

Studiengang

Chemistry
(Master of Science)

Modulhandbuch

SS 2022

WS 2021/2022

Prüfungsordnungsversion: 2020w

Modulhandbuch generiert aus *UnivIS*

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Chemistry (Master of Science)

SS 2022, WS 2021/2022; Prüfungsordnungsversion: 2020w

1 Fachliche Wahlpflichtmodule

1.1 Inorganic Chemistry

Inorganic Chemistry

- Inorganic Chemistry, 10 ECTS, Julien Bachmann, Nicolai Burzlaff, SS 2022, 2 Sem. 8

Inorganic Chemistry laboratory

- Inorganic Chemistry - Lab, 10 ECTS, Die Dozenten der Anorg. Chemie, SS 2022 9

1.2 Organic Chemistry

Organic Chemistry

- Organic Chemistry, 10 ECTS, Henry Dube, Andreas Hirsch, Dozenten der Organischen Chemie, SS 2022, 2 Sem. 11

Organic Chemistry laboratory

- Organic Chemistry - Lab, 10 ECTS, Svetlana Tsogoeva, WS 2021/2022 12

1.3 Physical Chemistry

Physical Chemistry

- Physical Chemistry, 10 ECTS, Thomas Drewello, Carola Kryschi, Jörg Libuda, SS 2022, 2 Sem. 14

Physical Chemistry laboratory

- Physical Chemistry - Lab, 10 ECTS, Guido Sauer, Assistenten, SS 2022 15

1.4 Quantum Chemistry

Quantum Chemistry

- Quantum Chemistry, 10 ECTS, Andreas Görling, Christian Neiß, WS 2021/2022, 2 Sem. 17

Quantum Chemistry laboratory

- Quantum Chemistry - Lab, 10 ECTS, Andreas Görling, Christian Neiß, Petra Imhof, Bernd Meyer, Dirk Zahn, WS 2021/2022, 2 Sem. 19

2 Ergänzende Wahlpflichtmodule

2.1 Inorganic Chemistry

Inorganic Chemistry

- Inorganic Chemistry, 10 ECTS, Julien Bachmann, Nicolai Burzlaff, SS 2022, 2 Sem. 8

Inorganic Chemistry laboratory

- Inorganic Chemistry - Lab, 10 ECTS, Die Dozenten der Anorg. Chemie, SS 2022 9

2.2 Organic Chemistry

Organic Chemistry

- Organic Chemistry, 10 ECTS, Henry Dube, Andreas Hirsch, Dozenten der Organischen Chemie, SS 2022, 2 Sem. 11

Organic Chemistry laboratory

- Organic Chemistry - Lab, 10 ECTS, Svetlana Tsogoeva, WS 2021/2022 12

2.3 Physical Chemistry

Physical Chemistry

- Physical Chemistry, 10 ECTS, Thomas Drewello, Carola Kryschi, Jörg Libuda, SS 2022, 14
2 Sem.

Physical Chemistry laboratory

- Physical Chemistry - Lab, 10 ECTS, Guido Sauer, Assistenten, SS 2022 15

2.4 Quantum Chemistry

Quantum Chemistry

- Quantum Chemistry, 10 ECTS, Andreas Görling, Christian Neiß, WS 2021/2022, 2 Sem. 17

Quantum Chemistry laboratory

- Quantum Chemistry - Lab, 10 ECTS, Andreas Görling, Christian Neiß, Petra Imhof, Bernd Meyer, Dirk Zahn, WS 2021/2022, 2 Sem. 19

2.5 Advances in Bio-Organic and Bio-Inorganic Chemistry

Advanced Bio-Organic and Bio-Inorganic Chemistry

- Advanced Bio-Organic and Bio-Inorganic Chemistry, 5 ECTS, Nicolai Burzlaff, Norbert Jux, WS 2021/2022 21

Bio-Organic and Bio-Inorganic Chemistry - Lab

- Lab Course Bioorganic & Bioinorganic Chemistry, 5 ECTS, Nicolai Burzlaff, Petra Imhof, Norbert Jux, Carola Kryschi, Andriy Mokhir, SS 2022 23

Metallic nanoparticles in Medicine

- Metallic Nanoparticles in Medicine, 5 ECTS, Carola Kryschi, Stefanie Klein, Olaf Prante, Christina Janko, und Mitarbeiter/innen, SS 2022 25

Special Aspects in Bio-Organic Chemistry

- Special Aspects in Bioorganic Chemistry, 5 ECTS, Petra Imhof, Andriy Mokhir, WS 2021/2022 26

2.6 Advances in Homogenous Catalysis

Homogeneous Catalysis - Lab

- Homogeneous Catalysis - Lab, 5 ECTS, Romano Dorta, Sjoerd Harder, Karsten Meyer, Andriy Mokhir, Svetlana Tsogoeva, SS 2022 27

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- Organocatalysis and Catalytic Reactions in Water, 5 ECTS, Andriy Mokhir, Svetlana Tsogoeva, SS 2022 29

Organometallic Catalysis

- Organometallic Catalysis, 5 ECTS, Romano Dorta, Sjoerd Harder, SS 2022 31

Small Molecule Activation

- Small Molecule Activation, 5 ECTS, Karsten Meyer, u.a., SS 2022 33

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- Heterogenous Catalysis and Kinetics, 5 ECTS, Jörg Libuda, SS 2022 35

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- Interfaces and Catalysis - Lab, 5 ECTS, Jörg Libuda, Dozenten der beteiligten Fachgebiete, SS 2022 37

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- Surface and Interface Science, 5 ECTS, Christian Papp, Marcus Bär, SS 2022 39

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- Research Module Organic Chemistry, 15 ECTS, Andreas Hirsch, Henry Dube, Norbert Jux, Andriy Mokhir, Svetlana Tsogoeva, Jürgen Schatz, Dozenten der Organischen Chemie, SS 2022 80

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- Research Module Physical chemistry, 15 ECTS, Hans-Peter Steinrück, Dirk M. Guldi, u. a. Hochschullehrer, SS 2022 82

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5 Masterarbeit

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Modulbezeichnung: **Inorganic Chemistry (CM-IC)** **10 ECTS**
 (Inorganic Chemistry)

Modulverantwortliche/r: Karsten Meyer

Lehrende: Julien Bachmann, Nicolai Burzlaff

Startsemester: SS 2022

Dauer: 2 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 90 Std.

Eigenstudium: 210 Std.

Sprache: Englisch

Lehrveranstaltungen:

Inorganic Chemistry (SS 2022, Vorlesung mit Übung, 3 SWS, Karl Mandel et al.)

Inorganic Chemistry (WS 2022/2023, Seminar, Julien Bachmann et al.)

Inhalt:

- Introduction to current research topics of Inorganic Chemistry
- establishing fundamental knowledge required for appreciation of more specialized topics in Inorganic Chemistry; the expected standard is based on a research oriented masters program.

Lernziele und Kompetenzen:

The students

- acquire knowledge and expertise required for danger evaluation and practical handling of novel inorganic compounds
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Inorganic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Inorganic Chemistry)

Studien-/Prüfungsleistungen:

Inorganic Chemistry (Prüfungsnummer: 65011)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 30

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O30(PL): Oral examination (30 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstabelleung: WS 2022/2023, 1. Wdh.: SS 2023

1. Prüfer: CM-IC (N70009)

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)!
- More information via Studon!

Bemerkungen:

Module compatibility:

- Lecture module within the **Core module** „Inorganic Chemistry“ in M. Sc. Chemistry
- Lecture module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Inorganic Chemistry - Lab (CM-IC-Lab)** **10 ECTS**
 (Inorganic Chemistry - Lab)

Modulverantwortliche/r: Karsten Meyer
 Lehrende: Die Dozenten der Anorg. Chemie

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 225 Std.	Eigenstudium: 75 Std.	Sprache: Englisch

Lehrveranstaltungen:

- Attendance in lab course is compulsory!
 - Attendance at safety instruction is compulsory!
 - Attendance in winter or summer term possible!
 - A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de
- Inorganic Chemistry - LAB (SS 2022, Praktikum, 15 SWS, Karsten Meyer et al.)

Inhalt:

- practical laboratory experience aiming at introducing students to current and state of the art inorganic research topics
- work experience in a team of researchers
- establishing fundamental knowledge required for addressing individual molecular research problems at a state of the art level
- independent and self-driven approach to problem solving in an assigned research project

Lernziele und Kompetenzen:

The students

- apply acquired fundamental knowledge and practical skills to an individual research problem that they work on independently
- manage and apply the fundamental safety regulations important to handling hazardous compounds and instruct other coworkers in relevant safety topics
- rank their own research results in the context of current literature and research papers in the field and record their results in appropriate scientific writing and documentation style
- give oral and written presentations of the results and acquired knowledge in an appropriate scientific style in English language

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Inorganic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Inorganic Chemistry)

Studien-/Prüfungsleistungen:

Inorganic Chemistry Laboratory (Prüfungsnummer: 65021)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: IC-Lab (N70010)

Organisatorisches:

Please note:

- Students have to register for the module in their first semester (check registration periods)!
- Lab course is held as an in-class-course
- Lab course can be chosen in winter or summer term
- Time and place by appointment (in one of the involved working groups of Inorganic chemistry)
- Registration / further information: please contact Dr. Achim Zahl (achim.zahl@fau.de)

Bemerkungen:

Module compatibility:

- Lab module within the **Core module „Inorganic Chemistry“** in M. Sc. Chemistry
- Lab module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Organic Chemistry (CM-OC)** **10 ECTS**
 (Organic Chemistry)

Modulverantwortliche/r: Henry Dube

Lehrende: Henry Dube, Dozenten der Organischen Chemie, Andreas Hirsch

Startsemester: SS 2022

Dauer: 2 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 90 Std.

Eigenstudium: 210 Std.

Sprache: Englisch

Lehrveranstaltungen:

Organic Chemistry (SS 2022, Vorlesung mit Übung, 3 SWS, Andreas Hirsch et al.)

Organic Chemistry (WS 2022/2023, Vorlesung mit Übung, Henry Dube et al.)

Inhalt:

- Introduction to current research topics of Organic Chemistry
- establishing fundamental knowledge required for appreciation of more specialized topics in Organic Chemistry; the expected standard is based on a research oriented Masters program

Lernziele und Kompetenzen:

Students

- acquire knowledge and expertise required for theoretical evaluation and practical handling of novel organic compounds
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Organic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Organic Chemistry)

Studien-/Prüfungsleistungen:

Organic Chemistry (Prüfungsnummer: 65031)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 30

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O30(PL): Oral examination (30 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2022/2023, 1. Wdh.: SS 2023

1. Prüfer: OC (N70011)

Organisatorisches:

Organic Chemistry (CM-PC) will be taught online (synchronous) - and please note: students have to register for the module (check registration periods)!

More information via studon!

Bemerkungen:

Module compatibility:

- Lecture module within the **Core module** „Organic Chemistry“ in M. Sc. Chemistry
- Lecture module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Organic Chemistry - Lab (CM-OC-Lab)** **10 ECTS**
(Organic Chemistry - Lab)

Modulverantwortliche/r: Henry Dube
Lehrende: Svetlana Tsogoeva

Startsemester: WS 2021/2022 Dauer: 1 Semester Turnus: jährlich (WS)
Präsenzzeit: 225 Std. Eigenstudium: 75 Std. Sprache: Englisch

Lehrveranstaltungen:

- Attendance at the preliminary briefing including 'safety instructions part 1': signature list serves as proof of attendance;
 - Attendance at the briefing 'safety instructions part 2' in the lab;
 - A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de
- Organic Chemistry - LAB (WS 2021/2022, Praktikum, 15 SWS, Svetlana Tsogoeva et al.)

Empfohlene Voraussetzungen:

Knowledge of the content of the lecture **Organic Chemistry (CM-OC)** is recommended.

Inhalt:

- Reactions / Synthesis: Oxidation reactions; Synthesis and application of Jacobsen Mn(III)-complex (Jacobsen epoxidation); Reductions; Reactions with lithium organic compounds; Cross-coupling reaction; Synthesis of the Evans-Auxiliary; Natural compounds; Heterocycles.
- Advanced practical lab work in organic chemistry, that includes molecular synthesis and use of state-of-the-art analytical tools.
- Instruction in laboratory safety regulations.

Lernziele und Kompetenzen:

The students are capable

- to use their theoretical and practical background to make an individual contribution to an independent, actual and realistic research project;
- to organize a small research/synthesis project in theory and practise
- to plan experiments to prove or reject a given hypothesis
- to provide a state-of-the-art documentation and discussion of results obtained as a member of a research team
- to present, communicate and discuss scientific results with experts in English.

Literatur:

- L. F. Tietze, Th. Eicher, Reaktionen und Synthesen in organisch-chemischen Praktikum und Forschungslaboratorium
- R. Brückner, et al., Praktikum Präparative Organische Chemie
- Organikum, Wiley-VCH

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

- [1] **Chemistry (Master of Science)**
(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Organic Chemistry)
- [2] **Chemistry (Master of Science)**
(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Organic Chemistry)

Studien-/Prüfungsleistungen:

Organic Chemistry Laboratory (Prüfungsnummer: 65041)
Prüfungsleistung, Praktikumsleistung
Anteil an der Berechnung der Modulnote: 100%
weitere Erläuterungen:
Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)
Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Svetlana Tsogoeva

Organisatorisches:

Please note:

- Lab course **Organic Chemistry laboratory** (CM-OC-Lab) is held as an in-class-course only in winter term (usually in February/March)!
- Students have to register for the module (check registration periods)!
- Registration/further information via StudOn: https://www.studon.fau.de/cat4182718.html_join.html

Bemerkungen:

Module compatibility:

- Lab module within the **Core module „Organic Chemistry“** in M. Sc. Chemistry
- Lab module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Physical Chemistry (CM-PC)** **10 ECTS**
 (Physical Chemistry)

Modulverantwortliche/r: Dirk M. Guldi

Lehrende: Jörg Libuda, Carola Kryschi, Thomas Drewello

Startsemester: SS 2022

Dauer: 2 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 90 Std.

Eigenstudium: 210 Std.

Sprache: Englisch

Lehrveranstaltungen:

Physical Chemistry (SS 2022, Vorlesung mit Übung, 3 SWS, Thomas Drewello et al.)

Physical Chemistry (WS 2022/2023, Vorlesung mit Übung, 3 SWS, Jörg Libuda)

Inhalt:

- introduction to the current topics of research in the field of physical chemistry
- developing the basics of physical chemistry at the level of a scientifically oriented Master's program
- deepening of knowledge in the specialized field of the lecturers involved in this module to the limit of current knowledge

Lernziele und Kompetenzen:

Students

- apply fundamental knowledge of physical chemistry to particular topics in research
- develop model-like descriptions for complex physicochemical systems and model experimental data

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Physical Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Physical Chemistry)

Studien-/Prüfungsleistungen:

Physical Chemistry (Prüfungsnummer: 65051)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 30

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O30(PL): Oral examination (30 min) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2022/2023, 1. Wdh.: SS 2023

1. Prüfer: CM-PC (N70012)

Organisatorisches:

Please note:

- Students have to register for module examination (check registration periods on meinCampus)!
- More information via studon!

Bemerkungen:

Module compatibility:

- Lecture module within the **Core module** „Physical Chemistry“ in M. Sc. Chemistry
- Lecture module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Physical Chemistry - Lab (CM-PC-Lab)** **10 ECTS**
 (Physical Chemistry - Lab)

Modulverantwortliche/r: Dirk M. Guldi
 Lehrende: Guido Sauer, Assistenten

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 120 Std.	Eigenstudium: 180 Std.	Sprache: Englisch

Lehrveranstaltungen:

- Attendance at lab-course is compulsory!
- Attendance at safety instruction is compulsory!
- Attendance in winter or summer term possible!
- A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Physical Chemistry - Lab (SS 2022, Praktikum, 15 SWS, Guido Sauer et al.)

Inhalt:

- Practical introduction to current and state-of-the-art research topics in the field of physical chemistry
- Advanced spectroscopic and image analysis
- Guided work on current research projects using methods of physical chemistry
- Documentation of experimental results

The practical part comprises 8 days in the physicochemical advanced practical course lab and, in addition, two 3-day practical projects in two different working groups of physical chemistry. The 3-day internships may be extended after consultation with the internship coordinator and the working group (in return the number of experiments in the practical lab course can be reduced).

Lernziele und Kompetenzen:

Students ...

- apply fundamental knowledge of physical chemistry to particular topics in research
- develop model-like descriptions for complex systems and model experimental data
- discover various modern experimental techniques and apply them systematically in practice
- apply and transfer knowledge acquired during their studies to handle and solve open questions in research projects in physical chemistry
- perform experiments/measurements, record and evaluate their results in appropriate scientific form and interpret results independently
- present their own results and acquired knowledge in an appropriate scientific style in English language in oral and written form
- evaluate the basic safety matters in handling hazardous materials and complex apparatus

Literatur:

- P. Atkins, J. De Paula, Atkins' Physical Chemistry, 10th edition, Oxford University Press, Oxford, 2014
 - Literature references provided in the guidelines of each experiment
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

- [1] **Chemistry (Master of Science)**
 (Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Physical Chemistry)
 - [2] **Chemistry (Master of Science)**
 (Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Physical Chemistry)
-

Studien-/Prüfungsleistungen:

Physical Chemistry Laboratory (Prüfungsnummer: 65061)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

SeL: Poster presentation, 20 - 30 min

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Guido Sauer

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)
- Lab course is held as an in-class-course
- Lab course can be chosen in winter or summer term
- Time and place by appointment
- Registration/further information available on studon https://www.studon.fau.de/crs397438__join.html

Bemerkungen:

Module compatibility:

- Lab module within the **Core module „Physical Chemistry“** in M. Sc. Chemistry
- Lab module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: Quantum Chemistry (CM-QC) (Quantum Chemistry)	10 ECTS
Modulverantwortliche/r: Andreas Görling	
Lehrende: Christian Neiß, Andreas Görling	
Startsemester: WS 2021/2022	Dauer: 2 Semester
Präsenzzeit: 90 Std.	Eigenstudium: 210 Std.
	Turnus: jährlich (WS)
	Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry - WS:

Winter Term:

1. Quantum Chemistry 1 (2V)
2. Quantum Chemistry 1 Seminar (1S)

Quantum Chemistry 1 (WS 2021/2022, Vorlesung mit Übung, Andreas Görling et al.)

Quantum Chemistry - SS:

Summer Term:

3. Quantum Chemistry 2 (2V)
4. Quantum Chemistry 2 Seminar (1S)

Quantum Chemistry 2 (SS 2022, Vorlesung mit Übung, 3 SWS, Andreas Görling)

Empfohlene Voraussetzungen:

Required Qualifications:

- good knowledge of basic quantum mechanics: axioms of QM, application to simple systems (particle in a box, harmonic oscillator, rigid rotator)
- good knowledge in mathematics: differential calculus of functions of several variables, basic linear algebra

Inhalt:

- Introduction to modern methods and current research issues in the field of quantum and computer chemistry
- Hartree-Fock, DFT, Many Body Perturbation Theory
- Configuration Interaction, Second Quantization, Coupled Cluster
- TD-HF, TD-DFT, RPA

Lernziele und Kompetenzen:

Students ...

- obtain sound knowledge in basic and advanced methods of quantum chemistry
- are able to solve mathematical problems occurring in quantum chemistry
- are able to understand and assess scientific reports in the field of quantum chemistry

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Quantum Chemistry)

[2] Chemistry (Master of Science)

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Quantum Chemistry)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Quantum Chemistry (Prüfungsnummer: 65071)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 30

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O30 (PL): Oral Examination (30 minutes) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Andreas Görling

Organisatorisches:

- The core module "Quantum Chemistry" starts only in winter term!
- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- Lecture module within the **Core module** „Quantum Chemistry“ in M. Sc. Chemistry
- Lecture module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: Quantum Chemistry - Lab (CM-QC-Lab) 10 ECTS
 (Quantum Chemistry - Lab)

Modulverantwortliche/r: Andreas Görling

Lehrende: Christian Neiß, Andreas Görling, Bernd Meyer, Petra Imhof, Dirk Zahn

Startsemester: WS 2021/2022

Dauer: 2 Semester

Turnus: jährlich (WS)

Präsenzzeit: 225 Std.

Eigenstudium: 75 Std.

Sprache: Englisch

Lehrveranstaltungen:

1. Scientific Programming 1 (5 SWS/Winter term):

Quantum Chemistry - Lab / Scientific Programming (WS 2021/2022, Seminar, 5 SWS, Christian Neiß et al.)

2. Scientific Programming 2 (5 SWS/Summer term):

Quantum Chemistry - Lab / Scientific Programming (SS 2022, Seminar, 5 SWS, Christian Neiß et al.)

3. Training in Applied Computational Chemistry (5 SWS/Winter or summer term):

- Internship in one of the Theoretical Chemistry groups (Profs Görling, Imhof, B. Meyer, Zahn), time and place by agreement (Winter or summer term)
- Training has to be taken only once: in winter **or** in summer term (time and place by agreement)

Training in Applied Computational Chemistry (WS 2021/2022, Praktikum, 5 SWS, Anwesenheitspflicht, Andreas Görling et al.)

Training in Applied Computational Chemistry (SS 2022, Praktikum, 5 SWS, Anwesenheitspflicht, Andreas Görling et al.)

Inhalt:

- Operating system Linux for high-performance computing (HPC)
- Scientific programming in Fortran and Python
- Using numerical and mathematical libraries/modules
- Introduction to parallel computing
- Exercises
- Programming project
- Training in applied computational chemistry

Lernziele und Kompetenzen:

Students

- get familiar with Linux as operating system for HPC
- are able to create computer programs for scientific purposes
- can use numerical and mathematical libraries/modules in home-made programs
- obtain knowledge about basic parallelization paradigms
- apply quantum chemical methods to scientific questions under guidance

Literatur:

- Stephen J. Chapman: Fortran for Scientists and Engineers, McGraw Hill 2017 (4th ed.)
 - Bernd Klein: Einführung in Python 3, Hanser 2017 (3rd ed.)
 - Stefan Gerlach: Computerphysik, Springer Spektrum 2019 (2nd ed.)
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Fachliche Wahlpflichtmodule | Quantum Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Quantum Chemistry)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Quantum Chemistry Laboratory (Prüfungsnummer: 65081)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol: Successful implementation of the programming project (working program) including Lab report (ca. 5 pages)

Grading procedure: 100% Graded Computer Program

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Andreas Görling

Organisatorisches:

Please note:

- The core module "Quantum Chemistry" starts only in winter term!
- Students have to register for the module
- Registration / further information via StudOn

Bemerkungen:

Module compatibility:

- Lab module within the **Core module** „Quantum Chemistry“ in M. Sc. Chemistry
- Lab module within the **Compulsory Elective Module** in M.Sc. Chemistry (if not chosen as Core module) or M. Sc. Molecular Science

Modulbezeichnung: **Advanced Bio-Organic and Bio-Inorganic Chemistry (BioIOC-1)** **5 ECTS**
(Advanced Bio-Organic and Bio-Inorganic Chemistry)

Modulverantwortliche/r: Nicolai Burzlaff
Lehrende: Norbert Jux, Nicolai Burzlaff

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Advanced Bioinorganic Chemistry, Metalloenzymes and Metals in Medicine (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Nicolai Burzlaff et al.)
Seminar Advanced Bioinorganic Chemistry, Metalloenzymes and Metals in Medicine (WS 2021/2022, Seminar, 1 SWS, Nicolai Burzlaff et al.)

Inhalt:

The students

- are introduced into recent activities and achievements in the fields of bioorganic and bioinorganic chemistry and metals in medicine

Lernziele und Kompetenzen:

The students

- are introduced into recent activities and achievements in the fields of bioorganic and bioinorganic chemistry and metals in medicine

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Bio-Organic and Bio-Inorganic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Advanced Bio-Organic and Bio-Inorganic Chemistry (Prüfungsnummer: 65111)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Bio-Organic and -Inorganic Chem-1 (N70005)

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Please note: The Compulsory Elective Module "**Advances in Bioorganic and Bioinorganic Chemistry**" can only be taken as a whole!

Module compatibility:

- Lecture module within the **Compulsory elective module** "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total)

- Lecture module as part of the **Elective Module** in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: **Lab Course Bioorganic & Bioinorganic Chemistry (BioIOC-Lab)** **5 ECTS**
 (Lab Course Bioorganic & Bioinorganic Chemistry)

Modulverantwortliche/r: Nicolai Burzlaff

Lehrende: Nicolai Burzlaff, Petra Imhof, Carola Krysch, Norbert Jux, Andriy Mokhir

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 105 Std.

Eigenstudium: 45 Std.

Sprache: Englisch

Lehrveranstaltungen:

Attendance at lab course is compulsory!

Bio-Organic & Bio-Inorganic LAB (SS 2022, Praktikum, Nicolai Burzlaff et al.)

Inhalt:

The students

- deepen their knowledge in special topics of bioorganic and bioinorganic chemistry and nanomedicine that are in the research focus of the involved research groups of the department depending on their own choice
- perform practical studies and small research projects regarding topics of the preparative, mechanistic or more biological bioorganic and bioinorganic chemistry and nanomedicine in an advanced level

Lernziele und Kompetenzen:

The students

- can characterise and evaluate bioinorganic models
 - manage the preparation of bioorganic compounds and bioinorganic models as well as synthesis of functionalized nanoparticles, their characterization as well as their application in mechanistic studies
 - carry out bioorganic and bioinorganic research projects largely independently using a wide range of bioorganic and bioinorganic theories and are able to reflect upon the gained results
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Bio-Organic and Bio-Inorganic Chemistry)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Bio-Organic and Bio-Inorganic Chemistry - Lab (Prüfungsnummer: 65141)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: BioIOC-Lab (N70017)

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)!
- Lab course **Advances in Bioorganic and Bioinorganic Chemistry Laboratory (BioIOC-Lab)** is held as an in-class-course in one of the participating research groups!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- Lab module within the **Compulsory elective module "Advances in Bioorganic and Bioinorganic Chemistry"** in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total)

Modulbezeichnung: **Metallic Nanoparticles in Medicine (BioIOC-2)** **5 ECTS**
 (Metallic Nanoparticles in Medicine)

Modulverantwortliche/r: Nicolai Burzlaff

Lehrende: Carola Kryschi, Christina Janko, Olaf Prante, und Mitarbeiter/innen, Stefanie Klein

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: jährlich (SS)

Präsenzzeit: 75 Std.

Eigenstudium: 75 Std.

Sprache: Englisch

Lehrveranstaltungen:

Metallic Nanoparticles in Medicine (SS 2022, Vorlesung mit Übung, 3 SWS, Carola Kryschi et al.)

Inhalt:

The students

- are introduced into recent research activities and achievements in the fields of nanomedicine
- evaluate and assess the basic theories, principles and concepts of bioorganic and bioinorganic chemistry and nanomedicine (in compliance with a research-orientated master course)

Lernziele und Kompetenzen:

The students

- can explain and reflect upon the bioorganic and bioinorganic nanochemistry aspects in medicinal chemistry and toxicology
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Bio-Organic and Bio-Inorganic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Metallic nanoparticles in Medicine (Prüfungsnummer: 65131)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

W60 (PL): Written Examination (60 minutes) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: SS 2023

1. Prüfer: Carola Kryschi

Organisatorisches:

- Students have to register for the module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Please note: The Compulsory elective module "**Advances in Bioorganic and Bioinorganic Chemistry**" has to be taken as a whole!

Module compatibility:

- Lecture module within the **Compulsory elective module** "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total)
- Lecture module as **Elective Module** in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: **Special Aspects in Bioorganic Chemistry (BioIOC-3)** **5 ECTS**
 (Special Aspects in Bioorganic Chemistry)

Modulverantwortliche/r: Nicolai Burzlaff
 Lehrende: Andriy Mokhir, Petra Imhof

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Special Aspects in Bio-Organic Chemistry (WS 2021/2022, Seminar, Andriy Mokhir et al.)

Inhalt:

The students

- deepen their knowledge in special topics of bioorganic and bioinorganic chemistry that are in the research focus of the involved research groups of the department depending on their own choice

Lernziele und Kompetenzen:

The students

- can explain, apply and reflect upon the theories, terminology, specialities, boundaries and different school of bioorganic and bioinorganic chemistry critically and in depth
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Bio-Organic and Bio-Inorganic Chemistry)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Special Aspects in Bio-Organic Chemistry (Prüfungsnummer: 65121)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Petra Imhof, 2. Prüfer: Andriy Mokhir

Organisatorisches:

- Students have to register for the module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Please note: The Compulsory Elective Module "**Advances in Bioorganic and Bioinorganic Chemistry**" can only be taken as a whole!

Module compatility:

- lecture module within the **Compulsory elective module** "Advances in Bioorganic and Bioinorganic Chemistry" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total)
- as **Elective Module** in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: **Homogeneous Catalysis - Lab (HomCatal-Lab)** **5 ECTS**
(Homogeneous Catalysis - Lab)

Modulverantwortliche/r: Sjoerd Harder

Lehrende: Svetlana Tsogoeva, Sjoerd Harder, Romano Dorta, Andriy Mokhir, Karsten Meyer

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: jährlich (SS)

Präsenzzeit: 105 Std.

Eigenstudium: 45 Std.

Sprache: Englisch

Lehrveranstaltungen:

- Attendance in lab course is compulsory!
- Attendance at safety instructions is compulsory!
- A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Homogeneous Catalysis - Lab (SS 2022, Praktikum, Sjoerd Harder et al.)

Inhalt:

Students

- Students get in touch with modern research topics in the field of homogenous catalysis & research tools or advanced spectroscopic tools (Practical work in one of the involved research groups!)
- deepens her/his knowledge in special topics of homogeneous catalysis that are in the research focus of the involved research groups
- will be trained in the practical aspects of advanced homogeneous catalysis

Lernziele und Kompetenzen:

Students

- get in touch with modern research topics in the field of homogenous catalysis & research tools or advanced spectroscopic tools
 - manage the preparation and full characterization of catalysts
 - learn methods to evaluate catalyst performance in a series of catalytic reactions and are able to discuss scope and relevance
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Homogenous Catalysis)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Homogeneous Catalysis - Lab (Prüfungsnummer: 65241)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: HomoCat-Lab (N70018)

Organisatorisches:

Homogenous Catalysis - Lab can only be taken in summer term!

Please note:

- Students have to register for the module (check registration periods)!
- Lab course Homogenous Catalysis - Lab (HomCatal-Lab) is held as an in-class-course!

The lab course takes place in one of the participating research groups!

Bemerkungen:

The compulsory elective module "Advances in Homogenous Catalysis" can only be taken as a whole (HomCatal-1 - 3 + HomCatal-Lab).

Module compability:

- Lab module within the Compulsory Elective Module (20 ECTS)!
- Lab module as part of the elective module (5 ECTS, not graded)!

Modulbezeichnung: **Organocatalysis and Catalytic Reactions in Water (HomCatal-2)** **5 ECTS**
(Organocatalysis and Catalytic Reactions in Water)

Modulverantwortliche/r: Sjoerd Harder
Lehrende: Andriy Mokhir, Svetlana Tsogoeva

Startsemester: SS 2022 Dauer: 1 Semester Turnus: jährlich (SS)
Präsenzzeit: 45 Std. Eigenstudium: 105 Std. Sprache: Englisch

Lehrveranstaltungen:

Organocatalysis and Catalytic Reactions in Water (SS 2022, Vorlesung mit Übung, 3 SWS, Andriy Mokhir et al.)

Inhalt:

- History and basic principles of organocatalysis,
- Different types of organocatalysts,
- Enantioselective organocatalysis,
- Domino reactions and important examples.
- Catalytic reactions in water: Important reactions in biological chemistry, Metabolism of biomolecules and artificial bioorthogonal reactions.

Lernziele und Kompetenzen:

The student

- can explain basic principles and underlying reaction mechanisms in organo- and organometallic catalysis and biological chemistry
- deepens her/his knowledge in special topics of homogeneous catalysis that are in the research focus of the involved research groups
- is able to construct important reaction mechanisms and catalytic cycles and can critically discuss each step.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Homogenous Catalysis)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Organocatalysis and Catalytic Reactions in Water (Prüfungsnummer: 65221)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral examination (20 minutes) or alternative examination according to FAU-Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Andriy Mokhir

Organisatorisches:

- **Organocatalysis and Catalytic Reactions in Water** will be taught only in summer term
- Students have to register for the module (check registration periods on MeinCampus)!
- Information/registration on studon!

Bemerkungen:

The compulsory elective module "Advances in Homogenous Catalysis" can only be taken as a whole (HomCatal-1 - 3 + HomCatal-Lab)!

Organocatalysis and Catalytic Reactions in Water can be taken

- within the Compulsory Elective Module "Advances in Homogenous Catalysis" (20 ECTS in total)
- as Elective Module (5 ECTS, not graded)

Modulbezeichnung: **Organometallic Catalysis (HomCatal-1)** **5 ECTS**
 (Organometallic Catalysis)

Modulverantwortliche/r: Sjoerd Harder
 Lehrende: Romano Dorta, Sjoerd Harder

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Metalorganic Catalysis (SS 2022, Vorlesung mit Übung, 3 SWS, Sjoerd Harder et al.)
 Organometallic Catalysis - Seminar (SS 2022, Seminar, 1 SWS, Sjoerd Harder et al.)

Inhalt:

- Harder: Introduction and basic principles of advanced catalysis, homogeneous vs. heterogeneous catalysis, mechanisms of substrate activation (C=C, C=O), control by ligand and metal choice, classical catalytic cycles: Wilkinson catalyst, C-C cross coupling, hydroformylation, polymerization catalysis, catalysis with main group metals.
- Dorta: Review of basic organometallic mechanisms & reactivity (elementary reactions, isolobality); Hydrogenation of alkenes and aromatics; C - C cross coupling; Atom-economical C - C formation (alkene hydroformylation & hydrocyanation, alkene oligomerization, methanol carbonylation); Synthetic fuels from CO (methanol, MTG, Fischer-Tropsch); Alkene metathesis; Selective C - O bond formation (epoxidations and Wacker-type oxidations)

Lernziele und Kompetenzen:

The student

- understands basic principles and underlying reaction mechanisms in organometallic catalysis
- is able to outline reaction mechanisms and catalytic cycles
- knows the tools for the characterization of catalysts and how to evaluate catalyst performance
- acquires knowledge on topics of current interest and recent breakthroughs in organometallic catalysis

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Homogenous Catalysis)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Metalorganic Catalysis (Prüfungsnummer: 65211)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral examination (20 minutes) or alternative examination according to FAU-Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Romano Dorta, 2. Prüfer: Sjoerd Harder

Organisatorisches:

- The module "Organometallic Catalysis" will be taught only in summer term!
- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- Lecture module within the Compulsory Elective module "Advances in Homogenous Catalysis" in M. Sc. Chemistry or Molecular Science (20 ECTS in total, graded)
- as Elective Module in M. Sc. Chemistry or Molecular Science (5 ECTS, ungraded)

Modulbezeichnung: **Small Molecule Activation (HomCatal-3)** **5 ECTS**
 (Small Molecule Activation)

Modulverantwortliche/r: Karsten Meyer
 Lehrende: u.a., Karsten Meyer

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:
 Small Molecule Activation (SS 2022, Seminar, Karsten Meyer)

Inhalt:

Lecture:

- Inorganic coordination chemistry, catalytic and electrocatalytic transformation of abundant small molecules N₂, O₂, CO or CO₂, H₂O and NH₃, into value-added commodities, fine-chemicals, active pharmaceutical ingredients and polymers.
- Selective oxidation reactions.
- CO₂ reduction to CO and subsequent Fischer-Tropsch catalysis for the production of carbon-based fuels.
- Reductive activation of atmospheric N₂ to NH₃ and the production of H₂ from H₂O splitting catalysis. Applications, e.g. fuel-cell technologies for carbon-free energy production.

Lernziele und Kompetenzen:

The student

- can explain basic principles and underlying reaction mechanisms in small molecule activation
- is able to construct important reaction mechanisms and catalytic cycles
- can critically discuss small-molecule activation

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Homogenous Catalysis)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Small Molecule Activation (Prüfungsnummer: 65231)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Written examination (60 minutes) or alternative examination according to FAU-Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Karsten Meyer

Organisatorisches:

Please note:

- **Small Molecule Activation** will be taught only in summer term
- students have to register for the module (check registration periods)!
- registration/further information via StudOn!

Bemerkungen:

The compulsory elective module **Advances in Homogenous Catalysis** can only be taken as a whole!

Module compability:

- Lecture module within the Compulsory Elective Module (20 ECTS in total!)
- Lecture module as part of the Elective Module (5 ECTS, not graded)!

Modulbezeichnung: **Heterogenous Catalysis and Kinetics (IntCat-1)** **5 ECTS**
 (Heterogenous Catalysis and Kinetics)

Modulverantwortliche/r: Jörg Libuda
 Lehrende: Jörg Libuda

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Heterogeneous Catalysis and Kinetics (SS 2022, Vorlesung mit Übung, 3 SWS, Jörg Libuda)

Inhalt:

Syllabus:

- Concepts in heterogeneous catalysis: definition of terms, industrial processes
- Characterization methods for real catalysts (in-situ and operando methods, TEM, SEM, XRD, EXAFS, XANES, XPS, SIMS, DRIFTS, Raman, TPR, etc.)
- Surface Reaction Dynamics: dynamics of adsorption, reaction, desorption, molecular beam experiments, laser spectroscopies
- Elementary Kinetics: microkinetics, transition-state theory, relaxation kinetics, rate-determining step; microkinetic experiments, TAP, SSITKA, etc.
- Model Catalysis: growth processes, preparation and characterization of model catalysts; kinetics on nanostructured surfaces
- Energy-related model catalysis (incl. examples from current research)

Lernziele und Kompetenzen:

Students ...

- acquire the professional competence in heterogeneous catalysis and respective topics
- obtain advanced knowledge in different experimental or theoretical models, their application to current problems, the corresponding data evaluation and interpretation using current research examples
- get familiar with various modern experimental techniques and are able to apply them in a targeted manner

Literatur:

O. Brummel, J. Libuda: "Electrifying Oxide Model Catalysis: Complex Electrodes based on Atomically-Defined Oxide Films", Catalysis Letters, 150 (2020) 1546-1560.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

- [1] **Chemistry (Master of Science)**
 (Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis A)
- [2] **Chemistry (Master of Science)**
 (Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis B)
- [3] **Chemistry (Master of Science)**
 (Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Heterogenous Catalysis and Kinetics (Prüfungsnummer: 65331)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral examination (20 minutes) or alternative examination according to the FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Jörg Libuda

Organisatorisches:

Please note:

- Students have to register for the module examination on MeinCampus (check registration periods)!
- Information/registration available on StudOn!

Bemerkungen:

Module compatibility:

- Lecture module within the **Compulsory Elective Module "Advances in Interface Science & Catalysis"** in M. Sc. Chemistry or M. Sc. Molecular Science
- as part of the **Elective Module** in M.Sc. Chemistry/MSc. Molecular Science

Modulbezeichnung: Interfaces and Catalysis - Lab (IntCat-Lab) **5 ECTS**
 (Interfaces and Catalysis - Lab)

Modulverantwortliche/r: Jörg Libuda

Lehrende: Dozenten der beteiligten Fachgebiete, Jörg Libuda

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 105 Std.

Eigenstudium: 45 Std.

Sprache: Englisch

Lehrveranstaltungen:

- Attendance in lab course is compulsory!
- Attendance at safety instructions is compulsory!
- Attendance in winter or summer term possible!
- A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Interface & Catalysis LAB (SS 2022, Vorlesung, 7 SWS, Jörg Libuda et al.)

Inhalt:

Practical introduction to state-of-the-art research in the fields of surface science, interface science, heterogeneous catalysis, electrocatalysis or materials characterization. Guided work on a current research project in a research group. Research topics may cover spectroscopy at surfaces, microscopy at surfaces, in-situ or operando spectroscopy, characterization of catalytic materials, in-situ methods in electrocatalysis, preparation and characterization of nanomaterials, modelling and simulation of interfaces and nanomaterials or similar. Practical laboratory experience to introduce state-of-the-art experimental tools in surface and catalysis research, among them:

- Electron spectroscopies
- Vibrational spectroscopies
- Microscopy at interfaces
- Other characterization methods for surfaces / interfaces
- In-situ and operando spectroscopy and microscopy
- Characterization of nanomaterials
- Electrochemical in-situ characterization
- Photochemical / photoelectrochemical in-situ characterization
- Modelling on processes at interfaces

Lernziele und Kompetenzen:

The students ...

- get familiar with the current state-of-knowledge for a specific research topic.
- apply fundamental knowledge of physical chemistry to a specific research topic.
- understand and test model-like descriptions for complex physicochemical problems.
- operate complex state-of-the-art instrumentation.
- get in contact with development of new methodologies to answer open questions in interface science and catalysis.
- analyze data with state-of-the-art methodologies.
- record, document, and analyze research data in in appropriate form.
- present and discuss experimental results and develop interpretations.
- present own results in written form and scientific style English language.

Literatur:

Will be provided by the supervising research group

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis A)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis B)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Interfaces and Catalysis - Lab (Prüfungsnummer: 65341)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Jörg Libuda

Organisatorisches:

Please note:

- Students contact the research research groups of their choice in the field of interface science, interface controlled materials, heterogeneous catalysis and electrocatalysis, nanomaterials characterization, or modelling and simulation of processes at interfaces at the Department of Chemistry and Pharmacy.
- Time and place by appointment (winter or summer term)
- Central Registration via Studon: https://www.studon.fau.de/crs4211909_join.html
- All organization information available vis Studon: <https://www.studon.fau.de/crs4211909.html>
- Module examination organized by supervising group
- Attendance in lab course is compulsory!
- Please check lab instructions (contact lab supervisor)
- Laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Bemerkungen:

Module compatibility:

- Obligatory lab course module (5 ECTS) within the Compulsory elective module **Interfaces and Catalysis** within the degree programmes M.Sc. Chemistry or M.Sc. Molecular Science

Modulbezeichnung: **Surface and Interface Science (IntCat-2)** **5 ECTS**
 (Surface and Interface Science)

Modulverantwortliche/r: Hans-Peter Steinrück

Lehrende: Christian Papp, Marcus Bär

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: jährlich (SS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Surfaces and Interface Science (SS 2022, Vorlesung mit Übung, 3 SWS, Christian Papp et al.)

Inhalt:

- Vacuum and pressure measurement (pumps, pressure and flow ranges)
- Lab-based and synchrotron-based light sources (principles, optics, insertion devices, etc.)
- Theory of photoemission and electronic structure
- XPS (elemental / chemical sensitivity, cross sections, quantification, examples)
- UPS (gas phase, adsorbates, 2D band structures, 3D band structures, orbital tomography)
- IPES (probing of unoccupied states, energy level alignment determination)
- HAXPES (depth-resolved photoemission measurements, examples)
- PEEM (spatially-resolved photoemission measurements, examples)
- NEXAFS (principle and examples)
- XES & RIXS (principle and examples)
- Structure of surfaces/ diffraction at surfaces (LEED, definitions and examples)
- X-ray spectroscopy - based materials research on energy conversion devices (examples from current research)

Lernziele und Kompetenzen:

Students ...

- understand the principles of photoemission variants and their applications
- can judge the quality of data evaluation and its pitfalls
- can deliberately select an X-ray spectroscopic analysis method to address given scientific question and are able to evaluate the collected data

Literatur:

- Hüfner: „Photoelectron Spectroscopy: Principles and Applications“ Springer-Verlag Berlin Heidelberg
- Ertl, Küppers: „Low Energy Electrons and Surface Chemistry“ VCH Weinheim
- D. Attwood, Soft X-rays and Extreme Ultraviolet Radiation, Cambridge University Press, 1999
- D. Briggs, M.P. Seah: Practical Surface Analysis: Auger and X-Ray Photoelectron Spectroscopy, Wiley, 1996
- M. Bär, L. Weinhardt, and C. Heske: Advanced Characterization Techniques for Thin Film Solar Cells, edited by D. Abou-Ras, T. Kirchartz, and U. Rau (Wiley VCH Verlag GmbH & Co KGaA, ISBN: 978-3-527-33992-1), 2nd Extended Edition, Volume 2, Chap. 18.
- A. Meisel, G. Leonhardt, R. Szargan: X-ray Spectra and Chemical Binding, Springer, 1989

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis A)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis B)

[3] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Surfaces and Interface Science (Prüfungsnummer: 65321)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Christian Papp

Organisatorisches:

Please note:

- Module can be taken only during summer term
- Students have to register for the module (check registration periods)
- registration/further information via StudOn

Bemerkungen:

Module compatibility:

- Lecture module within the Compulsory elective module "Advances in Interfaces and Catalysis" in M.Sc. Chemistry or M. Sc. Molecular Science (20 ECTS in total)
- Lecture module as part of the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: Theory of catalytical processes (IntCat-3A) 5 ECTS
 (Theory of catalytical processes)

Modulverantwortliche/r: Jörg Libuda
 Lehrende: Bernd Meyer

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Theory of Catalytic Processes (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Bernd Meyer)

Inhalt:

The module focuses on physical, chemical or technological aspects of modification, manipulation and characterization of interfaces. These aspects relate to the research of ideal model systems (surfaces and adsorbates on single crystal surfaces) or real systems, in which the interface plays a crucial role for the respective properties. In all cases, the local electronic and chemical interactions at the interface affect the geometric structure (e.g. adsorption geometry) and consequently the chemical and physical properties.

Lernziele und Kompetenzen:

Students

- deepen their knowledge in experimental methods and theoretical aspects to describe and characterize interface phenomena
 - are able to perform experiments independently and to analyse the data
 - are familiar with the model-type description of experimental data
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis A)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Theory of Catalytic Processes (Prüfungsnummer: 65311)

(englische Bezeichnung: Theory of catalytical processes)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Bernd Meyer

Organisatorisches:

Please note:

- students have to register for the module examination on MeinCampus (check registration periods)!
- registration/further information via StudOn

Bemerkungen:

Module compability:

- within the Compulsory Elective Module **Advances in Interfaces and Catalysis A (IntCat-3A)** (20 ECTS)!

- module can also be taken as part of the elective module (5 ECTS, not graded)!
- **MSc Molecular NANO Science students** have to attend the module **Advances in Interfaces and Catalysis A** (IntCat-3A) / **MSc Chemistry student** can choose between the module **Advances in Interfaces and Catalysis A** (IntCat-3A) and the module **Nanostructured Materials and Interfaces B** (IntCat-3B) of Prof. Bachmann

Modulbezeichnung: **Advanced Electrochemistry (EnMat-1)** **5 ECTS**
 (Advanced Electrochemistry)

Modulverantwortliche/r: Dirk M. Guldi
 Lehrende: Christian Ehli

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Advanced Electrochemistry (2V/1UE):

Advanced Electrochemistry (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Christian Ehli)

Inhalt:

- Comprehensive survey of the fundamentals for electrode processes (thermodynamics and kinetics)
- Introduction to electrochemical techniques (e.g. cyclic voltammetry, rotating disk voltammetry, differential pulse voltammetry, spectroelectrochemistry, electrochemical impedance spectroscopy)
- Applications of electrochemistry (e.g. corrosion prevention, batteries)
- Seminars will be based on the discussion of practical aspects and electrochemical exercises

Lernziele und Kompetenzen:

Students

- plan and perform own electrochemical experiments
- characterize electroactive materials by common electrochemical methods
- analyze, interpret and discuss electrochemical experimental results
- discuss and evaluate current electrochemical publications

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Energy Materials)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Advanced Electrochemistry (Prüfungsnummer: 65421)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

W60(PL): written examination (60 min)

Prüfungssprache: Englisch

Erstablesung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Dirk M. Guldi

Organisatorisches:

Please note:

- "Advanced Electrochemistry" will be taught only in winter term!
- Students have to register for the module on (check registration periods)!

Bemerkungen:

- Within the Compulsory Elective Module "Advances in Energy Materials" in M.Sc. Chemistry or M.Sc. Molecular Science (20 ECTS)!
- as part of the Elective Module in M.Sc. Chemistry or M.Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: Energy Materials - Lab (EnMat-Lab) **5 ECTS**
(Energy Materials - Lab)

Modulverantwortliche/r: Dirk M. Guldi
Lehrende: Christian Ehli, Dirk M. Guldi

Startsemester: SS 2022 Dauer: 1 Semester Turnus: halbjährlich (WS+SS)
Präsenzzeit: 105 Std. Eigenstudium: 45 Std. Sprache: Englisch

Lehrveranstaltungen:

- Attendance at lab course is compulsory!
 - Attendance at safety instructions is compulsory!
 - A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de
- Energy Materials - LAB (SS 2022, Praktikum, 7 SWS, Dirk M. Guldi et al.)

Inhalt:

- Practical introduction to electrochemical techniques
- Guided work on the characterization of electroactive materials
- Attempts to solve independently a scientific problem
- Documentation of experimental results

Lernziele und Kompetenzen:

Students

- plan and perform own electrochemical experiments
- characterize electroactive materials by common electrochemical methods
- analyze, interpret, and discuss electrochemical experimental results
- discuss and evaluate current electrochemical publications.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Energy Materials)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Energy Materials - Lab (Prüfungsnummer: 65441)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Graded Lab Protocol of 30 - 50 pages (plus raw data documentation)

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Dirk M. Guldi

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)!
- Lab course **Energy Materials - Lab (EnMat-Lab)** is held as an in-class-course!

The lab course takes place in one of the participating research groups!

Bemerkungen:

- Within the Compulsory Elective Module "Advances in Energy Materials" in M.Sc. Chemistry or M.Sc. Molecular Science (20 ECTS)!
- The module can be taken as part of the Elective Module (5 ECTS, not graded)!

Modulbezeichnung: **Semiconductor Materials for Energy Applications (EnMat-3)** **5 ECTS**
 (Semiconductor Materials for Energy Applications)

Modulverantwortliche/r: Dirk M. Guldi

Lehrende: Julien Bachmann, u. Mitarbeiter

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: jährlich (SS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Semiconductor Materials for Energy Applications (SS 2022, Seminar, Julien Bachmann)

Semiconductor Materials for Energy Applications - Seminar (SS 2022, Seminar, 1 SWS, Julien Bachmann et al.)

Inhalt:

- Fundamentals of semiconductors: Crystal structure, Electronic structure, Electrical transport, Interaction with light
- Semiconductor devices: Tunnelling, The pn junction, The transistor
- Photovoltaics: Principles, Types of solar cells
- The interface to a solution: Charged electrolytic interfaces, Electrocatalysis and photoelectrocatalysis

Lernziele und Kompetenzen:

The students

- are familiar with the fundamentals and modern developments in semiconductor science and applications
 - understand theoretical and practical aspects in state-of-the-art semiconductor devices
 - can present, communicate and discuss scientific results with experts in English.
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Energy Materials)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Semiconductor Materials for Energy Applications (Prüfungsnummer: 65411)

(englische Bezeichnung: Semiconductor materials for energy applications)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100% Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Julien Bachmann

Organisatorisches:

Please note:

- Students have to register for the module on StudOn (check registration periods)!
- Registration/further information via StudOn

Bemerkungen:

Module compatibility:

- within the Compulsory Elective Module "Advances in Energy Materials" in M. Sc. Chemistry or M. Sc. Molecular Science (20 ECTS)
- part of the Elective Module in M. Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: Solar Energy Conversion (EnMat-2) **5 ECTS**
 (Solar Energy Conversion)

Modulverantwortliche/r: Dirk M. Guldi
 Lehrende: Dirk M. Guldi

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Solar Energy Conversion (2V + 1S):

Solar Energy Conversion (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Dirk M. Guldi)

Inhalt:

- Demand and supply of energy
- Solar cells:
 1. Silicon solar cells
 2. dye-sensitized solar cells
 3. organic solar cells
 4. perovskite solar cells
 5. singlet fission
- Fundamentals of Electron Transfer
- Photosynthesis: natural photosynthesis, artificial photosynthesis

Lernziele und Kompetenzen:

The students . . .

- are familiar with the fundamentals and modern applications in solar energy research and applications
 - understand design principles in solar energy devices and can transfer this knowledge to related topics
 - can present, communicate and discuss scientific results with experts in English.
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Energy Materials)

[2] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Solar Energy Conversion (Prüfungsnummer: 65431)

Prüfungsleistung, Klausur, Dauer (in Minuten): 60

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

W60(PL): written examination (60 min) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Dirk M. Guldi

Organisatorisches:

Please note:

- "Solar Energy Conversion" will be taught only in winter term.
- Students have to register for the module (check registration periods)!

- Registration/further information via StudON

Bemerkungen:

- Within the Compulsory Elective Module "Advances in Energy Materials" MSc Chemistry and Molecular Science
- Module can be taken as part of the Elective Module, too!

Modulbezeichnung: **Nanostructured Materials and Interfaces (IntCat-3B)** **5 ECTS**
 (Nanostructured Materials and Interfaces)

Modulverantwortliche/r: Jörg Libuda

Lehrende: Julien Bachmann

Startsemester: WS 2021/2022

Dauer: 1 Semester

Turnus: jährlich (WS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Nanostructured Materials and Interfaces (WS 2021/2022, Seminar, 3 SWS, Julien Bachmann et al.)

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Ergänzende Wahlpflichtmodule | Advances in Interface Research and Catalysis B)

Studien-/Prüfungsleistungen:

Nanostructured Materials and Interfaces (Prüfungsnummer: 65371)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablesung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Julien Bachmann

Organisatorisches:

Please note:

- students have to register for the module examination on MeinCampus (check registration periods)!
- registration/further information via StudOn

Bemerkungen:

Module compability:

- within the Compulsory Elective Module **Advances in Interfaces and Catalysis B (IntCat-3B)** (20 ECTS)!
- module can also be taken as part of the elective module (5 ECTS, not graded)!
- MSc Chemistry student can choose between the compulsory elective module **Advances in Interfaces and Catalysis A (IntCat-3A)** and the compulsory elective module **Advances in Interfaces and Catalysis B (IntCat-3B)**

Modulbezeichnung: **Advanced Spectroscopic Techniques (ProSpec)** **5 ECTS**
(Advanced Spectroscopic Techniques)

Modulverantwortliche/r: Henry Dube

Lehrende: Alexander Scherer, Henry Dube

Startsemester: WS 2021/2022

Dauer: 1 Semester

Turnus: jährlich (WS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Advanced Spectroscopy in Organic Chemistry (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Henry Dube et al.)

Empfohlene Voraussetzungen:

Basic knowledge of spectroscopy is recommended.

Inhalt:

Fundamentals of spectroscopy in organic chemistry will be reviewed. More in-depth methods of molecular spectroscopy in organic chemistry are covered. Advanced methods of NMR-spectroscopy are also covered, such as NMR-spectroscopy of various nuclei (e.g., ¹H, ¹³C, ¹⁹F, ³¹P). Two-dimensional methods of NMR-spectroscopy using scalar spin-spin couplings (e.g., HSQC, HMBC) are discussed. Furthermore, NMR-spectroscopic methods relying on interactions between coupling nuclear dipoles, which are transmitted directly through space are covered (e.g., NOESY). In addition, other optical spectroscopic methods will be reviewed and discussed in more depth (e.g., UV/Vis-, CD-, IR-spectroscopy and Mass spectrometry).

Lernziele und Kompetenzen:

The students ...

- master the reliable use and gain an understanding of spectroscopic methods in organic chemistry, which are used to elucidate organic molecules;
- are able to characterize unknown molecules and to determine their structure as well as their dynamics and interactions (the correlations between the spectroscopic results and the characteristics of the molecules should become understandable and comprehensible);
- discuss practical examples of spectroscopic results and the related correlations in the exercises and practice the structure elucidation on examples.

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Advanced Spectroscopic Techniques (Prüfungsnummer: 65631)

Studienleistung, Übungsleistung

weitere Erläuterungen:

SL: practical exercise (homework assignment, 15- 20 pages), non-graded

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: keine Angabe

1. Prüfer: Alexander Scherer

Organisatorisches:

- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn: https://www.studon.fau.de/crs3726967_join.html

Bemerkungen:

Module compatibility:

- Elective Module within the degree programmes MSc Chemistry and Molecular Science, 5 ECTS/not graded

Modulbezeichnung: **Biological and Synthetic Molecular Switches and Machines (MolSwitch)** **5 ECTS**
 (Biological and Synthetic Molecular Switches and Machines)

Modulverantwortliche/r: Henry Dube
 Lehrende: Henry Dube

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Seminar (1UE): time and place by agreement
 Molecular Switches and Molecular Machines (SS 2022, Vorlesung, 2 SWS, Henry Dube)

Inhalt:

Examination of molecular triggers, switches and machines in biology and in synthetic systems as foundation of nanotechnology; working mechanisms; types of systems; design principles; seminal contributions; historical backgrounds are given. The material is ordered in introduction and context, basic principles, triggers, switches, machines, integrated systems, future prospective. The course will be updated to implement the newest developments yearly

Lernziele und Kompetenzen:

The Students ...

- acquire a fundamental understanding in the working mechanisms and design principles of molecular triggers, switches, and machines.
- will be able to develop strategies for implementing responsiveness into nanostructured biological or synthetic systems and will be equipped with an exhaustive overview of historical developments and current state of the art in the field by discussing representative examples in depth.
- will therefore be educated in one of the most prominent fields of modern (bio)chemistry and nanosciences.

Compulsory attendance will be necessary. The skills will be appropriate for Master's level and will partially repeat and build on knowhow from supramolecular, biological, and photochemistry as well as on fundamental physical organic chemistry, biochemistry, nanotechnology, and spectroscopy.

Literatur:

- "Molecular Switches", edited by Ben L. Feringa, Wiley-VCH
- "From Non-Covalent Assemblies to Molecular Machines", Edited by Jean-Pierre Sauvage & Pierre Gaspard, Wiley-VCH
- "Molecular Machines and Motors - Recent Advances and Perspectives" edited by Alberto Credi, Serena Silvi, Margherita Venturi, Springer

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Biological and Synthetic Molecular Switches and Machines (Prüfungsnummer: 65621)

Studienleistung, Übungsleistung, Dauer (in Minuten): 20

weitere Erläuterungen:

Assessment: 20 min oral examination in the form of a seminar talk presenting the content of a seminal original publication (Non-graded seminar presentation)

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: Henry Dube

Organisatorisches:

Please note:

- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- as Elective Module in MSc Molecular **Life** Science (not applicable for Molecular **Nanoscience**), 5 ECTS/not graded
- as Elective Module in MSc Chemistry, 5 ECTS/not graded

Modulbezeichnung: Economics (BWL) (Economics)	5 ECTS
Modulverantwortliche/r: Rainer Fink	
Lehrende: Andreas Späth, Gerhard Kranz	

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Deutsch

Lehrveranstaltungen:

- Economics A: Betriebswirtschaftslehre I (WS 2021/2022, Seminar, Anwesenheitspflicht, Gerhard Kranz)
- Economics B: Betriebswirtschaftslehre II (WS 2021/2022, Seminar, Anwesenheitspflicht, Gerhard Kranz)
- Economics C: Strategische Planung & Projektmanagement (WS 2021/2022, Seminar, Andreas Späth)

Inhalt:

Economics A: Betriebswirtschaftslehre I (BWL-I):

Einführung in ...

- Funktionsbereiche
- Unternehmensformen
- Bilanz/GuV/Kostenrechnung

Economics B: Betriebswirtschaftslehre II (BWL-II):

- Bilanzanalyse
- Kennzahlen
- Kostenrechnung

Economics C: Strategische Planung & Projektmanagement (BWL-III):

Einführung in ...

- Methoden der strategischen Analyse
- Innovationsstrategien
- F&E Projektmanagement
- Agiles Projektmanagement und Lean

Lernziele und Kompetenzen:

Die Studierenden ...

- erwerben Kenntnisse über Grundfragen der allgemeinen Betriebswirtschaftslehre
- kontrollieren ihr Wissen durch online Follow-Up Self-Assessments
- arbeiten erfolgreich mit gängigen Analysetools
- beherrschen grundlegende Techniken des Projektmanagements
- erarbeiten selbständig eine Unternehmensanalyse
- präsentieren die Ergebnisse

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Economics (Prüfungsnummer: 65481)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 15 - 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Prüfungsleistung: Erstellung und Präsentation einer Projektstudie (Vortrag ca. 15 - 20 min)

Prüfungssprache: Deutsch

Erstablingung: WS 2021/2022, 1. Wdh.: keine Angabe
1. Prüfer: Rainer Fink

Organisatorisches:

Bitte beachten Sie:

- Registrierung läuft über **StudOn** - der Anmeldezeitraum wird allen Studierenden rechtzeitig per E-Mail mitgeteilt
- die Teilnahme an den Präsenzveranstaltungen ist verpflichtend, wenn Präsenzveranstaltungen stattfinden können
- Aktuelle Informationen (z.B. zu Zeit und Raum) und Skripten finden Sie auf **StudOn!**

Bemerkungen:

- **Economics** ist ein **Wahlmodul** im MSc Chemistry oder MSc Molecular Science / 5 ECTS, unbenotet
- Für die Anrechnung des Wahlmoduls müssen alle 3 Lehrveranstaltungen (Economics 1-3) besucht werden!

Modulbezeichnung: Lebensmittelchemie (LmCh) **5 ECTS**
 (Food Chemistry)

Modulverantwortliche/r: Monika Pischetsrieder

Lehrende: Monika Pischetsrieder

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Deutsch

Lehrveranstaltungen:

Chemie und Technologie der Lebensmittel IV Bioaktive pflanzliche Lebensmittel (SS 2022, Vorlesung, 1 SWS, Monika Pischetsrieder)

Chemie und Technologie der Lebensmittel V - Proteine (SS 2022, Vorlesung, 1 SWS, Monika Pischetsrieder)

Instrumentelle Analytik für Lebensmittelchemiker und das Wahlmodul Lebensmittelchemie /Master Molecular Science (SS 2022, Seminar, 1 SWS, Monika Pischetsrieder)

Inhalt:

- Es werden toxikologisch, technologisch und physiologisch relevante Inhaltsstoffe von Lebensmitteln ausführlich vorgestellt und diskutiert.
- Ausgehend von den grundlegenden Kenntnissen der organischen Chemie werden Reaktionsmechanismen, die während der Prozessierung oder Entstehung von Lebensmitteln ablaufen, erläutert.
- Ausgehend von grundlegenden Kenntnissen der analytischen Chemie werden die wichtigsten weiterführenden und aktuellen instrumentellanalytischen und bioanalytischen Analysemethoden besprochen.

Lernziele und Kompetenzen:

Die Studierenden

- erarbeiten sich die Sachkompetenz zur theoretischen Beurteilung und praktischen Handhabung wichtiger Fragestellungen der Lebensmittelchemie
- sind in der Lage, die wichtigsten relevanten Arbeitstechniken aus dem Gebiet der Lebensmittelchemie und -analytik und eines anderen Gebiets der Lebensmittelwissenschaften selbständig anzuwenden
- können die wesentlichen Prinzipien der Lebensmittelanalytik auf praktische Probleme anwenden und kritisch reflektieren.

Literatur:

Wird von den Dozenten aktualisiert zur Verfügung gestellt.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Lebensmittelchemie (Prüfungsnummer: 65361)

Studienleistung, Seminarleistung, Dauer (in Minuten): 20

weitere Erläuterungen:

Seminarvortrag, 20 Minuten, unbenotet

Prüfungssprache: Deutsch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Monika Pischetsrieder

Organisatorisches:

Bitte beachten:

- das Seminar findet im zweijährigen Turnus statt (VL Lebensmittelchemie I - IX)
- alle Lehrveranstaltungen finden online über ZOOM statt
- Studierende müssen sich für das Modul und die Prüfung online registrieren (bitte beachten Sie die Registrierungsperiode auf MeinCampus!)

Bemerkungen:

Die Vorlesung **Lebensmittelchemie**

- hat je nach Semester unterschiedliche inhaltliche Schwerpunkte (Lebensmittelchemie I-XI)
- kann als Teil des Wahlmoduls/Elective module belegt werden (5 ECTS/unbenotet)

Modulbezeichnung: **Modern Methods in Mass Spectrometry (MaSpec)** **5 ECTS**
(Modern Methods in Mass Spectrometry)

Modulverantwortliche/r: Thomas Drewello
Lehrende: Thomas Drewello

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Modern Methods in Mass Spectrometry (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Thomas Drewello)

Empfohlene Voraussetzungen:

The course builds on the master module "Applied Spectroscopy" (Compulsory Module Physical Chemistry)

Inhalt:

- Advanced aspects of Soft Ionization methods (MALDI, ESI, related Atmospheric Pressure Ionization methods)
- Advanced aspects of mass analyzers (FT-ICR, orbitrap, hybrids: multi sector, BEqQ, QToF, QIT-ToF)
- Ion Activation (CID, BIRD, IRMPD, SID, ECID)
- Applications (thermochemistry, kinetic method, equilibrium methods, ion/molecule-reactions)
- "Omics" (proteomics, petroleomics, metabolomics)
- Further applications: ¹⁴C dating, accelerator MS, stable isotope MS, MS in space, ICP-MS.
- Seminars in form of problem solving classes

Lernziele und Kompetenzen:

Students ...

- gain insight into the different ion formation processes
- are able to decide on an ionization method for a given compound class
- are able to evaluate the use of different mass spectrometers
- gain understanding of ion activation processes in the gas phase

Literatur:

- Jürgen H. Groß: "Mass Spectrometry, a textbook" Springer, Heidelberg
- Edmond De Hoffmann: "Mass Spectrometry, principles and applications", Wiley

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Modern Methods in Mass Spectrometry (Prüfungsnummer: 65641)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100% Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: keine Angabe

1. Prüfer: Thomas Drewello

Organisatorisches:

Please note:

- Students have to register for the module (check registration periods)

- Information available on studon

Bemerkungen:

Module compatibility:

- Lecture module as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: Modern X-ray Structure Determination (MXD) **5 ECTS**
(Modern X-ray Structure Determination)

Modulverantwortliche/r: Frank Wilhelm Heinemann

Lehrende: Frank Wilhelm Heinemann

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Modern X-ray structure determination of single crystals (SS 2022, Vorlesung mit Übung, 3 SWS, Frank Wilhelm Heinemann)

Inhalt:

- Fundamentals of crystallization and polymorphism
- Structural description of single crystals, crystal systems, unit cell, symmetry and symmetry elements, space groups
- Diffraction power of crystals, diffraction conditions, structure factor
- Generation of X-rays, single crystal diffractometers, detection techniques
- Structure solution techniques and refinement procedures, software, problems and pitfalls, interpretation of results
- Anomalous dispersion and absolute structure
- Graphical representations, use of data bases

Lernziele und Kompetenzen:

Students ...

- get insight into thermodynamics of crystallization and crystallization techniques
- get fundamentals of the theory behind crystal structure determination
- get practice in crystal selection, mounting and measurement set-up
- get hands-on training in structure solution and refinement using up-to-date software
- are enabled to interpret and compare results of a single crystal structure determination

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Modern X-ray Structure Determination (Prüfungsnummer: 65581)

Prüfungsleistung, Übungsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Lab report in manuscript style (max. 2000 words plus raw data); module is ungraded, but has to be passed!

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: Frank Wilhelm Heinemann

Organisatorisches:

- Module can be taken in winter or in summer term
- Module will be taught in presence and/or online
- Students have to register for the module examination (check registration periods)
- Information/registration available on studon XXXXXXXX

Bemerkungen:

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: **Neurotech: Physics and Chemistry of Neuromodulation Technologies (Neurotech)** **5 ECTS**
 (Neurotech: Physics and Chemistry of Neuromodulation Technologies)

Modulverantwortliche/r: Danijela Gregurec
 Lehrende: Danijela Gregurec

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Neurotech: Physics and Chemistry of Neuromodulation Technologies (SS 2022, Vorlesung mit Übung, 3 SWS, Danijela Gregurec)

Inhalt:

- Introduction to neuromodulation technologies (definition, history, nervous anatomy, stimulation targets-ion channels, action potential)
- Imaging and spectroscopic concepts (MRI, EEG, Calcium imaging, electrophysiology)
- Current tech and principles (Invasive and noninvasive approaches, Deep brain stimulation, Transcranial magnetic stimulation, Pain management, BMI summary)
- Organic materials and approaches (viral vectors, optogenetics, Chemogenetics (DREED))
- Micro- and macroscale materials (Mechanical properties and compatibility of neural implants, Electrodes (Utah arrays, Neuralink. . .), Flexible electrodes, Optical fibers)
- Nanomaterials (Nanomaterial properties leveraged for neuromodulation (Importance of surface chemistry in bio(nano)materials, Quantum confinement and quantum dots, Plasmons and photothermal neuromodulation, Magnetism, Magnetolectric particles for electric stimulation, Magnetic nanoparticles for magnetothermal and magnetomechanical stimulation)

Lernziele und Kompetenzen:

Students will gain the knowledge, skills, and competences to be able to ...

- understand biophysical aspects of neuronal signaling and its correlation to cognition and behavior.
- learn physical foundations, biological concepts, and chemical approaches crucial for materials used in neuromodulation and neurotechnology.
- apply acquired knowledge to realize design criteria of technology that governs the modulation of neuronal signaling.

Literatur:

- Knotkova, Rasche; Springer-Verlag New York (2015) *Textbook of Neuromodulation: Principles, Methods and Clinical Applications*
- Luan et al, Front Neuroeng 7 (2014) *Neuromodulation: present and emerging methods*
- Frank, et al, Nat Biotech 37 (2019) *Next-generation interfaces for studying neural function*
- Chen et al, Nat Rev Mat 2 (2017) *Neural recording and modulation technologies*

**Literature will be updated with leading peer-reviewed papers during lectures*

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Neurotech: Physics and Chemistry of Neuromodulation Technologies (Prüfungsnummer: 65351)

Studienleistung, mündliche Prüfung, Dauer (in Minuten): 20

weitere Erläuterungen:

Oral examination (20 minutes, ungraded) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstabledung: SS 2022, 1. Wdh.: SS 2022

1. Prüfer: Danijela Gregurec

Organisatorisches:

Please note:

- The Neurotech-module starts only in summer term!
- Students have to register for the module examination (check registration periods on MeinCampus)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- Lecture module within the Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: **Organic thin films (OTF)** **5 ECTS**
 (Organic thin films)

Modulverantwortliche/r: Rainer Fink
 Lehrende: Rainer Fink

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Organic Thin Films (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Rainer Fink)
 Seminar Organic thin films (WS 2021/2022, Seminar, 1 SWS, Rainer Fink)

Inhalt:

- Molecular interactions and molecular self-organization
- Influence of molecular geometry and functionalization
- Thin film preparation techniques: Langmuir-Blodgett, Self-Assembled Monolayers (SAMs), other solvent-based techniques (e.g. spin-casting, doctor blading, etc.), vacuum sublimation
- Analytical techniques, in-situ analysis
- Effect of templates
- Organic thin film applications
- Seminars will be based on recent literature

Lernziele und Kompetenzen:

Students

- get insight into the major preparation techniques of organic thin films
- are able to evaluate to prepare organic thin film specimens
- know to analyse thin film specimens with respect to structural and electronic properties
- are aware of recent studies and modern applications of organic thin films

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Organic thin films (Prüfungsnummer: 65451)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral examination (20 minutes) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablesung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Rainer Fink

Organisatorisches:

Please note:

- Module will be taught only in winter term
- Students have to register for the module (check registration periods)
- Registration/further information available via **StudOn**

Bemerkungen:

Module compability:

- lecture module can be taken as part of the Elective Module!

Modulbezeichnung: Quantum Chemistry I (QuantCh-1) **5 ECTS**
(Quantum Chemistry I)

Modulverantwortliche/r: Andreas Görling

Lehrende: Andreas Görling

Startsemester: WS 2021/2022

Dauer: 1 Semester

Turnus: jährlich (WS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry 1 (WS 2021/2022, Vorlesung mit Übung, Andreas Görling et al.)

Empfohlene Voraussetzungen:

Required Qualifications:

- good knowledge of basic quantum mechanics: axioms of QM, application to simple systems (particle in a box, harmonic oscillator, rigid rotator)
- good knowledge in mathematics: differential calculus of functions of several variables, linear algebra

Inhalt:

- Mathematical concepts and current research issues in the field of quantum and computer chemistry
- Hartree-Fock, DFT

Lernziele und Kompetenzen:

Students ...

- obtain sound knowledge in basic methods of quantum chemistry
- are able to solve mathematical problems occurring in quantum chemistry
- are able to understand and assess scientific reports in the field of quantum chemistry

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Data Science (Master of Science)", "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Quantum Chemistry 1 (Prüfungsnummer: 65591)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral Examination (20 minutes, not graded: pass/fail) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Andreas Görling

Organisatorisches:

- The elective module "Quantum Chemistry I" will be taught only in winter term!
- Students have to register for this module (check registration periods)!

- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)

Modulbezeichnung: Quantum Chemistry II (QuantCh-2) 5 ECTS
 (Quantum Chemistry II)

Modulverantwortliche/r: Andreas Görling
 Lehrende: Andreas Görling

Startsemester: SS 2022	Dauer: 1 Semester	Turnus: jährlich (SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry 2 (SS 2022, Vorlesung mit Übung, 3 SWS, Andreas Görling)

Es wird empfohlen, folgende Module zu absolvieren, bevor dieses Modul belegt wird:

Quantum Chemistry I

Inhalt:

- Many-Body Perturbation Theory
- Configuration Interaction, Second Quantization, Coupled Cluster
- TD-HF, TD-DFT, RPA

Lernziele und Kompetenzen:

Students ...

- obtain sound knowledge in advanced methods of quantum chemistry
- are able to solve mathematical problems occurring in quantum chemistry
- are able to understand and assess scientific reports in the field of quantum chemistry

Literatur:

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

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Data Science (Master of Science)", "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Quantum Chemistry 2 (Prüfungsnummer: 65611)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral Examination (20 minutes, not graded: pass/fail) or alternative examination according to FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: Andreas Görling

Organisatorisches:

- The elective module "Quantum Chemistry II" will be taught only in summer term!
- Students have to register for this module (check registration periods)!
- Registration/further information via StudOn!

Bemerkungen:

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded) if **Quantum Chemistry I** was already chosen as Elective Module!

Modulbezeichnung: **Scientific Programming (ScP)** **5 ECTS**
 (Scientific Programming)

Modulverantwortliche/r: Andreas Görling

Lehrende: Christian Neiß

Startsemester: WS 2021/2022

Dauer: 2 Semester

Turnus: jährlich (WS)

Präsenzzeit: 150 Std.

Eigenstudium: k.A. Std.

Sprache: Englisch

Lehrveranstaltungen:

Quantum Chemistry - Lab / Scientific Programming (WS 2021/2022, Seminar, 5 SWS, Christian Neiß et al.)

Quantum Chemistry - Lab / Scientific Programming (SS 2022, Seminar, 5 SWS, Christian Neiß et al.)

Inhalt:

- Operating system Linux for high-performance computing (HPC)
- Scientific programming in Fortran and Python
- Using numerical and mathematical libraries/modules
- Introduction to parallel computing
- Exercises
- Programming project

Lernziele und Kompetenzen:

Students

- get familiar with Linux as operating system for HPC
- are able to create computer programs for scientific purposes
- can use numerical and mathematical libraries/modules in home-made programs
- obtain knowledge about basic parallelization paradigms

Literatur:

- Stephen J. Chapman: Fortran for Scientists and Engineers, McGraw Hill 2017 (4th ed.)
- Bernd Klein: Einführung in Python 3, Hanser 2017 (3rd ed.)
- Stefan Gerlach: Computerphysik, Springer Spektrum 2019 (2nd ed.)

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Data Science (Master of Science)", "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Scientific Programming (Prüfungsnummer: 65561)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

PL: Successful implementation of the programming project (working program), ungraded - module has to be passed

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: keine Angabe

1. Prüfer: Andreas Görling

Organisatorisches:

Please note:

- The module starts only in winter term! (Duration: 2 semesters)

- Students have to register for the module
- Registration / further information via StudOn

Bemerkungen:

Module compatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded) - please note: the module cannot be combined with the module **Quantum Chemistry - Lab**

Modulbezeichnung: Symmetry and Group Theory (SGT) (Symmetry and Group Theory)	5 ECTS
Modulverantwortliche/r: Jörg Libuda	
Lehrende: u. Mitarbeiter, Jörg Libuda	
Startsemester: WS 2021/2022	Dauer: 1 Semester
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.
	Turnus: jährlich (WS)
	Sprache: Englisch

Lehrveranstaltungen:

Seminar Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (WS 2021/2022, Seminar, 1 SWS, Jörg Libuda et al.)

Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Jörg Libuda)

Inhalt:

- Symmetry of Molecules (symmetry elements, operations, point groups, notations)
- Symmetry of Crystals, Surfaces and Interfaces (symmetry in 1, 2 and 3 dimensional periodic structures, lattices, crystal classes, space groups)
- Compact Course Group Theory (elements group theory, definitions, reducible and irreducible representations, orthogonality theorem, character tables)
- Group Theory and Quantum Mechanics (representations, operators and symmetry, matrix elements, direct product functions, projection operators)
- Symmetry of Organic Molecules: From Electronic Structure to Reactivity (symmetry adaption, cyclic groups, many electron systems, electronic transitions, configuration interaction, symmetry controlled reactions)
- Symmetry in Anorganic Chemistry: From Atoms to Complexes (MO models, transition metal complexes, direct product groups, rotation inversion group, angular momentum coupling, crystal field splitting, vibronically allowed transitions)
- Symmetry and Spectroscopy: Vibrational Spectroscopies (analysis of vibrational modes, normal coordinate analysis, symmetry of vibrational wave functions, vibrational spectroscopy, selection rules)
- Symmetry in Crystal Physics: Tensor Description of Physical Properties (tensors, axial, polar, representations, transformation properties, intrinsic symmetry, Neumann's principle, Curie's principle)
- Symmetry and Electronic Structure of Solids: Band Structures (translation group and irreps, reciprocal lattice, k-space, Bloch functions, Brillouin zones, symmetry of bands)

Lernziele und Kompetenzen:

Students

- acquire detailed understanding how to use symmetry properties and the mathematical tools of group theory in a broad range of application fields in chemistry, physics and materials science.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Symmetry and Group Theory (Prüfungsnummer: 65461)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral Examination (20 minutes) or alternativ examination according to FAU Corona Statutes, Date by agreement

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Jörg Libuda

Organisatorisches:

- lecture module will be taught **online** (synchronous)
- lecture module will be offered only in winter term
- Students have to register for the module (check registration periods)
- Registration/further information via **StudOn**

Bemerkungen:

Module compability:

- lecture module can be taken as part of the Elective module (5 ECTS, not graded)

Modulbezeichnung: Theory of Surface Phenomena (TheoSurf) 5 ECTS
(Theory of Surface Phenomena)

Modulverantwortliche/r: Bernd Meyer
Lehrende: Bernd Meyer

Startsemester: SS 2022 Dauer: 1 Semester Turnus: jährlich (SS)
Präsenzzeit: 45 Std. Eigenstudium: 105 Std. Sprache: Englisch

Lehrveranstaltungen:

Theory of Surface Phenomena / Theorie der Oberflächenphänomene (SS 2022, Vorlesung mit Übung, 3 SWS, Bernd Meyer)

Empfohlene Voraussetzungen:

Basic knowledge of quantum mechanics and quantum chemical calculations is strongly recommended

Inhalt:

- Brief introduction into quantum-chemical methods for surface science studies
- Introduction of basic nomenclature of how to describe the atomic and electronic structure of surfaces
- Basic concepts on how to understand the electronic properties of metal, semiconductor and insulator surfaces, such as surface states, dangling bonds, passivation, charge neutralization with respect to polar and nonpolar surfaces
- Thermodynamic analysis of the stability of surface structures; surface phase diagrams
- Methods for calculating STM and AFM data to support the analysis of experimental data from local probe measurements

Lernziele und Kompetenzen:

The students ...

- are familiar with the most common theoretical and experimental techniques for surface science studies
- have a sound knowledge in basic principles governing surface structure and reactivity
- can perform first quantum chemical calculations on their own and interpret the data

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | Wahlmodule)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Theory of Surface Phenomena (Prüfungsnummer: 65571)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: SS 2022

1. Prüfer: Bernd Meyer

Organisatorisches:

Please note:

- Lecture is taught only in summer term
- Registration for module examination (please check registration periods on meinCampus)
- Registration/Information via Studon

Bemerkungen:

Module compatibility:

- Elective module (5 ECTS, ungraded) within the M.Sc. degree programme Chemistry or M.Sc. Molecular Science (especially Molecular **NANO**science)

Modulbezeichnung: **Self-Assembly (Assembly)** **5 ECTS**
 (Self-Assembly)

Modulverantwortliche/r: Franziska Gröhn
 Lehrende: Franziska Gröhn

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: jährlich (WS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Self-Assembly: Molecular, Particulate and Hybrid Nanostructures (WS 2021/2022, Vorlesung, 2 SWS, Franziska Gröhn)
 Seminar Self-Assembly: Molecular, Particulate and Hybrid Nanostructures (WS 2021/2022, Seminar, 1 SWS, Franziska Gröhn)

Inhalt:

- Inspired by Mother Nature: Designing Structures on the Nanoscale
- Molecular Templates for Inorganic Nanostructures, Organic-Inorganic Hybrid Structures
- Self-Assembly of Amphiphilic Molecules
- Non-Covalent Interactions for Assembly and Particle Stabilization
- Characterization Tools for Nanoparticles, Polymers and Assemblies in Solution
- Dynamic Light Scattering
- The Form Factor as Key to Particle Shape: SAXS, SANS and Static Light Scattering
- Supramolecular Architectures through Combinations of Non-Covalent Interactions
- Electrostatic Self-Assembly
- Switchable Supramolecular Nanostructures: Light, pH- and Temperature Responsivity
- Molecular and Hybrid Nano-Assemblies for Catalysis, Solar Energy Conversion and Drug Delivery

Lernziele und Kompetenzen:

Students ...

- gain insight into structural design concepts on the nanoscale
- are able to evaluate the interplay of non-covalent interactions
- know how to approach the analysis of complex nanostructures in solution
- are aware of recent studies and applications of switchable and functional nano-assemblies

Literatur:

- Recent literature
- D. F. Evans, H. Wennerström: The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet, 2nd Edition, Wiley 1999
- O. Glatter: Scattering Methods and their Application in Colloid and Interface Science, Elsevier 2018

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | Wahlmodule)

Studien-/Prüfungsleistungen:

Self-assembly: molecular, particulate and hybrid nanostructures (Prüfungsnummer: 65651)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20 (PL): Oral examination (20 minutes) or alternative examination according FAU Corona Statutes!

Examination is ungraded, but must be passed!

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2022/2023

1. Prüfer: Franziska Gröhn

Organisatorisches:

Please note:

- Module will may be taught in presence or online (synchronous)- please check information on StudOn shortly before the start of the module!
- Students have to register for the module (check registration periods)
- Information available on StudOn: Link see below!

Bemerkungen:

Module compatibility:

- as Elective Module in MSc Chemistry, 5 ECTS/not graded

Modulbezeichnung: **Research Module Inorganic chemistry (IC-R-Lab)** **15 ECTS**
(Research Module Inorganic chemistry)

Modulverantwortliche/r: Karsten Meyer

Lehrende: Romano Dorta, Sjoerd Harder, Nicolai Burzlaff, Karsten Meyer, Die Dozenten der Anorg. Chemie

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 345 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Research lab course (23 SWS) in one of the work groups of Inorganic Chemistry

- Attendance at lab course is compulsory!
- Attendance at safety instructions is compulsory!
- Attendance in winter or summer term possible!
- A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Research module IC (SS 2022, Praktikum, 23 SWS, Anwesenheitspflicht, Die Dozenten der Anorg. Chemie)

Inhalt:

- practical laboratory experience aiming at introducing students to current and state of the art inorganic research topics
- work experience in a team of researchers
- establishing fundamental knowledge required for addressing individual molecular research problems at a state of the art level
- independent and self-driven approach to problem solving in an assigned research project

Lernziele und Kompetenzen:

The students

- apply acquired fundamental knowledge and practical skills to an individual research problem that they work on independently
 - manage and apply the fundamental safety regulations important to handling hazardous compounds and instruct other coworkers in relevant safety topics
 - rank their own research results in the context of current literature and research papers in the field and record their results in appropriate scientific writing and documentation style
 - give oral and written presentations of the results and acquired knowledge in an appropriate scientific style in English language
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] Chemistry (Master of Science)

(Po-Vers. 2020w | Forschungsmodul)

Studien-/Prüfungsleistungen:

Forschungsmodul Inorganic Chemistry (Prüfungsnummer: 65511)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Lab(PL): graded lab protocol of approx. 25 pages plus raw data documentation

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: IC-Lab (N70010)

Organisatorisches:

- Students have to register for the module examination on MeinCampus (check registration periods)!

- Lab course is held as an in-class-course
- Lab course can be chosen in winter or summer term
- Time and place by appointment (in one of the involved working groups of Inorganic chemistry), please contact the supervisor directly

Bemerkungen:

Please note:

- Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Inorganic Chemistry

Modulbezeichnung: **Research Module Organic Chemistry (OC-R-Lab)** **15 ECTS**
(Research Module Organic chemistry)

Modulverantwortliche/r: Andreas Hirsch

Lehrende: Andreas Hirsch, Henry Dube, Jürgen Schatz, Andriy Mokhir, Svetlana Tsogoeva, Norbert Jux, Dozenten der Organischen Chemie

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 345 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Research lab course (23 SWS) in one of the work groups of Organic Chemistry

- Attendance at lab course is compulsory!
 - Attendance at safety instructions is compulsory!
 - Attendance in winter or summer term possible!
 - A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de
- Research module OC (SS 2022, Praktikum, 23 SWS, Anwesenheitspflicht, Henry Dube et al.)

Inhalt:

- Integration of students in an actual research group
- self-organization of a research project both in theory and practice
- planning of experiments in order to prove (or reject) a given hypothesis

Lernziele und Kompetenzen:

The students are capable

- to use their theoretical and practical background to make an individual contribution to an independent, actual and realistic research project
- to provide a state-of-the-art documentation and discussion of results obtained as a member of a research team
- to present, communicate and discuss scientific results with experts in English.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Forschungsmodul)

Studien-/Prüfungsleistungen:

Forschungsmodul Organic Chemistry (Prüfungsnummer: 65521)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

Lab(PL): graded lab protocol of approx. 25 pages plus raw data documentation

Prüfungssprache: Englisch

Erstablingung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: OC (N70011)

Organisatorisches:

Please note:

- Students have to register for the module examination on MeinCampus (check registration periods)
- Lab course is held as an in-class-course
- Lab Course can be chosen in winter or summer term
- Time and place by appointment (in one of the involved working groups of Organic chemistry), please contact the supervisor directly

Bemerkungen:

Please note:

- Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Organic Chemistry

Modulbezeichnung: **Research Module Physical chemistry (PC-R-Lab)** **15 ECTS**
 (Research Module Physical chemistry)

Modulverantwortliche/r: Hans-Peter Steinrück

Lehrende: Dirk M. Guldi, Hans-Peter Steinrück, u. a. Hochschullehrer

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 225 Std.

Eigenstudium: 225 Std.

Sprache: Englisch

Lehrveranstaltungen:

Research project in Physical Chemistry (ca. 23 SWS/LAB) full time in a work group of the student's choice at a research group in Physical Chemistry

- Attendance at lab course is compulsory!
 - Attendance at safety instructions is compulsory!
 - Attendance in winter or summer term possible!
 - A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de
- Research module PC (SS 2022, Praktikum, 23 SWS, Anwesenheitspflicht, Dirk M. Guldi et al.)
-

Inhalt:

Research project in Physical Chemistry, lasting 6 weeks (ca. 15 SWS/LAB) full time in a work group of the student's choice at a research group in Physical Chemistry at the Department of Chemistry and Pharmacy (Attendance in lab course is compulsory!)

- introduction to the current issues of research in the field of Physical Chemistry
- integration in research group and instruction in scientific work
- familiarisation in fundamental concepts within a special subject of Physical Chemistry - to the limits of science
- finding answers to open questions in research project by means of experimental work

Lernziele und Kompetenzen:

Students

- apply and transfer knowledge acquired during their studies to handle and solve open questions in research project
 - interpret experimental data independently
 - compare and evaluate results with literature data
 - illustrate data in meaningful graphs
 - present and discuss scientific results referring to literature in verbal and written form
-

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Forschungsmodul)

Studien-/Prüfungsleistungen:

Forschungsmodul Physical Chemistry (Prüfungsnummer: 65531)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

LAB (PL): graded lab protocol of approx. 20 pages plus raw data documentation

Prüfungssprache: Englisch

Erstblegung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: PC-R-Lab (N70013)

Organisatorisches:

Please note:

- Students have to register for the module on MeinCampus (check registration periods)

- Lab course is held as an in-class-course
- Lab Course can be chosen in winter or summer term
- Time and place by appointment (in one of the involved working groups of Physical chemistry), please contact the supervisor directly

Bemerkungen:

Please note:

- Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Physical Chemistry

Modulbezeichnung: **Research Module Quantum Chemistry (QC-R-Lab)** **15 ECTS**
(Research Module Quantum Chemistry)

Modulverantwortliche/r: Andreas Görling

Lehrende: Dozenten, Dirk Zahn, Andreas Görling

Startsemester: SS 2022

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Präsenzzeit: 345 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Research lab course (23 SWS) in one of the work groups of Quantum Chemistry

- Attendance at lab course is compulsory!
- Attendance at safety instructions is compulsory!
- Attendance in winter or summer term possible!
- A valid laboratory insurance is mandatory for participation in the lab course - see: www.laborversicherung.de

Research Module QC (SS 2022, Praktikum, 23 SWS, Anwesenheitspflicht, Andreas Görling et al.)

Inhalt:

- Practical introduction to current and state- of- the- art research topics in the field of quantum and computer chemistry
- Integration into a research group
- Guided work on a current research project using the methods of quantum and computer chemistry
- Attempts to solve independently a scientific problem

Lernziele und Kompetenzen:

Students

- apply and transfer knowledge acquired during their studies to handle and solve open questions in research projects in quantum and computer chemistry
- put their own research results in relation to current literature and research papers in the field, and record their results in appropriate scientific writing and documentation style
- present their own results and acquired knowledge in an appropriate scientific style in English language

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science)**

(Po-Vers. 2020w | Forschungsmodul)

Studien-/Prüfungsleistungen:

Forschungsmodul Quantum Chemistry (Prüfungsnummer: 65541)

Prüfungsleistung, Praktikumsleistung

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

LAB (PL): graded lab protocol of approx. 20 pages plus raw data documentation

Prüfungssprache: Englisch

Erstablesung: SS 2022, 1. Wdh.: WS 2022/2023

1. Prüfer: QC-R-Lab (N70014)

Organisatorisches:

- Students have to register for the module (check registration periods)!
- Lab course is held as an in-class-course
- Lab course can be chosen in winter or summer term
- Time and place by appointment (in one of the involved working groups of Quantum chemistry), please contact the supervisor directly

Bemerkungen:

Please note:

- Research lab project (ca. 8 weeks: 21SWS LAB/2SWS Seminar) full time in a work group of the student's choice in Quantum Chemistry

Modulbezeichnung: Masterarbeit (Master's thesis)

30 ECTS

Modulverantwortliche/r Rainer Fink, Betreuer

Sprache: Englisch

Dauer: 1 Semester

Turnus: halbjährlich (WS+SS)

Empfohlene Voraussetzungen:

Prerequisites: Admission to the M. Sc. program Chemistry, successfully passed core modules, mandatory elective, elective and research modules

Inhalt:

Syllabus Outline:

Written elaboration in form of a scientific manuscript with a length of approx. 20,000 words. It describes the scientific findings as well as the way leading to these findings. It contains justifications for decisions regarding chosen methods for the thesis and discarded alternatives. The student's own substantial contribution to the achieved results has to be evident. In addition, the student presents his work in a seminar, in which the scientific quality and the scientific independence of his achievements are evaluated.

Lernziele und Kompetenzen:

Educational goals and Learning outcome:

Students

- demonstrate their ability to perform independent scientific work focusing on an adequately challenging research topic.
- rank their own research results in the context of current literature and research papers in the field and record their results in appropriate scientific writing and documentation style.
- give oral and written presentations of the results and acquired knowledge in an appropriate scientific style in English language.

Bemerkung:

Assessment and examinations:

Thesis (3 hard copies in bound form + electronic version) with a length of approx. 20,000 words;
Referee report, 2 experts

Calculation of the grade for the module:

Averaged grade of the two reports

Organisatorisches:

Workload: 900 h

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science): 4. Semester**

(Po-Vers. 2020w | Masterarbeit)