Description of Module Master of Science
733 Chemistry of Materials
PO-Version 2023

FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

Contents summary

Note : Please note that you can find the information on examinations, courses corresponding to the examinations, and examination dates in the portal Friedolin under the menu item ‘Browse module descriptions’. After logging in, please choose your degree, your study programme, and respective module. Any immediate changes made will be displayed promptly.

Explanations regarding the module catalogue

Compulsory modules with a total amount of **65 credit points** have to completed:

Code	Title	Semester	ECTS
MMC B001	Molecular Physics and Condensed Matter	1st Semester - winter	10
MMC B003	Structural Principles in Materials Science	1st Semester - winter	10
MMC B004	Materials Chemistry Laboratory Module: Synthesis & Characterization	1st Semester - winter	5
MMC W002	Foreign Language	1st Semester - winter	5
MMC P001	Functional Materials and Nanomaterials	2nd Semester - summer	10
MMC P002	Materials Synthesis	2nd Semester - summer	10
MMC P003	Research Laboratory Work	3rd Semester - winter	15

Compulsory elective modules as „required specialization" with a total amount of **10 credit points** have to be completed. Thereby students can choose, rather to complete simulation and computer science or characterization tools.

Code	Title	Semester
MMC W003	Multi-Scale Simulation and Computational Materials Science I	2nd Semester - summer
MMC W005	Multi-Scale Simulation and Computational Materials Science II	3rd Semester - winter
or		
MMC W004	Advanced Characterization Tools I	2nd Semester - summer
MMC W006	Advanced Characterization Tools II	3rd Semester - winter

Furthermore, students have to complete **elective modules as „individual specialization"** with a total amount of **15 credit points** during the second and third semester.

At the end of the study the **Master's Thesis** with an amount of **30 credit points** has to be completed.

Modul **MMC B001** Molecular Physics and Condensed Matter	
Module code	MMC B001
Module title (German)	Molecular Physics and Condensed Matter
Module title (English)	Molecular Physics and Condensed Matter
Person responsible for the module	Prof. Dr Benjamin Dietzek-Ivansic, Dr Martin Presselt, Prof. Dr Volker Deckert
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (5 SWS), seminar (3 SWS) (SWS stands for, hours per week per semester)
ECTS credits	10 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	300 h 120 h 180 h

Content	This adjustment module will present basic aspects of modern physics in the context of materials chemistry. Following the introduction of basic concepts of non-classical physics and conservative equations an introduction to experimental solid state and molecular physics will be given. This includes concepts of transport and structural dynamics (diffusion, charge conductivity, thermal transport, phonon transport, Drude model, plasmons). From this knowledge, in-depth considerations of the heat capacity of solids (e.g., Einstein and Debye models) will be deducted. Knowledge of lattice vibrations will be extended towards the fundamental principles of vibrational spectroscopy. Light-matter interactions, including the concept of waves and a reconsideration of geometrical and wave optics will be treated with a focus on the failure of the classical picture of matter (e.g. photo electrical effect, Stern-Gerlach). Based on the initial introduction of non-classical physics, the quantum theoretical approach to molecular bonds will be presented (valence bond theory, molecular orbital theory, variation principle, Hückel approximation etc.) and the consequences regarding structure, polarity and electronegativity will be discussed. A short outlook to computational and specialized /modern methods will be given. The lecture will conclude with an introduction to symmetry and how symmetry based arguments can be used to construct orbitals and support spectroscopic data.
Intended learning outcomes	The students will understand basic concepts of (experimental) physics with respect to the physical phenomena and experimental concepts for studying molecules and solids. They will be able to give an oral presentation of a selected topic and defend the content to other students.
Prerequisites for admission to the module examination	Oral presentation of a selected topic in the seminar.
Requirements for awarding credit points (type of examination)	Written or oral exam on the contents dealt with in the lecture and seminar (100%)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC B003** Structural Principles in Materials Science	
Module code	MMC B003
Module title (German)	Structural Principles in Materials Science
Module title (English)	Structural Principles in Materials Science
Person responsible for the module	Prof. Dr-Ing. Lothar Wondraczek;Dr. Alexander Knebel; Dr Zhiwen Pan; Dr Franziska Scheffler
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (4 SWS), seminar (2 SWS), exercises (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	10 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	300 h 120 h 180 h
Content	This module will introduce relations between thermodynamics, kinetics, structure and resulting physical properties of organic, inorganic and hybrid materials with a focus on the solid state. Starting from an overview of the technologically relevant classes of materials, students will learn to apply general principles of materials science and engineering to the design of advanced materials. Specifically, the introduction will cover (i) thermodynamics of the solid state, phase transitions, phase diagrams and non-equilibrium thermodynamics, (ii) principles of crystalline and amorphous structures and crystal chemistry, (iii) solid-state kinetics, and (iv) mechanical properties, corrosion and degradation of materials.

Intended learning outcomes	After successfully completing the module, students will know: 1) fundamental classes of materials: soft and hard materials, polymers and plastics, ceramics and glasses, metals, complex materials, hybrids and compounds, and can differentiate by states of bonding, topology and structural order 2) structural principles in materials science: ordered and disordered materials, bond localization, packing rules, structural dimensionality, structural hierarchy, material topology 3) solid-state thermodynamics: phase transitions, time-temperature-transformation diagrams, phase diagrams, non-equilibrium thermodynamics 4) structure-property correlations
Prerequisites for admission to the module examination	Oral presentation of a selected topic in the seminar.
Requirements for awarding credit points (type of examination)	Written or oral exam on the contents dealt with in the lecture and seminar (70%) Exercise Reports (30 %)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC B004** Materials Chemistry Laboratory: Synthesis & Characterization	
Module code	MMC B004
Module title (German)	Materials Chemistry Laboratory: Synthesis & Characterization
Module title (English)	Materials Chemistry Laboratory: Synthesis & Characterization
Person responsible for the module	Prof. Dr-Ing. Lothar Wondraczek, Prof. Dr Martin Oschatz, n.n. (IAAC)
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Exercises (2 SWS) and laboratory practical (4 SWS) as a block course during a lecture-free period (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	300 h 120 h 180 h
Content	The module covers fundamental laboratory training in materials chemistry, including chemical calculus, reaction design, results evaluation, error analysis, and safety.
Intended learning outcomes	With successfully completed module, students know basic chemical laboratory working methods, can independently execute and critically evaluate chemical experiments and analyses. They are able to perform independent quatitative observations.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Written laboratory reports (100 %)
Additional information on the module	The laboratroy practical will be performed as a group practical.
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC P001** Functional Materials and Nanomaterials	
Module code	MMC P001
Module title (German)	Functional Materials and Nanomaterials
Module title (English)	Functional Materials and Nanomaterials
Person responsible for the module	Prof. Dr Benjamin Dietzek-Ivansic, Prof. Dr Felix H. Schacher
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (3 SWS), seminar (1 SWS), laboratory practical (3 SWS) (SWS stands for, hours per week per semester)
ECTS credits	10 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	300 h 105 h 195 h
Content	This module focuses on preparative, structural and functional aspects of functional materials and nanomaterials. It includes: • preparation, properties, self-assembly, and characterization of nanostructured materials (e.g. amphiphiles, nanoparticles, composite materials, block copolymers, hybrid materials) • chemistry at surfaces and interfaces (e.g. self-assembled monolayers or SAMs, Langmuir-Blodgett films, membranes, sol-gel-chemistry, superhydrophobic/superhydrophilic surfaces) • suitable characterization methods to assess properties and structural details of such materials (e.g. scattering techniques, spectroscopic techniques, ellipsometry, quartz-crystal-microbalance) • optical properties of nanoparticles and functional materials • applications of nanostructured materials (e.g. lithography, sensing, theranostics, data storage)

Intended learning outcomes	Students understand the fundamental principles of functional materials and nanomaterials, their subdivision into different material classes, and have knowledge about various characterization techniques for the investigation of structure, morphology, surface or material properties. The laboratory practical enables students to independently solve problems regarding preparation and investigation of functional materials, and nanomaterials. Therefore, they will be introduced to modern laboratory techniques and combinations thereof. In addition, students are able to do literature research and to process, present and defend the results from the laboratory practical in front of an audience
Prerequisites for admission to the module examination	Laboratory course and oral presentation must be completed successfully prior to the exam.
Requirements for awarding credit points (type of examination)	Exam/test on the content dealt within the lecture and seminar (70%); laboratory report (30 %)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC P002** Materials Synthesis	
Module code	MMC P002
Module title (German)	Materials Synthesis
Module title (English)	Materials Synthesis
Person responsible for the module	Prof. Dr Delia Brauer, Dr Martin Hager
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (3 SWS), seminar (1 SWS), laboratory practical (3 SWS) (SWS stands for, hours per week per semester)
ECTS credits	10 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	300 h 105 h 195 h
Content	Core concepts of soft matter (e.g. polymers, hydrogels, polymer colloids), and hard matter (e.g. glass, ceramics, metals, concrete) will be presented. The students will be introduced to different methods for the preparation of different material classes. Specific attention will be given to the challenges of different length scales (from nanomaterials to surfaces and bulk materials), and throughput of manufacture. In addition, the design, fabrication and structural principles of hybrid materials, mesoporous materials, and of high-throughput approaches for materials synthesis will be discussed, including zeolitic powders, metal-organic frameworks (MOFs), and nanostructured polymeric materials.

Intended learning outcomes	After completing this module, students will have obtained an understanding of synthesis methods, structure and properties of various classes of materials across different scales of length, and fabrication throughput. In addition to theoretical knowledge from lectures and seminars, students will have obtained experimental knowledge from laboratory practical. During the practical, they will have learned how to plan the synthesis of different materials, and search for literature on methods of materials synthesis independently or in small groups. They will not only prepare selected materials but also learn how the atomic structure of a material determines its properties, and how this knowledge can be used to tailor such properties.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Exam/test on the content dealt with in the lecture, seminar, and laboratory content (70%); laboratory report (30%)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC P003** Research Laboratory Work	
Module code	MMC P003
Module title (German)	Research Laboratory Work
Module title (English)	Research Laboratory Work
Person responsible for the module	Dr Zhiwen Pan (organizational)
Prerequisites for admission to the module	733 MSc Chemistry of Materials: Minimum of 50 ECTS in the Master of Science Chemistry of Materials
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master' thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every semester
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Practical course
ECTS credits	15 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	450 h 250 h 200 h
Content	This module is conducted as an internship in a research group selected from among the teachers of the CoM program (alternative selections are possible, subject to evaluation and confirmation by the module responsible). Candidates will conduct a guided research project in materials chemistry.
Intended learning outcomes	Candidates will obtain introductory training in the practical aspects of scientific work. They will apply the knowledge and skills acquired during the first two semesters of the master's programme in the context of a specific research project. This includes : • carrying-out a scientific project on the field of materials chemistry • crtitical analysis of research findings and results • preparation and presentation of a scientific report • research integrity and scientific practice
Prerequisites for admission to the module examination	Interim oral presentation of the research project and initial results (15 min).

Requirements for awarding credit points (type of examination)	Written report (max. 30 pages) (100 %)
Additional information on the module	Total workload: 450 hours depending on the topic, the total workload should be divided into: • 50 hours: introduction to the research topic (study of relevant literature etc.) • 250 hours: research work (in the laboratory for experimental topics, and at the computer for theoretical topics) • 130 hours: preparation of final report • 20 hours: preparation and presentation of results The practical laboratory work can take place in the following working groups, all professors are examiners: Prof. Dr Delia S. Brauer, Prof. Dr Benjamin Dietzek, Prof. Dr Volker Deckert, Prof. Dr Wolfgang Fritzsche, Prof. Dr Stefanie Gräfe, Prof. Dr Thomas Heinze, Prof. Dr Jürgen Popp, Prof. Dr Felix H. Schacher, Prof. Dr Ulrich S. Schubert, Prof. Dr Andrey Turchanin, Prof. Dr Matthias Westerhausen, Prof. Dr-Ing. Lothar Wondraczek
Recommended reading	Will be recommended at the beginning of the laboratory work.
Language of instruction	English

Modul **MMC W001** Project Management	
Module code	MMC W001
Module title (German)	Project Management
Module title (English)	Project Management
Person responsible for the module	Prof. Dr-Ing. Lothar Wondraczek, Dr Zhiwen Pan
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual specializsation"
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (1 SWS), seminar (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 45 h 105 h
Content	Students will obtain a basic, hands-on introduction into project management tools applied to a scientific/research context. This will cover the formulation of a hypothesis, conception of work packages, GANT charts, considerations of research funding and proposal formulation, performance indicators and monitoring tools, risk mitigation, and innovation gateways.
Intended learning outcomes	With successful completion of the module, students have acquired basic knowledge and skills in practical project management with a scientific background. They know project management tools which can be applied in a scientific/research context. They can formulate hypothesis or research questions, formulate work packages, create diagrams, create a financing plan for the research and formulate performance indicators.
Prerequisites for admission to the module examination	none

Requirements for awarding credit points (type of examination)	Oral or poster pitch related on a personal (virtual or practical) research project (100 %)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W002** Foreign Language	
Module code	MMC W002
Module title (German)	Foreign Language
Module title (English)	Foreign Language
Person responsible for the module	Head of the Language Center (Dr Joachim Boldt), n/a
Prerequisites for admission to the module	Placement test
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: none
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module from PO 2023 733 MSc Chemistry of Materials: Elective module until PO 2023
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Seminar (4 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 60 h 90 h
Content	Students can choose a language at the Language Centre at the university. The recommended language is German. If sufficient German skills are already available, the student can choose another language. After having done the placement test, participants acquire basic skills in the chosen language. The four language skills (listening, reading, speaking and writing) are developed and practised systematically. Additionally, the study of phonetics plays an important role.
Intended learning outcomes	Students can communicate effectively in various situations
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Active participation (part I), written exam (part II, 90 min), oral exam (part III, 10-15 min); credit points will be recognized when all parts have been completed successfully passing at least 50 % in each part. Assessed with passed/ failed.
Additional information on the module	Students will not receive any grade for participating in this module. As a result, their performance will not contribute to their final grade.

Recommended reading	Will be recommended in the Language Centre.
Language of instruction	Chosen language

Modul **MMC W003** Multi-Scale Simulation and Computational Materials Science I	
Module code	MMC W003
Module title (German)	Multi-Scale Simulation and Computational Materials Science I
Module title (English)	Multi-Scale Simulation and Computational Materials Science I
Person responsible for the module	Prof. Dr Stefanie Gräfe, Dr Zhiwen Pan
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module in „required spezcialisation"
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (2 SWS), seminar (1 SWS), laboratory practical (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 75 h 75 h
Content	Introduction to the theoretical background of multi-electron systems: in the lectures and exercises, students will deal with basic sets and common ab initio methods, for example Hartree-Fock and higher level methods; introduction to the simulation of larger systems, including semi-empirical methods, and QM/MM calculations. The practical exercises focus on the realization of the theoretical concepts in different quantum chemical programme packages.
Intended learning outcomes	Basic concepts of various ab initio methods: quantum chemical calculations with applications in molecular structure calculations, chemical boning, molecular orbitals, coordination compounds, kinetics, thermodynamics, and spectroscopy; interpretation of results.
Prerequisites for admission to the module examination	Laboratory practical must be completed successfully prior to the exam.
Requirements for awarding credit points (type of examination)	Exam/test on the content dealt with in the lecture, seminar, and laboratory content (70%); laboratory report (30%)

Additional information on the module	If „Multi-Scale Simulation and Computational Materials Science I” is chosen, then „Multi-Scale Simulation and Computational Materials Science II” has to be chosen as well. The module can also be chosen as an elective module in „individual specialization”, if not already compled as „required specialization”.
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W004** Advanced Characterization Tools I	
Module code	MMC W004
Module title (German)	Advanced Characterization Tools I
Module title (English)	Advanced Characterization Tools I
Person responsible for the module	Prof. Dr Felix Schacher, Prof. Dr Lotar Wondraczek
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module in „required spezcialisation"
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Seminar (1 SWS), laboratory practical (4 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 75 h 75 h
Content	This module focuses on advanced characterization techniques for the investigation of morphology, size/size distribution or composition of nanostructured materials. Methods introduced to the students will include electron microscopy, i.e. transmission (TEM), scanning (SEM), and cryogenic transmission (cryo-TEM), scattering techniques (light or X-Ray, small and wide angle), powder diffraction, X-Ray spectroscopy etc.
Intended learning outcomes	At the end of the module, students are acquainted with advanced characterization methods of nanostructured materials, and are able to apply them and their combinations to state-of-the-art questions in this research field. Additionally, students learn how to solve problems in small groups, to present and defend their solutions in front of a larger audience.
Prerequisites for admission to the module examination	Regular participation in seminars and laboratory course during the semester
Requirements for awarding credit points (type of examination)	Written reports on laboratory practical (70%) and oral presentation with subsequent discussion (30%)

Additional information on the module	Laboratory practical in tandems A presentation or a written report graded as failed can be repeated once. If „Advanced Characterization Tools I" is chosen, then „Advanced Characterization Tools II" has to be chosen as well. The module can also be chosen as an elective module in „individual specialization", if not already compled as „required specialization".
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W005** Multi-Scale Simulation and Computational Materials Science II	
Module code	MMC W005
Module title (German)	Multi-Scale Simulation and Computational Materials Science II
Module title (English)	Multi-Scale Simulation and Computational Materials Science II
Person responsible for the module	Prof. Dr Lothar Wondraczek, Dr Zhiwen Pan
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module in „required spezcialisation"
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (2 SWS), seminar (1 SWS), laboratory practical (1 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 60 h 90 h
Content	In this module, mesoscale and larger-scale simulation approaches will be introduced and applied in a variety of real-world examples focusing on the area of materials synthesis, and processing. This will start with deviating relevant equations of state for use in finite element simulation methods. Applications will deal with problems of diffusion, thermal transport, fluid flow, reaction kinetics, optics and others.
Intended learning outcomes	Ability to apply mesoscale simulation techniques to problems in materials chemistry, synthesis, and large-scale processing, in particular FEM methods; knowledge of different software packages and tools
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Oral presentation of a mini project (30 min, 100%)

Additional information on the module	If „Multi-Scale Simulation and Computational Materials Science II” is chosen, then Multi-Scale Simulation and Computational Materials Science I” has to be chosen as well. The module can also be chosen as an elective module in „individual specialization”, if not already compled as „required specialization”.
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W006** Advanced Characterization Tools II	
Module code	MMC W006
Module title (German)	Advanced Characterization Tools II
Module title (English)	Advanced Characterization Tools II
Person responsible for the module	Prof. Dr Andrey Tuchanin, Prof. Dr Volker Deckert, Prof. Dr Benjamin Dietzek-Ivansic
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: Module required to complete master's thesis
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module in „required specialisation"
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Lecture (3 SWS), seminar (1 SWS), laboratory practical (1 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 75 h 75 h
Content	Spectroscopic and spectrometric characterization tools to characterize the chemical and electronic structure of materials. The module covers the physical and chemical basis underlying individual characterization tools, and derive the information content that can be obtained from the individual tools. In addition, the module also deals with UV/Vis absorption spectroscopy, emission spectroscopy (including FRET and confocal microscopy), Raman, resonance Raman and Brillouin scattering, IR absorption spectroscopy, X-ray absorption spectroscopy (XPS and XANES), Auger spectroscopy, photoelectron spectroscopy, and AFM and STM spectroscopy.

Intended learning outcomes	Upon successful completion of the module, students have advanced knowledge of concepts of spectroscopy and spectrometry to characterise materials. Through the lecture and seminar they know the theoretical background, including aspects of data analysis, while through the laboratory practical course they learn in-depth knowledge of data evaluation and the interpretation of experimental results using selected methods and are able to apply these.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Exam/test on the content dealt with in the lecture, seminar, and laboratory practical content (75%), laboratory reports (25%)
Additional information on the module	If „Advanced Characterization Tools II" is chosen, then Advanced Characterization Tools I" has to be chosen as well. The module can also be chosen as an elective module in „individual specialization", if not already completedas „required specialization".
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W007** Advanced Simulation Methods	
Module code	MMC W007
Module title (German)	Advanced Simulation Methods
Module title (English)	Advanced Simulation Methods
Person responsible for the module	Prof. Dr Stefanie Gräfe, Dr Stephan Kupfer
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: Fundamental simulation
Prerequisite for what other modules	733 MSc Chemistry of Materials: Elective module as „individual specialization”
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual specialization”
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, …)	Lecture (2 SWS), exercise (1 SWS), practical course (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 75 h 75 h
Content	Theoretical background of advanced multiscale simulation methods: in the lectures, foundations of density functional theory, molecular dynamics, and atomistic simulation methods will be discussed; practical exercises with focus on advanced multiscale simulations
Intended learning outcomes	Upon successful completion of the module, students will have advanced competences in computational materials science with a focus on bridging time and length scales. They have an overview of possible applications of computer simulations in academic research and industry.
Prerequisites for admission to the module examination	Successfully accomplished exercises and practical course
Requirements for awarding credit points (type of examination)	Written or oral exam covering the content dealt with in the lectures, exercises and practical courses (100%)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.

Language of instruction	English

Modul **MMC W008** Nanobiotechnology, Molecular Aspects of Nanotechnology	
Module code	MMC W008
Module title (German)	Nanobiotechnology, Molecular Aspects of Nanotechnology
Module title (English)	Nanobiotechnology, Molecular Aspects of Nanotechnology
Person responsible for the module	Prof. Dr Andrey Turchanin
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: none
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual spezcialization”
Frequency of offer (how often is the module offered?)	Every second semester (beginning in winter semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, …)	Lectures (2 SWS), seminar (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 60 h 90 h
Content	Fabrication of biofunctional surfaces and interfaces (molecular systems, self-assembly, soft lithography, biochemical functionalisation, and biorecognition). Basic experimental methods for the characterization of properties (selected spectroscopy and microscopy techniques); physico-chemical models for the description of biofunctional surfaces and interfaces. Biofunctional and bioinspired systems, and applications. Biochips (DNA-, protein-, cell-biochips), Lab-on-a-chip concepts, biosensors.
Intended learning outcomes	Upon successful completion of the module, students have in-depth knowledge of the production of biofunctional surfaces and interfaces and can apply concepts of nano- and nanobiotechnology. They can derive, characterise and describe processes. They can apply selected spectroscopy and microscopy techniques.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Written or oral exam on the contents dealt with in the lecture and seminar (100%)

Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W009** Advanced Polymer Synthesis	
Module code	MMC W009
Module title (German)	Advanced Polymer Synthesis
Module title (English)	Advanced Polymer Synthesis
Person responsible for the module	Prof. Dr Felix H. Schacher, Prof. Dr Ulrich S. Schubert
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: none
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual spezcialization”
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, …)	Lecture (2 SWS), seminar (1 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 45 h 105 h
Content	The module provides an introduction to a modern polymer chemistry starting with general principles of polymerization, and polymerization kinetics (step-growth and chain growth), but also advancing to controlled and living polymerization techniques, end functionalisation of polymers, and solution behaviour of different polymer classes. Students will also be introduced to different characterization tools for polymers, i.e. different techniques for molar mass determination. Furthermore, different subtopics will introduce important application fields of polymeric materials.
Intended learning outcomes	Students understand the fundamental principles of polymers and different important polymerization mechanisms, and have an understanding on various controlled/living polymerization techniques, and basic characterization methods for the investigation of molar mass, and polymer architecture. The laboratory practical enables students to prepare, isolate and purify polymeric materials using important polymerisation techniques, and to analyse materials regarding their molar mass and dispersity.

Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Exam/test on the content dealt within the lecture and seminar (100%)
Additional information on the module	none
Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W010** Batteries and Fuel Cells	
Module code	MMC W010
Module title (German)	Batteries and Fuel Cells
Module title (English)	Batteries and Fuel Cells
Person responsible for the module	Prof. Dr Andrea Balducci, Prof. Dr Martin Oschatz
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: none
Prerequisite for what other modules	733 MSc Chemistry of Materials: none
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual specialization”
Frequency of offer (how often is the module offered?)	Every second semester (beginning in summer semester)
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, …)	Lecture (2 SWS), seminar (1 SWS), laboratory practical (3 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 90 h 60 h
Content	Practical material-related aspects of batteries, supercapacitors and fuel cells will be discussed. The prime focus is on commercialized battery technologies, especially on the Li-ion battery technology. History, state-of-the art and future developments are discussed. This technology will be compared to sodium-ion batteries, supercapacitors and fuel cell technologies.
Intended learning outcomes	Students learn about material needs for designing batteries and fuel cells. Students learn to critically discuss changes and challenges of electrochemical storage, and of converter devices. They are able to describe their practical scientific works in a report and present seminar content adequately.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Written or oral exam (50%); laboratory practical, including report (30%); seminar presentation (20%)
Additional information on the module	none

Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC W011** Light-Matter Interactions and Optical Materials Design	
Module code	MMC W011
Module title (German)	Light-Matter Interactions and Optical Materials Design
Module title (English)	Light-Matter Interactions and Optical Materials Design
Person responsible for the module	Prof. Dr-Ing. Lothar Wondraczek
Prerequisites for admission to the module	733 MSc Chemistry of Materials: none
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: Fundamental physics
Prerequisite for what other modules	733 MSc Chemistry of Materials: none
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Elective module as „individual specialization”
Frequency of offer (how often is the module offered?)	Every semester
Duration of module	1 semester
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, …)	Lecture (2 SWS), seminar (2 SWS) (SWS stands for, hours per week per semester)
ECTS credits	5 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	150 h 60 h 90 h
Content	Theoretical background of light-mater interactions, distinguish between conductors, semi-conductors, and dielectric media; atomic polarization, optical refraction, and optical dispersion; length-scale dependence of light-matter interactions considering nanomaterials, plasmon interaction in particles, and thin layers; photonic band-gap; focus on inelastic light scattering at high and low frequencies; luminescence and phosphorescence; tailoring of optical properties through chemical bonds, material topology, dopants, and dopant interactions.
Intended learning outcomes	Students understand fundamental aspects of light-matter interaction, distinguish between electrical and magnetic field interactions, understand prominent resulting phenomena, and their tailoring through materials chemistry with a particular focus on inorganic materials.
Prerequisites for admission to the module examination	none
Requirements for awarding credit points (type of examination)	Written or oral exam covering the content dealt with in the lectures and seminar (100%)
Additional information on the module	none

Recommended reading	Will be recommended at the beginning of the module.
Language of instruction	English

Modul **MMC P005** Master's Thesis	
Module code	MMC P005
Module title (German)	Master's Thesis
Module title (English)	Master's Thesis
Person responsible for the module	Persons responsible for the modules in the Master of Science Chemistry of Materials
Prerequisites for admission to the module	733 MSc Chemistry of Materials: 60 ECTS and the completion of the practical module Reseach Laboratory Work or Scientific Internship
Recommended or expected prior knowledge	733 MSc Chemistry of Materials: knowledge of the compulsory modules
Prerequisite for what other modules	733 MSc Chemistry of Materials: finishing the study programme
Type of module (compulsory module, required elective module, elective module)	733 MSc Chemistry of Materials: Compulsory module
Frequency of offer (how often is the module offered?)	Every semester
Duration of module	6 month(s)
Module Components/Types of courses (lecture, practical course, lab, tutorial, exercise, seminar, internship, ...)	Practical course
ECTS credits	30 CP
Work load: - In-class studying - Independent studying (incl. preparations for examination)	900 h 20 h 880 h
Content	research in a laboratory
Intended learning outcomes	Independent research/laboratory work. The presentation of the thesis will be held during the last two months of thesis preparation
Prerequisites for admission to the module examination	Regular participation in the course
Requirements for awarding credit points (type of examination)	Written report, i.e. master's thesis (75%), and its oral presentation (25%) during the last two month of the master's thesis. The master's thesis should contain 30–60 pages. Candidates are expected to give an oral presentation (20–30 minutes) presenting the results of their thesis. It should be followed by a discussion. The final grade is determined according to the Examination Regulations.

Additional information on the module	Total workload: 900 hours depending on the topic, the total workload should be divided into: • 225 hours: introduction to the research topic (study of relevant literature etc.) • 450 hours: research work (in the laboratory for experimental topics, and at the computer for theoretical topics) • 200 hours: preparation of final report • 25 hours: preparation and presentation of results
Recommended reading	none
Language of instruction	English

Abbrevations:

Abbrevations of lectures

IL....	Inaugural lecture
WG....	Working group
AM....	Advanced module
Exh....	Exhibition
BM....	Basic module
BzPS....	Begleitveranstaltung zum Praxissemester
C....	Consulting
To....	Tour
M....	Meeting
Blo....	Blockage
BC....	Block course
DV....	Slide show
IN....	Introductory session
RS....	Registrations
EC....	Exam course
EX....	Excursion
Exp....	Experiment/survey
FE....	Celebration/festivity
MS....	Movie screening
FEx....	Field exercise
BC....	Basic course
MaS....	Main seminar
MS/ BC....	Main seminar/block course
MaS/ Ex....	Main seminar/exercise
Inf....	Information session
IDS/E....	Interdisciplinary main seminar/ exercise
E....	Exam
E/T....	Exam/test
C....	Colloquium
C/I....	Colloquium/practical work
CS....	Conference/symposium
kV....	Kulturelle Veranstaltung
Cu....	Course

Abbrevations of lectures

Co....	Course
Lag....	Lagerung
TRP....	Training research project
RC....	Reading course
M....	Module
ME....	Musical event
AS....	Advanced seminar
OnS....	Online seminar
OnL....	Online lecture
P....	Practical work
I/S....	Practical work/seminar
PM....	Practice module
Sa....	Sample
PJ....	Project
PPD....	Propaedeutic
PS....	Proseminar
EPr....	Exam preparation
CSA....	Cross-sectional area
RE....	Revision course
LS....	Lecture Series
TC....	Training course
S....	Seminar
S/E....	Seminar/Excursion
S/E....	Seminar/Exercise
ST....	Service time
SI....	Conference
SuSch....	Summer school
MISC....	Miscellaneous
OE....	Other event
LC....	Language course
Con....	Convention
TT....	Teleteaching
MN....	Meeting
Tu....	Tutorial
T....	Tutorial
E....	Exercise
E/BC....	Exercise/block course
E....	Exercises
E/I....	Exercise/interdisciplinary
E/I....	Exercise/practical work

Abbrevations of lectures

E/T....	Exercise/tutorial
Conf....	Conference
ViCo....	Video conference
L....	Lecture
L/C....	Lecture with colloquium
L/I....	Lecture/practical work
L/S....	Lecture/seminar
L/E....	Lecture/exercise
Sp....	Speech
TK....	Talk
OS....	Optional seminar
OL....	Optional lecture
Tr....	Training
Wo....	Workshop
WOS....	Workshop
CAC....	Certificate award ceremony

Other Abbrevations

Anm.....	Anmerkung
ASQ....	Allgemeine Schlüsselqualifikationen
AT....	Altes Testament
E....	Essay
FSQ....	Fachspezifische Schlüsselqualifikationen
FSV....	Fakultät für Sozial- und Verhaltenswissenschaften
GK....	Grundkurs
IAW....	Institut für Altertumswissenschaften
LP....	Leistungspunkte
NT....	Neues Testament
SQ....	Schlüsselqualifikationen
SS....	Sommersemester
SWS....	Semesterwochenstunden
TE....	Teilnahme
TP....	Thesenpublikation
ThULB....	Thüringer Universitäts- und Landesbibliothek
VVZ....	Vorlesungsverzeichnis
WS....	Wintersemester