</p>	
6	Learning objectives and skills	<p>Students ...</p> <ul style="list-style-type: none"> • describe the working principle of a synchrotron-based light source • explain basic photon-matter interactions • describe the principles of photoemission, diffraction, scattering based analysis method variants, photon-in - photon-out spectroscopic and microscopic techniques and their applications • deliberately select an X-ray based analysis method to address given scientific question and are able to evaluate the collected data • judge the quality of data evaluation and its pitfalls • represent their measurement results • are able to write a compelling beamtime proposal 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 1;2;3;4	
9	Module compatibility	Wahlmodule Master of Science Chemistry 20202	

		<ul style="list-style-type: none"> as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)
10	Method of examination	<p>Oral (20 minutes) PL (O20): Oral examination = Poster presentation (20 minutes)</p>
11	Grading procedure	<p>Oral (0%) Ungraded, module has to be passed only</p>
12	Module frequency	Only in winter semester
13	Workload in clock hours	<p>Contact hours: 60 h Independent study: 90 h</p>
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> 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 Ultraviolet Radiation, Cambridge University Press, 1999 D. Briggs, M.P. Seah: Practical Surface Analysis: Auger and X-Ray Photoelectron Spectroscopy, 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. Meisel, G. Leonhardt, R. Szargan: X-ray Spectra and Chemical Binding, Springer, 1989

1	Module name 46515	Sensory Sciences Lab	5 ECTS
2	Courses / lectures	<p>No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.</p> <p><u>Please note:</u></p> <ul style="list-style-type: none"> The module "Sensory Sciences Lab" is an interdisciplinary module with a limited number of participants: only 10 students from MSc Chemistry or MSc Molecular Science will be admitted! Students from Molecular LIFE Science will be given priority! The module "Sensory Sciences Lab" can be taken as part of the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" (20 ECTS in total, all modules have to be graded) or as an elective module (5 ECTS, ungraded)! 	
3	Lecturers		

4	Module coordinator	Prof. Dr. Andrea Büttner
5	Contents	<p>The field of Sensory Sciences investigates how animals and humans sense, neurally process and perceive their environment. This research-oriented interdisciplinary course provides important concepts, theories, and methods of the Sensory Sciences to advanced students from three disciplines (Psychology, Medicine and Chemistry - Molecular Science). These topics comprise human auditory, visual and olfactory perception, chemocommunication, psychophysics, neuroimaging, molecular sensory receptors and technologies for neuromodulation (among others). The students apply these concepts in interdisciplinary teams to develop, conduct and analyse their own small research project. While engaging in an interdisciplinary collaboration and exchange, students can share and deepen their discipline-specific perspectives and competencies as well as learn about concepts and methods from other disciplines.</p>
6	Learning objectives and skills	<p>The students are able to</p> <ul style="list-style-type: none"> explain fundamental concepts and methods of the Sensory Sciences develop an own (limited) research question and design an empirical data collection to investigate the research question collect data in the laboratory and analyse the data present their findings in oral and written form communicate effectively in interdisciplinary teams understand and reflect the challenges and chances of interdisciplinary collaborations.
7	Prerequisites	None
8	Integration in curriculum	semester: 1;2;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202
10	Method of examination	Seminar achievement

		Written project report (20-30 pages)
11	Grading procedure	Seminar achievement (100%) 100% project report <ul style="list-style-type: none"> • Part of the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" in M.Sc. Molecular Science (5 ECTS, graded; PO 2020) • elective module (5 ECTS, ungraded; PO 2020)
12	Module frequency	Only in winter semester
13	Workload in clock hours	Contact hours: 30 h Independent study: 120 h
14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • Literature will be announced in the first session • Scripts and materials will be provided via StudOn!

1	Module name 46516	Medical Life Sciences	5 ECTS
2	Courses / lectures	Vorlesung: Medical Life Sciences	5 ECTS
3	Lecturers	Prof. Dr. Stefan Lyer Dr. Stefanie Klein Prof. Dr. Ingrid Span Prof. Dr. Danijela Gregurec PD Dr. Christina Janko Prof. Dr. Olaf Prante PD Dr. Rainer Tietze	

4	Module coordinator	Prof. Dr. Ingrid Span
5	Contents	To lay the foundation for working in molecular disease research, the MedLife module provides knowledge in genetics, molecular biology, cell biology, nucleic acid and protein chemistry, enzymology, nuclear and nanomedicine.
6	Learning objectives and skills	The students <ul style="list-style-type: none"> • explain the basic principles and techniques of the various fields of research • engage with scientific texts • will be able to apply the essential principles to practical biological and chemical problems
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	Advances in Bio-Organic and Bio-Inorganic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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) <p>*If students want to take the compulsory elective module "Advances in Bio-Organic and Bio-Inorganic Chemistry" as a whole, they have to choose 3 out of the 4 lecture modules, the laboratory module "Bio-Organic and Bio-Inorganic Chemistry - Lab" (No.46514) must be taken compulsorily!</p>
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	

1	Module name 46538	Digital Chemistry	5 ECTS
2	Courses / lectures	Seminar: Digital chemistry (3.0 SWS)	5 ECTS
3	Lecturers	Prof. Dr. Carolin Müller Dr. Christian Neiß	

4	Module coordinator	Prof. Dr. Carolin Müller	
5	Contents	<ul style="list-style-type: none"> examination of practical application of data science methods in handling chemical data with a focus on both categorical or numerical data, such as catalytic turnover numbers or reaction yields, and discrete/continuous data, e.g., from spectroscopic experiments (such as, IR-, NMR- or UVvis absorption spectra); introduction to structural representations and electronic descriptors; practical introduction to computational methods for high-throughput generation of reference data (e.g., DFT, DFTB+, and MD simulations); curation and construction of a database and usage of database in practical applications 	
6	Learning objectives and skills	<p>Students are able to ...</p> <ul style="list-style-type: none"> apply data science methods effectively in handling chemical data. utilize structural representations and electronic descriptors to analyse chemical data and draw meaningful insights. employ computational methods for (high-throughput) generation of chemical reference data. construct and curate a database of (quantum) chemical data, and demonstrate the ability to utilize it in practical applications. independently apply the acquired expertise in data science and computational chemistry to address scientific questions. categorize their scientific results according to given instructions and articulate them accurately in written form, adhering to linguistic conventions. present their findings and the scientific context of their projects in graphically appealing presentations, communicating proficiently in English during discussions and presentations. 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	Wahlmodule Master of Science Chemistry 20202	
10	Method of examination	Variable pÜL: Completion of a programming project with submission of both code and documentation and 6-minute presentation (+20 minutes discussion) of the project	
11	Grading procedure	Variable (0%) pÜL 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	<ul style="list-style-type: none"> • T. Engel, Thomas and J. Gasteiger, "Chemoinformatics: Basic Concepts and Methods", Wiley-VCH, Weinheim 2018, ISBN 978-3-527-33109-3 (book) • A. Szabo and N. S. Ostlund, "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory", Courier Corporation, 2012, ISBN 0-486-69186-2 (book) • P. O. Dral, "Quantum Chemistry in the Age of Machine Learning", Elsevier 2022, DOI 10.1016/C2020-0-03124-5 (book)

1	Module name 46569	Stereoselective Synthesis	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Stereoselective Synthesis (3.0 SWS)	5 ECTS
3	Lecturers	apl. Prof. Evgeny Kataev	

4	Module coordinator	apl. Prof. Evgeny Kataev	
5	Contents	<p>The students are introduced to advanced aspects of stereoselective synthesis:</p> <ul style="list-style-type: none"> • General/Fundamental principles of stereochemistry. • Determination of absolute configuration and enantiomeric composition. • Various types of stereoselective reactions, including alkylation, aldol-related reactions, asymmetric Diels-Alder, and cyclization reactions • Stereo- and enantioselective metal-catalyzed reactions, organocatalytic transformation, and enzymatic reactions. • Historical and recent developments in the field are given. • Exemplary stereoselective syntheses of essential drugs and other molecules. 	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • understand mechanisms in terms of selectivities, conditions, additives, • are able to offer synthetic pathways to various chiral drugs and other molecules. 	
7	Prerequisites	None	
8	Integration in curriculum	semester: 2;3	
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Compulsory elective module "Advances in Organic 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	<p>Written examination (60 minutes) W60 (PL): Written examination (60 minutes)</p>	
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> • Written examination: 100 % • As part of the elective module: 0% - pass/fail 	
12	Module frequency	Only in summer semester	
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>	
14	Module duration	1 semester	
15	Teaching and examination language	english	

16	Bibliography	<ul style="list-style-type: none">• Eliel, Wilen, Doyle, Basic Organic Stereochemistry, WileySons 2001;• Lin, Li, Chan, Principles and application of asymmetric synthesis, WileySons, 2001;• Carreira, Kvaerno, Classics in Stereoselective Synthesis, Wiley-VCH 2009;• Carey, F. A.; Sundberg, R. J.; Organic Chemistry Part A and B, Springer, Berlin 2007.
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1	Module name 46571	Heterocyclic Chemistry	5 ECTS
2	Courses / lectures	Vorlesung mit Übung: Heterocyclic Chemistry (3.0 SWS)	5 ECTS
3	Lecturers	Norbert Jux	

4	Module coordinator	Norbert Jux
5	Contents	<p>The students are introduced to fundamental and advanced aspects of heterocyclic chemistry:</p> <ul style="list-style-type: none"> Nitrogen-, oxygen- and sulphur-containing heterocycles are discussed. Syntheses, characterization and properties of heterocycles with ring sizes from three to seven atoms are presented. Examples from pharmacy (drugs) and materials science underline the importance of heterocycles. Historical and recent developments in the field are given. Retrosynthetic analyses of heterocycles and drugs are described. Named reactions and important contributors to the field are presented.
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> understand the formation reactions of heterocycles are able to analyse drugs and other molecules in terms of their components, in particular, heterocycles are able to offer synthetic pathways to various heterocycle-containing drugs and other molecules
7	Prerequisites	None
8	Integration in curriculum	semester: 2;3
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> Lecture module within the Compulsory elective module "Advances in Organic 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	<p>Written examination (60 minutes) W60 (PL): Written examination (60 minutes)</p>
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> As part of the Compulsory Elective module "Advances in Organic Chemistry": W60, 100% As part of the elective module: 0% - pass/fail
12	Module frequency	Only in summer semester
13	Workload in clock hours	<p>Contact hours: 45 h Independent study: 105 h</p>

14	Module duration	1 semester
15	Teaching and examination language	english
16	Bibliography	<ul style="list-style-type: none"> • J. A. Joule, K. Mills, Heterocyclic Chemistry, Wiley-Blackwell, 5th Edition, 2010, ISBN-13: 978-1405133005. • T. L. Gilchrist, Heterocyclic Chemistry, Pearson Education Dorling Kindersley, 3rd Edition, 1997, ISBN: 978-8131707937. • Peter A. Jacobi, Introductory Heterocyclic Chemistry, Wiley, 1st Edition, 2018, ISBN: 978-1119417590. • T. Eicher, S. Hauptmann, A. Speicher, The Chemistry of Heterocycles, 3rd edition, Wiley 2013, ISBN: 978-3-527-66986-8.

1	Module name 46572	Advanced Spectroscopy in Organic Chemistry	5 ECTS
2	Courses / lectures	No teaching units are offered for the module in the current semester. For further information on teaching units please contact the module managers.	
3	Lecturers		

4	Module coordinator	Prof. Dr. Henry Dube	
5	Contents	<p>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, ^{13}C, ^{19}F, ^{31}P). 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).</p> <p>In addition, other optical spectroscopic methods will be reviewed and discussed in more depth (e.g., UV/Vis-, CD-, IR-spectroscopy and Mass spectrometry).</p>	
6	Learning objectives and skills	<p>The students</p> <ul style="list-style-type: none"> • 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: 1;2;3	
9	Module compatibility	<p>Advances in Organic Chemistry Master of Science Chemistry 20202 Wahlmodule Master of Science Chemistry 20202</p> <ul style="list-style-type: none"> • Lecture module within the Compulsory Elective module "Advances in Organic Chemistry" in M. Sc. Chemistry or Molecular Science (20 ECTS in total, graded) • As Elective Module in M. Sc. Chemistry or Molecular Science (5 ECTS, not graded) 	
10	Method of examination	Written examination (60 minutes)	
11	Grading procedure	<p>Written examination (100%)</p> <ul style="list-style-type: none"> • As part of the Compulsory Elective module "Advances in Organic Chemistry": W60, 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	<ul style="list-style-type: none"> • "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 46548	Economics	5 ECTS
2	Courses / lectures	Seminar: Economics - Chemistry (Blockveranstaltung) (3.0 SWS) Bitte beachten Sie: <ul style="list-style-type: none"> • Das Modul findet aktuell nur im Sommersemester 2024 (19. - 27.09.2024) statt! • Registrierung/aktuelle Informationen über StudOn - der Anmeldezeitraum wird allen Studierenden rechtzeitig per E-Mail mitgeteilt, falls das Modul angeboten werden kann! 	5 ECTS
3	Lecturers	Dr. Andreas Späth	

4	Module coordinator	Dr. Andreas Späth
5	Contents	Betriebswirtschaftslehre, Strategische Planung & Projektmanagement: Einführung in ... <ul style="list-style-type: none"> • Methoden der strategischen Analyse • Innovationsstrategien • F&E Projektmanagement • Agiles Projektmanagement und Lean
6	Learning objectives and skills	Die Studierenden ... <ul style="list-style-type: none"> • 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	Wahlmodule Master of Science Chemistry 20202 <ul style="list-style-type: none"> • 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%) SL: 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	german or english
16	Bibliography	