



Description of the degree program

Artificial Intelligence for Molecular Sciences (Master) PO 1

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Foundations			26 ECTS
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			



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

**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 Lebenswissenschaften
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 examination			
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 functionalities 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 Python for designing 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 synthesize 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	3,0	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 rechnerge- stützte 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 examina- tion	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 com- plex 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			15 ECTS
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 Bes-serve
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			



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.			



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

**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

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			



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 Maschinenbau
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 examination	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			37 ECTS
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 meaningful 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 Lebenswissenschaften
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 examination	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, transition metal hydrides and dihydrogen complexes, iso(valence)-electronic ligands to CO, metal-alkyl complexes, catalytic elementary reactions (oxidative addition, reductive elimination, insertions, hydride eliminations), catalytic processes (hydroformylation, acetic acid preparation, olefin polymerization, hydrogenations, Wacker process), carbene (alkylidene) and carbyne (alkylidyne) complexes, olefin and alkyne metathesis, complexes with π-ligands (olefin, alkyne, allyl, cyclopentadienyl, arene complexes), sandwich compounds, spectroscopic methods for structure elucidation in organometallic chemistry (IR, NMR), occurrence and biological functions of inorganic elements, 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 organometallic chemistry. They understand the role of metals in nature and are familiar with the fundamentals of bioinorganic and bioorganometallic chemistry. They can discuss and predict the structure and properties of metal complexes using modern bonding concepts and have knowledge of the use of transition metal complexes 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			



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, oligomerisation 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, industrial catalysis, polymerization with transition metal complexes, Ziegler-Natta polymerization, Phillips 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			



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 complexes 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 feature.			

ture (Hume-Rothery and Laves phases, alloys), polyhedra as a structural feature, symmetry 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



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 Compounds	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			



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
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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; exam can also be		
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



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 structural 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



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 multcale 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			



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 (unmarked) Practical work (marked)		
Contents			
Lecture and Computer Lab Advanced Quantum Chemistry: Mathematical Foundations of quantum-chemical methods, Hartree-Fock theory, perturbation 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, simulation 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 quantification, 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 independent projects.			
Objective qualification			
The students have acquired 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 suitable methods for their own research projects, to perform quantum-chemical calculations and to analyse, evaluate, and assess their results.			
Literature			



Related courses			
Rules for the choice of courses			
To complete the module one out of the three lectures and the associated exercise must be completed as well as the project lab. One of the three lectures and the associated exercise 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			



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			37 ECTS
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 Lebenswissenschaften
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 examination	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 experimental techniques in spectroscopy (UV-VIS spectroscopy, fluorescence spec-troscopy, IR, Raman and nonli-near spectroscopy).			
Excercise: 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 understand-ing 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 microscopy, 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 Chemistry: 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 elucidation 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 dynamic 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		Teaching unit	Fakultät für Lebenswissenschaften
Module duration		Institution	
Hours per Week / ECTS	0 / 8,0	Module owner	
Workload (h)			
Class attendance (h)		Self studying (h)	
Compulsory requirements			
Expected performance/ Type of examination			
Course achievement			
Contents			
Objective qualification			
Literature			



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 Lebenswissenschaften
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 examination	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 introduced, in particular machine learning, sequential optimization, and inverse design. It will be discussed how these methods can be applied 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 CO₂ and N₂ defines the focus of this lecture. Artificial Photosynthesis and CO₂ Activation: Introduction and working principle of molecular photosensitizers and catalysts, mechanisms of electron and energy transfer processes, artificial photosynthesis, solar fuels, molecular water splitting and CO₂ 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 interactions and synergies 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.



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
- Bornschlöggl, T. and Dietz, H., Biophysik in der Zelle
- Aktuelle Publikationen aus der Zell- und Infektionsbiologie, Biophysik in englischer Sprache (Zur Vorlesung und den Seminarvorträgen)



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 - successful 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



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			



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			



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			



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	37 ECTS
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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



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



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 semester, 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



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			



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

Network Biology	2,0	Lecture	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 reconstruction, 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 structured 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 potential 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 interactions.
- 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.

**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 application 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, infection 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 publications 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



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			12 ECTS
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



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



Related courses

Rules for the choice of courses

Compulsory attendance

Name of the course	SWS	Eventtype	Language
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Master's Thesis	30 ECTS
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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

