Description of the degree program

Artificial Intelligence for Molecular Sciences (Master)

PO 1

Date: 08.01.2026

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Foundations

Title	Introduction to AIMS		
Number	1498110 AM-P-1	**Module version**	
Shorttext		**Language**	english
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	Institut für Physikal. und Theoretische Chemie
Hours per Week / ECTS	3 / 5,0	**Module owner**	Prof. Dr. Christoph Jacob
Workload (h)	150		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination			
Course achievement	presentation (Referat, SL)		

Contents

Lecture Series: introduction to research data in molecular sciences: molecular representations, protein structure data, spectroscopic data, genomic databases, proteomics and other -omics data; research data management in different fields of the molecular sciences.
Seminar: student presentations of current topics and challenges related to artificial intelligence in molecular sciences (chemistry, pharmacy, biology)

Objective qualification

Students have an overview of current topics and challenges in the research field "Artificial Intelligence in Molecular Sciences". They are familiar with different types of research data generated in the molecular sciences and are able to carry out simple analyses of such data sets. They are familiar with the methods and tools of research data management in the molecular sciences.

Literature

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**

Introduction to AIMS		Lecture	english
Introduction to AIMS		Seminar	english

Title	Mathematics for Engineers A		
Number	1294250	**Module version**	V2
Shorttext	MAT-STD7-25	**Language**	english
Frequency of offer	only in the winter term	**Teaching unit**	Carl-Friedrich-Gauß-Fakultät
Module duration	1	**Institution**	Institut für Partielle Differentialgleichungen
Hours per Week / ECTS	6 / 8,0	**Module owner**	Studiendekan der Mathematik
Workload (h)	240		
Class attendance (h)	112	**Self studying (h)**	128
Compulsory requirements			
Expected performance/ Type of examination	1 written exam (180 minutes) After approval by the examination board mathematics (Prüfungsausschuss Mathematik), the examiner can also choose the take-home exam as the form of examination.		
Course achievement			

Contents

Mathematics for engineering students A (Calculus 1)
1 sequences and limit: definitions and concepts, e.g. monotony and bounds, convergence criteria of comparison and of monotony, typical limits, Euler's number e, accumulation point, limit superior, Bachmann-Landau notation, supremum, Cauchy sequence, basic properties of real numbers
2 series: convergence and absolute convergence, geometric, harmonic and exponential series, comparison test, ratio test, root test, alternating series test with proofs
3 functions: concepts, standard functions including hyperbolic and area functions, relation to trigonometric functions, inverse function, rational functions and partial fraction decomposition, graphical representation
4 limits of functions and continuity: definition, properties of continuous functions, classification of discontinuities, intermediate value theorem, extreme value theorem with proof
5 differentiation: difference and differential quotient, C^n-spaces and norms, product and chain rule, derivatives of standard functions, derivatives of inverse functions, mean value theorem, de l'Hospital's rule with proof, extreme values, curvature Taylor polynomials and series
6 integration: definit and indefinit integral (Riemann), fundamental theorem of calculus with proof, integration by parts, integration by substitution, integrals of standard functions, integrals of rational functions and power series, improper integrals, Gamma-unction

Mathematics for engineering students A (Linear Algebra)
1 algebraic structures: number domains, group, field, modulo, complex numbers, cartesian and polar form, Euler's identity, roots of complex numbers, polynomial division, linear factor decomposition, fundamental theorem of algebra without proof
2 vectors and vector spaces: linear independence, sub-space, basis, dimension, norm, scalar product, projection, ortho-normal basis, Cauchy Schwarz inequality
3 linear maps and matrices: definition of general linear maps, kernel, image, rank, inverse matrix, transposition, determinant, matrix norm
4 Gaussian algorithm: trapezoid form, underdetermined systems and parameter-dependent solutions, inverse matrix
5 eigenvalues and eigenvectors: diagonalizable matrices, eigenvalues and -vectors of symmetric matrices, Jordan form, similarity
6 vectors in geometry: lines and planes, Hesse normal form, vector product, triple product, transformation of coordinates

Objective qualification
The students combine the learnt mathematical methods of univariate calculus and linear algebra in the description and investigation of applied problems in the engineering sciences. They choose appropriate calculation techniques and appropriate methods of proof for the discussion of the mathematical fundamentals in the applied and engineering sciences, and they apply these techniques and methods. The students explain the formation of mathematical concepts and they derive the motivation of these concepts from applications and from the mathematical specification and delimitation of terms and definitions. The students reproduce and explain basic proofs and ideas of proofs in univariate calculus and linear algebra. They are able to identify and to test relations between the learnt concepts. The students are able to analyse mathematical problems occurring in applications and engineering lectures, to extract and to solve treatable sub-problems and to identify continuative difficulties. Finally, students use constructively modern tools for the treatment of computational problems.
Literature
Text books and lecture notes on calculus, linear algebra, mathematics for engineers, e.g. * Burg, Haf, Wille, Meister: Höhere Mathematik für Ingenieure, Band I & II, SpringerVieweg * Ansorge, Oberle, Rothe, Sonar: Mathematik in den Ingenieur- und Naturwissenschaften, Band I, Wiley * Langemann, Sommer: So einfach ist Mathematik, zwölf Herausforderungen im ersten Semester, SpringerSpektrum

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Related courses
Rules for the choice of courses
You can attend lectures in German or English. Participation in the small exercises is voluntary.
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Mathematics for Engineers A (Analysis 1)	1,0	Exercise	german
Mathematics for Engineers A (Analysis 1)	1,0	Exercise, small group	german
	2,0	Lecture/Exercise	german
	1,0	Exercise, small group	german
	2,0	Lecture/Exercise	english
	1,0	Exercise	english
	1,0	Exercise, small group	english
	2,0	Lecture/Exercise	english
	1,0	Exercise	english
	1,0	Exercise, small group	english

Mathematics for Engineers A (Linear Algebra)	1,0	Exercise	german
Mathematics for Engineers A (Linear Algebra)	2,0	Lecture/Exercise	german
Mathematics for Engineers	6,0	Lecture/Exercise	english german

Title	Programming in Python and Python Lab		
Number	1498130 AM-P-3	**Module version**	
Shorttext		**Language**	english
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswis-senschaften
Module duration	1 Semester	**Institution**	Institut für Physikal. und Theoretische Chemie
Hours per Week / ECTS	5 / 8,0	**Module owner**	Prof. Dr. Christoph Jacob
Workload (h)	240 h		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examina-tion			
Course achievement	team-based development and documentation of a data science software tool (Comp-Prog, SL)		

Contents

Programming in Python: This seminar covers an introduction to Python. The most important functionali-ties are presented, including matplotlib, numpy, scipy, and pandas. The planning, execution, documentation, and deposition of programming projects is explained.

Python Lab:
- Introduction to explorative data analysis in Python
- Statistical data analysis
- Unsupervised machine learning
- Supervised machine learning
- Critical assessment of machine learning

Objective qualification

After successful completion of this module, students will have the competence to apply Py-thon for desi-gning and implementing small to medium software projects and analytic workflows with a focus on statistics and machine learning. During an interactive learning phase during which the students will be able to apply common packages such as scikit-learn, and they will be able to syn-thesize analysis workflows for diverse data science questions. These workflows will be presented and discussed in a mini-conference among the students. After the mini-conference, students will form small teams to develop data science software tools which will be presented during the closing event. They will gain the competence to critically evaluate machine learning workflows.

Literature

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
Python Lab	4,0	Internship	english
	1,0	Colloquium	english
Programming in Python	1,0	Course	english

Title	Scientific Software Engineering – Lab		
Number	3325000040 AM-P-4	**Module version**	
Shorttext	AM-P-4	**Language**	english
Frequency of offer		**Teaching unit**	Fakultät Architektur, Bauingenieurwesen und Umweltwissenschaften
Module duration	1	**Institution**	Institut für rechnergestützte Modellierung im Bauingenieurwesen
Hours per Week / ECTS	/ 5,0	**Module owner**	
Workload (h)	150 h		
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements			
Recommended requirements	Algorithms & Programming (Lab)		
Expected performance/ Type of examination	written exam (60 min) or oral exam (30 min)		
Course achievement	Homework according to examiners specificatoins		
Contents			
Software Design Principles, Design Patterns, Software Quality Metrics, Agile Software Development, Test Driven Development (TDD)			
Objective qualification			
Students will be able to develop sustainable software solutions in the scientific contexts for moderately complex engineering problems using advanced design and implementation approaches. Furthermore, they will be able to evaluate software designs with respect to various quality aspects and to make independent design decisions and implement corresponding solutions.			
Literature			
Lecture script, scientific papers, books			

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
	4,0	Laboratory	english

Advanced Area

Title	Machine Learning for Data Science		
Number	4229000050	**Module version**	
Shorttext		**Language**	english german
Frequency of offer	irregular	**Teaching unit**	Carl-Friedrich-Gauß-Fakultät
Module duration	1	**Institution**	
Hours per Week / ECTS	3 / 5,0	**Module owner**	Prof. Dr. Michel Besserve
Workload (h)	150		
Class attendance (h)	42	**Self studying (h)**	108
Compulsory requirements			
Recommended requirements	The lectures and exercises require a good command of the knowledge from Bachelor level “Linear Algebra” and “Analysis” courses, and a background knowledge on probability theory and the python programming language is recommended.		
Expected performance/ Type of examination	1 examination: written exam, 90 minutes or oral exam, 30 minutes or take-home exam		
Course achievement	1 academic achievement: 50% of the exercises must be passed		

Contents

- Supervised Learning Algorithms
- Model Selection
- Unsupervised Learning Algorithms
- Deep Neural network architectures for data science
- Self-supervised learning and foundation models
- Uses and limitations of ML in data science projects

Objective qualification

After successfully completing this module, students should be able to
- understand and correctly apply basic concepts of machine learning algorithm design,
- master elementary tools for analyzing the performance of machine learning approaches,
- identify the most suited ML approaches for a particular application.

Literature

- Machine Learning, A Probabilistic Perspective, Murphy, 2012
- Deep Learning, Goodfellow et al., 2016
- Mathematics for Machine Learning, Deisenroth et al., 2020

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Machine Learning for Data Science	3,0	Lecture/Exercise	english

Title	Pattern Recognition		
Number	2424690	**Module version**	
Shorttext	ET-NT-69	**Language**	
Frequency of offer	every term	**Teaching unit**	Fakultät für Elektrotechnik, Informationstechnik, Physik
Module duration	1	**Institution**	Institut für Nachrichtentechnik
Hours per Week / ECTS	4 / 5,0	**Module owner**	Prof. Dr. Tim Fingscheidt
Workload (h)	150		
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements			
Expected performance/ Type of examination	Oral exam 30 min. or written exam 90 min.		
Course achievement			

Contents

- Bayesian decision rule
- Quality metrics in pattern recognition
- Supervised learning with parametric distributions
- Supervised learning with non-parametric distributions, classification
- Linear discriminant functions, single-layer perceptron
- Support vector machines (SVMs)
- Multi-layer perceptron, neural networks (NNs)
- Deep learning
- Unsupervised learning, clustering methods

Note: For pattern recognition using hidden Markov models (HMMs), a separate more in-depth module, Spoken Language Processing (ET-NT-68), is offered in the summer semester.

Objective qualification

Upon completion of this module, students gain fundamental knowledge about methods and algorithms for classification of data. They are capable to select the appropriate means for real-world problems, to design a solution and to evaluate it.

Literature

- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001
- C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006

Remark

Basic knowledge of statistics, such as acquired in the module "Probability Theory and Statistics", facilitates the understanding of the lecture.

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
	2,0	Lecture	english german
Literature			
- R. O. Duda, P. E. Hart, D. G. Stork: Pattern Classification, Wiley, 2001 - C. M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006			
	2,0	Seminar	english german
Literature			
- Vorlesungsfolien - R. O. Duda, P. E. Hart, D. G. Stork: Pattern Classification, Wiley, 2001 - C. M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006			

Title	Computer Lab Pattern Recognition		
Number	2424000020	**Module version**	
Shorttext		**Language**	
Frequency of offer	every term	**Teaching unit**	Fakultät für Elektrotechnik, Informationstechnik, Physik
Module duration	1	**Institution**	Institut für Nachrichtentechnik
Hours per Week / ECTS	4 / 5,0	**Module owner**	Prof. Dr. Tim Fingscheidt
Workload (h)			
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements			
Expected performance/ Type of examination			
Course achievement			

Contents

The course consists of hands-on programming tasks that are solved by the participants and subsequently evaluated in a semi-automated way. In total, seven units from the sub-fields (i) basics of hands-on application of machine learning methods, (ii) image processing (computer vision) and (iii) time series analysis have to be completed. The seven units are:

- Interactive introduction to Python fundamentals using Jupyter notebooks, fundamentals of data processing, preparation and visualization.
- Use of single-layer machine learning models to solve a two-class problem: Support vector machines (based on libsvm) and neural networks. Splitting and use of datasets, application of appropriate metrics for evaluation, use of high-level machine learning libraries such as Sci-Kit-Learn
- Use of deep neural networks to solve a multi-class classification problem, introduction to recognized academic datasets such as MNIST and CIFAR-10, introduction to the use of deep learning libraries PyTorch and Tensorflow, usage and adaptation of pre-trained models
- Use of convolutional neural networks to solve more challenging image processing problems such as semantic segmentation and depth estimation, use of regularization methods in training
- Use of diverse cost functions to optimize neural networks, implementation of generative models such as Generative Adversarial Networks (GANs)
- Use of recurrent neural networks to solve problems based on time series data, application of concepts for anomaly detection
- Use of recurrent neural networks for speech processing, e.g., for noise reduction, analysis of neural networks with respect to their complexity (FLOPs, number of parameters)

Six out of the seven units have to be successfully passed for the entire computer lab module to be passed, among these unit 4 (convolutional neural networks) and unit 7 (recurrent neural networks in speech processing).

Objective qualification

In this course, students acquire the competencies to independently select and apply appropriate machine learning and deep learning methods for complex problems. The students ...

- ... master the programming language Python as well as the basics of the deep learning libraries PyTorch and Tensorflow.
- ... evaluate the effectiveness of simple machine learning models and neuronal networks for classification and regression problems.
- ... evaluate the quality of deep learning models on appropriate data (sub)sets with meaningful metrics
- ... know and use different types of neural networks for problems in the areas of image processing, time series processing and generative problems
- ... know and use different strategies for data preprocessing and data augmentation
- ... know and use different training and regularization methods for the optimization of neural networks
- ... evaluate the complexity of a neural network on the basis of various parameters

Literature

- Christopher M. Bishop, Nasser M. Nasrabadi, “Pattern Recognition and Machine Learning”, Springer 2006
- Ian Goodfellow, Yoshua Bengio, Aaron Courville, “Deep Learning”, MIT Press 2016

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Computer Lab Pattern Recognition	3,0	Internship	english german

Literature

- Christopher M. Bishop, Nasser M. Nasrabadi, “Pattern Recognition and Machine Learning”, Springer 2006
- Ian Goodfellow, Yoshua Bengio, Aaron Courville, “Deep Learning”, MIT Press 2016

Name of the course	SWS	Eventtype	Language
Computer Lab Pattern Recognition	1,0	Colloquium	english german

Literature

- Christopher M. Bishop, Nasser M. Nasrabadi, “Pattern Recognition and Machine Learning”, Springer 2006
- Ian Goodfellow, Yoshua Bengio, Aaron Courville, “Deep Learning”, MIT Press 2016

Title	Deep Learning Lab		
Number	2424750	**Module version**	
Shorttext	ET-NT-75	**Language**	english german
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Elektrotechnik, Informationstechnik, Physik
Module duration	1	**Institution**	
Hours per Week / ECTS	4 / 5,0	**Module owner**	Prof. Dr. Tim Fingscheidt
Workload (h)	150		
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements			
Expected performance/ Type of examination			
Course achievement			

Contents
Objective qualification
Literature
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016

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Related courses
Rules for the choice of courses
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
	3,0	Internship	german

Literature
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016

	1,0	Colloquium	german

Literature

- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001 - C.M. Bishop: Pattern Recognition and Machine Learning, Springer, 2006 - I. Goodfellow, Y. Bengio, A. Courville: Deep Learning, MIT Press, 2016

Title	Methods of Uncertainty Analysis and Quantification		
Number	2540420 AM-V-5	**Module version**	
Shorttext	AM-V-5	**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Maschinen-bau
Module duration	1	**Institution**	
Hours per Week / ECTS	3 / 5,0	**Module owner**	Prof. Dr. Sabine Langer
Workload (h)	150		
Class attendance (h)	42	**Self studying (h)**	108
Compulsory requirements			
Recommended requirements	Basic knowledge of the finite element method, numerical procedures for quadrature and polynomial approximation as well as probability theory and statistics are helpful. Attending the course "Unsicherheiten in technischen Systemen" is not a requirement.		
Expected performance/ Type of examina-tion	1 examination element: Written exam (90 min) or oral exam (30 min)		
Course achievement			

Contents

Probability and random variables, advanced Monte Carlo methods, stochastic quadrature, stochastic spectral methods, global sensitivity analysis, data-driven uncertainty quantification

Objective qualification

Students can formulate and name elementary rules of probability theory and different ways to describe probability distributions. They can model technical/physical systems in a stochastic way using random variables. The students are further able to apply Monte Carlo and stochastic spectral methods to quantify uncertainties and also to assess the impact and propagation of uncertainties in models through global sensitivity analysis. Moreover, they are able to evaluate the numerical efficiency of the aforementioned methods. The students are also able to outline the principles of data-driven approaches to uncertainty analysis.

Literature

- O. Le Maitre, O.M. Knio: Spectral Methods for Uncertainty Quantification, Springer Netherlands, 2010
- D. Xiu: Numerical Methods for Stochastic Computations: A Spectral Method Approach, Princeton University Press, 2010
- G. J. Lord, C.E. Powell, T. Shardlow: An introduction to computational stochastic PDEs, Cambridge University Press, 2014

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
	2,0	Lecture	english
	1,0	Exercise	english

Profile Area Chemical Synthesis And Drug Design

Title	Reaction Mechanisms		
Number	1498570 AM-A-1	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	3 / 4,0	**Module owner**	Prof. Dr. Christopher Teskey
Workload (h)	120		
Class attendance (h)	42	**Self studying (h)**	78
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	oral or written exam (PL) nach BPO §5 (3)		
Course achievement	none		
Module grade composition	see expected performance		

Contents

Lecture: Orbitals and stereochemistry, enolate chemistry, radical reactions, photochemical reactions, pericyclic reactions, rearrangements, transition metal-catalyzed cross-coupling, C-H activation, metathesis, organocatalysis, photoredox catalysis, methods to elucidate reaction mechanisms, kinetics of organic chemical reactions.
Exercise: Deepening and consolidating the material presented in the lecture, working on exercises.

Objective qualification

The students understand the chemical reactivity of organic molecules and are able to apply chemical reactions specifically to modify molecules. They are able to formulate and classify the underlying organic chemical reaction mechanisms. With their help, they are able to make mean-ingful statements about the success of planned reaction paths from the starting molecule to the target molecule and to explain the main and by-products. The students know methods to explain reaction mechanisms and can assess and discuss their range of application and significance.

Literature

information in the courses

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Related courses			
Rules for the choice of courses			
none			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
Reaction mechanisms	2,0	Lecture	english
Reaction mechanisms	1,0	Exercise	english

Title	Organometallic Chemistry		
Number	1498590 AM-A-2	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswis-senschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	3 / 4,0	**Module owner**	Prof. Dr. Matthias Tamm
Workload (h)	120		
Class attendance (h)	42	**Self studying (h)**	78
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examina-tion	Oral or Written Exam		
Course achievement	none		
Module grade composition	see expected performance		
Contents			
Lecture: Coordination chemistry of transition metals, central atoms and ligand types, coordination numbers, geometries of complexes, bonding in transition metal complexes (valence bond theory, crystal field theory, molecular orbital theory), isolobal principle, carbonyl complexes, substitution and redox reactions, transi-tion metal hydrides and dihydrogen complexes, iso(valence)-electronic ligands to CO, metal-alkyl comple-xes, catalytic elementary reactions (oxidative addition, reductive elimina-tion, insertions, hydride eliminati-ons), catalytic processes (hydroformylation, acetic acid preparation, olefin polymerization, hydrogenations, Wacker process), carbene (alkylidene) and carbyne (alkyli-dyne) complexes, olefin and alkyne metathesis, complexes with #-ligands (olefin, alkyne, allyl, cy-clopentadienyl, arene complexes), sandwich compounds, spectroscopic methods for structure eluci-dation in organometallic chemistry (IR, NMR), occurrence and biological functions of inorganic ele-ments, especially the trace elements Co, Fe, Cu and Zn, cobalamins, hemoproteins, FeS clusters and non-heme iron, copper and zinc proteins. **Exercise:** Consolidation of the lecture material by examples and exercises, exam preparation			
Objective qualification			
Students will master advanced concepts in the chemistry of metals, coordination chemistry, and organo-metallic chemistry. They understand the role of metals in nature and are familiar with the fun-damentals of bioinorganic and bioorganometallic chemistry. They can discuss and predict the struc-ture and properties of metal complexes using modern bonding concepts and have knowledge of the use of transition metal com-plexes in industrial processes. They know the principles of homogeneous and heterogeneous catalysis and are able to combine important elementary reactions into catalytic cycles and formulate them.			
Literature			
information in the courses			

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Related courses
Rules for the choice of courses
none
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Organometallic Chemistry	2,0	Lecture	english
Organometallic Chemistry	1,0	Exercise	english

Title	Catalysis		
Number	1498750 AM-A-3	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Marc Walter
Workload (h)	150		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	Lab work (PL, expA, 25% of overall module mark) Lectures: oral or written exam according to BPO §5 (3) (PL, 75% of overall module mark)		
Course achievement	none		
Module grade composition	see expected performance		

Contents

Lecture Applied homogeneous catalysis: Societal relevance, metal-organic basics of catalysis, elementary reactions, catalytic cycles, industrial applications (Wacker process, acetic acid preparation, hydroformylation, hydrocyanation, hydrogenation, carbonylations, oligomerisati-on and polymerization of olefins and dienes, copolymerization of CO and olefins), recent developments (C-C cross-couplings, CH activation and functionalization, oxidation reactions, asymmetric catalysis, alkane, olefin and alkyne metathesis), contributions of homogeneous catalysis to sustainable and resource-efficient development of chemistry, elucidation of reaction mechanisms.
Lecture Applied Heterogeneous Catalysis and Catalytic Polymer Syntheses: Fundamentals of heterogeneous catalysis, adsorption and kinetics, theoretical concepts, preparation and characterization of catalysts, deactivation, mass transfer, reactors for catalysts, in-dustrial catalysis, polymerization with transition metal complexes, Ziegler-Natta polymerization, Phil-lips catalysts, metallocene and postmetallocene catalysts, metathesis polymerizations.
Practical course: Work on two projects; a) synthesis, characterization and use of a catalyst in homogeneous catalysis; b) synthesis of a polymer by metal catalysis.

Objective qualification

The students master the basic principles of homogeneous catalysis and the differentiation to heterogeneous catalysis and can confidently apply the underlying elementary reactions to catalytic processes. They have an overview of the most important metal-catalyzed industrial processes as well as of current developments and modern aspects of catalysis research. The students are familiar with methods of metal-catalyzed polymer synthesis and are able to evaluate and discuss the advantages of these methods compared to classical non-catalytic methods. They are familiar with methods for the characterization of polymers as well as their fields of application and are able to evaluate these methods.

Literature

information in the courses

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Related courses
Rules for the choice of courses
none
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Applied homogeneous catalysis	2,0	Lecture	german
Applied heterogeneous catalysis and catalytic polymer synthesis	2,0	Lecture	german
Lab Course metal catalysis	2,0	Internship	german

Title	Advanced Inorganic Chemistry		
Number	1499710 AM-A-4	**Module version**	
Shorttext		**Language**	english german
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Martin Bröring
Workload (h)	240		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	Presentation (PL, 25 % of overall module grade) Oral Exam or Written Exam (PL, 75 % of overall module grade) nach BPO §5 (3)		
Course achievement	none		
Module grade composition	see expected performance		

Contents

The module offers a versatile selection of topics, which are treated in a balanced way in lectures and exercises and prepare the students for independent research activities. The lecture block ‚Advanced Inorganic Chemistry‘ is composed of two of the following components, which change annually:
Lecture Modern Aspects of Coordination Chemistry: Ligand Field Theory: Strong field approach, weak field approach, atomic terms, correlation diagrams, interpretation of optical transitions, molecular magnetism, spin-only formula, orbital moments, orbital moment cancellation, spin-orbit coupling, trends in 3d and 4f elements, spin crossover, spin dynamics, magnetic communication, super-exchange, spin polarisation, spin delocalisation, double exchange, high spin molecules, zero field splitting, magnetic tunnelling, non-innocence, spectroscopy.
Lecture Supramolecular Coordination Chemistry: Classes of non-covalent interactions, energetics, dynamic and static behaviour, ordering principles, networks, MOFs (Metal Organic Frameworks), co-ordination polymers, brick-and-mortar processes, complex-as-ligand approach, molecules-to-materials, solvothermal syntheses, template syntheses, stacked compounds, surface functionalisation, aurophilicity as a control tool, nanostructuring.
Lecture Bioinorganic Model Systems: Historical overview of metalloproteins, mechanistic models, biogenic ligands, classification of model systems (speculative model, structural model, functional model), biological and chemical modelling, bioisomorphic substitution, site-specific mutagenesis, model com-plexes for iron sequestration, hydrolases, light collection, oxygen management, electron transfer, ni-trogen cycle, hydrogenases.
Lecture Synthesis of Inorganic Molecular Compounds: Symmetry, structure and bonding properties of molecules, hydrides of elements, polyhedral boranes and carboranes, silanes and hydrosilylation, car-bene, alkene and alkyne analogues of main group elements (element-element multiple bonds), coordination numbers > 4 for main group elements (hypervalency), Supramolecular chemistry (weak inter-actions), inorganic rings, chains and clusters, elementorganic compounds in organic synthesis and catalysis, frustrated Lewis acid-base pairs, modern methods for functionalisation of main group elements.
Lecture Structural Chemistry: History, overview of general methods for structure determination, description and models, ionic compounds (Madelung constants, radii quotients), sphere packing as a structural fea-

ture (Hume-Rothery and Laves phases, alloys), polyhedra as a structural feature, sym-metry as an ordering principle (group-subgroup relationships, phase transformations), physical properties of solids.
Lecture Chemistry of the f-elements: History; occurrence and separation; physical and chemical properties; differentiation from d-transition metals and s-block elements; chemical binding and role of f-orbitals; magnetism; current developments in coordination and organic metal chemistry; applications in technology, medicine, organic synthesis and small molecule activation.
Seminar: Recording, evaluation and processing of EPR and Mössbauer spectra as well as magnetic measurements on selected paramagnets; interpretation of the electronic structures in the synopsis of all the measurement data obtained; recording of the results and presentation in lecture form.

Objective qualification

The students are able to specifically build up inorganic molecular compounds and structures and to interpret and modify them with regard to their structure-activity relationships. Their understanding of the function of inorganic compounds in the biosphere as well as in supramolecular aggregates allows the students to discuss novel model compounds, switches, magnets and catalysts based on main group- and transition metals. Unusual structural and bonding relationships are competently evaluated. Students also have knowledge of interpreting and modelling spectra of paramagnetic compounds, and apply these independently.

Literature

information in the courses

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Related courses

Rules for the choice of courses

The following courses must be taken:
- Lectures with a minimum of 4 SWS
- Seminar Analysis of Paramagnetic Compounds **or** Seminar Practical X-Ray Structure Analysis

!The Seminar Analysis of Paramagnetic Compounds can only be taken in combination with the lecture “Modern Aspects of Coordination Chemistry!

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Molecular Main Group Chemistry	2,0	Lecture	english german
Pigments of Life	2,0	Lecture	english
Structural Chemistry	2,0	Lecture	english
Bioinorganic Model Systems	2,0	Lecture	english
Modern Aspects of Coordination Chemistry	2,0	Lecture	english
Paramagnetic Compunds	2,0	Seminar	english german
Seminar Paramagnets	2,0	Seminar	english

Title	Organic Synthesis Planning		
Number	1499160 AM-A-5	**Module version**	
Shorttext		**Language**	english
Frequency of offer	irregular	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	3 / 4,0	**Module owner**	Prof. Dr. Thomas Lindel
Workload (h)	120		
Class attendance (h)	42	**Self studying (h)**	78
Compulsory requirements	keine		
Recommended requirements	none		
Expected performance/ Type of examination	oral or written exam (PL)		
Course achievement	none		
Module grade composition	see expected performance		

Contents

Lecture: Reaction databases, retrosynthesis, functional group conversions, chemoselectivity, protecting group chemistry, atom-economic synthesis, multi-step sequences, biomimetic synthesis, natural product synthesis, current examples from the literature.

Objective qualification

Based on database-assisted retrosynthetic analysis, students are able to propose multi-step synthesis sequences for complex organic compounds, especially for natural and active ingredients.

Literature

information in the courses

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Related courses

Rules for the choice of courses

none

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Organic Synthesis Planning	2,0	Lecture	english

Organic Synthesis Planning	1,0	Exercise	english

Title	Enzyme Engineering		
Number	1601250 AM-A-6	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	9 / 10,0	**Module owner**	Prof. Dr. Anett Schallmey
Workload (h)	300 h		
Class attendance (h)	148 h	**Self studying (h)**	162 h
Compulsory requirements			
Recommended requirements	Participants need to have basic knowledge in molecular biology/genetics and protein biochemistry.		
Expected performance/ Type of examination	Oral examination (50 min) or written exam (200 min) according to BPO §5 (3)		
Course achievement	Practical Exercise including experimental work.		
Module grade composition	Oral examination or written exam (PL) according to BPO §5 (3). Examination: 90 min. written exam or 25 min. oral exam.		

Contents

(en)
Lecture: General principles and methods for enzyme engineering via protein design and directed evolution using literature examples; introduction of computational tools for identification of mutational hotspots; discussion of different genetic methods for the generation of mutant libraries and suitable assay systems for library screening.
Practical exercise: Promoting a deeper understanding of lecture contents, application of selected computational tools for enzyme engineering, practical skills for generating and screening mutant libraries.

Objective qualification

The students know different genetic and bioinformatics methods for targeted adaptation of enzyme-specific characteristics via enzyme engineering. Starting from the amino acid sequence of an enzyme, they are able to predict mutational hotspots using computational tools, to generate corresponding mutant libraries, and to select suitable assay systems for library screening.
After completing the module, students will be able to
- explain various genetic and bioinformatic methods for the targeted modification of enzyme-specific properties.
- select suitable mutations based on the amino acid sequence of an enzyme to improve a desired enzyme property using digital tools.
- practically create mutant libraries using molecular biology methods.
- select and practically apply suitable assay systems for screening mutant libraries.
- carry out computer-aided modelling.

- assess the presentation of scientific results (protocols) of others in the context of a peer review.

Literature

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Attendance is compulsory for the practical exercise.			
Name of the course	**SWS**	**Eventtype**	**Language**
Enzyme Engineering (Bt-MM 11, Bt-MB 12, AM-A-6, CM-A-5)	2,0	Lecture	german
Enzyme Engineering (Bt-MM 11, Bt-MB 12, AM-A-6, CM-A-5)	7,0	Practical exercise	english

Title	Fundamentals of Protein Structure Analysis		
Number	1399640 AM-A-7	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	9 / 10,0	**Module owner**	Prof. Dr. Wulf Blankenfeldt
Workload (h)	300		
Class attendance (h)	126	**Self studying (h)**	174
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	written exam (ca. 200 min.)		
Course achievement	- experimental work - successful participation in the seminar - presentation (45 minutes in groups or two or three students)		

Contents

Lecture:
Protein structures, common principles of protein structures, methods in structural biology, protein crystallization, characterization of crystals, X-ray diffraction data collection, the phase problem and its solutions, model building and refinement, interpretation of protein structures.

Practical course:
Protein crystallization, X-ray diffraction data collection, protein structure analysis (molecular replacement), model building, refinement and validation, protein structure analysis and interpretation.

Seminar:
Recent publications in structural biology.

Objective qualification

After completing this module students will be able to
- name forces that lead to the formation of the stable three-dimensional structures of proteins.
- name methods that can be used to determine three-dimensional structures and to explain their underlying physical principles.
- name the most important steps in structure determination with crystallographic methods and to explain their background.
- judge the quality of published protein structures.
- suggest subsequent experiments that utilize the information contained in three-dimensional structures.
- plan scientific projects in the field of structural biology.
- grasp the content of scientific publications in the field of structural biology.
- critically analyze the content of scientific publications in the field of structura biology.
- search, present and discuss relevant scientific content.
- contribute to controversial discussions of scientific topics.

Literature

- Rupp, Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology, Garland Science
- Rhodes, Crystallography Made Crystal Clear, Academic Press
- Klostermeier & Rudolph, Biophysical Chemistry, CRC Press

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, Bt-MM 05, AM-A-7)	1,0	Lecture	english
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, AM-A-7)		Seminar	english
Fundamentals of Protein Structure Analysis (Bio-BB 22, Bio-SB 22, Bt-MM 05, AM-A-7)		Internship	

Title	Biomolecular Modelling		
Number	1499680 AM-A-8	**Module version**	
Shorttext		**Language**	english
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Christoph Jacob
Workload (h)	240		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	Oral or written exam+ (30% of the practical work mark are taken into account in the overall module mark)		
Course achievement	Practical work (marked)		
Module grade composition	see expected performance		

Contents

Lecture: Introduction to the basics of simulations of biomacromolecules - BornOppenheimer approximation, potential energy surface, basics of statistical thermodynamics, empirical force fields and their efficient implementation - geometry optimization, molecular dynamics methods, thermodynamic and static description of (bio)chemical processes, analysis of molecular dynamics simulations, calculation of free energies, multiscale simulation methods - implicit solvent models, coarsegrained models, hybrid QM/MM methods, quantum-chemical embedding methods.
Computer Lab: Use of force field programs, visualization of crystal structures, geometry optimization, molecular dynamics and normal mode analysis of polypeptides, simulation of (bio)molecules) with different computational methods and their analysis, analysis of dynamical and entropic effects.
Project Lab: Molecular Dynamics Simulations of Biomolecules.

Objective qualification

The students are familiar with modern methods for modelling the structure of biomacromolecules and for simulating their thermodynamic properties. The know empirical force field methods, methods for performing molecular dynamics simulations, as well as modern multicale simulation methods. The students are able to judge the applicability and the limitations of such methods, to choose suitable simulation methods for their own research projects and to perform, analyze, and evaluate molecular dynamics simulations.

Literature

information in the courses

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Related courses

Rules for the choice of courses

none

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Biomolecular Modelling	2,0	Lecture	english german
Computer Lab Biomolecular Modelling	2,0	Exercise	english german
Project Lab Biomolecular Modelling	2,0	Internship	english

Title	Advanced Theoretical Chemistry		
Number	1499170 AM-A-9	**Module version**	
Shorttext		**Language**	english
Frequency of offer	irregular	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Christoph Jacob
Workload (h)	240		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements			
Expected performance/ Type of examination	Oral or Written Exam+ (20% of the coursework and 20% of the practical work mark are taken into account in the overall module mark)		
Course achievement	Solve coursework problems (umarked) Practical work (marked)		

Contents

Lecture and Computer Lab Advanced Quantum Chemistry: Mathematical Foundations of quantum-chemical methods, Hartree-Fock theory, perturbati-on theory and configuration interaction, coupled-cluster theory, density-functional theory.

Lecture and Computer Lab Theoretical Spectroscopy: Time-dependent quantum mechanics, interaction of electromagnetic radiation with molecules, basics of Hartree-Fock and density-functional theory, quantum-chemical calculation of spectroscopic data (Infrared and Raman spectroscopy, UV/Vis spectroscopy, ESR and NMR, simulati-on of spectra.

Lecture and Computer Lab Artificial Molecular Intelligence: Molecular quantum mechanics in a nutshell: Hartree–Fock (HF) theory, post-HF methods, density functional theory; Molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantifi-cation, active learning; Applications: structure–property relationships, chemical space exploration, molecular design.

Project Lab Theoretical Biophysical Chemistry: Introduction to scientific programming and in-depth study of selected quantum-chemical methods. Application of quantum-chemical methods that usually cannot be used as "black-box" methods in own independet projects.

Objective qualification

The students have aquired knowledge on modern methods of quantum chemistry. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the limits of different quantum-chemical methods and to use choose suita-ble methods for their own research projects, to perform quantum-chemical calculations and to analyse, evaluate, and assess their results.

Literature

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Related courses
Rules for the choice of courses
To complete the module one out of the three lectures and the associated excercise must be completes as well as the project lab. One of the three lectures and the associated excercise is offered every winter term. The project lab is offered every winter term.
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Advanced Quantum Chemistry	3,0	Lecture	english german
Computer Lab Advanced Quantum Chemistry	1,0	Exercise	english
Project Lab Advanced Quantum Chemistry	2,0	Internship	english

Title	Machine Learning in Computational Chemistry		
Number	1499180 AM-A-10	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Jonny Proppe
Workload (h)	240 h		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements			
Expected performance/ Type of examination	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
Course achievement	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		
Contents			
Lecture and Computer Lab Artificial Molecular Intelligence: Molecular quantum mechanics in a nutshell: Hartree–Fock (HF) theory, post-HF methods, density functional theory; molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantification, active learning; Applications: structure–property relationships, chemical space exploration, molecular design. **Project Lab:** In-depth study of molecular machine learning methods, application of methods of artificial molecular intelligence in own independent projects.			
Objective qualification			
The students have acquired knowledge on modern methods of molecular machine learning and molecular artificial intelligence. They are familiar with the foundations of important methods and possess an overview of commonly used methods, their implementation, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose and apply suitable methods for their own research projects and to analyse, evaluate, and assess their results.			
Literature			

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**

Machine Learning in Computational Chemistry	3,0	Lecture	english
Computer Lab Machine Learning in Computational Chemistry	1,0	Exercise	english
Project Lab Machine Learning in Computational Chemistry	2,0	Internship	english

Title	Research Lab Chemical Synthesis and Drug Design		
Number	1499230 AM-A-RP	**Module version**	
Shorttext		**Language**	english
Frequency of offer	every term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	/	**Module owner**	Prof. Dr. Marc Walter
Workload (h)	360 - 510		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	study research project including report and presentation (StA)		
Course achievement			

Contents
Research Lab: Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points. **Seminar:** Participation in scientific colloquia, presentation and discussion of current research results
Objective qualification
Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.
Literature

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Related courses			
Rules for the choice of courses			
the number of credit points assigned for this module depends on the duration of the research project: 13 LP = 390 h 14 LP = 420 h 15 LP = 450 h 16 LP = 480 h 17 LP = 510 h			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**

Research Lab Chemical Synthesis and Drug Design		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

Profile Area Spectroscopy and Imaging

Title	Molecular Spectroscopy		
Number	1498560 AM-B-1	**Module version**	1
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswis-senschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	4 / 5,0	**Module owner**	Prof. Dr. Peter Jomo Walla
Workload (h)	150		
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements	none		
Expected performance/ Type of examina-tion	Oral exam or written exam (PL) nach BPO §5 (3)		
Course achievement	Completing Exercises (SL)		

Contents

Lecture: Introduction to quantum mechanical description of chemical bonding, transition dipole moment and density. Selection rules, symmetry of orbitals, theory of atomic and molecular spec-tra, modern experimen-tal techniques in spectroscopy (UV-VIS spectroscopy, fluorescence spec-troscopy, IR, Raman and nonli-near spectroscopy).

Excersise: Reinforcement and consolidating the material presented in the lecture, working on exercises.

Objective qualification

Students understand the concept of chemical bonding on a quantum chemical basis and are able to explain the structure of molecules. They understand the influence of alternating elec-tromagnetic fields on atoms and molecules and are able to make independent quantitative state-ments about the absorption and emis-sion of light using transition dipole moments and densities. They will have a thorough theoretical understan-ding of the spectroscopic properties of atoms and molecules and of modern spectroscopic techniques, and will be able to plan and evaluate their use to determine molecular structures.

Literature

Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
Molecular Spectroscopy	3,0	Lecture	english
Exercise Molecular Spectroscopy	1,0	Exercise	english

Title	Biophysical Chemistry		
Number	1498670 AM-B-2	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	4 / 8,0	**Module owner**	Prof. Dr. Peter Jomo Walla
Workload (h)	240		
Class attendance (h)	66	**Self studying (h)**	174
Compulsory requirements			
Expected performance/ Type of examination	oral exam or written exam (PL) nach BPO §5 (3)		
Course achievement	completing exercises (SL)		

Contents

Lecture Biophysical Chemistry: Brief review of biochemical and microbiological basics, traditional methods such as fluorescence and absorption spectroscopy, light scattering, Raman spectroscopy, NMR, ESR and mass spectrometry on biomolecules. Modern methods such as fluorescence mi-croscopy, single molecule detection, nonlinear and ultrafast spectroscopy or nanotechnology to study biomolecules. Prospects for industrial applications and drug discovery.

Exercise: Independent calculation and answering of questions with corrections by instructors and assistants, discussion of solution methods in the exercise.

Applied Biophysical Chemisty: In this course, the knowledge gained will be deepened through guest lectures on concrete examples of industrial research, e.g. in combination with an excursion to a pharmaceutical company, or from basic research, e.g. at Max Planck Institutes.

Objective qualification

The students know the basics of the most important physicochemical methods for the elucida-tion of biomolecular interactions and structures and are able to decide which modern or traditional method is most efficient to answer such biochemical questions. They know the limitations and dy-namic range of these methods and the importance of structure and dynamics of biomolecules for their function. Students will be able to classify which methods are suitable for studying biomolecules and answering biomolecular questions in the different environments of industrial or basic research.

Literature

Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Biophysical Chemistry	3,0	Lecture	english german
Biophysical Chemistry	1,0	Exercise	english german
Applied Biophysical Chemistry	0,7	Seminar	english german

Title	Modern Optical Methods and Imaging		
Number	1499190 AM-B-3	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	0 / 8,0	**Module owner**	Prof. Dr. Peter Jomo Walla
Workload (h)	240 h		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination			
Course achievement			
Contents			
Objective qualification			
Literature			

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**
Modern Optical Methods and Imaging	2,0	Lecture	english
	1,0	Exercise	english
Modern Optical Methods and Imaging - Lecture/Demonstration/Course Microscopy	1,0	Lecture	english

Title	Solar and Chemical Energy Conversion		
Number	1497800 AM-B-4	**Module version**	
Shorttext		**Language**	
Frequency of offer	irregular	**Teaching unit**	Fakultät für Lebenswis-senschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	8 / 8,0	**Module owner**	Prof. Dr. Stefanie Tschierlei
Workload (h)	240		
Class attendance (h)	112	**Self studying (h)**	128
Compulsory requirements			
Expected performance/ Type of examina-tion	Oral exam (marked, 30 minutes) or written exam (marked, 90 minutes)		
Course achievement	Practical work including written report and oral exam (unmarked)		

Contents

Selected Aspects of Energy Conversion: The lecture covers fundamental areas of physical chemistry (such as thermodynamics, transport processes, fluid mechanics, electrochemistry) and connects them with the main renewable energies (biomass, wind, thermosolar, photovoltaic) and their conversion, transport and storage techniques. The lecture may have different emphases: Hydrogen applications, fuel cells, chemical energy storage, hydrogen economics, natural and artificial light harvesting systems.

Molecular design: Artificial intelligence and data science methods will be intro-duced, in particular machine learning, sequential optimization, and inverse design. It will be dis-cussed how these methods can be app-lied in a fully automated fashion to design functional molecules and materials on a computer. The search for reactive species and catalysts for the activation of small molecules such as CO_2 and N_2 defines the focus of this lecture.

Artificial Photosynthesis and CO_2 Activation: Introduction and working principle of molecular photosensiti-zers and catalysts, mechanisms of electron and energy transfer processes, artificial photosynthesis, solar fuels, molecular water splitting and CO_2 activation, photoelectro-chemistry, structure-activity relationships.

Spectroscopic Methods: Methods for the investigation of light-driven processes and the activation of CO2, time-resolved and stationary spectroscopy (e.g. X-ray, UV/vis, IR, Raman), spectroelectrochemistry, spectra evaluation using theory, overview of current spectra analysis methods.

Practical course: Work on a practical project related to the respective lecture or seminar content.

Objective qualification

Students will be enabled to understand and competently discuss current research and application areas of solar and chemical energy conversion. They will further be enabled to recognize the in-teractions and syner-gies of the topics represented and to establish interdisciplinary references. Finally, the students are able to read scientific publications in the field of solar and chemical energy conversion and to classify and evaluate experiments and calculations described therein.

Literature

Wird über Stud.IP vor Vorlesungsbeginn bekannt gegeben.

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Related courses

Rules for the choice of courses

Choose from a-d with a combined workload of 240 h / 8 CP:

a) Selected aspects of energy conversion (2 LP)
b) Molecular design + Lab course on molecular design (1 + 2 LP)
c) Artificial photosynthesis and CO_2 activation + Lab course on artificial photosynthesis (2 + 1 LP)
d) Spectroscopic Methods + Lab course on spectroscopic methods (1 + 2 LP)

Note: It is recommended to attend the lab courses associated with the selected theoretical courses. A lab course can only be completed in combination with the corresponding lecture.

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Selected aspects of energy conversion	2,0	Lecture	english german
Molecular Design	1,0	Lecture	english german
Lab Course on Molecular Design	2,0	Internship	english german
Artificial photosynthesis and CO_2 activation	2,0	Lecture	english german
Lab course on artificial photosynthesis	1,0	Internship	english german
Spectroscopic Methods	1,0	Lecture	english german
Lab course on spectroscopic methods	2,0	Internship	english german

Title	Physical Biology of the Cell		
Number	1398890 AM-B-5	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1 Semester	**Institution**	
Hours per Week / ECTS	8 / 10,0	**Module owner**	Prof. Dr. Christian Sieben
Workload (h)	300		
Class attendance (h)	112 h	**Self studying (h)**	188 h
Compulsory requirements	none		
Recommended requirements	uccessfully finished modules Bio-IB 21 or Bio-IB 23		
Expected performance/ Type of examination	- Seminar presentation (1, ca. 15 min) - Course report (1)		
Course achievement	- Experimental work in the practical course - Successfull participation in exercise and seminar		

Contents

Lecture: Students get practical-oriented insights into the field of cell biophysics. The lecture series provides a broad overview of various topics in quantitative biology and cell biophysics. At the beginning, basic concepts, scales and principles of cellular organization (tissue, cells, organelles) will be considered. In addition, the cellular components and their properties are discussed not only biochemically, but also from a biophysical perspective (e.g. polymers such as DNA or the cytoskeleton). In addition, topics such as membranes, diffusion, electrophysiology, structural biology as well as mechanics and kinetics of cell biological processes are covered in depth. A biophysical approach will be chosen in order to understand and predict processes using models. In order to provide a practical perspective, examples from primary literature will be presented alongside content from textbooks. In particular, topics from cell and infection biology will be used.

Practical course: Cell biological processes such as diffusion, cell mobility and the cell cycle are investigated using various model systems. Both bacteria and mammalian cells will be examined using various spectroscopic and microscopic methods. The students should plan, carry out and analyze their experiments themselves. The protocols should be prepared in the form of a short publications according to scientific standards.
Seminar: During the seminar, students will present and compare both classical (seminal papers) and current
publications. We will compare the scientific methods in both cases in order to give students the opportunity to recognize the appeal of a classical (historical) approach as well.

Exercise: During the exercise, students will work through a publication independently in preparation for the upcoming lecture.

Objective qualification

After completing the module, students will be able to
- Understand fundamental orders of magnitude of cellular processes and from this develop their own intuition
towards the measurable framework in which biological processes take place.
- understand basic terms and concepts of biophysics in cellular and molecular biological systems.

- develop interdisciplinary approaches to specific experimental problems from the quantitative methods learned in
cell biophysics.
- deal intensively with data analysis up to the generation of computer models. Apply quantitative methods to cell
biological preparations, analyze structures and kinetics and make predictions based on biophysical models.
- measure and analyze the function of specific cellular components.
- document, analyze and critically discuss their own results

Literature

• Phillips, R., Kondev, J., Theriot, J., Garcia, H.G. and Orme, N., 2012. Physical biology of the cell. Garland Science
• Bornschlögl, T. and Dietz, H., Biophysik in der Zelle
• Aktuelle Publikationen aus der Zell- und Infektionsbiologie, Biophysik in englischer Sprache (Zur Vorlesung und den Seminarvorträgen)

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	2,0	Lecture	english german
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	1,0	Seminar	english
Physical Biology of the Cell (Bio-ZB 26, Bio-ZN 32, Bt-MZ 05, AM-B-5)	5,0	Internship	english german

Title	Sophisticated Imaging		
Number	1301260 AM-B-6	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	10 / 10,0	**Module owner**	Manfred Rohde
Workload (h)	300		
Class attendance (h)	140	**Self studying (h)**	160
Compulsory requirements			
Expected performance/ Type of examination	- Seminar presentation (1, approx. 20 min) and lab report (1) - The report summarizes the background (from the lecture) and the results of the practical work during the internship		
Course achievement	- Experimental work in the practical course - succeccfull participation in seminar The lecture conveys all contents that are important for the successful completion of the practical course including the protocol.		
Contents			

Lecture: The lecture series provides an overview of the most important imaging and analysis methods in the life
sciences. The physical basics of these techniques as well as many application examples from infection biology are
taught. One focus is on the presentation of light and electron-optical methods and the corresponding sample preparation. In particular, fluorescence microscopy, confocal microscopy, super-resolution microscopy and high-resolution transmission (TEM) and field emission scanning electron microscopy (FESEM) are covered. In LM, a strong focus is placed on live cell imaging for tracking dynamic processes, as well as the various super-resolution microscopy methods and their areas of application. FESEM and TEM are treated as the methods that allow us to penetrate into the submicroscopic range. Special applications such as the immuno-gold detection of proteins as well as recent developments in the field of cryo-EM will be presented. In addition to visualization methods, the lecture will also cover the acquisition, evaluation and further processing of images and films in order to show which methods are suitable or unsuitable for further processing of images taken with fluorescence and confocal microscopy and to optimize the quality of the images without violating current good scientific practice with regard to image processing. In addition to these techniques, laser dissection microscopy will also be presented, a method that can be used to precisely isolate specific cell components or individual cells from mixed populations. This technique allows target structures to be precisely defined under the microscope and then extracted using a laser beam, which is particularly used in cellular and molecular research.

Practical course: Easy-to-perform experiments are chosen to focus on the operation and functionality of the available equipment. The students will independently acquire images at different magnification levels and process them with the help of various image processing tools learned in the practical course. The focus is on the visualization of pathogens (TEM) and host-pathogen interactions (LM/FESEM). In TEM, students will learn how to prepare samples and visualize bacteria, viruses and proteins using the negative-staining method. In addition, a self-conducted infection experiment is designed to illustrate the correlation of LM and FESEM technologies. Immunolabelled samples will also be examined. In LM, mammalian cells are first examined structurally and then infected in order to visualize infected cells and affected organelles. Both high-resolution and super-resolution microscopy methods will be used. In addition to super-resolution and high-resolution microscopy, students will have the opportunity to experience the principles and techniques

of laser microdissection in practical applications and learn how to use this method to isolate specific cells or cell regions for subsequent molecular analysis. Seminar: In the accompanying seminar, the latest microscopic techniques that are not available in the module will be presented in seminar lectures.
Objective qualification
After completing the module, students will be able to - apply basic and advanced knowledge of modern light microscopy (LM), fluorescence microscopy, photo-manipulation and electron microscopy (EM) to their scientific questions. - understand which relevant questions in the life sciences they can best work on with which imaging or analysis method. - recognize and assess the advantages and disadvantages of a method. - recognize what new insights can be gained by combining imaging methods with different resolution and magnification ranges (cross-technology) (correlative microscopy). - present and discuss scientific content. - engage controversially with scientific topics and issues in a group discussion.
Literature
current microscopy-oriented publications in English to accompany the seminar lectures

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Related courses
Rules for the choice of courses
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Lecture	german
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Internship	german
Sophisticated Imaging (Bio-IB 27, Bio-MI 34, AM-B-6)		Seminar	german

Title	Chemometrics		
Number	4011200 AM-B-7	**Module version**	
Shorttext		**Language**	english
Frequency of offer		**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	3 / 5,0	**Module owner**	
Workload (h)	150		
Class attendance (h)	42	**Self studying (h)**	108
Compulsory requirements			
Expected performance/ Type of examination	oral exam (30 min)		
Course achievement	project report on practical course		

Contents

Chemical data and their statistical data analysis; Data pretreatment; Dimensionality reduction; Univariate and multivariate regression and calibration; Validation of univariate and multivariate calibration; Design of experiments applied to chemical data; Univariate and multivariate statistical process control.

Objective qualification

Knowledge, understanding and application of chemometric methods to pharmaceutical engineering. Critical evaluation of the performance of chemometric methods in practice.

Literature

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Introduction to Chemometrics	2,0	Lecture	english german
Introduction to Chemometrics	1,0	Internship	english german

Title	Theoretical Spectroscopy		
Number	1498120 AM-B-8	**Module version**	
Shorttext		**Language**	english
Frequency of offer	irregular	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	Institut für Physikal. und Theoretische Chemie
Hours per Week / ECTS	/ 8,0	**Module owner**	Prof. Dr. Christoph Jacob
Workload (h)			
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
Course achievement	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		

Contents

Lecture and Computer Lab Theoretical Spectroscopy: Time-dependent quantum mechanics, interaction of electromagnetic radiation with molecules, basics of Hartree-Fock and density-functional theory, quantum-chemical calculation of spectroscopic data (Infrared and Raman spectroscopy, UV/Vis spectroscopy, ESR and NMR), simulation of spectra.
Project Lab: Introduction to scientific programming and in-depth study of selected quantum-chemical methods. Application of quantum-chemical methods that usually cannot be used as "black-box" methods in own independent projects.

Objective qualification

The students have acquired knowledge in time-dependent quantum mechanics and on modern methods of theoretical spectroscopy. They are familiar with the foundations of important methods and possess an overview of commonly used quantum-chemical methods in theoretical spectroscopy, their implementation in scientific software, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose suitable methods for their own research projects, to perform calculations and to analyse, evaluate, and assess their results.

Literature

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**

Theoretical Spectroscopy	3,0	Lecture	english german
Computer Lab Theoretical Spectroscopy	1,0	Exercise	english
Project Lab Theoretical Spectroscopy	2,0	Internship	english

Title	Machine Learning in Computational Chemistry		
Number	1499180 AM-A-10	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	6 / 8,0	**Module owner**	Prof. Dr. Jonny Proppe
Workload (h)	240 h		
Class attendance (h)	84	**Self studying (h)**	156
Compulsory requirements			
Expected performance/ Type of examination	oral or written exam+ (PL, 20% of the coursework and 20% of the practical work mark are taken into account in the overall module grade)		
Course achievement	solve coursework problems (ÜbA, SL unmarked) practical work (expA, SL marked)		
Contents			
Lecture and Computer Lab Artificial Molecular Intelligence: Molecular quantum mechanics in a nutshell: Hartree–Fock (HF) theory, post-HF methods, density functional theory; molecular machine learning in a nutshell: molecular representations, deep learning and kernel methods, generative models, uncertainty quantification, active learning; Applications: structure–property relationships, chemical space exploration, molecular design. **Project Lab:** In-depth study of molecular machine learning methods, application of methods of artificial molecular intelligence in own independent projects.			
Objective qualification			
The students have acquired knowledge on modern methods of molecular machine learning and molecular artificial intelligence. They are familiar with the foundations of important methods and possess an overview of commonly used methods, their implementation, and their use in chemistry. They are able to judge the applicability and the limits of different methods and to use choose and apply suitable methods for their own research projects and to analyse, evaluate, and assess their results.			
Literature			

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**

Machine Learning in Computational Chemistry	3,0	Lecture	english
Computer Lab Machine Learning in Computational Chemistry	1,0	Exercise	english
Project Lab Machine Learning in Computational Chemistry	2,0	Internship	english

Title	Research Lab Spectroscopy and Imaging		
Number	1499240 AM-B-RP	**Module version**	
Shorttext		**Language**	english
Frequency of offer	every term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	/	**Module owner**	Prof. Dr. Marc Walter
Workload (h)	360 - 510		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	study research project including report and presentation (StA)		
Course achievement			

Contents
Research Lab: Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points. **Seminar:** Participation in scientific colloquia, presentation and discussion of current research results
Objective qualification
Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.
Literature

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Related courses			
Rules for the choice of courses			
the number of credit points assigned for this module depends on the duration of the research project: 12 LP = 360 h 13 LP = 390 h 14 LP = 420 h 15 LP = 450 h 16 LP = 480 h			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**

Research Lab Spectroscopy and Imaging		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

Profile Area Data-Driven Biology

Title	Molecular Microbial Evolution and Diversity		
Number	1399900 AM-C-1	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	9 / 10,0	**Module owner**	Dr. Jörn Petersen
Workload (h)	300		
Class attendance (h)	126	**Self studying (h)**	174
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	written exam (ca. 200 min.)		
Course achievement	- experimental work - protocol (1) - written exam (ca. 90 min.)		

Contents

Lectures:
Functional diversity of bacterial communities and relevance for global element cycling, ways to quantify microbial diversity, methods of comparative genomics, population genetics and speciation, the polyphasic bacterial species concept, phylogenetic concepts, evolution of the prokaryotic and eukaryotic cell, multicellularity, symbiosis and pathogenesis, biodiversity informatics, organization of sequence databases, biotechnological utilization of microbial diversity, microbiological ressource centers.

Practical Course:
Work in the accompanying practical course focuses on the application of a suite of laboratory methods and is supervised by resident scientists at the Leibniz Institute DSMZ. The methods introduced comprise molecular biological techniques (high throughput sequencing, PCR, cloning), epifluorescence microscopy, bioinformatics (annotations, sequence comparisons, different phylogenetic analyses), state-of-the-art methods for the high-throuput cultivation of novel types of bacteria, chemotaxonomical methods (fatty acid profiles, cell wall chemistry), and the long-term conservation of bacterial strains.

Objective qualification

After completing the module, students are able to
- determining and interpreting microbial diversity based on high throughput sequence datasets
- analyzing microbial functional diversity by culture-independent approaches (including field methods)
- cultivating and isolating bacterial strains from complex communities, determining their 16S rRNA gene sequences and evaluating the taxonomy of the isolates
- characterizing bacterial isolates by physiological and chemotaxonomical methods
- conducting phylogenetic analyses and interpreting their results

- interpreting morphological, physiological, and phylogenetic diversity in the context of existing information from genome sequence
- quantifying mutation rates and interpret their implications for bacterial evolution
- elucidating the role of accessory genes under natural conditions (by plasmid curing, competition experiments)
- integrating heterogenous datasets from own experiments, literature searches and bioinformatic analysis
- contextualize the integrated data considering the actual state of scientific knowledge.

Literature

Madigan et al., Brock Biology of Microorganisms, 2014

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Molecular Microbial Evolution and Diversity (Bio-MI 22, Bio-BD 22, AM-C-1)		Lecture	
Molecular Microbial Evolution and Diversity (Bio-MI 22, Bio-BD 22, AM-C-1)		Internship	english

Title	Immunometabolism		
Number	1398590 AM-C-2	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	8 / 10,0	**Module owner**	Prof. Dr. Karsten Hiller
Workload (h)	300		
Class attendance (h)	112	**Self studying (h)**	188
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	- term paper - oral presentation		
Course achievement	Successful participation in the practical course and seminar		
Module grade composition	The module grade corresponds to the grade for the examination performance.		

Contents

The seminar gives an introduction into the metabolism of macrophages and how to analyze it by using isotope-labeling experiments and modeling. Especially the role of itaconic acid, ROS, NO and glutathione is discussed. Afterwards, different analytical methods for studying the Immunometabolism of different cell lines will be presented by the students. The students will plan themselves the workflow for the practical course to answer different biological questions. The
students will present their work by using different presentation concepts (talk, poster, etc).
Practical course: Students will apply their theoretical knowledge to answer different biological questions by using the methods discussed in the seminar. The students will apply several methods, covering cell cultivation, metabolite extraction, seahorse measurements, GC-MS measurements and data analysis, metabolic flux analysis with stable isotopes, etc.

Objective qualification

After completing the module, students are able to
- explain the importance of the metabolism of immune cells during infection/inflammation.
- apply modern analytical techniques, such as isotope labelling, mass spectrometry and metabolic flux analysis - evaluate and interpret GC-MS data.
- interpret the energy metabolism by means of respiration measurements.
- develop concepts for solving systems biology problems with the help of different methods.
- present and discuss scientific work.
- discuss controversial scientific topics and questions.

- search, present and discuss relevant scientific content.
- contribute to controversial discussions of scientific topics.
- work successfully and independently in a team, organize a team and communicate efficiently with different target groups.
- carry out advanced practical and scientific work independently and analyze experimental data.
- apply in-depth foreign language skills (usually English).

Literature

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Attendance is compulsory for practicals, exercises, seminars, and excursions.			
Name of the course	**SWS**	**Eventtype**	**Language**
Immunmetabolism (Bio-BB 31, Bio-SB 31, AM-C-2)		Seminar	english german
Immunmetabolism (Bio-BB 31, Bio-SB 31, AM-C-2)		Practical exercise	english german

Title	Applied bioinformatics: biomarkers for diagnosis		
Number	1303600 AM-C-3	**Module version**	
Shorttext		**Language**	english
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	/ 10,0	**Module owner**	Prof. Dr. Karsten Hiller
Workload (h)	300		
Class attendance (h)	188	**Self studying (h)**	112
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	written exam (ca. 200 min.)		
Course achievement	- Successful participation in the seminar - Experimental work		
Module grade composition	The module grade corresponds to the grade for the examination performance.		

Contents

Seminar:
1 week course “Introduction to R”.
Integrated Lecture, computational Workshops and Experimental course (whole semster, 4h per week):
Lecture, Workshops: Introduction into mass-spectrometry driven metabolome analysis, understanding the selection of suitable mass units to ensure reproducible measurements, understanding the relevance of measurement traceability and uncertainty for data interpretation. Introduction to algorithms for machine learning based biomarker prediction, correction for multiple testing, basics of logistic regression and neuronal networks, training and evaluating a machine learning based prediction model, receiver operating characteristics, data normalization. Understanding the relevance of quality controls for data backup and safety. Designing a crossover intervention study.

Experimental course: Isolation of metabolites from saliva and/or blood followed by analysis via mass spectrometry. The method will be optimized for specific metabolites and quantification of these performed via isotope dilution. Acquisition of different methods for optimization of sample withdrawal and sample processing as well as data analysis. Determination of biomarker signatures, e.g. based on saliva samples to distinguish whether donor was case or control.

Objective qualification

After completing the module, students are able to
- Perform a simple crossover intervention study and collect samples
- Perform metabolome analyses of human saliva and/or blood samples by mass spectrometry
- Analyze the raw data with the help of bioinformatics to determine quantitative and semi-quantitative metabolite concentrations
- Identify biomarker signatures by application of machine learning algorithms (logistic regression, lasso (least absolute shrinkage and selection operator)
- Quantify selected biomarkers with high precision and reproducibility
- Apply basic concepts of metrology and standardization
- Perform statistical analyses in R.

- Understand the relevance of standardization for experimental design and performance.
- Understand the concept of a clinical crossover study / trial to evaluate the efficacy or effects of a drug.

- search, present and discuss relevant scientific content.
- contribute to controversial discussions of scientific topics.
- work successfully and independently in a team, organize a team and communicate efficiently with different target groups.
- carry out advanced practical and scientific work independently and analyze experimental data.
- apply in-depth foreign language skills (usually English).

Literature

will be announced in the lecture

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Related courses

Rules for the choice of courses

Compulsory attendance

Attendance is compulsory for practicals, exercises, seminars, and excursions.

Name of the course	SWS	Eventtype	Language
Navigating the Metabolic Maze: Machine Learning for Biomarker Detection and Quantification (Bio-BB 32, Bio-SB 32, AM-C-3)		Seminar	english
Navigating the Metabolic Maze: Machine Learning for Biomarker Detection and Quantification (Bio-BB 32, Bio-SB 32, AM-C-3)		Internship	english

Title	Network Biology		
Number	4217840	**Module version**	V2
Shorttext	INF-MI-84	**Language**	english
Frequency of offer	only in the summer term	**Teaching unit**	Carl-Friedrich-Gauß-Fakultät
Module duration	1	**Institution**	Peter L. Reichertz Institut für Medizinische Informatik
Hours per Week / ECTS	4 / 5,0	**Module owner**	Prof. Dr. Tim Kacprowski
Workload (h)	150		
Class attendance (h)	56	**Self studying (h)**	94
Compulsory requirements			
Expected performance/ Type of examination	1 graded work: written exam, 90 minutes, or oral exam, 30 minutes or Take-Home-Exam.		
Course achievement	1 non-graded work: 50% of exercises must be passed		

Contents

- Introduction graph theory
- Biological networks
- Biological network databases
- Statistical network analysis
- Graph algorithms
- Graph-based machine learning

Objective qualification

After successful completion of this module, students will have a basic understanding of graph theory and its applications for the analysis of biomedical data. They will be able to use network biology tools and critically assess network analyses. They will be capable to devise new graph-based strategies for the analysis of biomedical data.

Literature

wird noch bekanntgegeben

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**

Network Biology	4,0	Lecture/Exercise	english
Literature			
to be announced			

	2,0	Exercise	english

Title	Functional Genomics in Infection Biology		
Number	1398580 AM-C-8	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	0 / 10,0	**Module owner**	Prof. Dr. Susanne Engelmann
Workload (h)	300		
Class attendance (h)	140	**Self studying (h)**	160
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	Oral presentation (1)		
Course achievement	- Successful participation in the practical course - Protocols (1) - Oral presentation (1)		

Contents

Lecture:
The Lecture will provide an overview of the potential of functional genomics in infection biology, as well as its limitations.
Further topics are:
- Detailed overview of functional genomics methods (genome sequencing, mutagenesis, mutation analysis, transcriptomics, proteomics, metabolomics).
- Introduction to systems biology models of infection biology and microbial pathophysiology (e.g. stochastic models of gene expression, thermodynamic models of metabolism).
- Introduction to complex omics datasets and their analysis (standard methods of genome recon-struction, annotation, comparative genome analysis and differential gene expression analysis).
- Examples of how functional genomics can be used to gain a more complex understanding of host-pathogen interactions.
- Microbiome structure and physiology.
- Biomarkers as diagnostic tools.

Practical course:
- Provide skills for designing experiments in genomics, transcriptomics and proteomics
- Present analysis strategies using local and web-based databases and analysis tools

Seminar:
- Presentation of a talk on a current topic in functional genomics
- Experience in advanced literature review
- Acquisition of knowledge in the independent development of a limited, scientifically relevant topic from functional genome research on the basis of original works in English, in order to give an overview of the current state of research and to present and critically discuss it in a clearly struc-tured lecture of approx. 30 minutes duration with appropriate visualisations.

Objective qualification
After completing this module students are able to - understand the concepts of functional genomics. In particular, they will be able to recognise the poten-tial and limitations of molecular genetic methods and OMICs technologies in basic and applied research and medical diagnostics. - apply a wide range of infection genetics and functional genomics techniques to study host-pathogen inter-actions. - design experiments to comprehensively answer a scientific question. - critically analyse the advantages and disadvantages of a method and the results obtained. - place results in a scientific context. - present and discuss researched scientific content. - discuss controversial scientific topics and issues in a group discussion.
Literature
wird in der Vorlesung bekanntgegeben.

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Related courses
Rules for the choice of courses
Compulsory attendance

Name of the course	**SWS**	**Eventtype**	**Language**
Functional Genomics in Infection Biology (Bio-IB 28, Bio-MI 33, AM-C-8)		Lecture	english
Functional Genomics in Infection Biology (Bio-IB 28, Bio-MI 33, AM-C-8)		Internship	

Title	Microbial Proteomics		
Number	1301290 AM-C-9	**Module version**	
Shorttext		**Language**	
Frequency of offer	only in the summer term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	6 / 10,0	**Module owner**	Prof. Dr. Susanne Engelmann
Workload (h)	300		
Class attendance (h)	148	**Self studying (h)**	152
Compulsory requirements	none		
Recommended requirements	none		
Expected performance/ Type of examination	presentation (ca. 40 min.)		
Course achievement	- Experimental work - Successful participation in the seminar - protocol (1) - presentation (ca. 30 min.)		

Contents

Lecture:
The lecture "Microbial Proteomics" provides an overview of proteomics methods and their applica-tion in microbiology. Based on an introduction to methods for the identification and quantification of proteins in highly complex protein mixtures, modern experimental approaches for the qualitative and quantitative characterisation of the entirety of proteins (proteome) of a microorganism or a community of microorganisms (metaproteome) will be presented. In addition, possibilities for the detection of protein modifications and the visualisation of protein complexes will be demonstrated.

Practical course:
In the practical course "Microbial Proteomics", students should apply the methods taught in the lecture under supervision to answer a question in the field of physiology of microorganisms, infec-tion biology or the elucidation of the mode of action of antibacterial natural products.

Seminar:
In the 'Microbial Proteomics' seminar, students are required to independently analyse recent publi-cations on research in this field, present them in a short talk, and critically question and discuss them.

Objective qualification

After completing the module, students are able to
- describe the basic principles of proteomic methods and critically evaluate the advantages and disadvantages of the methods.
- identify and quantify proteins from complex protein mixtures.
- analyse large data sets and visualise the results.
- design experiments to comprehensively answer a scientific question.
- critically analyse the advantages and disadvantages of a method and the results obtained.
- place results in a scientific context.

- present and discuss researched scientific content.
- discuss controversial scientific issues in a group.

Literature

- H. Rehm und T. Letzel, Der Experimentator Proteinbiochemie/Proteomics
- F. Lottspeich und J. W. Engels, Bioanalytik
- aktuelle englischsprachige Fachliteratur

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Lecture	english
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Seminar	english
Microbial Proteomics (Bio-MI 26, Bio-SB 35, AM-C-9)		Internship	english

Title	Research Lab Data-Driven Biology		
Number	1499250 AM-C-RP	**Module version**	
Shorttext		**Language**	english
Frequency of offer	every term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	/	**Module owner**	Prof. Dr. Marc Walter
Workload (h)	360 - 510		
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	study research project including report and presentation (StA)		
Course achievement			

Contents

Research Lab: Conduction and scientific documentation of (parts of) a current research project. The duration of the research project depends on the number of required credit points.
Seminar: Participation in scientific colloquia, presentation and discussion of current research results

Objective qualification

Students are able to work independently on a scientific question in the field of "Artificial Intelligence for Molecular Sciences" and apply their skills in data-based methods and methods of artificial intelligence in a sub-area of molecular sciences. They possess advanced skills required for their research project and are able to plan, perform, analyze and document advanced data analysis. They have an overview of the current research in a selected research area and are familiar with its theoretical foundations. They are able to adequately present their research results and to engage in scientific discussions.

Literature

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Related courses

Rules for the choice of courses

the number of credit points assigned for this module depends on the duration of the research project:
12 LP = 360 h
13 LP = 390 h
14 LP = 420 h
15 LP = 450 h
16 LP = 480 h
17 LP = 510 h

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Research Lab Data-Driven Biology		Internship	english
Seminar Research Lab Artificial Intelligence for Molecular Sciences		Seminar	english

Key Qualifications

Title	Ethics and Epistemology		
Number	4411440 AM-KQ-1	**Module version**	
Shorttext	GE-Phil-44	**Language**	
Frequency of offer	only in the winter term	**Teaching unit**	Fakultät für Geistes- und Erziehungswissenschaften
Module duration	1	**Institution**	
Hours per Week / ECTS	2 / 5,0	**Module owner**	Prof. Dr. Hans-Christoph Schmidt am Busch
Workload (h)	Präsenzzeit: 30 h Selbststudium: 120 h Gesamtworkload: 150 h		
Class attendance (h)	30	**Self studying (h)**	120
Compulsory requirements			
Expected performance/ Type of examination	1 graded examination (Prüfungsleistung): written exam, 120 minutes		
Course achievement	1 non graded examination (Studienleistung): Protokoll, 2 pages		

Contents

This course provides students with philosophical knowledge in order to reason thoughtfully, judge effectively and act morally in the field of data science. Students learn to differentiate between concepts, phenomena and actions, which is relevant for understanding the presuppositions and implications of machine ethics. This new field is, on the one hand, concerned with established ethical approaches (Kant, Utilitarianism); on the other hand, with giving machines ethical principles, i.e. programs and operations for discovering a way to resolve ethical dilemmas they might encounter. Whereas enabling machines to function in an ethically responsible manner through their own ethical decision making is a long wished-for in AI and robotics, philosophers and society highlight basic questions still in need for an answer; for example: can machines be moral agents? When adopting norms and values, who should they take as paradigmatic role model? Who has the right to judge about that, and why? Students will learn the preconditions and limits of modeling the world according to machines. Not last, which kind of world machines face by means of artificial sensory perception matters for understanding the difficult questions of embodiment, and really being in the world instead of only having one.

Objective qualification

The course:
- provides a philosophical framework and moral compass for guiding the judgement of students regarding data science and its applications (artificial intelligence, robotics, etc.).
- aims to develop communication skills, social and civic competences,
- reassures students on the limits of machines, machinery settings, and machine ethics,
- strengthens personal development in the light of digit(al)ization and related claims of social change.

The students will be able to recognize and interpret social and technical problems in technology and information processingn based in classical and recent position in theoretical and practical philosophy. They will be able to interpret these problems ethically and support their position with arguments from machine ethics.

Literature

Anderson, Michael/Anderson, Susan Leigh (eds.): Machine Ethics, 2011

Misselhorn, Catrin: Grundfragen der Maschinenethik, 3rd ed. 2018
Nagel, Thomas: What is it like to be a Bat? Englisch/Deutsch, Reclam 2016

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Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
Ethics and Epistemology	2,0		english german

Literature

Literatur:
- Misselhorn, Catrin: Grundfragen der Maschinenethik, 3rd ed. 2018
- Anderson, Michael/Anderson, Susan Leigh (eds.): Machine Ethics, 2011
- Nagel, Thomas: What is it like to be a Bat? Englisch/Deutsch, Reclam 2016

Title	Professionalization		
Number	1499410	**Module version**	
Shorttext		**Language**	english german
Frequency of offer	every term	**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	/ 7,0	**Module owner**	Prof. Dr. Marc Walter
Workload (h)			
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	The examination modalities vary depending on the selected courses, see BPO.		
Course achievement	The examination modalities vary depending on the selected courses, see BPO.		

Contents

The interdisciplinary courses can be selected from the overall program, see also BPO.

Objective qualification

The learning outcomes of the interdisciplinary courses related to key qualifications are divided into three sub-areas:

Overarching reference: Embedding the subject of study: Students are enabled to embed their subject of study in social, historical, legal or professional contexts (depending on the focus of the course). They are able to recognize, analyze and evaluate overarching subject-related connections and their significance. The students gain an insight into the networking possibilities of the subject and application possibilities of their field of study in professional life.

Scientific cultures: Students become familiar with the theories and methods of other scientific cultures, learn to deal and work interdisciplinarily with students from other fields of study, can discuss and evaluate current controversies from individual disciplines, recognize the importance of cultural framework conditions for different scientific understandings and applications, know gender-related perspectives on different subject areas and the effects of gender differences, and can deal intensively with application examples from foreign disciplines.

Action-oriented courses: Students are enabled to apply theoretical knowledge in an action-oriented manner. They acquire procedural knowledge (knowledge of procedures and courses of action, application criteria for certain procedures and courses of action) as well as metacognitive knowledge (including knowledge of their own strengths and weaknesses).

Depending on the focus of the course, students acquire the ability to
- impart knowledge and apply communication techniques,
- conduct discussions and negotiations effectively, reflect on themselves and evaluate themselves appropriately,
- work cooperatively in a team, manage conflicts,
- lead teams,
- use information and communication media or
- express themselves in another language.

The action-oriented courses enable students to use knowledge acquired in other areas more effectively, to work more easily and constructively with other people and thus to facilitate the acquisition and development of new knowledge. They acquire key qualifications that facilitate their entry into professional life and contribute to success in all professional situations.
Literature

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**

Master's Thesis

Title	Master's Thesis		
Number	1499420	**Module version**	
Shorttext		**Language**	english
Frequency of offer		**Teaching unit**	Fakultät für Lebenswissenschaften
Module duration		**Institution**	
Hours per Week / ECTS	/ 30,0	**Module owner**	
Workload (h)			
Class attendance (h)		**Self studying (h)**	
Compulsory requirements			
Expected performance/ Type of examination	master thesis (see APO §14 and BPO §8)		
Course achievement			
Contents			
The topic of the master's thesis must address an issue from the field of "Artificial Intelligence for Molecular Sciences" in the broader sense and should be chosen in such a way that it matches the chosen specialization.			
Objective qualification			
Students are able to work independently on a scientific question from a sub-field of "Artificial Intelligence for Molecular Sciences" within a specified period of time and to present their research results adequately in written form. They are familiar with the relevant conventions of their field of research and have an insight into current topics of research.			
Literature			

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Related courses			
Rules for the choice of courses			
Compulsory attendance			
Name of the course	**SWS**	**Eventtype**	**Language**