Module Guide / Modulhandbuch

TECHNISCHE UNIVERSITÄT DARMSTADT

Fachbereich Material- und Geowissenschaften
Institut für Materialwissenschaft
Peter-Grünberg-Straße 2
64287 Darmstadt

Course of Studies / Studiengang
Master of Science
Materials Science
Examination Regulations 2024 / Prüfungsordnung 2024

Final Module

Module name Master Thesis					
Module no.	**Credit Points** 30 CP	**Workload** 900 h	**Self-study** 900 h	**Duration** 1 Semester	**Frequency** Every semester
Language of Instruction English and German			**Person responsible for the Module** Dean of studies Materials Science		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week

2 Course Content

Current research topic from the general research area of the administering research group. Examination: Every full-time professor of the Institute of Material Science.

Tasks:

- Familiarization with the subject and setup of a work schedule.
- Experimental and/or theoretical work on a scientific subject.
- Documentation of the results by authoring the Master Thesis.
- Presentation of the results with subsequent scientific discussion.

3 Learning Outcomes

On successful completion of the Master Thesis, students are able to:

1. translate challenges from practice into a problem to be solved by using state of the art methods of engineering and natural sciences;
2. independently solve scientific questions in a structured manner based on accepted standards in science and engineering;
3. explain structure and composition of scientific publications;
4. apply acquired knowledge and qualifications to specific scientific topics in order to independently work on scientific problems in a sufficient depth and breadth;
5. extend existing knowledge with their results;
6. work within a team and to coordinate collaborative teams;
7. take up problems from other disciplines and recognize target-oriented scientific approaches;
8. autonomously create documentations and presentations about their research work and results;
9. set realistic but also very demanding goals, to realize them within a reasonable period of time and to reflect on the results and the way to achieve them;
10. to critically scrutinize material-scientific or material-relevant statements and theories and to confidently represent one's own point of view in written and oral form in front of professional colleagues and laypersons.

4	**Requirements for Participation** Completion of all mandatory modules (lectures) and individual obligations. For a detailed list of the required mandatory modules please refer to the regulations of the degree programme M.Sc. Materials Science section 23 (2). The topic has to be approved by the examination board.
5	**Form of Examination** Thesis: Written thesis and an oral exam (30 min)
6	**Requirements on the Award of Credit Points** Passing the examinations
7	**Grading** Technical examination; written thesis (100%) default (number grades) and Study achievement: oral exam passed/not passed grading system
8	**Associated study programme** M.Sc. Materials Science: Master Thesis
9	**Literature** will depend on topic
10	**Comment** Cycle: A Master thesis may be started at any time.

Module name					
Functional Materials					
Module no. 11-01-4104	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Andreas Klein		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-1036-vl	Functional Materials	6	Lecture	4

2 Course Content

Functional Materials and specific devices:

- Conductivity in metals,
- Semiconductors,
- Thermoelectricity,
- Organic semiconductors,
- Ionic conductors,
- Dielectric and ferroelectric materials,
- Introduction to magnetism and magnetic materials,
- Magnetic materials and their applications (permanent and soft magnets),
- Magnetocaloric materials,
- Metal Hydrides,
- Superconductors.

3 Learning Outcomes

On successful completion of the module, students are able to:

1. understand the most important physical principles of the relevant material classes and can explain the physical fundamentals for materials' functionality.
2. explain with materials synthesis and application of the most important functional materials. They critically evaluate the applications of these material classes.
3. to model and explain the characterization of simple devices constructed from the above-mentioned materials.

4 Requirements for Participation

Recommended: Good knowledge of basic solid-state physics

Students who have an obligation to pass the module "Concepts in Materials Physics" are strongly advised to take the module "Functional Materials" parallel to or after the module "Concepts in Materials Physics".

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book) 90 min
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: mandatory domain.
9	**Literature** 1. K.Nitzsche, H.-J.Ullrich, „Funktionswerkstoffe der Elektrotechnik und Elektronik“, Deutscher Verlag für Grundstoffindustrie, Leipzig (1993). 2. O. Kasap, “Principles of Electronic Materials and Devices”, Mcgraw-Hill Publ. Comp. (2005). 3. Rolf E.Hummel, „Electronic properties of materials“, Springer Verlag (1993). 4. J.C.Anderson et al., „Materials Science“, Chapman & Hall Verlag (1990). 5. C.Kittel, „Einführung in die Festkörperphysik“, 14. Auflage, Oldenburg Verlag, München (2006). 6. H.Ibach, H.Lüth, "Festkörperphysik", 6. Auflage, Springer Verlag, Berlin (2002). 7. E.A.Silinsh, V.Capek, "Organic molecular crystals" , AIP Press (1994). 8. W.Brütting, "Physics of organic semiconductors", Wiley- VCH (2005). 9. W.Buckel, R.Kleiner „Supraleitung“, 6. Auflage, Wiley-VCH Verlagsgesellschaft (2004). 10. J. M. D. Coey, “Magnetism and Magnetic Materials”, Cambridge University Press (2010). 11. B. D. Cullity, “Introduction to Magnetic Materials”, Wiley-IEEE Press (2008). 12. O’Handley, “Modern magnetic materials: principles and applications”, Wiley & Sons (2000) 13. Darren P. Broom, “Hydrogen Storage Materials: The characterisation of Their Storage Properties (Green Energy and Technology)”, Springer (2011).
10	**Comment** Cycle: each winter semester

Module name					
Sustainable Materials					
Module no. 11-01-4110	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr.-Ing. Oliver Gutfleisch		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4110-vl	Sustainable Materials	6	Lecture	4

2 Course Content

The course introduces the current challenges related to sustainability and circular economy of materials.

The sustainable synthesis, and scalable production of materials from waste/recyclates/secondary raw materials, recycling and zero emission industrial preparation, as well as the application of clean energy will be topic of this course.

Further keywords: Green chemistry, plastic recycling, de-fossilisation, waste water recycling, life cycle assessment.

3 Learning Outcomes

On successful completion of the module, students are able to:

1. analyze the property profiles of materials in a differentiated manner, assess materials with regard to socio-economic, environmental and further sustainability aspects and select materials appropriately.
2. recognize social challenges and to assess the consequences of their activities with regard to social, economic, safety-related and environmental aspects.
3. critically reflected their professional activities in these dimensions and thus to play a significant role in shaping social processes with a sense of responsibility and democratic public spirit, even beyond the narrowly specialized area of responsibility.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book) 90 min.

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

	Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: mandatory domain.
9	**Literature** Will be announced.
10	**Comment** Cycle: each summer semester

Module name					
Surfaces and Interfaces					
Module no. 11-01-4105	**Credit Points** 5 CP	**Workload** 150 h	**Self-study** 105 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Jan Philipp Hofmann		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7922-vl	Surfaces and Interfaces	5	Lecture	3

2 Course Content

- Surfaces of solids: thermodynamics of surface formation, structure of surfaces, electronic structure of surface and surface potentials.
- Kinetics of surface reactions: physisorption and chemisorption, surface diffusion, surface reactions and catalysis.
- Internal surfaces: structural models, thermodynamics of internal surfaces, epitaxy and growth modes.
- Solid/liquid interfaces: thermodynamics and electrochemical double layers, thermodynamics of electrochemical reactions, kinetics of electrochemical reactions, corrosion and corrosion modes

3 Learning Outcomes

On successful completion of the module, students are able to:

1. understand and treat the specific effects of surfaces and interfaces in materials science,
2. differentiate between thermodynamically and kinetically determined properties,
3. describe the important terms and definitions and related theoretical concepts used in surface/interface science and electrochemistry,
4. explain how surfaces/interfaces affect the properties of presented devices,
5. discuss material science related aspects of electrochemical processes,
6. transfer this knowledge to any future envisaged problems and materials,
7. differentiate between bulk and surface effects in devices and to correlate them with material's properties,
8. evaluate experimental and theoretical methods in their possible future research involving surface/interface effects and electrolyte interfaces,
9. follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: basic knowledge in quantum mechanics and good knowledge in solid state physics

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: mandatory domain
9	**Literature** 1. H. Lüth, Solid Surfaces, Interfaces and Thin Films, Springer (2015) 2. H. Ibach, Physics of Surfaces and Interfaces, Springer (2006) 3. K. Oura et al., Surface Science – An Introduction, Springer (2003) 4. F. Bechstedt, Principles of Surface Physics, Springer (2003) 5. J. T. Yates, Jr., Experimental Innovations in Surface Science, Springer (2015) 6. J. W. Niemantsverdriet, Spectroscopy in Catalysis, Wiley-VCH (2007) 7. W. Schmickler and E. Santos, Interfacial Electrochemistry, Springer (2010) 8. K. W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, Wiley (2020)
10	**Comment** Cycle: each winter semester

Module name					
Theoretical Methods in Materials Science					
Module no. 11-01-4106	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Karsten Albe		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-9314-ue	Exercises Theoretical Methods in Materials Science	0	Exercise	1
11-01-9314-vl	Theoretical Methods in Materials Science	6	Lecture	3

2 Course Content

- Balance equations of mechanics and thermodynamics.
- Free energy of non-uniform materials
- Fluctuations and stability
- Linear non-equilibrium thermodynamics
- Transition state theory and transport processes
- Statistical mechanics models for materials
- Quantum statistical mechanics
- Optimization techniques
- Partial differential equations in materials science
- Boundary value problems in materials science

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the key concepts of non-equilibrium thermodynamics, continuum mechanics and (quantum) statistical mechanics relevant for materials science and can apply these principles to specific problems.
2. identify and apply appropriate theoretical concepts for solving materials science problems related to properties and processing of materials.
3. Critically apply numerical methods and solve boundary value problems, ordinary differential equations and transport equations.
4. follow advanced textbooks and scientific literature on theoretical methods in materials science and thus to extend their knowledge independently.

4 Requirements for Participation

recommended: module „Quantum Mechanics for Materials Science” or module "Micromechanics for Materials Science"

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book) 90 min The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: mandatory domain
9	**Literature** 1. R.B. Balluffi, S.M. Allen, W. C. Carter, Kinetics of Materials, Wiley (2005) 2. P. Haupt, Continuum Mechanics and Theory of Material, Springer 3. JR. Acton, P.T. Squire, Solving Equations with Physical Understanding, Adam Hilger, Bristol (1985) 4. D. Kondepudi, I. Prigogine, Modern Thermodynamics: From heat engines to dissipative structures, Wiley (1998) 5. D. C. Wallace, Thermodynamics of Crystals, Dover (1998) 6. R.K. Pathria, Statistical Mechanics, Elevier Butterworth-Heinemann (2005) 7. Rob Philips, Crystals, Defects and Microstructures, Cambridge (2001)
10	**Comment** Cycle: each summer semester

Module name					
Advanced Characterization Methods of Materials Science					
Module no. 11-01-4107	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Wolfgang Donner		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-9313-ue	Exercises Advanced Characterization Methods of Materials Science	0	Exercise	1
11-01-9313-vl	Advanced Characterization Methods of Materials Science	6	Lecture	3

2 Course Content

- Small Angle Scattering
- Scattering from Amorphous Materials
- Diffraction from Nanocrystals
- Thin Film Diffraction
- Photoelectron Spectroscopy
- Spectral Photometry
- Atomic Absorption Spectrometry
- Optical Emission Spectrometry
- X-ray Fluorescence Analysis
- Neutron Activation Analysis
- Proton-Induced X-Ray Emission
- Rutherford Backscattering Spectrometry
- Nuclear Reaction Analysis
- Elastic Recoil Detection

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the fundamentals of various methods of structural and elemental analysis, their advantages and disadvantages.
2. select and apply an appropriate technique for a given analytical problem.
3. perform analytical experiments on their own.
4. critically judge the validity of experimental results in the scientific literature.

4 Requirements for Participation

recommended: module „Quantum Mechanics for Materials Science"

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book) 90 min The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: mandatory domain
9	**Literature** 1. Small Angle Scattering, Glatter & Kratky, ebook 2. Underneath the Bragg Peaks, Egami & Billinge, ebook 3. High Resolution X-ray Scattering, Holy, Pietsch, Baumbach, Springer 4. Structural and Chemical Analysis of Materials, Eberhard, Wiley 5. An Introduction to Surface Analysis by XPS and AES, Wolstenholme, ebook 6. Handbook of X-Ray Spectrometry, Marcel Dekker 7. Atomic and Nuclear Analytical Methods, Verma, Springer 8. Quantitative Chemical Analysis, Harris, Palgrave Mcmillan 9. Chemical Analysis, modern Instrumentation, Methods and Techniques, Rousseac
10	**Comment** Cycle: each summer semester

Module name					
Quantum Mechanics for Materials Science					
Module no. 11-01-4108	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Hongbin Zhang		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4004-ue	Exercises Quantum Mechanics for Materials Science	0	Exercise	1
11-01-4004-vl	Quantum Mechanics for Materials Science	6	Lecture	3

2 Course Content

- Historical background
- Diffraction experiments
- Schrödinger equation and quantum mechanical properties
- The H- atom and H2-molecule, tunneling, harmonic oscillator
- LCAO model: from finite to infinite systems, the Bloch function
- Density of states in two and three dimensions, population density, Fermi statistics
- Bandgaps and their origin
- Transport equation of electrons in external fields
- Theory of free electrons

3 Learning Outcomes

On successful completion of the module, students are able to:

1. recognize basic quantum mechanical phenomena.
2. derive and calculate simple quantum mechanical problems and are able to use them in daily problems.
3. understand the nature of binding and the electronic structure of atoms, molecules and solids.
4. apply the theory to the evaluation of the electronic structure of atoms, molecules and solids and are able to describe charge transport in a quantum mechanical manner.
5. Understand and discuss modern research in quantum mechanics and their knowledge allows them to follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: Bachelor modules “Physical Chemistry I” and “Materials Science VI & VII”

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book) 90 min In this course lecture-accompanying achievements (e.g. written homework assignments and/or written or online assessments) can be credited, which can lead to a grade improvement of up to 1.0 grade points according to §25(2) of "6. Novelle der Allgemeinen Prüfungsbestimmungen" of TU Darmstadt. The form of examination and the specific bonus regulations will be announced within two weeks after the first lectures.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: Quantum mechanics or Micromechanics
9	**Literature** 1. Ch. Kittel: Introduction into solid state physics, John Wiley and Sons (1996) 2. H. Ibach, H. Lüth: Solid state physics, Springer Verlag (2002) 3. A. Sutton: Electronic structure of materias, Clarendon Press (1993) 4. P.W. Atkins, R.S.Friedman: Molecular Quantum Mechanics, Oxford University Press (2000) 5. R. Feynman: The Feynman lectures Vol. III, Addision-Wesley Publishing Company (1989). 6. Franz Schwabl, Advanced Quantum Mechanics, Springer Verlag (2008)
10	**Comment** Cycle: each winter semester

Module name					
Micromechanics for Materials Science					
Module no. 11-01-4109	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Bai-Xiang Xu		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7050-ue	Exercises in Micromechanics for Materials Science	0	Exercise	1
11-01-7050-vl	Micromechanics for Materials Science	6	Lecture	3

2 Course Content

This lecture deals with fundamentals of micromechanics in the framework of elasticity and plasticity theory. Important topics include: Basics of elasticity, defect mechanics, plasticity, crystal plasticity, Theory of configurational force, Micro-macro transition and homogenization, and phase-field theory and phase-field fracture modeling.

3 Learning Outcomes

On successful completion of the module, students are able to:

1. mathematically interpret the elastic and plastic behavior of a material using the continuum theory, and describe the stress situation around certain microstructure e.g. at crack tips and near defects.
2. apply the basic concept of homogenization to calculate the effective properties of heterogeneous materials.
3. read and understand advanced textbooks and scientific literature on nonlinear continuum mechanics and composite mechanics and widen their knowledge to tackle specific problems.

4 Requirements for Participation

recommended: basics of mathematics and elastomechanics

5 Form of Examination

Written exam (120 min), oral exam (30 min), or remote exam (open book) 120 min

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

Passing the examination

7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: Quantum mechanics or Micromechanics
9	**Literature** 1. Cai W., & W.D. Nix; Imperfections in Crystalline Solids, Cambridge, 2016 2. Gross D., Seelig T.; Fracture Mechanics with an Introduction to Micromechanics, 3. 2nd Edi. 2011 4. Le, Khan Chau; Introduction to Micromechanics, Nova Science Publ, 2010 5. Mura, T.; Micromechanics of Defects in Solids, Martinus Nijho_ Publishers 1982 6. Zohdi T.I., &Wriggers P.; An Introduction to Computational Micromechanics, Springer, 2004 7. Weertman, J.; Dislocation based fracture mechanics, World Scienti_c 1996 8. Provatas, N., Elder, K.; Phase-Field Methods in Materials Science and Engineering, 9. Wiley-VCH Verlag GmbH & Co. KGaA, 2010
10	**Comment** Cycle: each winter semester

Module name					
Concepts in Materials Physics					
Module no. 11-01-2009	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English and German (optional)			**Person responsible for the Module** Prof. Dr. rer. nat. Robert Stark		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2009-ue	Exercises Concepts in Materials Physics	0	Exercise	1
11-01-2009-vl	Concepts in Materials Physics	6	Lecture	3

2 Course Content

- Properties of crystalline solids: orientation dependence, lattice and reciprocal lattice, semiconductors, metals and isolators.
- Lattice dynamics: lattice with monatomic and diatomic basis, dispersion relation, Brillouin zones, acoustic and optical modes, phonons, density of states, specific heat, thermal transport, thermal expansion.
- Metals: electronic structure, band model, free electron gas, density of states, Fermi-Dirac statistics, Bloch functions
- Electronic transport: Drude model, Drude-Sommerfeld model, thermal properties of the electron gas.
- Semiconductors: synthesis (examples), doping, electronic transport, effective mass, chemical potential, optical properties, density of states, diodes.
- Solid state ionics: ionic and mixed transport.
- Dielectric properties: polarisation and polarizability, electronic and ionic polarization, optical properties, electro-elastic properties
- Magnetism: para, dia- and ferromagnetism, magnetism of solids.

3 Learning Outcomes

On successful completion of the module, students are able to:

1. describe crystals as the combination of a lattice with a pattern and can explain interference phenomena using the concept of the reciprocal lattice;
2. explain diffraction of electromagnetic waves, electron waves or collective excitations in a lattice;
3. critically discuss electrical and thermal transport properties based on crystal structure, phononic and/or electronic structure;
4. explain fundamental material properties in appropriate pictures of quasi-particles and collective excitations based on a quantum mechanical approach;
5. explain ionic transport in solid;
6. explain the interaction of electromagnetic fields and waves with materials;

	7. explain the magnetism of materials;
4	**Requirements for Participation** Individual obligation or individual permission by the examination board. Adjustment course (individual obligation). This module cannot be selected by graduates holding a Bachelor's degree in Materials Science from TU Darmstadt.
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book) (90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Associated study programme** M.Sc. Materials Science: individual obligation
9	**Literature** 1. Philipp Hofmann; Solid state physics : an Introduction 2. John J. Quinn, Kyung-Soo Yi; Solid State Physics : Principles and Modern Applications 3. Harald Ibach, Hans Lüth; Solid-State, Physics : An Introduction to Principles of Materials Science 4. Charles Kittel; Introduction into solid state physics, John Wiley and Sons (1996) 5. Neil Ashcroft, N- David Mermin; Solid state physics (1977)
10	**Comment** Cycle: each winter semester.

Module name					
Research Lab I					
Module no. 11-01-4101	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 60 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Dean of studies Materials Science		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4011-pr	Research Lab I	4	Practical / Lab / Internship	4

2 Course Content

During the laboratory course, students will learn advanced material synthesis, material modelling and/or characterization methods in a practice-oriented way. This is done by means of selected experiments from the field of material science by research grade instruments and software. The experiments are performed hands-on using the equipment of the involved research groups, making sure that every student is exposed to scientific research groups. Within the course, students learn the systematic procedure in all phases of an experiment (hypothesis - planning - measuring - evaluating - assessing). Instructions in occupational safety are given and applied in practice.

3 Learning Outcomes

On successful completion of the research lab, students are able to:

1. independently operate modern state-of-the-art scientific equipment for materials synthesis, characterization, and modelling;
2. implement occupational safety rules in their practical work;
3. plan and realize materials synthesis and characterization experiments self-reliantly in a team.
4. analyze data with complex data analysis programs and apply research data management (FAIR - principles, data life cycle and data quality).
5. analyse and critically discuss experimental results in a complex material context and evaluate the result with respect to specific applications.

4 Requirements for Participation

none

5 Form of Examination

Report for each experiment (content, scope and assessment criteria will be communicated at the beginning of the course)

6	**Requirements on the Award of Credit Points** 1. Attestations for all experiments. 2. Attendance for at least 75% of contact hours. Compulsory attendance is required for the acquisition of following competencies: Students are taught hands-on skills to operate modern state-of-the-art scientific equipment for materials synthesis, characterization, and modelling in a safe and responsible manner. They learn to operate the instruments in a way that the experimental results are repeatable, reliable and well documented. Students learn to adhere the specific occupational safety rules and implement the rules in their practical work in a laboratory environment.
7	**Grading** Study achievements (100%); bnb (passed/not passed grading system)
8	**Associated study programme** M.Sc. Materials Science: compulsory module
9	**Literature** to be provided in the introduction to each experiment
10	**Comment** Cycle: each winter semester

Module name					
Research Lab II					
Module no. 11-01-4102	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 60 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Dean of studies Materials Science		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4012-pr	Research Lab II	4	Practical / Lab / Internship	4

2 Course Content

During the laboratory course, students will learn advanced material synthesis, material modelling and/or characterization methods in a practice-oriented way. This is done by means of selected experiments from the field of material science by research grade instruments and software. The experiments are performed hands-on using the equipment of the involved research groups, making sure that every student is exposed to scientific research groups. Within the course, students learn the systematic procedure in all phases of an experiment (hypothesis - planning - measuring - evaluating - assessing). Instructions in occupational safety are given and applied in practice.

3 Learning Outcomes

On successful completion of the research lab, students are able to:

1. independently operate modern state-of-the-art scientific equipment for materials synthesis, characterization, and modelling;
2. implement occupational safety rules in their practical work;
3. plan and realize materials synthesis and characterization experiments self-reliantly in a team.
4. analyze data with complex data analysis programs and apply research data management (FAIR - principles, data life cycle and data quality).
5. analyse and critically discuss experimental results in a complex material context and evaluate the result with respect to specific applications.

4 Requirements for Participation

none

5 Form of Examination

Report for each experiment (content, scope and assessment criteria will be communicated at the beginning of the course)

6 Requirements on the Award of Credit Points

	1. Attestations for all experiments. **2.** Attendance for at least 75% of contact hours. Compulsory attendance is required for the acquisition of following competencies: Students are taught hands-on skills to operate modern state-of-the-art scientific equipment for materials synthesis, characterization, and modelling in a safe and responsible manner. They learn to operate the instruments in a way that the experimental results are repeatable, reliable and well documented. Students learn to adhere the specific occupational safety rules and implement the rules in their practical work in a laboratory environment.
7	**Grading** Study achievements (100%); bnb (passed/not passed grading system)
8	**Associated study programme** M.Sc. Materials Science: compulsory module
9	**Literature** to be provided in the introduction to each experiment
10	**Comment** Cycle: each summer semester

Module name					
Advanced Research Lab					
Module no. 11-01-4113	**Credit Points** 15 CP	**Workload** 450 h	**Self-study** 450 h	**Duration** 1 Semester	**Frequency** Every semester
Language of Instruction English			**Person responsible for the Module** Dean of studies Materials Science		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4013-se	Advanced Research Lab	15	Seminar	0

2 Course Content

Current research topic from the general research area of the administering research group at the materials science department or in industry. Examination: Every full-time professor of the Institute of Material Science.

Tasks:

- Familiarization with the subject and setup of a work schedule.
- Experimental and/or theoretical work on a scientific subject.
- Documentation of the results by authoring the report.
- Presentation of the results with subsequent scientific discussion.

3 Learning Outcomes

On successful completion of the ARL, students are able to:

1. solve scientific questions in a structured manner based on accepted standards in science and engineering guided by a supervisor;
2. implement occupational safety rules in their practical work;
3. understand structure and composition of scientific publications;
4. apply acquired knowledge and qualifications to specific scientific topics with state of the art methods and means in order to work on scientific problems in a sufficient depth and breadth;
5. deepen existing knowledge with their results;
6. work in collaborative teams;
7. create documentations and presentations about their research work and results;
8. present their work in written and oral form in a scientifical manner.

4 Requirements for Participation

none

5 Form of Examination

	Written report and oral exam (30 min).
6	**Requirements on the Award of Credit Points** passing of report and of oral talk
7	**Grading** Study achievements: written report (100%) Default (Number grades) and oral exam Passed/not passed Grading
8	**Associated study programme** M.Sc. Materials Science: compulsory module
9	**Literature** will depend on topic
10	**Comment** Cycle: The Advanced Research Lab (ARL) may be started at any time. Shorter versions of this ARL module are offered for some double degree students: 11-01-4198 with 12 ECTS (workload 360h) for AMIR M2 and FAME M1 students 11-01-4197 with 8 ECTS (workload 240h) for FAME M1 students 11-01-4199 with 7 ECTS (workload 210h) for AMIS M1 students

Elective Courses Materials Science

Elective courses materials science can be selected from the technical subjects (Master level) of the course catalogue of TU Darmstadt. You find a list of courses offered by the Institute of Materials Science below, for further courses in other departments please refer to the course catalogue.

Your individual selection of elective courses has to be approved by the examination board. Please contact your mentor and discuss your individual choice of courses (discussion with mentor).

The Institute of Materials Science offers the following elective courses:

Module name					
Electrochemistry for Energy Applications					
Module no. 11-01-7302	**Credit Points** 8 CP	**Workload** 240 h	**Self-study** 180 h	**Duration** 2 Semesters	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Jan Philipp Hofmann, Prof. Dr. Ulrike I. Kramm		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7300-vl	Electrochemistry for Energy Applications I: Fundamentals	4	Lecture	2
11-01-7301-vl	Electrochemistry for Energy Applications II: Devices and Technology	4	Lecture	2

2 Study Content

- Electrochemical Thermodynamics
- Electrochemical Kinetics
- Electrochemical Methods
- Solid State Ionics
- Electrocatalysis
- Water Electrolysis
- Fuel Cells
- Battery Fundamentals
- Li-Ion Batteries
- Semiconductor Electrochemistry
- Photocatalysis
- Photoelectrochemical Hydrogen Production
- Industrial Electrochemical Processes

3	**Learning Outcomes** On successful completion of the module, students are able to: 1. explain to the fundamental concepts of heterogeneous electrochemistry (electrodics), basic electrochemical methods and main materials science questions related to the use and application of electrochemical converter and storage devices. 2. evaluate experimental and theoretical results obtained with different electrochemical, surface science and theoretical techniques, 3. assess modern electrodics applied for continuing experimental work in this field. 4. explain and detail current energy conversion and storage device concepts and related technological aspects in the second part of the module. 5. discuss and link fundamental electrochemical phenomena, processes, and mechanisms as well as materials science related questions with device concepts, function and failure. 6. evaluate electrocatalysis in fuel cells, electrolyzers and photoelectrochemical /-catalytic applications and contemporary battery concepts with respect to stability and life-time limitations. 7. explain and discuss major industrial electrochemical processes in the light of the energy transition. 8. follow advanced textbooks and scientific literature.
4	**Requirements for Participation** recommended: modules “Surfaces and Interfaces” and “Quantum Mechanics for Materials Science”
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M. Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. P. Atkins et al., Atkins’ Physical Chemistry, Oxford University Press, 2018. 2. C. H. Hamann et al. Electrochemistry, Wiley, 2007. 3. J. Maier, Physical Chemistry of Ionic Materials: Ions and Electrons in Solids, Wiley, 2004. 4. D. Linden, T. B. Reddy, Handbook of batteries, McGraw-Hill, 2002. 5. M. Wakihara, O. Yamamoto (eds.), Lithium Ion Batteries, Fundamentals and

	Performance, Wiley, 2008. 6. R. Memming; Semiconductor Electrochemistry, Wiley, 2015. 7. C.A. Grimes, O.K. Varghese, S. Ranjan; Light, Water, Hydrogen, Springer, 2008. 8. G. Hoogers (ed.), Fuel Cell Technology Handbook, Taylor and Francis, 2003.
10	**Comment** Cycle: each year This module cannot be taken together with 11-01-7300 Electrochemistry for Energy Applications I (4 CP) or 11-01-7301Electrochemistry for Energy Applications II (4 CP)

Module name					
Polymer Materials					
Module no. 11-01-3031	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 135 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr.-Ing. Jürgen Wieser		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-3031-vl	Polymer Materials	6	Lecture	3

2 Study Content

Molecular structures and morphologies in polymers; Basics of polymer synthesis; mechanisms of additives, fillers and fibres in polymer compounds; viscoelasticity; creep and relaxation; rheology of polymer melts, glass transition and crystallisation of polymers; mechanical, thermal, optical and electrical properties of polymer compounds; longterm behavior of polymers; characterization methods and procedures for polymers.

3 Learning Outcomes

The student has gained an overview on typical morphologies in polymers and is able to discuss structure-property relationships and also the influence of kinetic parameters on the morphology. He/she can explain the role and the mechanisms of the most important classes of additives, fillers and fibres in polymer compounds. He/she can identify the appropriate characterization methods, testing devices and testing procedures for typical applications.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of exam

7 Grading

Technical Examination (100%); Default (Number grades)

8 Usability of the Module

	M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. G. Menges, Menges Werkstoffkunde der Kunststoffe, Hanser, München, 2011. 2. M. Schiller, Plastic Additives Handbook, Hanser, München, 2009. 3. T. Osswald, G. Menges, Material Science of Polymers for Engineers, Hanser, München, 2012.
10	**Comment** Cycle: each winter semester

Module name					
Finite Element Simulation for Material Science					
Module no. 11-01-2027	**Credit Points** 5 CP	**Workload** 150 h	**Self-study** 105 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Bai-Xiang Xu		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2027-vl	Finite Element Simulation in Material Science	5	Lecture	2
11-01-2027-ue	Excecises Finite Element Simulation in Material Science	0	Exercises	1

2 Study Content

The lecture covers the fundamentals of the finite element methods and its application in material science. Specifically, the focus is on strong and weak forms of linear elasticity and heat conduction problems. Finite element formulations as well as its implementation for linear elasticity and heat conduction problems will be discussed.
1. Review of Basics of tensor calculus, Linear algebra, Continuum mechanics (kinematics) and Material mechanics (Hook's law)
2. Weak form construction for 1D bar and "truss-based" FE problem
3. Learning about the Galerkin approach for a general solid and construction of the weak form for a general PDE
4. Finite element (1): concept of Shape functions and discretised version of the weak form
5. Finite element (2): construction of residual vector and Stiffness matrix
6. Finite element (3): learning about numerical integration and post-processing.
7. Multiphysics problems: focusing on a simple thermo-mechanical problem (Strong form + Weak form)
8. Thermo-mechanical problem (finite element discretization)
9. Discussions towards nonlinear FE (simple plasticity model)
If time permits:
10. Multi-scaling and Machine learning in FE

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the fundamental concept behind the finite element method as one of the most promising and wide-used computational schemes at different scales.
2. develop a mathematical representation of material behavior within a computational framework.
3. explain how a finite element code in a simple program works and how they can

	3. implement their own coding for new problems. 4. apply their understanding to further governing equations in different branches and applications of material science. 5. understand and discuss future and more advance topics in computational material mechanics and science, such as studies on plasticity and damage progression in solids.
4	**Requirements for Participation** Knowledge on basic material and continuum mechanics is a plus.
5	**Form of Examination** Report (content, scope and assessment criteria will be communicated at the beginning of the course)
6	**Requirements on the Award of Credit Points** Passing of examination
7	**Grading** (A) home project; report (100%) In this course lecture-accompanying achievements (e.g. written homework assignments and/or written or online assessments) can be credited, which can lead to a grade improvement of up to 1.0 grade points according to the General Examination Regulations of Technical University of Darmstadt (APB) section 25(2). The form of examination and the specific bonus regulations will be announced within two weeks after the first lecture.
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. T. I. Zohdi and P. Wriggers, An Introduction to Computational Micromechanics. Springer, 2010. 2.Zienkiewicz OC, Taylor RL, Zhu JZ. The finite element method: its basis and fundamentals. Elsevier; 2005. 3. Jacob, Fish, and Belytschko Ted. A first course in finite elements. Wiley, 2007. 4.Lecture notes on FE
10	**Comment**

Module name Machine Learning for Materials Science					
Module no. 11-01-2031	**Credit Points** 6 CP	**Workload** 180 h	**Self-study** 120 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Hongbin Zhang Prof. Dr. Bai-Xiang Xu		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2031-vl	Machine Learning for Materials Science	5	Lecture	3
11-01-2031-ue	Exercises Machine Learning in Materials Science	0	Exercises	1

2 Study Content

Basics in python programming; Exploratory data analysis and visualization; Ordinary machine learning methods; Neural network and deep Learning methods; Gaussian process, Bayesian optimization and adaptive design; Forward prediction models and inverse design models. Applications to materials science problems with hands-on tutorials

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain and differentiate the most relevant machine learning algorithms for experimental characterization, theoretical simulations, and in general statistical analysis in materials science;
2. choose and apply appropriate methods to basic materials science problems;
3. work with available packages within Python to develop their own simple machine learning based programs;
4. tackle a challenging project in team work.

4 Requirements for Participation

recommended: basics of mathematics and materials science

5 Form of Examination

Report (content, scope and assessment criteria will be communicated at the beginning of the course)

6 Requirements on the Award of Credit Points

	Passing of examination
7	**Grading** (A) home project; report (100%) In this course lecture-accompanying achievements (e.g. written homework assignments and/or written or online assessments) can be credited, which can lead to a grade improvement of up to 1.0 grade points according to the General Examination Regulations of Technical University of Darmstadt (APB) section 25(2). The form of examination and the specific bonus regulations will be announced within two weeks after the first lecture.
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Goodfellow, Bengio, Courville. Deep Learning. MIT Press. 2016 2. Raschka, Mirjalili. Python Machine Learning. Packt. 3. Murphy. Machine Learning: a Probabilistic Perspective. MIT Presse. 2012 4. Bishop. Pattern Recognition and Machine Learning. Springer. 2006 5. Rasmussen, Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006
10	**Comment**

Module name					
Scanning Probe Microscopy in Materials Science					
Module no. 11-01-7060	**Credit Points** 5 CP	**Workload** 150 h	**Self-study** 105 h	**Duration** 1 Semester	**Frequency** Every 2. semester

Language of Instruction	**Person responsible for the Module**
English	PD Dr. Christian Dietz

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7060-vl	Scanning Probe Microscopy in Materials Science	5	Lecture	2 SWS
11-01-7060-ü	Exercises Scanning Probe Microscopy in Materials Science		Exercise	1 SWS

2 Study Content

Introduction into Nanoscience and Nanotechnology
- Concepts of nanomanufacturing
- Surface forces

Introduction into Scanning Probe Microscopy
- Scanning Force Microscopy
- Scanning Tunneling Microscopy
- Scanning Near-Field Optical Microscopy

Scanning Force Microscopy
- Instrumentation
- Theory of feedback control systems
- High resolution imaging
- Force spectroscopy
- Static and dynamic measurement modes
- Surface characterization in liquids, air, and vacuum
- Amplitude and frequency modulation
- Advanced force microscopy methods for materials scientists

Scanning Tunneling Microscopy
- The tunneling effect
- Surface characterization
- Tunneling spectroscopy

Scanning Near-Field Optical Microscopy
- The optical near-field
- Fiber-based methods
- Scattering methods
- Nanospectroscopy

3	**Learning Outcomes** On successful completion of the module, students are able to: 1. explain the basic concepts of nano- and microfabrication techniques. 2. Explain contact mechanics and surface forces and is able to apply the appropriate model to a nanomechanical experiment. 3. The students have achieved an extensive overview on established surface characterization techniques based on scanning probe microscopy including the physical principle, instrumentation, modes of operation and can explain underlying physical principles. 4. explain the interplay between manufacturing and evaluation/characterization in nanoscience. 5. analyze and explain physical phenomena at solid liquid interfaces. 6. select the adequate methods and to apply an appropriate but yet simple model to study nanophysical properties of soft and hard matter. 7. make themselves familiar with a current topic in scanning probe microscopy in materials science and summarize the content in a short presentation.
4	**Requirements for Participation** none
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. B. Bhushan (Ed.), Handbook of Nanotechnology, Springer, Berlin Heidelberg, 2010. 2. E. Meyer, H. J. Hug, R. Bennewitz, Scanning Probe Microscopy, Springer, Berlin Heidelberg, 2004. 3. R. Garcia, Amplitude Modulation Atomic Force Microscopy, WILEY-VCH, Weinheim, 2010. 4. J. Israelachvili, Intermolecular & Surface Forces, Academic Press, London, 1992. 5. H.-J. Butt, M. Kappl, Surface and Interfacial Forces, WILEY-VCH, Weinheim, 2010.
10	**Comment** Cycle: each summer semester

Module name					
Computational Materials Science					
Module no. 11-01-7562	**Credit Points** 5 CP	**Workload** 150 h	**Self-study** 105 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Karsten Albe		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7562-ue	Exercises Computational Materials Science	0	Exercise	1
11-01-7562-vl	Computational Materials Science	5	Lecture	2

2 Study Content

- Introduction to Basic Concepts of Thermodynamics and Statistics
- Molecular Dynamics Method: Principles
- Equilibrium Thermodynamics and MD-Simulations
- Overview of Analytic Potentials
- Transport Processes and MD-Simulations
- Monte-Carlo Methods
- Kinetic Monte-Carlo Methods
- Bridging Time Scales: Accelerated Dynamics
- Foundations of Density Functional Theory
- Kohn-Sham Ansatz
- Functionals for Exchange and Correlation

Electronic Structure Calculations: PlaneWaves, LCAO, …

3 Learning Outcomes

The student knows fundamentals, possible applications and limitations of computational methods relevant in materials science. He/she has a basic understanding of the underlying numerical methods and algorithms and has gained practical experience with standard software packages like LAMMPS for molecular dynamics simulations. ABINIT for electronic structure calculations and software tools for data analysis (OVITO). He/she will have the competence to follow advanced textbooks and scientific literature on atomistic methods in materials science.

4 Requirements for Participation

recommended: modules “Quantum Mechanics for Materials Science” and “Theoretical Materials Science”

5 Form of Examination

	Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.)
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. R.B. Balluffi, S.M. Allen, W. C. Carter, Kinetics of Materials, Wiley (2005) 2. P. Haupt, Continuum Mechanics and Theory of Material, Springer 3. JR. Acton, P.T. Squire, Solving Equations with Physical Understanding, Adam Hilger, Bristol (1985) 4. D. Kondepudi, I. Prigogine, Modern Thermodynamics: From heat engines to dissipative structures, Wiley (1998) 5. D. C. Wallace, Thermodynamics of Crystals, Dover (1998) 6. R.K. Pathria, Statistical Mechanics, Elevier Butterworth-Heinemann (2005) 7. Rob Philips, Crystals, Defects and Microstructures, Cambridge (2001)
10	**Comment** Cycle: each winter semester

Module name					
Density Functional Theory: A Practical Introduction					
Module no. 11-01-8291	**Credit Points** 5 CP	**Workload** 150 h	**Self-study** 105 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Karsten Albe		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8291-ue	Exercises: Density Functional Theory: A Practical Introduction	0	Exercise	1
11-01-8291-vl	Density Functional Theory: A Practical Introduction	5	Lecture	2

2 Study Content

Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids, and material interfaces, including surfaces.
In this lecture the basic theoretical concepts underlying DFT calculations are introduced. Practical applications of DFT, focusing on planewave DFT, are discussed and hands-on training is provided using the open-source code ABINIT.
The course is a practical introduction for students of materials science, physics and chemistry who want to use DFT in their work.
- Short repetition of Quantum Mechanics (infinitely deep well, harmonic oscillator, H atom, Hartree-Fock approximation for interacting systems)
- Basic concepts in DFT (Hohenberg-Kohn theorems, Kohn-Sham ansatz, local-density approximation)
- Functioning of DFT planewave pseudopotential codes
- Tools for electronic-structure analysis (density, density of states, Bader charge analysis, band structure)
- Calculating bulk properties
- Calculating defect (free) energies (surfaces, interfaces, point defects)
- Calculating kinetic energy barriers (nudged-elastic-band method)
- Modeling complex structure: ab initio molecular dynamics, simulated annealing, basin hopping and other structure search techniques.
- Density-functional perturbation theory: application to phonon band-structures
- Improved band-structure methods: LDA+U, hybrid functionals and the GW method.

3 Learning Outcomes

After successfully completing this course, the students will be in the position to independently run DFT calculations using the ABINIT code and the PYTHON based Atomic Simulation Environment package. Specifically they will learn how to compute bulk elastic properties, surface/interface/defect (free) energies, electron and phonon

	band-structures and transition barriers for chemical reactions. In addition, the students will learn how to use density-of-states, electron densities and Kohn-Sham orbitals as tools for electronic-structure analysis. Thus, they will be able to apply basic concepts of DFT (Hohenberg-Kohn theorems, Kohn-Sham ansatz, local density approximation of the exchange-correlation functional) and of the functioning of planewave-pseudopotential codes.
4	**Requirements for Participation** recommended: background in materials science, physics, or chemistry on the bachelor level
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. R.B. Balluffi, S.M. Allen, W. C. Carter, Kinetics of Materials, Wiley (2005) 2. P. Haupt, Continuum Mechanics and Theory of Material, Springer 3. JR. Acton, P.T. Squire, Solving Equations with Physical Understanding, Adam Hilger, Bristol (1985) 4. D. Kondepudi, I. Prigogine, Modern Thermodynamics: From heat engines to dissipative structures, Wiley (1998) 5. D. C. Wallace, Thermodynamics of Crystals, Dover (1998) 6. R.K. Pathria, Statistical Mechanics, Elevier Butterworth-Heinemann (2005) 7. Rob Philips, Crystals, Defects and Microstructures, Cambridge (2001)
10	**Comment** Cycle: each summer semester

Module name					
Mechanical Properties of Metals					
Module no. 11-01-2006	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester

Language of Instruction	**Person responsible for the Module**
English	Prof. Dr.-Ing. Karsten Durst

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-9092-vl	Mechanical Properties of Metals	4	Lecture	2

2 Syllabus

This lecture deals with the mechanical behaviour of metals and crystalline solids across different length scales from small scale to macroscopic mechanical behaviour

- Strengthening mechanism and microstructure property relationships
- Stress-strain tensor, yield criterion, stiffness
- Uniaxial testing, Hart criterion
- Indentation testing, Sneddon, Oliver-Pharr method, influencing factors
- Correlation between uniaxial and indentation testing: Constraint and representative strain
- Indentation size effect and strain gradient plasticity
- Thermally activated deformation mechanism: bcc plasticity and high temperature creep, Larson Miller and Norton
- Fracture mechanics: elastic and elastic plastic, size effects
- Fatigue: cyclic stress strain diagram, Wöhler stress strain controlled, cyclic crack growth, Paris law

3 Learning Outcomes

1. The successful students can describe the elastic and plastic deformation behavior of materials for various loading conditions ranging from small scale mechanical testing to the macroscopic materials response.
2. Based on dislocation theory, the students can explain size effects in the mechanical response of crystalline materials.
3. Successful students can read and understand advanced textbooks and scientific literature on mechanical behaviour of metals and crystalline solids.

4 Requirements for Participation

recommended: basics of defects in crystalline solids, mechanical behavior

5 Form of Examination

Written exam (90 min), oral exam (25 min), presentation (30 min) or remote exam (open book) 90 min.

	The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** Passing the examination
7	**Grading** Technical Examination (100%); Standard (Number grades)
8	**Associated Study Programme** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Mechanical Behavior of Engineering Materials, J. Rösler, Springer Verlag 2. Mechanical metallurgy, G. Dieter, McGrow Hill 3. Deformation and Fracture Mechanics of Engineering Materials, R.W. Hertzberg, John Wiley & Sons, Inc 4. Werkstoffkunde und Werkstoffprüfung, W. Domke. Verlag W. Girardet, Essen 5. A.C. Fischer Cripps: Nanoindentation, Springer 6. D. Tabor: The Hardness of metals, Oxford University Press 7. K.L. Johnson: Contact mechanics, Cambridge University Press 8. W. C. Oliver, G. M. Pharr., Beschreibung der Oliver-Pharr Methode, J Mater Res, 7(6):1564–1580, 1992 9. E. Arzt: Review der Größeneffekte, Acta Mater, 46(16):5611–5626, 1998
10	**Comment** Cycle: each winter semester

Module name Advanced Light Microscopy					
Module no. 11-01-3029	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Robert Stark		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-3029-vl	Advanced Light Microscopy	4	Lecture	2

2 Study Content

The lecture covers topics in materials optics and gives an overview on how to use light in order to characterize materials. Conventional light microscopy methods are discussed with respect to their applications in (bio)materials science. Theoretical and practical aspects of modern super-resolution techniques are discussed.

- Electromagnetic Waves at interfaces (Electromagnetic waves; Reflection and transmission: External reflection, Internal reflection, Frustrated total internal reflection (FTIR), Total internal reflection microscopy), Electromagnetic properties of materials (The dielectric response; The Lorentz model of dielectrics; Drude's model for metals)
- Birefringence (Optical Anisotropy; Anisotropic dispersion; Uniaxial Materials; Biaxial and other Materials), Optical Activity, Electro Optics, and Magneto Optics (Optical activity; Electro-Optics; Magneto-Optic Effects)
- Paraxial Optics: Thin Lenses, Thick Lenses, and ABCD Formalism (Curved mirrors; Thin Lenses; Thick Lenses; ABCD Matrices) Optical aberrations and stops (Aberrations; Stops in Optical Systems; Optical devices)
- Widefield Microscopy (The compound microscope; Resolution; Bright field microscopy; Dark field; Phase contrast; Differential Interference Contrast (DIC); Polarisation microscopy; Fluorescence microscopy) Confocal Microscopy (The confocal principle; Scanning; The pinhole; Airy Scanning)
- Super resolution microscopy – Beating Abbe's limit (3-D methods based on nonlinear optical phenomena, Common ideas, 2-photon excitation, Second harmonic generation; 4Pi-microscopy: Looking at the specimen from both sides; Structured illumination microscopy (SIM); Stimulated emission depletion (STED) microscopy; Stochastic optical reconstruction microscopy (STORM) or (fluorescence) photoactivation localization microscopy ((F)PALM))
- Scanning nearfield optical microscopy (SNOM/NSOM) (The basic idea; Near field probes; Aperture SNOM; Scattering SNOM (s-SNOM))

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the interaction of electromagnetic waves with ordered materials, in

	particular with non-isotropic materials in terms of polarization, electro- and magneto optics, optical activity and photon-phonon interaction; 2. to design a simple optical device in order to perform optical measurements on materials, in terms of defining position and quality of lenses, filters, stops, mirrors, light sources and detectors; 3. explain and handle a light microscope in order to achieve a homogenously exposed image with high contrast in various modalies of light microscopy (e.g. darkfield, DIC, phase contrast) of typical specimen in (bio)materials science; 4. explain the reason for Abbe's resolution limit and knows how this limitation can be overcome in specific cases; 5. choose the appropriate super-resolution technique for a specific problem in (bio)materials science and to critically discuss experimental results.
4	**Requirements for Participation** none
5	**Form of Examination** Written exam (90 min), oral exam (30 min), presentation (30 min) or remote exam (open book) 90 min The specific modalities of the examination will be announced 14 days after the first lecture
6	**Requirements on the Award of Credit Points** passing of examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Eugene Hecht, Optics, Pearson, 5th Ed 2017 2. John Ferraro et al., Introductory Raman Spectroscopy, Academic Press, 2nd Ed. 2003 3. Jerome Mertz, Introduction to Optical Microscopy, Roberts and Co., 2009 4. Jörg Haus, Optische Mikroskopie: Funktionsweise und Kontrastierverfahren, Wiley-VCH 2014
10	**Comment** Cycle: each summer semester

Module name					
Soft Matter and Interfacial Phenomena					
Module no. 11-01-2016	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Robert Stark		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2016-vl	Soft Matter and Interfacial Phenomena	4	Lecture	2

2 Study Content

Phenomena at the fluid-solid boundary play an important role in many technical applications such as lubrication, microfluidics, biotechnology or printing. The lecture focuses on the fundamental aspects. Topics include:

- Liquid surfaces,
- thermodynamics of interfaces,
- the electric double layer,
- surface forces,
- contact angle, wetting,
- evaporation and condensation,
- Surface active agents,
- surface modification,
- colloids,
- microfluidics,
- cleaning.

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the thermodynamics of soft matter interfaces;
2. explain phenomena at the liquid solid interface in terms of physical and chemical properties;
3. select materials and explain how to modify their surfaces in order to achieve the desired wetting behavior in a technical environment.

4 Requirements for Participation

recommended: basic physical chemistry and physics

5 Form of Examination

	Written exam (90 min), oral exam (30 min), presentation (30 min), or remote exam (open book) 90 min The specific modalities of the examination will be announced 14 days after the first lecture
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Butt, Graf, Kappl, Physics and Chemistry of Interfaces, Weinheim 2003. 2. Israelachvili, Intermolecular & Surface Forces, San Diego 1991. 3. Persson, Sliding Friction – Physical Principles and Applications, Berlin 2000.
10	**Comment** Cycle: each winter semester

Module name

Applied Fluoroorganic Chemistry: Synthesis, Functional Materials, Pharmaceuticals

Module no.	Credit Points	Workload	Self-study	Duration	Frequency
11-01-2030	4 CP	120 h	90 h	1 Semester	Every 2. semester

Language of Instruction	Person responsible for the Module
English	Prof. Dr. rer. nat. Peer Kirsch

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2030-vl	Applied Fluoroorganic Chemistry: Synthesis, Functional Materials, Pharmaceuticals	4	Lecture	2

2 Syllabus

Introduction into the methods for the lab-scale und preparation of fluoroorganic compounds. The focus will also be on the unique property profile of fluorochemicals, and how that can be utilized for the design of functional materials, industrial chemicals and pharmaceuticals:

- Properties of fluoroorganic compounds
- Environmental impact of fluoroorganic chemistry
- Survey of synthetic methods and reactivity
- Fluoroorganic materials: the chemistry of liquid crystals
- Fluoropharmaceuticals and diagnostics: structure-property relationships
- Fluorous synthesis and catalysis

3 Learning Outcomes

1. The students understand and analyse the physical and chemical property profile of fluoroorganic compounds.
2. They have developed an overview on the synthetic toolbox for the synthesis of fluoroorganic compounds and select appropriate methods.
3. They critically analyse various current applications which depend critically on fluoroorganic compounds.
4. They analyze the property profiles of materials in a differentiated manner, assess materials with regard to sustainability aspects and select materials appropriately.

4 Requirements for Participation

Recommended: good background of general and organic chemistry.

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

	The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Standard (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1.P. Kirsch. Modern Fluoroorganic Chemistry: Synthesis, Reactivity, Applications (2nd ed). Wiley-VCH, Weinheim (2013) (doi: 10.1002/9783527651351) 2.A. Haupt. Organic and Inorganic Fluorine Chemistry: Methods and Applications. De Gruyter, Berlin (2021) (doi: 10.1515/9783110659337) 3.J. Han, A. M. Remete, L. S. Dobson, L. Kiss, K. Izawa, H. Moriwaki, V. A. Soloshonok, D. O'Hagan. Next generation organofluorine containing blockbuster drugs. J. Fluorine Chem. 239, 109639 (2020) (doi: 10.1016/j.jfluchem.2020.109639) 4.Y. Ogawa, E. Tokunaga, O. Kobayashi, K. Hirai, N. Shibata. Current contributions of organofluorine compounds to the agrochemical industry. iScience (2020) (doi: 10.1016/j.isci.2020.101467)
10	**Comment** Cycle: each summer semester

Module name					
Organic Functional Materials: From LCD to Molecular Circuits					
Module no. 11-01-2026	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Peer Kirsch		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2026-vl	Organic Functional Materials: From LCD to Molecular Circuits	4	Lecture	2

2 Syllabus

Introduction into chemistry, physics, applications and industrial aspects of organic functional materials for electronics industry. The focus of the course is on small molecules and their supramolecular chemistry:

- Materials for liquid crystal displays (LCD): design, synthesis and structure-property relationships
- Basics of organic electronics: physics and structures of organic conductors, semiconductors and superconductors
- Materials for organic light emitting diode (OLED) displays and their function
- Organic semiconductors for printed field effect transistors (OFET)
- Organic photovoltaics (OPV) and dye-sensitized solar cells (DSC)
- Basics of molecular nanoelectronics: physics, structures and methods
- Unimolecular wires, diodes, transistors, memory and circuits

3 Learning Outcomes

1. The students can analyse and explain the design and structure-property relationships of functional materials based on organic small molecules.
2. They understand, analyse and explain of the physics and function of organic electronic devices: OLED, OFET, OPV
3. They understand, analyse and explain physics, materials, design and functional limitations of devices based on single molecules and self-assembled monolayers

4 Requirements for Participation

Recommended: good background in basic solid state physics and organic chemistry.

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6	**Requirements on the Award of Credit Points** passing of examination
7	**Grading** Technical Examination (100%); Standard (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. D. Dunmur, T. Sluckin, Soap, Science, & Flat-Screen TVs: A History of Liquid Crystals, Oxford University Press, 2010. 2. J. A. Castellano, Liquid Gold: The Story of Liquid Crystal Displays and the Creation of an Industry, World Scientific, 2005. 3. S. Hunklinger, Festkörperphysik, De Gruyter, 2018 4. P. Kirsch, M. Bremer, Angew. Chem. Int. Ed. 2000, 39, 4216-4235. 5. P. Kirsch, M. Bremer, M. Klasen-Memmer, K. Tarumi, Angew. Chem. Int. Ed. 2013, 52, 8880-8896. 6. H. E. Katz, Z. Bao, S. L. Gilat, Acc. Chem. Res. 2001, 34, 359-369. 7. J.-L. Brédas, D. Beljonne, V. Coropceanu, J. Cornil, Chem. Rev. 2004, 104, 4971-5003. 8. V. Coropceanu, J. Cornil, D. A. Da Silva Filho, Y. Olivier, R. Silbey, J.-L. Brédas, Chem. Rev. 2007, 107, 926-952. 9. D. Hertel, C. D. Müller, K. Meerholz, Chem. Unserer Zeit 2005, 39, 336-347. 10. D. Wöhrle, O. R. Wild, Chem. Unser Zeit 2010, 44, 174-189. 11. D. Xiang, X. Wang, C. Jia, T. Lee, X. Guo, Chem. Rev. 2016, 116, 4318-4440. 12. M. Elbing, J. U. Würfel, M. Di Leo, H. B. Weber, M. Mayor, Nachrichten – Forschungszentrum Karlsruhe 2005, 37, 24-29.
10	**Comment** Cycle: each winter semester

Module name					
Characterization Methods in Materials Science: Neutrons and Synchrotron					
Module no. 11-01-9811	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** On request
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Wolfgang Donner		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-9811-vl	Characterization Methods in Materials Science: Neutrons and Synchrotron	0	Lecture	2

2 Study Content

- Synchrotron and Neutron Sources
- Neutron Reflectivity
- Crystal Truncation Rod Diffraction
- Diffuse Scattering
- Inelastic Scattering
- Quasi-elastic Scattering
- Coherent Diffraction and Reconstruction
- Selected topics from current research

3 Learning Outcomes

The students learn about the technology and possibilities of large research facilities. They are able to relate the specific advantages of Neutron and Synchrotron sources over conventional lab-based radiation sources to modern analytical methods. The course enables the students to associate specific problems in Materials Science to analytical techniques that are available at large scale facilities. The students are qualified to design specific experiments at Neutron and Synchrotron sources and evaluate the resulting data. They acquired a competence to critically evaluate the outcome of large scale experiments and to comment on results presented in the literature.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

	passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Elements of Modern X-ray Physics, Als-Nielsen & McMorrow 2. Diffuse X-ray Scattering and Models of Disorder, Welberry 3. Diffuse X-ray Scattering from Crystalline Materials, Nield & Keen
10	**Comment** Cycle: on request

Module name					
Electrochemistry for Energy Applications I: Fundamentals					
Module no. 11-01-7300	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Jan Philipp Hofmann Prof. Dr. Ulrike I. Kramm		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7300-vl	Electrochemistry for Energy Applications I: Fundamentals	4	Lecture	2

2 Study Content

- Electrochemical Thermodynamics
- Electrochemical Kinetics
- Electrochemical Methods
- Fuel cells
- Electrolysis

3 Learning Outcomes

The student will be introduced to the fundamental concepts of heterogeneous electrochemistry (electrodics), basic electrochemical methods and main materials science questions related to the use and application of electrochemical converter devices. He/she will learn to evaluate experimental and theoretical results obtained with different electrochemical, surface science and theoretical methods and obtain a first insight in modern electrodics applied for continuing experimental work in this field. Moreover, he/she obtains basic competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: modules “Surfaces and Interfaces” and “Quantum Mechanics for Materials Science”

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of examination

7 Grading

	Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. P. Atkins et al., Atkins' Physical Chemistry, Oxford University Press, 2018. 2. C.H. Hamann et al. Electrochemistry, Wiley, 2007. 3. J. Maier, Physical Chemistry of Ionic Materials: Ions and Electrons in Solids, Wiley, 2004. 4. D. Linden, T. B. Reddy, Handbook of batteries, McGraw-Hill, 2002. 5. M. Wakihara, O. Yamamoto (eds.), Lithium Ion Batteries, Fundamentals and Performance, Wiley, 2008. 6. R. Memming; Semiconductor Electrochemistry, Wiley, 2015. 7. C.A. Grimes, O.K. Varghese, S. Ranjan; Light, Water, Hydrogen, Springer, 2008. 8. G. Hoogers (ed.), Fuel Cell Technology Handbook, Taylor and Francis, 2003.
10	**Comment** Cycle: each summer semester This module cannot be taken in combination with 11-01-7302 Electrochemistry for Energy Applications (8 CP)

Module name					
Electrochemistry for Energy Applications II: Devices and Technology					
Module no. 11-01-7301	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Jan Philipp Hofmann Prof. Dr. Ulrike I. Kramm		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-7301-vl	Electrochemistry for Energy Applications II: Devices and Technology	4	Lecture	2

2 Study Content

- Solid State Ionics
- Battery Fundamentals
- Li-Ion Batteries
- Semiconductor Electrochemistry
-
- Photocatalysis
- Photoelectrochemical Hydrogen Production
- Electrocatalysis
- Water Electrolysis
- Fuel Cells
- Industrial Electrochemical Processes

3 Learning Outcomes

The student will be introduced to the main concepts of heterogeneous electrochemistry (electrodics), solid state ionics and main materials science questions related to the use and application of electrochemical storage and converter devices. He/she will learn to combine electrochemical concepts and solid-state concepts for dealing with energy devices and electrochemical technology and to evaluate experimental and theoretical results obtained with different electrochemical, surface science and theoretical methods and obtain a first insight in modern electrodics applied for continuing experimental work in this field. Moreover, he/she obtains basic competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: modules “Surfaces and Interfaces”, “Quantum Mechanics for Materials Science” and “Electrochemistry in Energy Applications I: Fundamentals”

5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. P. Atkins et al., Atkins' Physical Chemistry, Oxford University Press, 2018. 2. C.H. Hamann et al. Electrochemistry, Wiley, 2007. 3. J. Maier, Physical Chemistry of Ionic Materials: Ions and Electrons in Solids, Wiley, 2004. 4. D. Linden, T. B. Reddy, Handbook of batteries, McGraw-Hill, 2002. 5. M. Wakihara, O. Yamamoto (eds.), Lithium Ion Batteries, Fundamentals and Performance, Wiley, 2008. 6. R. Memming; Semiconductor Electrochemistry, Wiley, 2015. 7. C.A. Grimes, O.K. Varghese, S. Ranjan; Light, Water, Hydrogen, Springer, 2008.
10	**Comment** Cycle: each winter semester This module cannot be taken in combination with 11-01-7302 Electrochemistry for Energy Applications (8 CP)

Module name

Fundamentals and Technology of Solar Cells

Module no.	Credit Points	Workload	Self-study	Duration	Frequency
11-01-2005	4 CP	120 h	90 h	1 Semester	Every 2. semester

Language of Instruction	Person responsible for the Module
English	Prof. Dr. rer. nat. Jan Philipp Hofmann

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8401-vl	Fundamentals and Technology of Solar Cells	4	Lecture	2

2 Study Content

- energy resources and scenarios
- fundamentals of semiconductor and device physics
- preparation and properties of single crystalline Si cells, compound semiconductor cells, high performance cells, thin film solar cells, perovskite solar cells
- technological and economic aspects of photovoltaics in a renewable energy system

3 Learning Outcomes

The student has gained the information to address and judge energy topics in their relevance for future technology areas, he/she has gained a broad understanding of semiconductor physics as background of the working principles of solar cells, he/she has been introduced to the materials science challenges given for the different cell technologies, he/she has learned which preparation and processing techniques are involved in the manufacturing and improvement of solar cells, he/she is qualified to evaluate experimental and theoretical methods for possible future research in solar cell basic science and technology, he/she has obtained the competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: modules “Surfaces and Interfaces”, “Quantum Mechanics for Materials Science”

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of examination

7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Solar cells: operating principles, technology, and system applications / Martin A. Green, Englewood Cliffs: Prentice Hall, 1982. (Prentice Hall series in solid state physical electronics) 2. Fundamentals of solar cells: photovoltaic solar energy conversion / Alan L. Fahrenbruch ; Richard H. Bube. Boston: Academic Press, 1983. 3. Organic Inorganic Halide Perovskite Photovoltaics, N. G. Park, M. Grätzel , T. Miyasaka (eds.) Springer, 2016. 4. S. M. Sze: Semiconductor Devices: Physics and Technology, Wiley, 2002.
10	**Comment** Cycle: each summer semester

Module name					
Graphen and Carbon Nanotubes - from fundamentals to applications					
Module no. 11-01-2008	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Ralph Michael Krupke		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2008-vl	Graphen and Carbon Nanotubes - from fundamentals to applications	0	Lecture	2

2 Study Content

- Synthesis of graphene and carbon nanotubes
- Structure – property correlation
- Electrical and optical properties
- Device fabrication
- Potential applications

3 Learning Outcomes

The student has gained a basic knowledge in the fundamentals of graphene and carbon nanotubes. He/she is able to understand how the atomic structure of a carbon allotrope determines its properties. He/she is able to understand the electrical and optical properties of nanocarbons and its implications for future applications. He/she is qualified in characterisation techniques and device fabrication techniques. The student has the competence to follow scientific literature and the knowledge that is required to conduct research in the field.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of exam

7 Grading

Technical Examination (100%); Default (Number grades)

8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science	
9	**Literature** 1. S. Reich, C. Thomsen, J. Mautzsch, Carbon Nanotubes: Basic Concepts and Physical Properties, WILEY-VCH, 2004. 2. A. Jorio, G. Dresselhaus, M. Dresselhaus (Eds.), Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties and Applications, Series: Topics in Applied Physics Vol 111, Springer, 2008. 3. S. Heinze, J. Tersoff, P. Avouris, Carbon nanotube electronics and optoelectronics, Materials Today Vol 9, Page 46-54, 2006. 4. P. Avouris, M. Freitag, V. Perebeinos, Carbon-nanotube photonics and optoelectronics, Nature Photonics Vol 2, Page 341-350, 2008. 5. F. Bonaccorso, A. Lombardo, T. Hasan, Z. Sun, L. Colombo, A. Ferrari, Production and processing of graphene and 2d crystals, MaterialsToday Vol15, Page 564-589, 2012. 6. F. Bonaccorso, Z. Sun, T. Hasan, A. Ferrari, Graphene Photonics and Optoelectronics, Nature Photonics Vol 4, Page 611-622, 2010.	
10	**Comment** Cycle: each summer semester	

Module name					
Hysteresis in Magnetic Materials					
Module no. 11-01-2024	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr.-Ing. Oliver Gutfleisch		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2024-vl	Hysteresis in Magnetic Materials	4	Lecture	2

2 Study Content

This lecture covers first some fundamental theory of magnetic materials, then design principles, and (micro)structure-property-relations in connection with the resulting thermal and magnetic hystereses. It covers the ground from intrinsic to extrinsic magnetic properties and develops strategies for the processing and fabrication of various functional magnets leading to variety of applications in energy technologies, sensors and actuators in robotics and biomedicine.

The main topics that will be studied in framework of this course are:
· Magnetism and hysteresis
· Physics of magnetic materials: from isolated moments to ordered arrangements
· Thermodynamics of magnetic solids
· Magnetic domains
· Micromagnetic theory
· Coercivity mechanisms
· Hard magnetic materials: maximizing hysteresis
· Hysteresis in fine particles and nanostructured materials: below the critical single-domain size
· Soft magnetic materials: minimizing hysteresis
· Magnetoelastic materials: magneto-structural coupling
· Magnetocaloric materials: balancing near the critical point
· Magnetic materials for efficient energy conversion, sensors and actuators
· Hysteresis in magnetic multiferroics and heterostructures: combining magnetism with additional functionalities
· Magnetic materials for recording and computers
· Magnetic Materials in Medicine and Biology

3 Learning Outcomes

Students will be able apply their acquired knowledge on magnetic hysteresis to the understanding of advanced functional principles of magnetic materials, which are key components of modern technologies with broad spectra of applications. The students will understand the basic principles of high coercivity in advanced permanent magnet (Nd-Fe-

	B, Sm-Zr-Co-Cu-Fe, Ferrites etc.). The students will understand the basics of materials with magneto-structural first-order phase transitions (La(FeSi)13-based, FeRh, Heusler alloys etc) and they will understand the critical role of thermal and magnetic hysteresis in solid state magnetic refrigeration. Further, the important role of magnetic hysteresis optimization in soft magnetic materials and fine magnetic particles for medicine and biology will be elucidated. The knowledge and skills gained in this course will help the students to work with advanced textbooks and scientific literature on functional magnetic materials and will qualify them to assess magnetic materials as key energy and technology enablers for wind energy and electromobility.
4	**Requirements for Participation** recommended: modules "Functional Materials" and "Magnetism and Magnetic Materials"
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. J. M. D. Coey, "Magnetism and Magnetic Materials", Cambridge University Press, 2010 2. B.D. Cullity and C.D. Graham, "Introduction to Magnetic Materials", John Wiley &Sons, 2009 3. R. O’Handley, "Modern Magnetic Materials", John Wiley &Sons, 2000, 4. R. Hilzinger and W. Rodewald, "Magnetic Materials", VAC, 2013 5. A. Hubert and R. Schäfer, "Magnetic Domains", Springer, 2000 6. S. Chikazumi, "Physics of Ferromagnetism", Oxford Science Publ., 1997 7. S. Blundell, "Magnetism in condensed matter", Oxford master Series in Cond Matt Phys., 2012 8. D. Jiles, "Magnetism and magnetic materials", Chapman & Hall, 1991
10	**Comment** Cycle: each summer semester

Module name

In-situ Transmission Electron Microscopy

Module no.	Credit Points	Workload	Self-study	Duration	Frequency
11-01-2017	5 CP	150 h	105 h	1 Semester	Every 2. semester

Language of Instruction	Person responsible for the Module
English	Prof. Dr. rer. nat. Christian Klaus Ulrich Kübel

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2017-vl	In-situ Transmission Electron Microscopy	4	Lecture	2
11-01-2017-vl	Exercises In-situ Transmission Electron Microscopy	1	Exercise	1

2 Study Content

In-situ electron microscopy techniques are becoming increasingly established to understand fundamental processes during synthesis, processing and application of functional materials at the atomic and nanometer scale. Different stimuli ranging from heating or electrical biasing to mechanical deformation and various liquid and gas environments are used to model selected processes and follow the structural changes with the full range of advanced imaging techniques in the TEM to correlate structure and properties of materials and identify transient states in reactions.
This lecture will (a) review the most important imaging techniques in the TEM (BF-/DF-/HRTEM, STEM), analytical techniques (EELS, EDX) and recent developments such as ACOM orientation mapping and other 4D-STEM techniques, (b) discuss electron beam effects in materials, (c) introduce various in-situ thermal, electrical, mechanical, liquid and gas phase setups, and (d) their application to understand processes in (nanostructured) materials. The aim is to provide the student with tools for advanced atomic and nanoscale characterization of materials and processes.

3 Learning Outcomes

The students are able to assess to the possibilities that modern electron microscopy imaging and spectroscopy techniques offer for advanced atomic/nanoscale structural and chemical characterization and the different in-situ approaches that can be implemented to follow complex processes in materials.

They can explain how materials research can benefit from (in-situ) electron microscopy and can interpret (in-situ) electron microscopy data and recognize challenges and pitfalls, enabling independent critical analysis of their own experimental research and published structural characterization.

4 Requirements for Participation

recommended: module “Transmission Electron Microscopy (TEM)”

	recommended: module “Scanning Transmission Electron Microscopy for Materials Science”
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Transmission Electron Microscopy, D.B. Williams and C.B. Carter, (2nd Ed.) Springer Verlag 2. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM, R. Egerton, Springer Verlag 3. Stephen J. Pennycook, Peter D. Nellist (Eds.): Scanning Transmission Electron Microscopy - Imaging and Analysis 4. G. Dehm, J.M. Howe, J. Zweck (Eds.): In-situ Electron Microscopy, Wiley-VCH 5. T.W. Hansen, J.B. Wagner (Eds.): Controlled Atmosphere Transmission Electron Microscopy, Springer 6. A. Ziegler, H. Graafsma, X.F. Zhang, J.W.M. Frenken (Eds.): In-situ Materials Characterization – Across Spatial and Temporal Scales, Springer
10	**Comment** Cycle: each summer semester

Module name					
Magnetism and Magnetic Materials					
Module no. 11-01-2001	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Lambert Alff		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2001-vl	Magnetism and Magnetic Materials	0	Lecture	2

2 Study Content

- Basic notions of magnetism
- Magnetism in atoms and ions
- Magnetism in metallic materials
- Crystal field symmetry and Exchange Interaction
- Magnetically ordered structures
- Magnetic order, symmetry and phase transitions
- Micromagnetism and domain behavior
- Experimental methods in magnetism
- Selected (hot) topics from current research

3 Learning Outcomes

The student is able to remember the basic notions of magnetism for a broad range of situations and materials. The student has the competence to differentiate different types of magnetism and their origin, and to correlate them with materials properties. He/she is qualified to evaluate experimental and theoretical methods for goal-oriented research in the area of magnetism and magnetic materials. The student remembers modern magnetic materials and their use in current applications. The student has a first insight in modern research in magnetism and magnetic materials and a beginner's competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

recommended: module „Quantum Mechanics for Materials Science”

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

	passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. S. Blundell: Magnetism in Condensed Matter, Oxford University Press (2001) 2. J. M.D. Coey: Magnetism and Magnetic Materials, Cambridge University Press (2009) 3. D. Jiles: Introduction to Magnetism and Magnetic Materials, Chapman & Hall (2001) 4. R. Skomski: Simple Models of Magnetism, Oxford University Press (2008) 5. N. Spaldin, Magnetic Materials, Cambridge University Press (2006) 6. L. Alff, Magnetismus und magnetische Materialien, Lecture notes (2004)
10	**Comment** Cycle: each winter semester

Module name					
Materials Science of Thin Films					
Module no. 11-01-2004	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Lambert Alff		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2004-vl	Thin Film Fabrication and Surface Techniques	4	Lecture	2

2 Study Content

- Introduction to thin film technology
- Nucleation: Thermodynamics and kinetics
- Structure and strain
- Thermal Evaporation
- Sputtering
- Chemical vapor deposition (CVD)
- Molecular beam epitaxy (MBE)
- Pulsed laser deposition (PLD)
- Thin film deposition of oxides
- Thin films for solar cells

3 Learning Outcomes

The student has gained a broad overview on and remembers relevant thin film deposition methods. He/she is able to identify the advantages and disadvantages of each deposition method for different applications and needs. The student has the competence to apply fundamental thin film science to novel materials. The student has the competence to differentiate different types of deposition methods according to their physical and chemical principles. He/she is qualified to evaluate thin film methods for goal-oriented research in the diverse fields of thin film applications. The student has a first insight in modern research in thin films and a beginner's competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. M. Ohring: Materials Science of Thin Films, Academic Press (2002) 2. L. B. Freund and S. Suresh: Thin Film Materialss, Cambridge University Press (2003). 3. R. Eason (Ed.): Pulsed Laser Deposition of Thin Films, Wiley (2007) 4. 17. IFF-Ferienkurs: Dünne Schichten und Schichtsysteme, Forschungszentrum Jülich (1986)
10	**Comment** Cycle: each summer semester

Module name					
Mathematical Methods in Materials Science					
Module no. 11-01-3018	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Apl. Prof. Dr. rer. nat. Yuri Genenko		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8662-vl	Mathematical Methods in Materials Science	0	Lecture	2

2 Study Content

- Linear ordinary differential equations: constant and variable coefficients
- Relaxation processes and oscillations in electrical circuits, parametric resonance
- Normal vibrational modes of polyatomic molecules: Lagrangian mechanics
- Linear partial differential equations: elliptic, hyperbolic, and parabolic equations
- Method of Fourier and Laplace transforms
- Diffusion in composite media: interface resistance
- Diffusion of foreign atoms to cylindrical and spherical precipitates
- Diffusion of magnetic field in a metal
- Solidification processes in an undercooled melt: Stefan problem
- Injection of electrons into dielectrics and organic semiconductors
- Green's function technique
- Bifurcations and phase transitions in open biological and chemical systems
- Self-organization in nonlinear active media

3 Learning Outcomes

The student is able to use advanced mathematical techniques for exactly, or approximately, solving linear ordinary and partial differential equations. He/she is able to implement these techniques for dealing with a variety of typical problems in materials science. He/she is able to follow sophisticated texts on these techniques and to address complex issues of that sort him- or herself.

4 Requirements for Participation

recommended: basic knowledge in mathematics, physics, and materials science

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. G.B. Arfken, H.J. Weber: Mathematical Methods for Physicists, Academic Press, New York (1995) 2. H.S. Carslaw, J.C. Jaeger: Conduction of Heat in Solids, Clarendon Press, Oxford (1993) 3. J. Crank: The Mathematics of Diffusion, Clarendon Press, Oxford (1994) 4. H. Heuser: Gewöhnliche Differentialgleichungen – Einführung in Lehre und Gebrauch, Teubner, Stuttgart (1995) 5. G. Lehner: Elektromagnetische Feldtheorie für Ingenieure und Physiker, Springer, Berlin (1996) 6. W. Richter: Einführung in Theorie und Praxis der partiellen Differentialgleichungen, Spektrum, Heidelberg (1995)
10	**Comment** Cycle: each winter semester

Module name					
Phase Transitions in Materials					
Module no. 11-01-9812	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Wolfgang Donner		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-9812-vl	Phase Transitions in Materials	4	Lecture	2

2 Study Content

- Basic Thermodynamics
- Nucleation and Diffusion
- Energy nad Entropy
- Melting
- Precipitation
- Diffusionless Transformations
- Ordering Transformations
- Magnetic Transitions
- Critical Phenomena

3 Learning Outcomes

Phase transitions are ubiquitous in Materials Science; close to such a transition, the response functions (i.e. physical properties) are enhanced. After taking this course, the student will be able to:

1. Classify phase transitions,
2. Relate the changes inside the materials to changes in their physical properties,
3. Choose appropriate characterization methods for phase transitions,
4. Critically review the literature about phase transitions,
5. Use the knowledge about phase transitions for his/her own scientific project.

4 Requirements for Participation

recommended: BSc in Materials Science, Physics or Chemistry; Course in Thermodynamics; Course in Scattering Methods

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

	passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Brent Fultz: Phase Transitions in Materials. Cambridge University Press 2014 2. Minoru Fujimoto: The Physics of Structural Phase Transitions. Springer 2005 also at: https://link.springer.com/book/10.1007%2Fb138153 3. P. Papon, L. Leblond, P.H.E. Meijer: The Physics of Phase Transitions. Springer 2006 also at: https://link.springer.com/book/10.1007%2F3-540-33390-8
10	**Comment** Cycle: each summer semester

Module name

Polymer Processing

Module no.	Credit Points	Workload	Self-study	Duration	Frequency
11-01-3030	4 CP	120 h	90 h	1 Semester	Every 2. semester

Language of Instruction	Person responsible for the Module
English	Prof. Dr.-Ing. Jürgen Wieser

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-3030-vl	Polymer Processing	0	Lecture	2

2 Study Content

Processing of Polymers: Compounding, extrusion, injection moulding, thermoforming, blow moulding, welding, glueing and typical surface decorations and treatments

3 Learning Outcomes

The student has gained an overview on typical processing technologies for polymers. He/she is able to identify processing technologies for different applications. He/she can explain the plastification, the melt flow and the solidification characteristics of a thermoplastic resin and how the materials morphology develops during processing. He/she can identify typical failures which can result of inappropriate processing. The student is able to describe the most important machines and process steps.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of exam

7 Grading

Technical Examination (100%); Default (Number grades)

8 Usability of the Module

M.Sc. Materials Science: Elective Courses Materials Science

9	**Literature** 1. W. Michaeli, Einführung in die Kunststoffverarbeitung, Hanser, München, 2010. 2. W. Knappe, Kunststoff-Verarbeitung und Werkzeugbau, Hanser, München, 1992. 3. F. Johannaber, W. Michaeli, Handbuch Spritzgießen, Hanser, München, 2004.
10	**Comment** Cycle: each summer semester

Module name					
Quantum Materials: Theory, Numerics, and Applications					
Module no. 11-01-2019	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Hongbin Zhang		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2019-vl	Quantum Materials: Theory, Numerics, and Applications	4	Lecture	2

2 Study Content

In this course, we will focus on several fundamental aspects of Quantum Materials where Quantum Mechanics can be applied to get the physical properties, including but not limited to

* Crystallography based on symmetry
* Computational thermodynamics: Thermodynamic stability
* Theory of elasticity: Mechanical properties
* Lattice dynamics: Phonons and anharmonicity
* Graphene and its electronic structure
* Modern theory of ferroelectric polarization
* Magnetism
* Linear-response theory

All the topics in this course will be discussed by solving simple models numerically, with Python modules prepared for/developed during the courses. Hands-on tutorials will be arranged with access to clusters where calculations can be done.

3 Learning Outcomes

The students develop a fundamental understanding on the quantum origin of various physical properties, in close connection to their future researches. They obtain a deep understanding of the theory behind each class of phenomena.

4 Requirements for Participation

recommended: basic quantum mechanics and basic knowledge of programming

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** Learning materials will be distributed during the lectures, with detailed theory, guide for numerical implementation, and further literature
10	**Comment** Cycle: each summer semester

Module name					
Semiconductor Interfaces					
Module no. 11-01-8162	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Andreas Klein		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8162-vl	Semiconductor Interfaces	4	Lecture	2

2 Study Content

- Carrier concentrations in semiconductors
- Defect properties and self-compensation
- Origin of the difference between semiconductors and insulators
- Excess carriers and carrier recombination
- Direct and indirect energy gaps
- Space charge layers
- Schottky diodes and p/n-junctions
- Charge transport characteristics of semiconductor diodes
- Solar cells, light emitting diodes, semiconductor lasers, field effect transistors
- Barrier formation at semiconductor interfaces

3 Learning Outcomes

The student is able to remember the basic notions of semiconductor physics including carrier concentrations in thermal equilibrium and non-equilibrium situations. The student has the competence to develop energy band diagrams and understand the function of all basic semiconductor structures. He/she is qualified to evaluate semiconductor devices and remembers most important semiconductor materials, their properties and their use in current applications. The student is aware of several materials limitations of semiconductor devices.

4 Requirements for Participation

recommended: basic knowledge in solid state physics

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

	passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. Klein, Semiconductor Interface, Lecture Notes (2009) 2. S.M. Sze, and K.K. Ng: Physics of Semiconductor Devices, John Wiley & Sons, Hoboken (2007) 3. P.Y. Yu, and M. Cardona: Fundamentals of Semiconductors. Physics and Materials Properties, Springer, Berlin (2001)
10	**Comment** Cycle: each winter semester

Module name					
Spintronics					
Module no. 11-01-2002	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Lambert Alff		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-2002-vl	Spintronics	4	Lecture	2

2 Study Content

- Introduction and basic notions of spintronics
- Spin dependent transport
- Magneto resistive (MR) effects, anisotropic magneto resistance (AMR)
- Giant magneto resistance (GMR)
- Spin dependent tunneling and tunneling magneto resistance (TMR)
- Materials for Spintronics, colossal magneto resistance (CMR)
- Spin transport in semiconductors
- Spintronic devices
- Meso and nanomagnetism
- Magnetic storage
- Selected (hot) topics from current research

3 Learning Outcomes

The student is able to adapt the concepts of spintronics to a broad range of situations and materials. The student has the competence to differentiate different types of magneto-resistive effects and their origin, and to correlate them with materials properties. He/she is qualified to evaluate experimental and theoretical methods for goal-oriented research in the area of spintronics. The student remembers modern spintronic materials and their use in current applications. The student has a first insight into modern research in spintronics and its device applications. He/she has a beginner's competence to follow advanced textbooks and scientific literature.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6	**Requirements on the Award of Credit Points** passing of exam
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. M. Ziese, M. J. Thornton (Eds.), Spin Electronics, Springer (2001) 2. D. D. Awschalom et al. (Eds.), Spin Electronics, Kluwer (2004) 3. S. Maekawa, Spin Electronics, Oxford University Press (2006) 4. S. Bandyopadhyay and M. Cahay, Introduction to Spintronics, Crc Pr Inc (2008) 5. L. Alff, Spintronics, Lecture Material (latest version 2010)
10	**Comment** Cycle: each summer semester

Module name					
Thermodynamics and Kinetics of Defects					
Module no. 11-01-3577	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. rer. nat. Andreas Klein		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-3577-vl	Thermodynamics and Kinetics of Defects	0	Lecture	2

2 Study Content

- Basic thermodynamics of solids
- Thermodynamics of point defects
- Defect reactions and concentrations
- Kröger-Vink notation and Brouwer approximation
- Fermi energy and defect concentrations
- Boundary layers: Mott-Schottky and Guy-Chapman profiles
- Diffusion processes
- Chemical, electrical- and electrochemical potential gradients
- Ambipolar diffusion and oxidation of metals
- Experimental determination of diffusion coefficients
- Fuel cells and batteries

3 Learning Outcomes

The student is able to remember the relevance of point defects for the electronic properties of materials. He/she has the competence to identify conditions under which point defects define material properties and to develop strategies how these can be modified. The student has a basic qualification to make materials selections for electronic and ionic applications.

4 Requirements for Participation

none

5 Form of Examination

Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min)

The form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

passing of exam

7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. A. Klein, T. Frömling, Lecture Notes 2. M.W. Barsoum, Fundamentals of Ceramics, IOP Publishing (2003) 3. J. Maier, Physical Chemistry of Ionic Materials, Wiley (2004)
10	**Comment** Cycle: each summer semester

Module name					
Fundamentals and Techniques of Modern Surface Science					
Module no. 11-01-8202	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Jan Philipp Hofmann		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8202-vl	Fundamentals and Techniques of Modern Surface Science	4	Lecture	2

2 Study Content

- Vacuum techniques
- Auger-electron spectroscopy (AES)
- X-ray photoelectron spectroscopy (XPS)
- Ultraviolett photoelectron spectroscopy (UPS)
- Inverse photoemission spectroscopy (IPE, BIS)
- Electron energy loss spectroscopy (ELS,HREELS)
- X-ray absorption spectroscopy (XAS, NEXAFS)
- Thermal desorption spectroscopy (TDS)
- High energy electron diffraction (LEED)
- Ion scattering (ISS, LEISS)}
- Scanning tunneling microscopy (STM)
- Atomic force microscopy (AFM)

3 Learning Outcomes

On successful completion of the module, students are able to:

1. explain the main experimental methods used in modern surface science,
2. explain the basic physical principles which are relevant for surface analytic techniques,
3. analyse surface science related problems and select appropriate analysis techniques,
4. understand the main materials science questions related to the use and application of these analytic techniques,
5. critically assess to which extent the application of certain surface analytic techniques is of use for a given scientific problem,
6. evaluate experimental and theoretical results obtained with these techniques,
7. understand modern surface science research and techniques applied for continuing experimental work in this field,
8. read and understand advanced textbooks and scientific literature.

4	**Requirements for Participation** recommended: modules “Quantum Mechanics for Materials Science”, “Surfaces and Interfaces” (can be followed in parallel)
5	**Form of Examination** Written exam (90 min), oral exam (30 min), or remote exam (open book, 90 min) The form of examination will be specified within two weeks after the first lecture.
6	**Requirements on the Award of Credit Points** passing of examination
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature** 1. W. Mönch: Semiconductor Surfaces and Interfaces (Springer, 2001) 2. G. Ertl, J. Küppers: Low Energy Electrons and Surface Chemistry (VCH, 1974) 3. M. A. van Hove, S.Y. Tong: Surface Crystallography by LEED (Springer, 1979) 4. D.P. Woodruff, T.A. Delchar: Modern Techniques in Surface Science (Cambridge University Press, 1986) 5. D. Briggs, M. P. Seah: Practical Surface Analysis (Wiley, 1996) 6. S. Hüfner: Photoelectron Spectroscopy (Springer, 1994) 7. M. Cardona, L. Ley: Photoemission in Solids I + II (Springer) 8. C. D. Wagner et al.: Handbook of X-ray Photoelectron Spectroscopy (Perkin-Elmer 1992) 9. H.-J. Güntherodt, R. Wiesendanger: Scanning Tunneling Microscopy I-III (Springer, 1994) 10. J. T. Yates: Experimental Innovations in Surface Science (Springer, 2015)
10	**Comment** Cycle: each winter semester

Module name					
Seminar Research Topics in Materials Science					
Module no. 11-01-4055	**Credit Points** 2 CP	**Workload** 60 h	**Self-study** 30 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr. Hongbin Zhang Dr. Wenjie Xie		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-4005-se	Seminar: Research Topics in Materials Science	2	Seminar	2

2 Study Content

- Topics are given to elaborate on in a seminar talk. These topic are related to actual research areas in materials science. Each set of topics is coherent within a certain field of materials science. The seminar is designed to help to bridge the gap between the scientific education and textbooks and scientific reseach and published papers.
- In the discussion section, students have to defend their seminar and should actively contribute to the discussion of other seminars. In the discussion the link between the talks should be reflected.

3 Learning Outcomes

The student gains the ability to approach a scientific topic by accumulating information from textbooks and scientific literature. Ability to sort the information and present it to other students at a similar level of knowledge in a useful way. Learning to ask useful and the right questions to scientific talks. Drive to participate in discussion and drawing lines between different talks.

4 Requirements for Participation

none

5 Form of Examination

Presentation (30 min)

The specific form of examination will be specified within two weeks after the first lecture.

6 Requirements on the Award of Credit Points

Attendance for at least 75% of the contact hours.

Compulsory attendance is required for the acquisition of following competencies: students are able to meaningfully contribute to scientific discussions, interact with fellow scientists, criticise scientific talks/presentations in a respectful and constructive manner,

	and realistically evaluate the quality of scientific presentations.
7	**Grading** Technical Examination (100%); Default (Number grades)
8	**Usability of the Module** M.Sc. Materials Science: Elective Courses Materials Science
9	**Literature**
10	**Comment** Cycle: each semester

Module name					
Engineering Microstructures					
Module no. 11-01-8131	**Credit Points** 4 CP	**Workload** 120 h	**Self-study** 90 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr.-Ing. Karsten Durst		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
11-01-8131-vl	Engineering Microstructures	4	Lecture	2

2 Syllabus

This lecture approaches microstructures of metallic materials from different perspectives including their characterization / quantification as well as their design. An emphasis is put on the underlying processes during thermomechanical treatments and related driving and dragging forces. The main chapters cover the following topics:

- Microstructural defects and their correlation with material properties
- Microstructural analysis (stereology and microscopic methods)
- Recovery, recrystallization and grain growth
- Severe plastic deformation
- Current trends in microstructural engineering

3 Learning Outcomes

1. The students can indentify appropriate microstructural characterization methods to quantify microstructural defects based on the potential and limitations of state-of-the-art microscopic methods.
2. The students are capable to perform basic stereologic analyses on micrographs.
3. The students can illustrate the stages of recovery and recrystallization processes. They are capable to relate driving forces to microstructural processes during thermal and thermomechanical treatments of metals.
4. The students can explain the concepts and working principle of severe plastic deformation processes.

4 Requirements for Participation

recommended: basics of defects in crystalline solids, mechanical behavior

5 Form of Examination

Oral exam (20 min)

6 Requirements on the Award of Credit Points

Passing the examination

7 Grading

Technical Examination (100%); Standard (Number grades)

8	**Associated Study Programme**
9	**Literature** 1. R.W. Cahn, P. Haasen: Physical Metallurgy, Elsevier Science B.V. (1996) 2. F.J. Humphreys, M. Hatherly: Recrystallization and Related Annealing Phenomena, Elsevier (2004) 3. G. Gottstein, Physical Foundations of Materials Science, Springer (2004)
10	**Comment** Cycle: each winter semester

Module name					
Current Topics in Physical Metallurgy					
Module no.	**Credit Points** 2 CP	**Workload** 60 h	**Self-study** 30 h	**Duration** 1 Semester	**Frequency** Every 2. semester
Language of Instruction English			**Person responsible for the Module** Prof. Dr.-Ing. Karsten Durst		

1 Courses of the Module

Course no.	Course name	Workload (CP)	Form of Teaching	Contact Hours per Week
	Current Topics in Physical Metallurgy	2	Seminar	2

2 Syllabus

The seminar is held in an inverted classroom format, consisting of bi-weekly seminar sessions with lecture videos for self-study in preparation of each session. During the seminar sessions, a specific topic will be discussed from a theoretical and application point of view followed by practical exercises that students will be working on individually or in small groups. The seminar covers a variety of current topics in physical metallurgy such as:

- Uniaxial and small-scale mechanical testing
- Imaging and quantification of dislocations
- Finite element simulations
- Severe plastic deformation

3 Learning Outcomes

1. The students are familiar with mechanical testing procedures across different length scales and the evaluation of such experiments.
2. The students can explain the basic concepts of geometrically necessary and statistically stored dislocations and provide examples as well as suitable characterization methods.
3. The students are capable to extract the key concepts and insights of research articles and pre-sent them to peers.

4 Requirements for Participation

Knowledge on mechanical properties of metals including strengthening mechanisms. Attendance of "Mechanical Properties of Metals" and/or "Engineering Microstructures" lectures recommended.

5 Form of Examination

Presentation (20 min)

6 Requirements on the Award of Credit Points

Passing the examination

7	**Grading** Technical Examination (100%); Standard (Number grades)
8	**Associated Study Programme**
9	**Literature** 10. Mechanical Behavior of Engineering Materials, J. Rösler, Springer Verlag 11. Mechanical metallurgy, G. Dieter, McGrow Hill 12. Deformation and Fracture Mechanics of Engineering Materials, R.W. Hertzberg, John Wiley & Sons, Inc 13. Werkstoffkunde und Werkstoffprüfung, W. Domke. Verlag W. Girardet, Essen 14. A.C. Fischer Cripps: Nanoindentation, Springer 15. D. Tabor: The Hardness of metals, Oxford University Press 16. K.L. Johnson: Contact mechanics, Cambridge University Press 17. Oliver and Pharr An improved technique for determining hardness and elastic modulus using load and displacement sensing indentation experiments. J. Mater. Res. 1992;7:1564–83. 18. Ast et al. A review of experimental approaches to fracture toughness evaluation at the micro-scale. Materials & Design. 2019;173:107762.
10	**Comment** Cycle: each winter semester