

### Modulhandbuch für den Master-Studiengang Chemie

### Studienplan für den Master-Studiengang Chemie

Der folgende Studienplan gilt in Verbindung mit der Prüfungsordnung des Master-Studiengangs der Fakultät für Chemie und Biochemie.

(1) Die Gliederung des Studienplans beruht auf dem Studienjahr mit Studienbeginn im Wintersemester.

(2) Es wird empfohlen, die Lehrveranstaltungen in der angegebenen Reihenfolge zu besuchen. Für einzelne Praktika ist die erfolgreiche Teilnahme an vorhergehenden Lehrveranstaltungen entsprechend Abs. 3 erforderlich.

(3) Die Zulassung zu den nachstehend genannten Lehrveranstaltungen ist abhängig von dem Vorliegen eines Leistungsnachweises für die im Ausbildungsgang vorhergehenden Lehrveranstaltungen (Vorleistungen) gemäß folgender Zusammenstellung:

Lehrveranstaltung	Vorleistung
Spezialisierungspraktikum	"Practical Science and
	Communication" und
	Vertiefungspraktika I - III
Master-Arbeit	Spezialisierungspraktikum

(4) Kennzeichnung der Lehrveranstaltungen

Com = Compulsory Module

Elec = Elective Module

CP = Credit Points für den jeweiligen Leistungsnachweis

(5) Die Vertiefungspraktika I bis III müssen jeweils aus unterschiedlichen Lehrveranstaltungen stammen.

(6) Wahlfreiheit. Wahlpflichtmodule und Vertiefungspraktika können frei aus dem gesamten Lehrangebot der Fakultät für Chemie und Biochemie für den Master-Studiengang gewählt werden. Die Wahl vergleichbarer Module aus anderen Fakultäten kann gegebenenfalls auf Antrag durch den Prüfungsausschuss genehmigt werden.

Master of Science Chemistry (M. Sc. Chemistry)



Sem.	Module	L	E/S	Pr	Туре	СР
1. (WS)	Physical Chemistry V	2	Ι	-	Com	5
	Practical Science and Communication	-	2	6	Com	6
	Elective Lecture I	2	Ι	-	Elec	5
	Elective Lecture II	2	I	-	Elec	5
	In-Depth Practical I	-	-	9	Elec	8
26 HpW	Total: 1st Semester	6	5	15		29
2.(SS)	Elective Lecture III	2	Ι	-	Elec	5
	Organic Chemistry IV	2	I	-	Com	5
	Inorganic Chemistry IV	2	Ι	-	Com	5
	In-Depth Practical II	-	-	9	Elec	8
	In-Depth Practical III	-	-	9	Elec	8
30 HpW	Total: 2nd Semester	8	4	18		3I
3.(WS)	Elective Lecture IV	2	Ι	-	Elec	5
	Elective Lecture V	2	Ι	-	Elec	5
	Elective Lecture VI	2	Ι	-	Elec	5
	Focal Point Practical	-	-	15	Com	15
21 HpW	Total: 3rd Semester	6	3	15		30
4. (SS)	Master Thesis				Com	30
77 HpW	Total: 1. – 4. Sem.	18	II	48		120

Master of Science Chemistry (M. Sc. Chemistry)



### Modulliste Masterstudiengang Chemie

Lfd. Nr.	Module Masterstudiengang Chemie	Seite
1	Pflichtveranstaltungen	
1.1	Inorganic Chemistry IV	6
1.2	Organic Chemistry IV	7
1.3	Physical Chemistry V: Molecular Reaction Dynamics	8
1.4	Introduction to Scientific Communication (ITSC)	9
	Master Wahlvorlesungen	
2	Analytische Chemie	
2.1	Advanced Electrochemistry: From Fundamentals to Applications I	10
2.2	Advanced Electrochemistry: From Fundamentals to Applications II	11
2.3	Research practical in the focal point programme	12
2.4	In-depth Practical "Biointerfaces"	13
2.5	In-depth Practical "Advanced Electrochemistry – From Fundamental to Applications"	14
2.6	In-depth Practical: Micro-Electrochemistry & Scanning Electrochemical Microscopy	15
2.7	In-depth Practical "Sensors and Bioanalytics"	16
2.8	In-depth Practical "Nanomaterials – Synthesis, Characterization and Application"	17
2.9	In-depth Practical: Electrocatalysis and energy conversion	18
3	Anorganische Chemie	
3.1	Bioinorganic Chemistry	19
3.2	Crystal Engineering – Chemistry beyond the molecule	20
3.3	Medicinal Inorganic Chemistry	21
3.4	Main Group Chemistry: From Curiosities to Catalysis	22
3.5	Green and Sustainable Chemistry	23
3.6	In-depth Practical: Green and Sustainable Chemistry	24
3.7	In-depth Practical: Computational Chemistry in Inorganic Chemistry	25
3.8	In-depth practical: Analytical Methods in Inorganic Chemistry	26
3.9	In-depth practical: Bioinorganic Chemistry	27
3.10	In-depth Practical: Molecular Chemistry and Synthesis	28
3.11	Research Practical: Inorganic Chemistry	29

Master of Science Chemistry (M. Sc. Chemistry)



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Master of Science Chemistry (M. Sc. Chemistry)

Lfd. Nr.	Nr. Module Masterstudiengang Chemie (Fortsetzung)		
8	Technische Chemie		
8.1	Heterogeneous Catalysis	69	
8.2	Industrial Chemistry II: Chemical Reaction Engineering	70	
8.3	Modern Microkinetics	71	
8.4	Processes in Chemical Production - Past, Present and Future	72	
8.5	In-depth Practical: "Characterization of Heterogenous Catalysts"	73	
8.6	In-depth Practical: Industrial Catalysis	74	
8.7	In-depth Practical: Reaction Engineering of Heterogeneously Catalyzed Reactions	75	
9	Theoretische Chemie		
9.1	Computational Chemistry I: Structure and Dynamics of Molecules	76	
9.2	Computational Chemistry II: Quantitative Structure-Activity Relations in Drug Design	77	
9.3	Theoretical Chemistry II: Dynamics and Simulation	78	
9.4	Biomolecular Simulation: Understanding Experiments at the Molecular Level	79	
9.5	Theoretical Chemistry III: Electronic and Molecular Structure Theory (Chemistry)	80	
9.6	Atomistic Simulations with Machine Learning	81	
9.7	Theoretical Spectroscopy (Chemistry)	82	
9.8	Industrial Computational Chemistry I: Fundamentals	83	
9.9	Industrial Computational Chemistry II: Applications in Process Development	84	
9.10	Scientific Programming Methods for Chemists	85	
9.11	Electronic and Molecular Structure Theory	86	
9.12	In-depth Practical in Theoretical Chemistry, Part I, II, III	87	
9.13	Focal-point Research Practical in Theoretical Chemistry	89	
10	Crossdisciplinary Lectures and Practicals		
10.1	Introduction to Computational Chemistry	90	
9.8	Industrial Computational Chemistry I: Fundamentals	83	
3.7	In-depth Practical: Computational Chemistry in Inorganic Chemistry	25	
5.2	Introduction to Chemistry of Materials	38	
7.2	Biophysical Chemistry II	58	
7.6	Compact Course: "Scanning Probe Microscopy"	62	
10.2	From top-level science to top-level business	91	
7.5	Compact Course: "Laser and Optics"	61	
11	Masterarbeit	92	

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## Pflichtveranstaltungen

Inorganic Chemistry IV							
Module	Credits	Workload	Term	Frequency	Duration		
1.1	5 CP	150 h	2. Sem.	Each SuS	1 Semester		
Courses Inorganic Chemistry IV a) Lecture b) Exercise		Contact hours a) 2SWS/30 h b) 1 SWS/15 h	<b>Self-Study</b> 105 h	<b>Group size</b> All students of the respective semester, ca. 50			

#### Prerequisites

Admission to the Master Course Program; basic knowledge general in synthetic chemistry (organic and inorganic chemistry) and the structure of molecular compounds, complexes (molecular orbitals, Lewis structures) is recommended

#### Learning outcomes

After the successful completion of the module

- Students have acquired advanced knowledge of the interpretation of the electronic structure, properties and reactivities of organometallic, inorganic molecular and solid state compounds and systems of higher and lower dimensionality.
- Students will be able to apply their knowledge independently on current, and intellectually demanding research problems in modern inorganic chemistry
- Students will be able to analyze research questions and develop solutions and solution strategies.

#### Content

The module focusses on the reactivity, properties and electronic structure of organometallic, inorganic and bioinorganic compounds. Content may include one or several of the following topics:

- Concepts of organometallic chemistry: Stabilization of reactive intermediates, control of electronic and steric properties of ligands, applications in homogenous catalysis, trends in the periodic table
- Concepts of bioinorganic chemistry and medicinal chemistry
- Concepts in inorganic solid state and materials chemistry
- Application of spectroscopic methods for the characterization of inorganic solid state materials, molecular compounds and complexes and the elucidation of reaction mechanisms; computational methods in structure elucidation and mechanistic studies
- Modern trends in organometallic, inorganic and/or bioinorganic chemistry

#### **Teaching methods** Lecture with exercises und accompanying e-learning moduls **Mode of assessment**

end-of-term written exam

### Requirement for the award of credit points

Passing the written examination

Module applicability

Chemistry (Master), IMOS

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

Prof. Dr. Däschlein-Gessner

V. Däschlein-Gessner, N. Metzler-Nolte, A. Devi and lecturers from inorganic chemistry

#### **Further information**



Organic Chemistry IV						
	Credits	Workload	Term	Frequency	Duration	
1 2	5 CP	150 h	2. Sem.	nur SS	1 Semester	
Courses			Contact	Self-Study	Group size	
a) lecture			hours	100 h	60 Studierende	
b) exercise			3+1 SWS			
Prerequisites						
-General knowl	edge of therm	odynamics, sta	itistical mechan	ics, and quantum n	nechanics.	
Learning outcom	mes					
<ul> <li>student</li> </ul>	s aquire kno	wledge on the	theory of adva	nced topics and c	oncepts of organic	
chemist	try such as p	ericyclic reacti	ons, heterocycl	es and supramoleo	cular chemistry. In	
additior	n links are d	rawn to theore	etical, physical	and spectroscopica	al aspects of these	
concept	s.					
Content						
<ul> <li>The co backgro reaction</li> </ul>	ncept of aro ound, electroo	maticity; perio cyclic reactions	cyclic reactions s, sitmatropic	: Molecular orbita reactions, cycloado	lls and theoretical litions, cheletropic	
heteroc	vcles: nomei	nclature, satur	rated heterocyc	les, aromatic he	terocvcles, natural	
heteroc	, ycles and thei	r role in bioche	mistry, synthes	is of heterocycles	<b>,</b> ,	
• fundam	ientals of sup	ramolecular ch	emistry and mo	lecular recognition		
<ul> <li>organoo</li> </ul>	catalysis			-		
<ul> <li>natural</li> </ul>	compounds: s	sugars and carl	oohydrates			
Teaching metho	ods					
a) lecture b	) exercise					
Mode of assess	ment		-			
Pequirement fo	r the award o	f credit points	e			
Passing the writt	en evan	r creati points				
Module applica	Pussing the written exam					
M Sc. Chemistry						
Weight of the mark for the final score						
Module coordin	nator and lectu	irer(s) Prof. Dr	. Lukas Gooßen	, Prof. Dr. Stefan H	Iuber, Dr. Wolf	
Matthias Panka	u, Dr. Dirk G	rote				
Further inform	ation					



Physical Ch	emistrv V:	Molecular R	Reaction Dvn	amics			
Module	Credits	Workload	Term	Frequency	Duration		
1.3	5 CP	120 h	1. or 3 Sem.	nur WS	1 Semester		
Courses			Contact	Self-Study	Group size		
a) lecture			hours	75 h	20 Studierende		
b) exercise			3 SWS				
Prerequisites	Prerequisites						
-							
Learning outco	mes						
• Student	ts acquire a	broad overvi	ew over exper	imental techniques	s and theoretical		
approac	thes aiming at	t the determina	ition and predic	tion of reaction rate	coefficients in the		
gas pha	se and in solu	ition.					
Content			h:	ationa in the as a nles	as and in aslution.		
Reaction     Reaction	n rate coefficie	ents of uni- and	ndomann Hind	ctions in the gas pha	Master equation;		
approa	h. Temperatu	re dependence	· Arrhenius equ	ation Transition St	te Theory: Energy		
depend	ence: RRK and	d RRKM theori	es other Transi	tion State Theory de	rivatives: Viscosity		
depend	ence: Kramer	s theory Time	- and frequence	v-domain spectrosc	opic experiments		
molecu	lar beam metl	ods: femtosec	ond nump-prob	e laser spectroscopy	opie experiments.		
Teaching meth	ods	1045, 101110500					
Lecture, exercise							
Mode of assess	ment						
Written exam (12	20 min) at the e	nd of the modul	e				
Requirement for	or the award o	f credit points					
Passing the writh	ten exam	_					
Module applica	bility						
M. Sc. Chemistr	γ						
Weight of the n	nark for the fi	nal score					
Weighted accord	Weighted according to CPs						
Module coordir	nator and lectu	ırer(s)					
lecturers Physic	cal Chemistry						
Further inform	ation						
The lectures are	e recorded to y	video and audio	, and posted on	the electronic Black	board with		
password prote	ction as an e-l	earning modul	e. The screencas	sts can also be used	tor inverted		
classroom sessi	ons.						



Introduction to Scientific Communication (ITSC)						
Module	Credits	Workload	Term	Frequency	Duration	
1 4	6 CP	180 h	1. Sem.	WiSe	2 Semester	
Courses			Contact	Self-Study	Group size	
Introduction to	Scientific Co	ommunication	hours	120 h	60 students	
			1 SWS			
Prerequisites						
General knowle	edge in chem	istry				
Learning outco	mes					
The students ga	ain skills in c	ommon scientif	ic presentation	n formats using th	eir own research	
results from Ba	chelor theses	s and in-depth p	racticals	_		
Content						
Abstract writing	. Students lea	arn to write a sh	ort abstract on	their own work, w	which is peer-	
reviewed by oth	ner students o	of the course and	d subsequently	revised.		
Short communit	cations. Stude	ents write a total	of two short c	ommunications (2	pages) on their own	
work, which is	peer-reviewe	d by other stude	nts of the cour	se and subsequen	tly revised. After the	
first round of re	eviews, an ad	ditional semina	r on common	mistakes during re	eviewing stages	
further teaches	good review	ing practices.				
Oral presentatio	ns. Using ow	n research resul	lts as topics, ea	ch student gives a	15 minutes oral	
presentation w	hich is review	ved by means of	an evaluation	sheet that the aud	ience fills out.	
Thereby, the st	udents get fe	edback on their	presentation s	tyle.		
Poster presentati	<i>ions</i> . In a pos	ter symposium,	all students pr	esent posters on t	he research done	
during their in-	-depth practio	cals, thus genera	iting a first fee	ling for poster ses	sions.	
Self-managemer	<i>it</i> . The stude	nts manage the e	entire submiss	ion and peer-revie	ewing (editorial office)	
and the schedu	ling of lectur	es and the poste	er symposium	(conference organ	ization team)	
themselves and	l thereby acqu	uire important s	oft-skills in tea	im management a	nd organization.	
Teaching meth	ods					
a) Semina	rs b) Peer	r-review assisted u	vriting			
Mode of assess	ment					
Peer-review by st	tudents of the	course				
Requirement for	or the award	of credit points				
Passing abstract	and short cor	nmunications rei	viewing phases,	active participation	,	
Module applica	bility					
M.Sc. Chemistry	Y					
Weight of the n	nark for the f	final score				
	. 11					
Module coordin	nator and lect	turer(s)				
C. Merten						
Further information						



## Master Wahlvorlesungen Analytical Chemistry

Advanced E	lectrochem	istry: From	Fundamenta	als to Applicatio	ons I	
Module	Credits	Workload	Term	Frequency	Duration	
2.1	5 CP	150 h	1.,3. Sem.	WS	1 Semester	
Courses		1	Contact	Self-Study	Group size	
a) Elective Cour	se		hours	108 h	30 Students	
b) Elective Lectu	ure I-VI		a) 2 SWS			
,			b) 1 SWS			
Prerequisites			-			
Knowledge of ba	sic electrochem	nistry				
Learning outco	mes					
The students sho	ould gain an ad <sup>,</sup>	vanced understar	nding of theory ar	nd practice of modern	electrochemical	
techniques, appl	ications, and po	ossible combinati	ions with other m	ethods like e.g. spect	roscopic methods.	
Content						
General Principl	<u>es in Electroch</u>	<u>emistry</u> (Electroc	hemical Thermod	lynamics; Mass Trans	sport in Solution	
(Fundamentals)	; The Electroch	emical Double La	ayer)		_1 1 .	
Kinetics of Electr	rochemical Rea	ctions (Activation	n Energies and Th	eir Consequences for	r Electrochemistry,	
Tatel analysis; C	V Shapes as Me	eans to Identify R	Reaction Mechani	sms; The Marcus The	eory in	
Electrochemistry	' and Beyond) Maga Tuanga	t and its Tills at as	. Valtanan stren E		tin a Dian Electro de a	
and Potating Pir	Mass Transpor	es: Electrocataly	ris: Fundamental	undamentals of Rota	ling Disc Electrodes	
Flectrochemical	Impedance Spe	ectroscopy (Intro	duction to Flectro	chemical Impedance	Spectroscopy:	
Revision on Imp	edance Charact	teristics of Electri	ical Circuits: Equi	ivalent Circuit Models	s in Electrochemistry	
and Data Acquis	ition)		iour officiality, 24u		, 2.000.00.00.00.00.00.00.00.00.00.00.00.0	
Teaching meth	ods					
a)Lecture; b) Exe	rcise					
Mode of assess	ment					
30 - 45 min end-	of-term oral exa	ım				
Requirement for	or the award o	f credit points				
Passing the oral	exam					
Module applica	ıbility					
Master of Scienc	e Chemistry					
Weight of the r	nark for the fi	nal score				
Weighted accord	ing to CPs					
Module coordin	nator and lectu	urer(s)				
K. Tschulik, C. J.	Bondue, H. A	min, J. Linnemar	nn			
Further inform	Further information					



Advanced Electro	ochem	istry: From	Fundamenta	als to Applicatio	ons II
Module Cred	its	Workload	Term	Frequency	Duration
2.2 5 CP		150 h	2. Sem.	SoSe	1 Semester
Courses			Contact hours	Self-Study	Group size
a) Elective Course			a) 2 SWS	108 h	30 Students
b) Elective Lecture I-V	VI		b) 1 SWS		
,					
Prerequisites					
Knowledge of basic elec	trochem	istry; attending A	Advanced Electroo	chemistry I beforehan	d is recommended
Learning outcomes					
The students should gai	in an adv	vanced understar	nding of theory ar	nd practice of modern	electroanalytical
techniques, applications	s, and po	ssible combinati	ons with other m	ethods like e.g. spectr	oscopic methods.
Content					
Local and Nanoscale Ele	ectrochei	<u>mistry</u> (Mass trar	nsport at microele	ectrodes; Mass transpo	ort at heterogeneous
and nanoparticle modif	ied elect	rodes; Electroche	mical scanning p	robe techniques)	
Electrochemical Adsorp	tion Pro	<u>cesses (</u> Adsorptio	on Isotherms and	competitive adsorpti	on; Exploiting
electrochemical adsorpt	101 to de	termine surface	areas, underpote	ntial deposition: Mecl	nanisms of
Flectrocatalysis II (Facto	igiiiuii-i	alling electrocate	l Eley-Ridal mech	allisiii)	
Advanced Flectrochemi	cal Impe	edance Spectrosci	opy ( Flectrochem	vical impedance chara	cteristics for
different modes of mas	s transpo	ort: Electrochemi	cal impedance ch	aracteristics for adsor	ption processes and
porous electrodes)	o transpe		eur mig euunee en		priori processes una
Teaching methods					
Lecture and Seminar					
Mode of assessment					
30 - 45 min end-of-term	oral exa	m			
Requirement for the a	award o	f credit points			
Passing the oral exam					
Module applicability					
Master of Science Chen	nistry				
Weight of the mark for	or the fi	nal score			
Weighted according to (	CPs				
Module coordinator a	nd lectu	ırer(s)			
K. Tschulik, C. J. Bondu	ıe, H. Ar	nin, J. Linnemar	n		
Further information					

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1,10uuic	Credits	Workload	Term	Frequency	Duration	
2.3	15 CP	450 h	3. Sem.	Every semester	1 Semester	
Courses	1		Contact hours	Self-Study	Group size	
Practical lab cou	arse (15 hours	per week)	15 h per week	240 h	1	
within research	projects.					
Prerequisites						
Knowledge of analytical and/or electrochemical methods						
Learning outco	mes					
The students sho	ould gain an a	dvanced theoretic	al and practical un	derstanding of surfa	ce analytical	
techniques, elect	rochemical m	ethodology inclu	ding micro- and na	anoelectrochemistry,	and electrocatalysis	
for energy conve	rsion embedd	ed within actual	research projects in	n the research groups	s of the chairs of	
analytical chemi	stry. They gain	n insight into mo	dern research metl	hods and topics in th	e actual research	
projects. The stu	dents should	develop skills to s	elf-reliantly plan, s	set up, work up and a	nalyze experiments.	
Contents:						
<ul> <li>Surface functi</li> </ul>	onalization ar	nd characterization	n of biointerfaces			
Bioelectrocher	nistry with ap	plications in bios	ensors and biofuel	cells		
<ul> <li>Electrocatalysi</li> </ul>	s for energy c	onversion in fuel	cells and electrolyz	zers		
• High-through	put electroche	mical materials s	creening			
• Synthesis and	characterizati	on of electrocatal	ysts for energy con	version reactions		
<ul> <li>Microelectroch</li> </ul>	nemistry and a	single-entity elect	rochemistry			
Battery researcher	ch					
<ul> <li>Electrodeposit</li> </ul>	ion, magneto	electrochemistry,				
Scanning elect	trochemical m	nicroscopy; scann	ing electrochemica	ll cell microscopy		
Teaching methods						
Teaching meth	ods					
<b>Teaching meth</b> Practical lab cou	ods rse					
Teaching meth Practical lab cou Mode of assess	ods <sup>rse</sup> ment					
Teaching meth Practical lab cou Mode of assess Lab report	ods rse ment					
Teaching meth Practical lab cou Mode of assess Lab report Requirement for	ods rse ment or the award	of credit points				
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments	ods rse ment or the award are completed	<b>of credit points</b> I successfully and	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a	ods rse ment or the award are completed a written repo	<b>of credit points</b> l successfully and rt.	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica	ods rse ment or the award are completed written repo ibility	<b>of credit points</b> l successfully and rt.	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica Master of Science	ods rse ment or the award are completed a written repo ibility e Chemistry	<b>of credit points</b> l successfully and rt.	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica Master of Science Weight of the r	ods rse ment or the award are completed written repo ibility e Chemistry nark for the	of credit points l successfully and rt. final score	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica Master of Science Weight of the report Weighted accord	ods rse ment or the award are completed a written repo ibility e Chemistry nark for the ing to CPs	of credit points l successfully and rt. final score	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica Master of Science Weight of the r Weighted accord Module coordin	ods rse ment or the award are completed written repo ibility e Chemistry nark for the ing to CPs nator and lec	of credit points I successfully and rt. final score turer(s)	available in the ele	ectronic lab book. Th	e results are	
Teaching meth Practical lab cou Mode of assess Lab report Requirement for All experiments summarized in a Module applica Master of Science Weight of the r Weighted accord Module coordin Research group	ods rse ment or the award are completed written repo- bility e Chemistry nark for the ing to CPs nator and lec leaders of the	of credit points I successfully and rt. final score iturer(s) chair of analytica	available in the ele	ectronic lab book. Th	e results are	



In-depth Practical "Biointerfaces"						
Module	Credits	Workload	Term	Frequency	Duration	
2.4	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester	
Courses			Contact hours	Self-Study	Group size	
Lab course with			a) 30 h		Individuals or	
a) 30 hours per week for 5 to 6 weeks lab work				b) 60 h	small teams	
b) 2 weeks for w	riting of the re	port and			(<5 students)	
preparation of the oral presentation						
Prerequisites						
Fundamental kn	owledge about	spectroscopy				
Learning outco	mes					
The in-depth cou	irse is a practica	al introduction to	the preparation a	and characterization of	of (bio-) functional	
interfaces. Funct	ional coatings v	will be prepared t	by self-assembly,	grafting and surface i	nitiated synthesis. A	
training in differ	ent optical, infr specific adsorpt	ion as well as bio	g techniques is p	rovided. Besides surfa	rt of the training	
Content	specific ausorpt		logical attachine	in experiments are pa	it of the training.	
Self assembly, ch	nemical grafting	z. surface initiate	d polymerization	reactions, spectral ell	ipsometry, contact	
angle goniometr	y, ATR-FTIR, S	PR, Fluorescence	e microscopy, mic	crofluidics.	1p50111011), contact	
Teaching meth	ods		17			
Lab course and S	Seminar					
Mode of assess	ment					
Lab report and o	ral presentation	l				
Requirement for	or the award o	f credit points				
The course is suc	ccessfully comp	leted with the ap	proved written re	port and oral present	ation (20 min)	
Module applicability						
Master of Scienc	e Chemistry					
Weight of the r	nark for the fi	nal score				
Weighted accord	ing to CPs					
Module coordin	nator and lectu	ırer(s)				
A. Rosenhahn	ation					
Further inform	ation					



Module	Credits	Workload	Term	Frequency	Duration			
2.5	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester			
Courses			Contact	Self-Study	Group size			
a) Elective Cor	irse		nours	b) 60 b	1 Student			
b) Elective Lec	ture I-VI		a) 50 11	b) 00 11				
Prerequisites								
Knowledge of ba	sic electrochei	mistry						
Learning outco	mes							
The students wil	l gain a high-le	evel understandir	ng and practical ex	pertise in advanced n	nethods in electro-			
chemistry. This i	ncludes electr	ode preparation,	modification and	characterization, perf	orming of			
electrochemical	measurement	s, data analysis ar	nd interpretation o	f data. Students will l	earn to plan,			
perform and inte	erpret experim	ents as a means t	to solve analytical a	and physical-chemist	ry problems.			
Content	1							
Individual researce	<u>n projects are c</u>	<u>offerea, covering on</u> rocatalusta and ai	<u>e or more topics.</u> ngla antitiog: Surf	a characterization 1	Electrogunthogic for			
the sustainable r	vroduction of y	rocatarysts and sr	ical and renewable	e fuels: Electrodeposi	tion of metals allows			
and conducting i	olymers: Mag	metic field enhan	iced electrochemis	stry: Electrochemical e	energy conversion			
and storage: batt	eries, superco	nductors, redox-fl	low batteries; Deve	elopment of electroch	emical sensors.			
In these projects o	ne or more of th	he following techni	ques will be employ	ed:				
Standard Techni	ques of Electro	ochemistry: poter	ntial step experime	ents, impedance spect	roscopy,			
voltammetry at c	atalyst-modifi	ed electrodes incl	uding rotating (rir	ng) disk electrode (R(l	R)DE)			
measurements; S	Single particle	electrochemistry	, Electrochemical	quartz crystal microb	alance			
measurements.	Combined	ith Advanced And	lucic Technicues	Floctrochomistry cou	plad to Daman ID			
Hyperspectral in	Lonnondark fie	eld microscopy: F	lectrochemical ato	mic force microscopy	<i>r</i> : Differential			
electrochemical	mass spectron	netry (DEMS): Sci	anning electroche	mical techniques	, Differential			
Numerical Simu	lations: Beside	es these experime	ental courses, theo	ry practicals are offer	ed on numerical			
simulation of ma	uss transport in	n electrochemical	systems	, I				
Teaching meth	ods							
lab course a) 30 l	nours per wee	k for 5-6 weeks b	) 2-3 weeks for wr	iting and preparation	of the oral			
presentation								
Mode of assess	ment							
Lab report and oral presentation								
	Requirement for the award of credit points							
Requirement fo		All experiments are completed successfully and written up in a lab report, oral presentation (15 minutes)						
Requirement for All experiments	are completed	successfully and	written up in a lal	o report, oral presenta	ation (15 minutes)			
Requirement for All experiments a Module applica	are completed bility	successfully and	written up in a lal	o report, oral presenta	ation (15 minutes)			
Requirement for All experiments : Module applica Master of Science	are completed bility e Chemistry	successfully and	written up in a lal	o report, oral presenta	ation (15 minutes)			
Requirement for All experiments a Module applica Master of Science Weight of the m	are completed bility e Chemistry nark for the f	successfully and final score	written up in a lal	o report, oral presenta	ation (15 minutes)			
Requirement for All experiments Module applica Master of Science Weight of the m Weighted accord	are completed bility e Chemistry nark for the f ing to CPs	successfully and	written up in a lal	o report, oral presenta	ation (15 minutes)			
Requirement for All experiments of Module applica Master of Science Weight of the m Weighted accord Module coordin K. Tschulik I. Li	are completed bility e Chemistry nark for the f ing to CPs nator and lect	successfully and final score turer(s) Bondue	written up in a lal	o report, oral presenta	ation (15 minutes)			

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In-depth Practical "Scanning Electrochemical Microscopy and								
Microelectrochemistry"								
Module	Credits	Workload	Term	Frequency	Duration			
2.6	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester			
Courses		1	Contact	Self-Study	Group size			
Elective Course			hours		· · · ·			
Elective Lecture	I-VI		a) 30 h	b) 60 h				
			,	,				
Prerequisites								
Basics in electroc	chemistry							
Learning outcom	mes							
The students sho	ould gain an adv	vanced theroretic	al and practical u	nderstanding on the j	preparation and			
application of ult	ra-microelectro	des and electroly	te-filled capillarie	es and their positionin	ig in scanning			
electrochemical r	microscopes (S	ECM), scanning	electrochemical c	ell microscopes (SEC	CM). And scanning			
droplet cells (SD	C). This contair	ns knowledge of t	the control softwa	re, different operation	n modi of the			
SECM, SDC and	SECCM. The s	tudents should le	earn to plan, perf	orm and interpret SE	CM, SECCM and			
SDC experiments	s to solve analy	tical problems.						
Content								
Microelectrodes,	preparation of	micro- and nano	electrodes (Pt, ca	rbon fibers), SECM, S	ECCM, SDC,			
operation modi, o	control softwar	e, application of s	SECM, SDC and	SECCM.				
Teaching meth	ods							
Lab course with								
a) 30 hours per w	veek for 5 to 6 v	veeks lab work	C.1 1					
b) 2 weeks for wr	iting of the rep	ort and preparati	ion of the oral pre	esentation				
Mode of assess	ment							
Lab report and of	ral presentation							
Requirement in	or the award o	n creati points	lotod succossfully	and available in the e	loctronic lab book			
The regults are su	ummarized in a	written report	Oral presentation	(20 min)	TECHOTIC IAD DOOK.			
Modulo applica	bility	a willien report.	Ofai presentation					
Master of Science	e Chemistry							
Weight of the n	nark for the fi	nal score						
Weighted accord	ing to CPs							
Module coordin	nator and lect	irer(s)						
K. Tschulik: W. S	Schuhmann	(5)						
Further inform	ation							



In-depth Pra	actical "Ser	nsors and Bi	oanalytics"		
Module	Credits	Workload	Term	Frequency	Duration
2.7	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester
Courses			Contact	Self-Study	Group size
Elective Course			hours		1
Elective Lecture	I-VI		a) 30 h	b) 60 h	
				-,	
Prerequisites			•		
Basics in electroo	chemistry				
Learning outco	mes				
The students sho	ould gain an ad	vanced theoretica	l and practical ur	derstanding of the pr	eparation and
application of bio	osensors. This o	contains the syntl	hesis and use of 1	edox polymers in am	perometric
biosensors, as we	ell as the immo	bilisation of enzy	mes on electrode	e surfaces. The studen	ts should learn to
plan, perform an	d interpret me	asurements for th	ne solution of ana	lytical problems by m	eans of
amperometric bi	osensors.				
Content			_		
Amperometric b	iosensors, elect	ron transfer betw	veen redox enzyn	ies and electrodes, red	lox mediators, redox
polymers, electro	deposition pair	nts, immobilizati	on of enzymes in	polymer layers and o	n self-assembled
monolayers, chro	noamperomet	ry, flow injection	analytics, sequer	itial injection analytics	S
Teaching meth	ods				
Lab course with	reals for E to C r	malra lab marlı			
b) 2 weeks for w	riting of the rer	veeks lab work	on of the oral pre	esentation	
Mode of assess	ment	ort and preparati		scillation	
Lab report and or	ral presentation	1			
Requirement for	or the award o	f credit points			
All experiments a	are completed s	successfully and a	available in the el	ectronic lab book. The	e results are
summarized in a	written report	. Oral presentatio	on (20 min)		
Module applica	bility	*	, , , , , , , , , , , , , , , , , , ,		
Master of Scienc	e Chemistry				
Weight of the n	nark for the fi	nal score			
Weighted accord	ing to CPs				
Module coordin	nator and lect	urer(s)			
W. Schuhmann					
Further inform	ation				



Modulo	Cradita	Workload	Term	Frequency	Duration			
7 8	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester			
Courses Elective Course Elective Lecture I-VI		Contact hours a) 30 h	Self-Study b) 60 h	Group size 1 Student				
Prerequisites Knowledge of b	Prerequisites Knowledge of basic electrochemistry							
characterization synthesis, modi physical and ch electrocatalysis world sample.	n of functional n fication of nanc emical characte and electrosynt	anoparticles and sub omaterials and sub rization methods hesis to sensing o	nanostructured n face-immobilizat of nanomaterials f molecules, nano	naterials. Methods in tion will be complen . Applications will ra oparticles and micro	n nanoparticle nented with different ange from -organisms in real-			
<b>Content</b> <ol> <li>Wet-chemical nanoparticle synthesis of: core/shell nanoparticles, alloys, nanowires, and nanocubes;</li> <li>surface immobilization of nanoparticles including electrodeposition of nanowires;</li> <li>Nanoparticle modification by: ligand exchange, underpotential deposition and electrochemical dealloying;</li> <li>Single nanoparticle electrochemistry;</li> <li>Combined electrochemical and microscopy analysis of nanoparticles includingidentical location electron microscopy and atomic force microscopy.</li> <li>electrocatalytic activity testing also in the context of electrosynthesis.</li> <li>Nanoparticle corrosion and aggregation studies,</li> <li>Spectroscopic nanomaterial characterization to deterimine size- and shape-depend reactivity</li> </ol>								
(7) Spectroscop in(electro)cataly	he context of ele ic nanomaterial ysis	ectrosynthesis. (6) characterization t	and atomic force Nanoparticle cor to deterimine size	microscopy. (6) elect rosion and aggregat e- and shape-depend	rocatalytic activity ion studies, reactivity			
(7) Spectroscop in(electro)cataly	he context of ele ic nanomaterial rsis <b>hods</b>	ctrosynthesis. (6) characterization t	and atomic force Nanoparticle cor to deterimine size	microscopy. (6) elect rosion and aggregat e- and shape-depend	rocatalytic activity ion studies, reactivity			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for	he context of ele ic nanomaterial rsis hods week for 5-6 we writing and pre	ectrosynthesis. (6) characterization t eeks eparation of the o	and atomic force Nanoparticle cor to deterimine size	microscopy. (6) elect rosion and aggregat e- and shape-depend	rocatalytic activity ion studies, reactivity			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b>	he context of ele ic nanomaterial vsis hods week for 5-6 we writing and pre sment	ectrosynthesis. (6) characterization t eeks eparation of the or	and atomic force Nanoparticle cor to deterimine size	microscopy. (6) elect rosion and aggregat e- and shape-depend	rocatalytic activity ion studies, reactivity			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and	he context of ele ic nanomaterial rsis hods week for 5-6 we writing and pre- sment oral presentation	ectrosynthesis. (6) characterization t eeks eparation of the or n	and atomic force Nanoparticle cor to deterimine size	microscopy. (6) elect rosion and aggregat e- and shape-depend	rocatalytic activity ion studies, reactivity			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b>	he context of ele ic nanomaterial ysis hods week for 5-6 we writing and pre- sment oral presentation for the award of are completed	ectrosynthesis. (6) characterization t eeks eparation of the or n of credit points	and atomic force Nanoparticle cor to deterimine size ral presentation	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b> All experiments <b>Module applie</b>	he context of ele ic nanomaterial rsis hods week for 5-6 we writing and pre- sment oral presentation for the award of are completed rability	ectrosynthesis. (6) characterization t eeks eparation of the or n of credit points successfully and v	and atomic force Nanoparticle cor to deterimine size ral presentation written up in a lal	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b> All experiments <b>Module applic</b> Master of Scien	he context of ele ic nanomaterial ysis hods week for 5-6 we writing and pre- sment oral presentation for the award of are completed ability ce Chemistry	ectrosynthesis. (6) characterization t eeks eparation of the or n of credit points successfully and v	and atomic force Nanoparticle cor to deterimine size ral presentation	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b> All experiments <b>Module applic</b> Master of Scien <b>Weight of the</b>	he context of ele ic nanomaterial sis hods week for 5-6 we writing and pre sment oral presentation for the award of are completed cability ce Chemistry mark for the f	ectrosynthesis. (6) characterization t eeks eparation of the or n of credit points successfully and v	and atomic force Nanoparticle cor to deterimine size ral presentation written up in a lal	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b> All experiments <b>Module applic</b> Master of Scient <b>Weight of the</b> Weighted accor	he context of ele ic nanomaterial vsis hods week for 5-6 we writing and pre- sment oral presentation for the award of are completed cability ce Chemistry mark for the f ding to CPs	ectrosynthesis. (6) characterization t eeks eparation of the or of credit points successfully and v	and atomic force Nanoparticle cor to deterimine size ral presentation	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and <b>Requirement</b> All experiments <b>Module applic</b> Master of Scient <b>Weight of the</b> Weighted accord	he context of ele ic nanomaterial rsis hods week for 5-6 we writing and pre sment oral presentation for the award of are completed ability ce Chemistry mark for the finding to CPs inator and lect	ectrosynthesis. (6) characterization t eeks eparation of the or of credit points successfully and v inal score urer(s)	and atomic force Nanoparticle cor to deterimine size ral presentation	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			
testing also in t (7) Spectroscop in(electro)cataly <b>Teaching met</b> lab course a) 30 hours per b) 2-3 weeks for <b>Mode of asses</b> Lab report and of <b>Requirement</b> All experiments <b>Module applic</b> Master of Scien <b>Weight of the</b> Weighted accord <b>K.</b> Tschulik, W.	he context of ele ic nanomaterial sis hods week for 5-6 we writing and pre- sment oral presentation for the award of are completed cability ce Chemistry mark for the f ding to CPs inator and lect Schuhmann	ectrosynthesis. (6) characterization t eeks eparation of the or n of credit points successfully and v inal score urer(s)	and atomic force Nanoparticle cor to deterimine size ral presentation written up in a la	microscopy. (6) elect rosion and aggregat e- and shape-depend	tation (15 min)			



In-depth Pra	actical "Ele	ctrocatalysis	and Energy	Conversion"			
Module	Credits	Workload	Term	Frequency	Duration		
2.9	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester		
<b>Courses</b> Elective Course Elective Lecture	I-VI		Contact hours a) 30 h	Self-Study b) 60 h	Group size		
Prerequisites Basics in electroo	chemistry				-		
Learning outco The students sho optimization of r preparation proce students should voltammetry, im model electrolyze	Learning outcomes The students should gain an advanced theoretical and practical understanding of the characterization and optimization of materials for energy conversion and electrocatalysis. This contains knowledge of the preparation procedures as well as of the practical performance of electrochemical measurements. The students should learn to plan, perform and interpret electrochemical experiments including cyclic voltammetry, impedance spectroscopy, rotating disc and rotating ring-disk measurements, operation of						
<b>Content</b> Electrocatalysis: o electrodes fabrica	optimization of	f the activity of el talyst synthesis a	ectrocatalysts; cat nd characterizatio	alyst ink preparation,	gas diffusion		
Teaching meth	ods						
Lab course with							
a) 30 hours per w	veek for 5 to 6 v	weeks lab work					
b) 2 weeks for wr	riting of the rep	oort and preparat	ion of the oral pre	esentation			
Mode of assess	ment						
Lab report and or	ral presentation	1					
Requirement for All experiments a summarized in a	or the award of are completed a written report	of credit points successfully and Oral presentation	available in the el on (20 min)	ectronic lab book. Th	e results are		
Module applica	bility						
Master of Science	e Chemistry						
Weight of the n	nark for the fi	inal score					
Weighted accord	ing to CPs						
Module coordin	nator and lect	urer(s)					
K. Tschulik; W. S	Schuhmann						
Further inform	ation						



## Inorganic Chemistry

Bioinorganic	Chemist	rv I			
Module 3.1	<b>Credits</b> 5 CP	Workload 150 h	Term 1 <sup>st</sup> or 3 <sup>rd</sup> Sem.	<b>Frequency</b> Only WS	<b>Duration</b> 1 Semester
Courses a) Bioinorgani (Lecture and	c Chemistr l Seminar)	y I	Contact hours 3 SWS	<b>Self-Study</b> 105 h	Group size
<b>Prerequisites</b> Basic Understan	ding of gen	eral chemistry,	coordination of	hemistry and bioch	nemistry
Learning outcom After successful - A basic u - Knowled	nes completion inderstandi ge about th	of this module ng of the role o e structure, fur	e, the students l f metals in a b action and prop	have iological environme perties of metalloen	ent Izymes
The students are - Identify, - Find, rea Chemist	able to solve, and c ad, and crit ry	liscuss problen fically commen	ns related to th at on pertinen	e role of metal cent t literature in the	ers in biomolecules field of Bioinorganic
Content The lecture cover following: Occur homeostasis, me centers in biomo metalloenzymes metalloenzymes	rs classical l rrence of me etals as activ elecules, rea , activation (e.g. H <sub>2</sub> , O	bioinorganic ch etal ions and co re sites in metal ction mechanis and metabolism 2, N2, CH4, etc.)	nemistry topics ompounds in the lloenzymes, sp sms of metalloo n of small moleo.	, including but not ne environment, me ectroscopic charact enzymes, model co ecules by metal cen	restricted to the etal ion uptake and erization of metal mpounds for tters and
<b>Teaching metho</b> Lecture and Sem such as project d	<b>ds</b> linar with st lraft or gran	tudent contribu t application)	itions (e.g. pres	sentation, video, wr	itten contribution
Mode of assessm Written exam an	nent d grading o	f student contr	ibutions		
Requirement for Active participati	the award of ion in stude	of credit points ent contributior	n, successful co	mpletion of writter	n exam
Master Chemistr	ry, Master E ark for the f	iochemistry, N	laster Biology		
Weighted accord Module coordina	ing to CP ator and lect	turer(s)			
Nils Metzler-Nol Further informa	te, Ulf-Pete tion	r Apfel and Me	mbers of Inorg	ganic Chemistry I	

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Crystal Engineering – Chemistry beyond the molecule								
Module	Credits	Workload	Term	Frequency	Duration			
3.2	5 CP	150 h	2. Sem.	Each SuS	1 Semester			
Courses	•	·	Contact hours	Self-Study	Group size			
c) Lecture			c) 2SWS/30 h		Students of the			
d) Exercise			d) 1 SWS/15 h	105 h	respective			
semester, ca. 2								
<b>Prerequisites</b> After successfu behavior of sma	<b>Prerequisites</b> After successful completion of the module, students have a basic knowledge of the aggregation behavior of small organic molecules in crystal structures.							
Learning outco	mes							
After the succes	ssful completi	ion of the modu	ıle					
• Student	ts will have ad	vanced knowle	dge of supramolecu	ılar synthons, i	ntermolecular			
interact	tions, and the	design of crysta	al structures with s	mall organic mo	olecules			
• Student	ts will be able	to specifically d	lesign polymorphic	c forms as well a	as multi-			
compor	nent crystals b	ased on crystal	structure predictio	ns.				
Content								
<ul> <li>Aggregation</li> </ul>	ation phenom	ena of organic	molecules in solid	state (crystal pa	cking)			
• Crystal	Design Strate	gies with organ	ic molecules					
Strong	and weak inte	ermolecular Inte	eractions (focusing	most of lecture	s series)			
Supram	iolecular Synt	hons						
<ul> <li>Crystal</li> </ul>	Structure pre	diction (CSP)						
<ul> <li>Polymo</li> </ul>	orphism							
Multi-ce	omponent cry	stals						
<ul> <li>Applica</li> </ul>	tions							
Special	crystallization	1 techniques						
Teaching meth	ods							
Lecture with ex	ercises							
Mode of assess	ment							
end-of-term wr	itten exam an	d talks on selec	ted topics					
Requirement fo	or the award o	f credit points						
Passing the wri	tten examinat	tion and talks of	n selected topics					
Module applica	bility							
Chemistry (Ma	ster), IMOS							
Weight of the n	nark for the fi	nal score						
Weighted accor	aing to CPs							
Module coordin	lator and lect	urer(s)						
Dr. Klaus Merz								
Further information								



Module	Credits	Workload	Term	Frequency	Duration	
3.3	5 CP	150 h	$2^{nd}$ or $4^{th}$	Only SoS	1 Semester	
			Sem.			
Courses	1		Contact	Self-Study	Group size	
b) Medicinal Inorganic Chemistry			hours	105 h		
(Lecture	and Seminar)		3 5 8 5			
Prerequisites	3			<b>I</b>		
Basic Under	standing of gen	neral chemistry,	, coordination c	hemistry and bioc	hemistry	
Learning out	comes					
After success	ful completion	n of this module	e, the students l	nave		
- An a	dvanced under	standing of the	role of metal ic	ons in health and d	isease	
- Knov	vledge about tl	he most importa	ant metallodrug	s and their mode	of action	
The students	are able to					
- Ident	tify, solve, and	discuss probler	ns related to the	e role of metal con	pounds in health and	
disea	se					
- Find, read, and critically comment on pertinent literature in the field of Medicinal						
- Find,	read, and c	ritically comme	ent on pertine	nt literature in th	ne field of Medicina	
- Find Inorg	, read, and cr ganic Chemist	ritically comme ry	ent on pertine	nt literature in th	ne field of Medicina	
- Find Inorg Content	read, and cr ganic Chemist	ritically comme	ent on pertine	nt literature in th	ne field of Medicina	
- Find Inorg Content The lecture c	vread, and cr ganic Chemistr overs medicin	ritically comme ry al inorganic che	ent on pertiner	nt literature in th	estricted to the	
Find Inorg Content The lecture c following: Co	v read, and cr ganic Chemist overs medicin oncepts of drug	ritically comme ry al inorganic che g discovery and	ent on pertiner emistry topics, i development; F	nt literature in th ncluding but not r Health and disease	estricted to the	
- Find Inorg Content The lecture c following: Co homeostasis;	vers medicin overs medicin oncepts of drug Toxicity of me	ritically comme ry al inorganic che g discovery and etals and metal	ent on pertiner emistry topics, i development; F compounds; Sy	nt literature in th ncluding but not r Health and disease onthesis, properties	e field of Medicina estricted to the s in metal ion s and mode of action	
- Find Inorg Content The lecture c following: Co homeostasis; of metallodru	read, and cr ganic Chemist overs medicin oncepts of drug Toxicity of me ugs (e.g. metal	ritically comme ry al inorganic che g discovery and etals and metal complexes as as	ent on pertiner emistry topics, i development; F compounds; Sy nti-cancer drug	nt literature in th including but not r Health and disease withesis, properties s, as anti-infectives	ne field of Medicina estricted to the s in metal ion s and mode of action s, in	
- Find Inorş Content The lecture c following: Co homeostasis; of metallodru neurodegene	v read, and cr ganic Chemist overs medicin oncepts of drug Toxicity of me ags (e.g. metal trative diseases	ritically comme ry al inorganic che g discovery and etals and metal complexes as as s, etc.).	ent on pertiner emistry topics, i development; F compounds; Sy nti-cancer drug	nt literature in th ncluding but not r Health and disease mthesis, properties s, as anti-infectives	ne field of Medicina estricted to the s in metal ion s and mode of action s, in	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me	read, and cu ganic Chemist overs medicin oncepts of drug Toxicity of me ugs (e.g. metal trative diseases thods	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.).	emistry topics, i development; H compounds; Sy nti-cancer drug	nt literature in th including but not r Health and disease onthesis, properties s, as anti-infectives	estricted to the s in metal ion s and mode of action s, in	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S	read, and cr ganic Chemistr overs medicin oncepts of drug Toxicity of me ugs (e.g. metal erative diseases thods Seminar with s	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wi	estricted to the s in metal ion s and mode of action s, in	
- Find Inors Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje	read, and cr ganic Chemist overs medicin oncepts of drug Toxicity of me ags (e.g. metal erative diseases ethods Seminar with s ect draft or gran	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application)	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wi	ne field of Medicina estricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse	read, and cu ganic Chemistr overs medicin oncepts of drug Toxicity of me ugs (e.g. metal erative diseases thods Seminar with s ect draft or grad ssment	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application)	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres	nt literature in th including but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wi	estricted to the s in metal ion s and mode of action s, in	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exam	read, and cu ganic Chemists overs medicin oncepts of drug Toxicity of me ugs (e.g. metal erative diseases thods Seminar with s ect draft or gras ssment n and grading	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contr	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa	ne field of Medicina estricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inors Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exan Requirement	read, and cu ganic Chemistr overs medicin oncepts of drug Toxicity of me ags (e.g. metal erative diseases thods Seminar with s ect draft or grad sessment n and grading t for the award	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contr of credit points	emistry topics, i development; F compounds; Sy nti-cancer drug ations (e.g. pres	nt literature in th including but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa	ne field of Medicina estricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exan Requirement Active partici	read, and cr ganic Chemistr overs medicin oncepts of drug Toxicity of me ugs (e.g. metal erative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contri of credit points ent contribution	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, was mpletion of writte	ne field of Medicina estricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inorş Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exam Active partici Module appli Master Chen	read, and cu ganic Chemisti overs medicin oncepts of drug Toxicity of me ugs (e.g. metal rative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contr of credit points ent contribution	emistry topics, i development; H compounds; Sy nti-cancer drug utions (e.g. pres <u>ributions</u> <u>n, successful co</u> Master Biology	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa mpletion of writte	ne field of Medicina restricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inors Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exam Active partici Module appli Master Chem	vers medicin overs medicin overs medicin oncepts of drug Toxicity of me ags (e.g. metal erative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability nistry, Master	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contri- of credit points ent contribution Biochemistry, M final score	emistry topics, i development; H compounds; Sy nti-cancer drug utions (e.g. pres <u>ributions</u> n, successful co <u>Master Biology</u>	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa mpletion of writte	ne field of Medicina estricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inorg Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exan Active particit Module appli Master Chen Weight of the	read, and cr ganic Chemistr overs medicin oncepts of drug Toxicity of me ugs (e.g. metal erative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability nistry, Master e mark for the cording to CP	ritically comme ry al inorganic che g discovery and etals and metal complexes as an s, etc.). student contribu nt application) of student contri- of credit points ent contribution <u>Biochemistry, M</u> final score	ent on pertiner emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres <u>ributions</u> n, successful co <u>faster Biology</u>	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa mpletion of writte	ne field of Medicina restricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inorş Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exan Active partici Module appli Master Chen Weight of the Weighted aco	read, and cu ganic Chemistr overs medicin oncepts of drug Toxicity of me ags (e.g. metal rative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability nistry, Master e mark for the cording to CP dinator and lea	ritically comme ry al inorganic che g discovery and etals and metal complexes as an s, etc.). student contribu nt application) of student contri- of credit points ent contribution Biochemistry, M final score	emistry topics, i development; F compounds; Sy nti-cancer drug utions (e.g. pres ributions n, successful co faster Biology	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, was mpletion of writte	ne field of Medicina restricted to the s in metal ion s and mode of action s, in ritten contribution	
- Find Inors Content The lecture of following: Co homeostasis; of metallodru neurodegene Teaching me Lecture and S such as proje Mode of asse Written exan Active partici Module appli Master Chen Weight of the Weighted acc Nols Metzler	overs medicin overs medicin oncepts of drug Toxicity of me ags (e.g. metal erative diseases thods Seminar with s ect draft or grat ssment n and grading t for the award pation in stud icability nistry, Master e mark for the cording to CP dinator and lea	ritically comme ry al inorganic che g discovery and etals and metal complexes as a s, etc.). student contribu nt application) of student contri- of credit points ent contribution Biochemistry, M final score	emistry topics, i development; H compounds; Sy nti-cancer drug utions (e.g. pres <u>cibutions</u> <u>n, successful co</u> <u>faster Biology</u>	nt literature in th ncluding but not r Health and disease onthesis, properties s, as anti-infectives sentation, video, wa mpletion of writte	ne field of Medicina restricted to the s in metal ion s and mode of action s, in ritten contribution	





Main Grour	Chemist	rv. From Cui	riosities to (	Catalysis	
Module	Credits	Workload	Term	Frequency	Duration
	5 CP	150 h	1 <sup>st</sup> or 3 <sup>rd</sup>	Only WS	1 Semester
5.4	5.01	150 11	Sem.		i bennester
Courses			Contact	Self-Study	Group size
Main Group	o Chemistry: F	From Curiosities	hours	105 h	1
to Catalysis	(Lecture and	Seminar)	3 SWS		
Prerequisites					
Basic Understa	nding of gen	eral chemistry, o	organometalli	c chemistry and ca	talysis.
Learning outco	mes				
After successfu	l completion	of this module,	the students l	have a basic unders	standing
- of the r	eactivity of o	rganometallic co	mpounds of t	he s- and p-block e	lements
- of struc	cture reactivi	ty relationships	and application	ons in the activatio	on of small molecules
(H2, N2	, CO, CO2) a1	nd strong bonds	as well as in I	homogeneous catal	lysis.
The students ar	e able to				
- Identify	, solve, and	discuss problem	ms related to	the bonding situa	tion, properties and
reactivit	ty of s- and p	-block element o	compounds		0.11 0
- Find, r	ead, and crit	tically comment	t on pertinen	t literature in the	field of main group
chemis	try				
Content			1 1	a analan ah analatan	with former and the
I ne lecture cov	ers recent de	velopments in n	1 b an din a site	n group chemistry	with focus on the
Stabilization of	reactive spec	les with unusua	l bonding sitt	lations and applica	tions in catalysis.
I ne following t	opics may be	e coverea:	f 1 1 1	un bla alt alamant a	
- Synthes	inda includir	s and reactivities	s of iow-valent	t p-block element o	ompounds and
Synthese	unus incluun	ig ionnal eleme	nt multiple bo	onus. otal organylg and h	vdridog
- Synthes	on of strong	bonds and smal	l molecules w	rith main group cou	mounds including
differer	off of strong	ich as Friistrate	d Lewis pairs	and cooperative eff	ects as well different
mechar	isms le g ov	vidative addition	metathesis)		cets as well uniferent
- Applica	tions in hom	logeneous cataly	sis		
rippiicu		logeneous cutury	515		
The lecture will	particularly	focus on underl	ving concepts	(Structure-activity	relationships, acidity
and basicity, tre	ends in the p	eriodic table etc.	) and molecul	lar design strategies	S.
Teaching meth	ods			<u> </u>	
Lecture and ser	ninar with st	udent contribut	ions (e.g. pres	entation, video, con	mputational studies,
written contrib	ution such as	s project draft or	grant applica	tion)	
Mode of assess	ment				
Written exam a	nd grading o	of student contri	butions		
Requirement for	or the award	of credit points			
Active participa	tion in stude	ent contribution,	successful co	mpletion of written	n exam
Module applica	bility				
Master Chemis	try				
Weight of the n	nark for the f	inal score			
Weighted accor	ding to CP				
Module coordin	hator and lec	turer(s)	<b>C .</b>	1	
Viktoria Däschl	lein-Gessner	and Members o	t Inorganic C	hemistry II	
Further inform	ation				



Creen and S	Justainabla	Chamistry			
Module	Credits	Workload	Term	Frequency	Duration
3 5	5 CP	150 h	1 <sup>st</sup> or 3 <sup>rd</sup>	Only WS	1 Semester
5.5	5 01	150 11	Sem.	· · · · ·	i beinester
Courses	I		Contact	Self-Study	Group size
Green and Sus	stainable Cher	nistry	hours	105 h	1
(Lecture)			2 SWS		
Prerequisites	1. 6				
Basic Understa	nding of gene	ral chemistry			
Learning outcom	mes				
After successfu	l completion o	of this module,	the students h	nave	
- A basic	understandin	g of the princip	oles of green a	nd sustainable che	emistry
- Concep	ts for mechan	ochemistry as v	well as technic	al electrochemistr	У
- Implem	nentation of no	ew technologies	s in an industi	rial context	
71					
The students ar	e able to	11	1.1.	. • 11	
- Identify	, solve, and di	scuss problem	s related to su	stainable processes	S Cold of our out
- Find, r	ead, and crit	ically commen	t on pertinen	it literature in th	e field of green and
sustaina	able chemistry	/			
Content	ora chomistry	topica includi	a hut not roat	wisted to the fellow	ring The 10
nrinciples of gr	oon chomistry	topics, including	ant and nocos	ricled to the follow	and sustainable
principles of gr	tilization of g	olvent reduced	or froe chomi	sily to create green	and sustainable
chemical process	sees (includin	g Power to X p	or free cherring	ries /redox flow ba	tteries fuel cells etc.)
Teaching meth	ode	g I Ower-to-X p	iocesses, Dalle	lies/iedox-iiow ba	itteries, ruer cens etc.j.
Lecture	ous				
Mode of assess	ment				
Written or oral	exam				
Requirement fo	or the award o	f credit points			
Successful com	pletion of wri	tten exam			
Module applica	bility				
Master Chemis	try, Master Bi	ochemistry, Ma	aster Biology, I	Master Engineerin	g
Weight of the n	nark for the fi	nal score	07	0	0
Weighted accor	ding to CP				
Module coordin	nator and lectu	ırer(s)			
Lars Borchardt,	Ulf-Peter Apt	fel			
Further inform	ation				





In-depth pr	actical: Gre	en and Sust	ainable Cher	mistrv	
Modulo	Crodite	Workload	Term	Frequency	Duration
3.6	7 5 CP	225 h	1 <sup>st</sup> to 3 <sup>rd</sup>	WS and SoS	6 Weeks
5.0	7.5 CI	225 11	Sem.		0 WCCR5
Courses			Contact	Self-Study	Group size
Green ar	Green and Sustainable Chemistry		hours	65 h	Individual
(Lab practi	(Lab practical)		160 h		
V I	,				
Prerequisites			•	•	
Basic Understa	nding of gene	ral chemistry, i	norganic chemi	istry and analytical r	nethods
Learning outco	mes		0		
After successfu	l completion o	of this practical.	the students h	ave	
- Hands-	on experience	e in performin	g selected ana	lvtical methods fre	equently used and
runnin	g the respectiv	e instruments	ig sciected and	ilytical incurous in	equentity used and
- A pract	ical understan	ding of parame	ters defining g	reen and sustainable	e processes
11 prace		ang or parame			e processes
The students a	re able to				
- Apply s	uitable metho	ds to solve prol	plems or answe	r questions in the fi	eld
- Analyse	and profession	onally report / d	locument analy	tical data	
- Correla	te the princi	ples of green	chemistry to	individual problet	n sets and from
experin	nental data, an	d critically com	ment on those	Problem	
Content					
In this lab prac	tical. the stude	ents will identif	v and then perf	orm suitable experi	ments to answer
research questi	ons related to	a scientific pro	iect under the s	upervision of their 1	mentor. Typically.
the lab practica	l will involve f	irst the synthes	is of a new or k	nown compound or	: material or
reaction impler	nenting the p	rinciples of gree	en chemistry, a	nd then comprise ru	inning the
necessary expension	riments. The r	esearch topic w	vill be in the sci	entific (PhD or post	doc) project of the
supervisor, incl	uding but not	limited to area	s such as mech	anochemistry, catal	vsis and
electrochemisti	y.				, ,
Teaching meth	ods				
Lab practical					
Mode of assess	ment				
Written report,	typically in th	e form of a scie	entific publication	on	
Requirement for	or the award o	f credit points			
Active participa	ition in lab wo	rk, successful c	completion of w	ritten report	
Module applica	bility				
Master Chemis	try, Master Bi	ochemistry, Ma	ster Physics, M	aster Engineering	
Weight of the r	nark for the fi	nal score			
Weighted accor	ding to CP				
Module coordin	nator and lectu	ırer(s)			
All professors a	ind Independe	ent Group Lead	ers in Inorganie	c Chemistry	
Further inform	ation				



In-depth Pra	actical: Co	mputational	Chemistry	in Inorganic C	hemistry			
Module	Credits	Workload	Term	Frequency	Duration			
3.7	7.5 CP	225 h	$1^{st}$ to $3^{rd}$	WS and SoS	6 Weeks			
5.7			Sem.					
Courses	•	•	Contact	Self-Study	Group size			
Computati	onal Chemis	try	hours	65 h	Individual			
(Lab/office	practical)	,	160 h					
Prerequisites Basic Knowledg	<b>Prerequisites</b> Basic Knowledge of Theoretical Methods and computer skills							
Learning outco	mes		F					
After successfu - Hands- used to - A basic comput The students an	<ul> <li>Learning outcomes</li> <li>After successful completion of this practical, the students have <ul> <li>Hands-on experience in performing the current state-of-the-art computational methods used to theoretically model molecular and/or solid systems.</li> <li>A basic practical understanding of computational chemistry and the application of computational methods and programs</li> </ul> </li> <li>The students are sheats.</li> </ul>							
- apply st	ate-of-the-art	computational	methods used	l to theoretically mo	del molecular			
and/or - analyse question - search t to the s	solid systems , interpret an n. he literature tate-of-the-ar	s. .d document co , related to the g t.	mputational re	esults to answer a gi question, and relate	ven research their research results			
Content								
In this practical relationships an UNIX type envi- be trained in ap of - density - force fie molecu method spectros - Machin These computa research projec organometallic <b>Teaching meth</b>	<ul> <li>to the state-of-the-art.</li> <li>Content In this practical, the students will perform theoretical calculations to deduce structure-activity relationships and understand chemical properties and reactivities. They will learn how to use a UNIX type environment, edit input files and visualize chemical systems. Furthermore, they will be trained in applying different computational methods. Topics my include for example the use of <ul> <li>density functional theory approaches to elucidate reaction profiles and bonding situations</li> <li>force field calculations of inorganic systems including structural optimizations and molecular dynamics, first principles calculations with DFT or wave function based methods for molecular systems and extended solids (structural analysis and/or spectroscopic properties like normal modes). <ul> <li>Machine learning methods to quantitatively describe structure activity relationships</li> </ul> These computational methods are applied within a scientific context, connected to the current research projects of the supervisor, including but not limited to materials chemistry, connected to the supervisor.</li></ul></li></ul>							
Computational	practical							
Mode of assess	ment							
Written report	typically in t	he form of a sci	entific publica	tion				
Requirement fo	or the award	of credit points	pablica					
Active participa	tion in com	utational work	successful co	mpletion of written	report			
Module applica	hility		, 54000514100					
Master Chemis	trv							
Weight of the n	<u>uy</u> nark for the f	inal score						
Weighted accor	ding to CP							
Module coordin	uning in Cl	turor(s)						
Prof Dr Doch	is Schmid D	rof Dr Vilstori	n Däschlein C	acenar				
FIOL DI. KOCHU	ation		a Dascillelii-Ge	2551101				
r urmer inform	at1011							





In double and		aal Masha da in	In an anti- Ch				
In-depth pract	Credits	Cal Methods In Workload	Term	Frequency	Duration		
3.8	7.5 CP	225 h	1 <sup>st</sup> to 3 <sup>rd</sup>	WS and SoS	6 Weeks		
5.0			Sem.				
Courses		·	Contact	Self-Study	Group size		
Analytical	Methods	in Inorganic	hours	65 h	Individual		
Chemistry	(Lab practica	1)	160 h				
Prerequisites							
Basic Understa	nding of gen	eral chemistry, i	norganic chemi	istry and analytical	methods		
Learning outco	mes						
After successfu	l completion	of this practical,	, the students h	ave			
- Hands-	on experient	ce in performin	ng selected an	alytical methods	frequently used in		
inorgar	nic chemistry,	, and running th	e respective ins	truments			
- A pract	ical understa	nding of analytic	al methods in i	norganic chemisti	У		
The students a	re able to						
- Apply s	suitable analy	rtical methods t	to solve problem	ms or answer que	estions in inorganic		
chemis	try						
- Analyse	e and professi	ionally report / c	locument analy	tical data			
- Deduce	e structure an	d properties from	m analytical dat	a, and critically co	mment on those		
Content			· 1.1 C				
In this lab prac	tical, the stud	lents will identif	y and then perf	orm suitable analy	tical experiments to		
answer researc	n questions r	elated to a scient	tific project und	ler the supervision	of their mentor.		
Typically, the la	ab practical w	ill involve first ti	ne synthesis of a	a new or known co	mpound or		
advanced apost	romotorg or o	ther equipment	The recess	ary analytical expe	aciontific (DhD or		
auvaliceu speci	t of the super	nier equipment	but not limited	to aroas such as r	scientific (PhD of		
chemistry org	nometallic or	r coordination cl	peristry cataly	sig or materials of	reen and medicinal		
inorganic chem	nistry		lielilistiy, cataly	sis, of materials, g			
Teaching meth	nstry.						
Lab practical	Jous						
Mode of assess	ment						
Written report,	typically in th	ne form of a scie	entific publication	on			
Requirement for	or the award o	of credit points	<b>r</b>	-			
Active participa	Active participation in lab work, successful completion of written report						
Module applica	bility	·	1	1			
Master Chemis	stry, Master B	iochemistry					
Weight of the r	nark for the f	inal score					
Weighted accor	rding to CP						
Module coordin	nator and lect	urer(s)					
All professors a	and Independ	ent Group Lead	ers in Inorganio	c Chemistry			
Further inform	Further information						



In-depth Pra	actical: Bioind	organic Chemi	stry					
Module 3.9	Credits 7.5 CP	Workload 225 h	Term 1 <sup>st</sup> to 3 <sup>rd</sup> Sem.	<b>Frequency</b> WS and SoS	Duration 6 Weeks			
Courses Bioinorg (Lab pra	ganic Chemistr ctical)	у	Contact hours 160 h	Self-Study 65 h	<b>Group size</b> Individual			
Prerequisites Pagic Understanding of general chemistry, increasic chemistry and biochemistry								
Learning out After success - Hand used - A bas	comes ful completior ls-on experience in bioinorgani sic practical un	n of this practica ce in performin c or medicinal i derstanding of	al, the students g chemical syn inorganic chem bioinorganic cl	have thesis and analytica nistry nemistry	l methods typically			
<ul> <li>The students are able to</li> <li>Synthesize compounds of bioinorganic interest and analyze their properties (including biological), or otherwise study a biological system of interest to bioinorganic chemistry</li> <li>Analyse and document analytical data to deduce the answers to a given research question in bioinorganic chemistry</li> <li>Search the literature related to the given research question, and critically comment on the regulta</li> </ul>								
<b>Content</b> In this lab practical, the students will perform chemical synthesis, analytical measurements, or otherwise lab experiments (e.g. including cell biology or microbiology work) as part of an ongoing research project in the broad area of bioinorganic chemistry. Data will be analyzed to deduce structure-activity relationship, and compared to published scholarly information. The research topic will be in the scientific (PhD or postdoc) project of the supervisor, including but not limited to areas such as organometallic or coordination chemistry, catalysis, enzyme or medicinal inorganic chemistry.								
<b>Teaching me</b> Lab practical	thods							
Mode of asse Written repor	<b>ssment</b> rt, typically in t	the form of a sc	ientific publica	tion				
Requirement for the award of credit points Active participation in lab work, successful completion of written report								
Module appli Master Chem	cability	Biochemistry						
Weight of the Weighted acc	e mark for the cording to CP	tinal score						
Module coore	dinator and lects and Indepen	t <b>urer(s)</b> dent Group Lea	ders in Inorga	nic Chemistry				
Further infor	mation							

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In-depth Practical: Molecular Chemistry and Synthesis							
Module	Credits	Workload	Term	Frequency	Duration		
3.10	7.5 CP	225 h	Sem	w 5 and 505	6 Weeks		
Courses			Contact	Self-Study	Group size		
Molecular	Chemistry a	nd Synthesis	hours	65 h	Individual		
(Lab practi	ical)		160 h				
Prerequisites	u din a of ann	anal ala anai atmu	:	بمناعدت ويتروك ويتبع	, ma atla a da		
Learning outco	mang of gen	ierai chemistry,	inorganic che	mistry and symmests	s methods		
After successfu	ll completion	of this practica	1 the students	have			
- Hands-	on experienc	re in performing	r, the students o chemical syn	thesis by methods f	requently used in		
inorgar	ic chemistry	, and suitable n	ethods of cha	racterization of the i	new compound or		
materia	l energy	, 4114 20114210 1			ion compound of		
- A pract	ical understa	nding of synthe	esis methods in	n inorganic chemist	ry		
The students a	re able to						
- Synthes	size new ino	rganic chemistr	у		<u>.</u>		
- Analyse	e and docum	ent analytical da	ata to establish	identity and purity	of inorganic		
compot	unds and ma	terials	• 11 .1	• .1 1 1	·.· 11 .		
- Search	the chemica	I literature for s	suitable synthe	esis methods, and ci	ritically comment on		
Content							
In this lab prac	tical the stu	lents will perfo	rm chemical s	unthesis of known o	r new compounds		
or materials as	part of an or	igoing research	project. Identi	ity and purity of the	product will be		
established by s	suitable meth	nods. and the pr	operties of the	e new compound / n	naterial will be		
analyzed. The r	esearch topi	c will be in the s	scientific (PhD	or postdoc) project	of the supervisor,		
including but n	not limited to	areas such as r	nain group cho	emistry, organometa	llic or coordination		
chemistry, cata	lysis, or mate	erials, green and	d medicinal in	organic chemistry.			
Teaching meth	ods						
Lab practical							
Mode of assess	ment						
Written report,	typically in t	he form of a sci	entific publica	ition			
Requirement fo	or the award	of credit points	1	· ·			
Active participa	110n 1n lab w	ork, successful	completion of	written report			
Module applica	ID111ty	Diachomistry					
Waster Chemis	nark for the	final score					
Weighted accor	rding to CP	linal score					
Module coordi	nator and lec	turer(s)					
All professors a	and Independ	lent Group Lea	ders in Inorga	nic Chemistry			
Further inform	ation	eroup deu					



Module	Credits	Workload	Term	Frequency	Duration	
3.11	13 CP	450 fi			5 Months	
Courses	<u>C</u> 1		Contact	Self-Study	Group size	
Inorganic	Chemistry		hours	130 h	Individual	
(Lab practical) 320 h						
Prerequisites						
Advanced Un	derstanding o	f Inorganic Che	emistry, includi	ng synthesis and ar	halytical methods	
Learning outc	omes					
After successf	ul completion	n of this practica	al, the students	have		
- Advan	ced expertise	in inorganic ch	emistry, includ	ing synthesis, analy	rtical or	
compu	utational meth	rods as applical	ole to the projec	t		
- A goo	d practical uno	derstanding of i	inorganic chem	iistry		
The students :	are able to					
- Search	1 the chemical	l literature for s	uitable method	s to address a giver	problem	
- Select	suitable meth	nods and plan th	neir research to	solve the given pro	blem	
- Execu	te their resear	ch independent	tly, but under s	upervision of a mer	ntor	
- Profes	sionally analy	vse and docume	nt their data ac	cording to the estab	lished scholarly	
standa	irds in inorga	nic chemistry				
Content						
The research	practical will b	pe performed as	s part of an ong	oing research proje	ct, forming by itself	
a small indepe	endent project	t. Content will i	nclude a literat	ure search, identific	ation and	
application of	suitable meth	ods (e.g. synthe	esis, analytical,	computational), an	d independent	
execution of tl	ne work, in clo	ose interaction	with the superv	isor / mentor. The	research topic will	
be in the scier	itific project o	of the supervisor	r, including but	not limited to area	s such as main	
group chemis	try, organome	etallic or coordin	nation chemistr	y, catalysis, or mate	erials, green and	
medicinal ino	rganic chemis	stry.				
Teaching met	hods					
Lab practical						
Mode of asses	sment					
Written repor	t, typically in t	the form of a pr	oject proposal			
Requirement	for the award	of credit points	completion of	writton roport		
Active particip	-alion in lab w	ork, successiui	completion of	witten iepoit		
Module annli	aunity					
Module applic	stry Master I	Riochemistry				
Module applic Master Chem	istry, Master I	Biochemistry				
Module applic Master Chem Weight of the	istry, Master I mark for the	Biochemistry final score				
Module applic Master Chemi Weight of the Weighted acco	istry, Master I mark for the ording to CP	Biochemistry final score				
Module applic Master Chem Weight of the Weighted acco Module coord All professors	istry, Master I mark for the ording to CP inator and lec	Biochemistry final score turer(s)	ders in Inorgan	nic Chemistry		



## Biochemie

Introduction to Bioinformatics							
Module	Credits	Workload	Term	Frequency	Duration		
And Course       a) Lecture: Introduction to Bioinformatics       b) Computer Practical: Introduction to Bioinformatics			Contact hours 28 h	Self-study 122 h	a) unlimited b) maximum 40 students in parallel sessions		
Prerequisites: Knowledge of h	Prerequisites: Knowledge of basic concepts of Biochemistry, Genetics and Molecular Biology lectures						
Learning outco In this combine Bioinformatics interpretation of prediction meti- techniques. Th strong focus lie enabling the str to make use of laboratory work <b>Content</b> a) Lecture Introduce Genomes Database Binary Se Local Ali Global M Molecula Molecula Molecula Database Validatio Phyloger Structure RNA ana Machine b) Exercise and Database Virtual C Phyloger Transcrij Validatio Structure Molecula	mes ed lecture/pra . The topics co of 3D structure hods for RNA e algorithmic es on the exten- udent to becon- them for the tec- tion and Overs s and Genome es I – Literatur equence Com- gnmentsLocal fultiple Seque- tr Dynamics S ar Dynamics S ar Dynamics S ar Dynamics S ar I - Protein n of ProteinSt and some ly sis -Transcri- Learning in E . Computer Pro- es cloning hetic Analysis production ar pynamics S ar Dynamics S	ctical module the wered range from ess of proteins. S and proteins, be principles are te sision of theoretic ne familiar with heoretical plant cts are further essent view of Bioinfor e Analysis – New e Search - Virtue parison and Global Alian ince Alignments imulation II – S Structure Base ructures and Gene Findin aptome Analysis Gioinformatics actical	ne students are om basic sequer strong emphasis eing also compleached as neces ical knowledge to h tools available ning and experi- engrossed by the cmatics st Generation Second al Cloning gnments - Moti sualization of p Structure Predic - Visualization	introducted to the bace analysis to the visit is given to classical lemented to novel and sary for a basic under to development of profiles of charge from mental interpretation exercises and complex from the profiles of Proteins using of Biomolecules	asic concepts of sualization and l structure ctifical intelligence erstanding. A ractical skills, the internet, and on of their own <u>puter practicals.</u>		

Master of Science Chemistry (M. Sc. Chemistry)



b) Exercises and Computer Practical. Home work on selected assignments and supervision of
script-based practical work at the computer pool of the university
Mode of assessment
Written exam
Requirement for the award of credit points
Passing the exam
Module applicability
Master of Science Biochemistry, also open to M. Sc. students of Stem Cell Biology, Applied
Informatics, Physics, Medical Physics, and to B. Sc. students of Biology
Weight of the mark for the final score
Weighted by CP
Module coordinator and lecturer(s)
M. Lübben, R. Stoll, T. Rudack, A. Mosig
Further information

Further information

AKULTÄT FÜ aster of Scien	R CHEMIE UND ce Chemistry (M	<b>BIOCHEMIE</b> I. Sc. Chemistry)		RUHR UNIVE BOCHU	IRSITÄT RU
Biochemi	strv III				
Module 4.2	Credits 5 CP	<b>Workload</b> 120 h	<b>Term</b> 5. Sem.	<b>Frequency</b> nur WS	<b>Duration</b> 1 Semester
<b>Courses</b> Biochemistr	y III (184500)		Contact hours 32 h	Self-Study 88 h	<b>Group size</b> ca. 55 students
Prerequisite none	S				
Learning outo The lecture is that play a ro Furthermore cell cycle reg participants simultaneous have an over English-lang	omes imparts knowled ole in the expre- e, the regulator gulation and the are introduced asly showing Ge- view of the reg- guage terms of	edge about the c ssion of genetic y mechanisms of e molecular base to the scientific erman-language ulatory mechan biochemistry.	omplex regula information f of the targeting is of the immu alanguage Eng e slides. After of isms in eukary	tory processes spec rom the chromoson g of proteins transp ine system are taug lish by using the E completing the lect yotes and an under	tific to eukaryotic cells me to the mRNA. Forted within the cell, wht. In addition, the nglish language while ure, the participants standing of the basic
Content The lecture of Structure of Chromosof Replication topoisomera Recombina gene conve Transposal TY, Drosop Reassociati repetitive I Transcripti RNA class RNA polyn RNA polyn binding pr RNA polyn binding pr RNA polyn splice varia Ribozymes Regulation modular tr Translocati of membra Cell cycle: p	deals with the c of eukaryotic ce me structure: p in eukaryotes: ses, telomera ation mechanis ersion, transgen ole elements: p <i>bhila</i> FB elemer ion of nucleic a DNA on in eukaryot es nerase I: riboso nerase II: gene oteins, zinc fin nerase II: prom ants : self-splicing i of gene express ranscription fac ion of proteins; ane proteins, in phases of the co ystem: immuno	complex regulate lls: differences to olyteny, nucleos mechanism, D se ms: DNA repain nic animals seudogene and nts cids: stability of es: nuclear struc- mal RNA, prome estructure, tRN ger proteins, leu noter structure, 1 ntrons, ribozym sion: transcript stors, 2-hybrid sy signaling hypo nport into organ ell cycle, cyclins e cells, antibody	ory mechanism to prokaryotes, somes, chroma NA polymeras r, heteroduples processed gen double-strand cture, transpor noter, processi A structure, pr ucine zipper, r RNA capping, nes, tetrahymen ion initiation, o ystem, steroid thesis, SRP, do nelles , CDKs, regula structure, ant	ns in eukaryotes: organelles atin structure ses, DNA topology, a, Holliday structur es, transposons, re- led nucleic acids, T t through nuclear p ng, nucleolus comoter structure, I egulation of transc: polyadenylation, sp na, RNase, editing of enhancer/silencer, receptors ocking proteins, int tion ibody diversity, T co	e, recA protein, troposons, yeast m value, pores, capping, DNA ription factors bliceosome, of RNA regration
Compleme     Teaching me	ecules ent system: com ethods	nplement activat	tion, amplifica	tion cascade, MAC	
Lecture	· · · ·				
Mode of asse Written exar	e <b>ssment</b> n				
<b>Requiremen</b> Passing the	<b>t for the award</b> exam	of credit points			

RUHR

Master of Science Chemistry (M. Sc. Chemistry)



Biochemistry IV - Biochemistry of Membrane Receptors									
Module	Credits	Workload	Term	Frequency	Duration				
4.3	7 CP	210 h	2nd	only summer	1 semester				
			semester	term					
Courses			Contact	Self-Study	Group size				
Biochemistry	IV – Biochem	istry of	hours	182 h	45 students				
Membrane Re	ceptors (1858	20)	28 h						
Prerequisites									
Familiarity wi	Familiarity with the contents of the Bachelor studies course lectures Biochemistry 0, I, II, and III.								
Learning outco Students will g structure-funce receptors are of different signal Students are s have for cell p and understar reference will considered cru Content • Cell-cell co	omes gain an overvi tion relations connected to I transduction upposed to gr hysiology and d basic conce be made to th ucial for an in-	ew of the variou hips, and the int A further focus v n pathways as we asp the wide-ran the organism as pts in biochemis ose basic concep depth understan	s membrane rec rracellular signa will be on under ell as the regula nging implicatio s a whole. Furth stry. In the cont ots of previous 1 nding of the prin	ceptors and ion cha l transduction path standing the interp tory principles gove ons that signal trans ermore, students a ext of the specific t ectures (Biochemis nciples of biochem	nnels, their ways these blay between erning them. sduction pathways re expected to learn opics listed below, etry I-III) that are istry.				
<ul> <li>gap junctio</li> <li>Cell-cell ac endothelial tenascin. In from withi fertilization</li> <li>Voltage-act currents, p technique.</li> <li>Presynaptio complex fo</li> <li>Ligand-acti transcriptio modulation acetylcholin</li> </ul>	ns. Ihesion: Cell cells, extrace ntegrin recept n the cell, re- ivated ion ch ootassium cu c function an rmation, fusio vated ion cha onal modifica a, molecular co ne release, por	migration, N-0 llular matrix pro ors: MIDAS mo gulation of the nannels: Resting rrents, action p d vesicle releas on pore formation nnels: Glutamations, structure prrelates of mem- re opening. GAE	CAMs, cadherin oteins: FGF, cho otif, I-domain, s cytoskeleton, fo g membrane p potential; single e: Life cycle of on, NSF and SN te receptors (NN -function relation ory formation, I BA and glycine r	ns, selectins, integondroitin sulfate, la ignal transduction; ocal adhesion kina otential, signal pre e channel conduct a vesicle, vesicula ARE complex disso MDA, kainate, AM onship, ligand bir LTP. Acetylcholine eceptors: structure	grins, activation of aminin, fibronectin, integrin regulation se, function during copagation, sodium tivity, patch clamp ar proteins, SNARE blution. PA receptors), post- nding site, receptor receptors: structure, and function.				
Structure of structure of postsynapt	of the synaps f the nerve-r c potentials	<b>e:</b> Presynaptic nuscle synapse,	chemical vs. e	le release, postsyr electrical synapses	aptic organization, EPSPs, miniature				



- **Signal transduction pathways:** Introduction, protein kinase A, structure-function relationship in the catalytic center.
- **Receptor protein tyrosine kinases**: Subclasses. Insulin receptor and FGF receptor: extra- and intracellular domains, heparin, EGF-receptor, PDGF receptor. Signaling modules SH2 domain, SH3 domain, TRK and GDNF receptors. Protein-protein interaction domains: SHC-GRB2, IRS-1, protein tyrosine phosphate binding domain (PTB), pleckstrin homology domain (PH), phospholipase C-g.
- **Signal transduction of cellular survival:** PI-3 kinase: P85 subunits, a, b, g, d subunits, catalytic subunits; Bcl-2 protein family: Bcl-xl, Bak; Ras protein, MAP kinase; serine-threonine kinases: TGF-b receptors, structure of the cytoplasmic domain, comparison to PKA, SMAD.
- Phosphotyrosine phosphatases: Mechanism, PTP-BL, PDZ domains, catalytic center
- Non-receptor tyrosine kinases: Src kinase family, structure-function relationship.
- Cytokines: Families I through IV of cytokine receptors. Class I: growth hormone, erythropoietin, and prolactin receptors, janus kinases (JAKs), STATs, IL-6 receptor family: signal transduction, II-2 receptor family, gene therapy. Class II: Interferon alpha (ligand), signal transduction of the interferon alpha receptor. Class III: Tumor necrosis factor receptor family (p55), TRAFs, TRADD, FAAD, RIP, death domain (Fas, TNFRI, p75NTR), caspases (9.3.I), and their inhibition. Class IV: Interleukin-I receptor, IRAP.
- Seven-transmembrane receptors/G proteins: (GPCRs): Classification, GTP-ase cycle, transducin, regulation of GDP/GTP exchange activity, rhodopsin, regulation of guanylate cyclase, calcium-dependent proteins, Ca/calmodulin, arrestin, photo transduction, G proteins

Teaching methods
Lecture
Mode of assessment
Written exam
Requirement for the award of credit points
Passing the exam
Module applicability (in other studies courses)
Weight of the mark for the final score
Weighted by CP
Module coordinator and lecturer(s)

M. Hollmann, T. Günther-Pomorski, S. Neumann

#### Further information

The PowerPoint slides shown are available on disc and/or deposited in the corresponding Moodle course. Note-taking during lectures is encouraged. Independent post-preparation of module contents as well as independent consultation of course material is recommended to prepare for the exam.



1/10/4/14/11				Eroquerer		
Module	Credits	Workload	1 erm	Frequency	Duration	
4.4	16 CP	480 h	Tst semester		1 semester	
Courses		C	Contact	Self-Study	Group size	
Four modulat	r practicals fro	m four	hours	224 h	1–4 students	
different foca	I points. The i	ndividual	256 h			
courses offere	ed are listed of	n the following				
pages.						
Prerequisites						
none						
Learning outo	comes					
Students lear	n advanced te	chniques applied	in research lab	s of the different	focal points involved	
in the studies	course as wel	I as theoretical a	spects of the top	oics investigated i	in these labs.	
Details on the	e learning out	comes of the ind	ividual courses o	can be found on	the following pages.	
Content						
See individua	l course descr	iptions.				
Teaching me	thods					
Practical						
Mode of asses	ssment		<u> </u>			
Varies betwee	en courses, us	ually active and s	successful partic	ipation in the pr	actical and either a	
written projec	t report, a pre	esentation or a po	ster to present	the results of the	practical. Details for	
each individu	al course can	be found on the	tollowing pages.	•		
Requirement	tor the award	of credit points				
See individua	l course descr	iptions.				
Module appli	<b>cability</b> (in oth	er studies cours	es)			
Weight of the	mark for the	final score				
Each of the fo	ur courses we	eighted by its CP	s (4 CP for each	course)		
Module coord	linator and lec	cturer(s)				
Module coord	linator: I. Diet	zel-Meyer				
Lecturers: See individual course descriptions.						
Further information						



Research Practical in the Focal Point Programme								
Module	Credits	Workload	Term	Frequency	Duration			
4 5	14 CP	420 h	3. Sem.	WS	1 Semester			
Courses	11 01	120 11	Contact	Self-Study	Group size			
a) Lab course			hours	Self Study	Individual			
b) Seminar			a) $3 \times 16h$	196 h	training			
,			b) $1 \times 16 h$	17011	0			
Droroquigitog								
Both Advanced F	Practicals of Ma	ster semester 2 h	ave to be passed					
Learning outco Students, coache a topic that is lin system. Students thus practicing e experimental dat Finally, they sho practicing how to they will develop written in the sty described as prel volume, which sl exposé is graded	mes d by their chose ked, in the wide then proceed t xperimentation a. Finally they p w their data in t present experi- their Research le of a regular I iminary work. The hould be around by the supervise	en supervisor, are est sense, to the l o carry out the est in a research lab practive how to w the lab seminar o mental data to an Practical topic in DFG grant propo The work program d 10 pages (half t or to provide the	e expected to lear piochemistry and operiments indep operiments indep operite a protocol the of their supervisor of audience. They not a Master thesi sal, with the worl mme should com he size of a regul grade for the Res	n how to plan a re molecular neurol endently over the perly evaluate and at contains all nec in an oral or post also write a Maste s project. This Ma c done during the prise at least one ar DFG grant pro- search Practical.	esearch project related to piology of the nervous course of one semester, document essary information. ter presentation, thereby er exposé detailing how aster exposé is to be Research Practical third of the total exposé posal). The Master			
<b>Content</b> Research projects are provided by the members of the Focal Point Programme "Biochemistry of the Nervous System". Topicwise, any current research question within the wide area of the biochemistry of the nervous system, neurobiochemistry, or molecular neuroscience can be offered as a project Seminar: Students participate in the seminars of the research group of their practical supervisor, and at the end of								
Teaching meth	ods							
Lab course and S	Seminar							
Mode of assess	ment							
A protocol, and a	Master exposé	in the style of a 1	DFG grant applic	ation, which is lin	nited to 10 pages			
Requirement for	or the award o	f credit points	~ **		* *			
The protocol and the Master exposé have to be submitted and accepted								
Module applica	bility			*				
Master of Scienc	e Biochemistry;	; Master of Scien	ce Chemistry					
Weight of the n	nark for the fi	nal score						
Weighted accord	ing to CPs							
Module coordin	nator and lectu	ırer(s)						
All members of t	he Focal Point	Programme "Bio	chemistry of the	Nervous System"				
Further inform	ation							
Г



### Funktionale Materialien

Materials Synthesis: Fundamentals and Applications of Modern Processing							
Routes for Creating Functional Materials							
Module	Credits	Workload	Term	Frequency	Duration		
5.1	5 CP	150 h	1, 2, 3, Sem.	Each SuS	1 Semester		
Courses			Contact hours	Self-Study	Group size		
e) Lecture			e) 2SWS/30 h		Students of the		
f) Exercise	as seminars		f) I SWS/15 h	65 h	respective		
,			, , , , ,	-	semester, ca. 50		
Prerequisites Admission to M physical chemis	Master Course stry).	e Program: Bas	sic knowledge in c	hemistry (inor	ganic, analytical and		
Learning outcom	mes						
After the succes	ssful completi	on of the modu	ıle				
<ul> <li>Student</li> </ul>	s will have ad	vanced knowle	dge on processing	of functional m	naterials, material		
properti	ies and advan	ced technologic	cal applications				
<ul> <li>Student</li> </ul>	s will be able	to apply their k	nowledge on curre	ent research top	oics in processing of		
advance	ed functional i	materials					
Define	topics for rese	arch projects in	n the field of mater	ials chemistry			
Content							
<ul> <li>Fundan</li> </ul>	nental princip	les in materials	s processing				
<ul> <li>Theoret</li> </ul>	ical models fo	or prediction of	material formation	n and propertie	S		
<ul> <li>Mechan</li> </ul>	nism of mater	ials processing	via solid-state and	gas phase proc	essing		
Routes	to material sy	nthesis: wet ch	emical processes, p	precursor route	s, metal vapor and		
gas pha	se synthesis						
<ul> <li>Materia</li> </ul>	ls characteriz	ation to elucida	te structure, morp	hology, compos	sition		
<ul> <li>Applica</li> </ul>	tion: Case stu	dies					
Teaching metho	ods						
Lecture with set	minars						
Mode of assess	ment						
End-of-term wr	itten exam						
Requirement for	or the award o	f credit points					
Passing the wri	Passing the written examination and talks on selected topics						
Module applicability							
Chemistry (Mas	Chemistry (Master), Materials Science and Simulation (MSS-ICAMS)						
Weight of the n	nark for the fi	nal score					
Weighted according to CPs							
Module coordin	Module coordinator and lecturer(s)						
Anjana Devi							
Further inform	ation						



Introduction to Chemistry of Materials (lecture series)							
Module	Credits	Workload	Term	Frequency	Duration		
5.2	5 CP	150 h	1, 3	Each WS	1 Semester		
Courses			Contact hours	Self-Study	Group size		
g) Lecture	series		g) 150 h	,	Students of the		
h) Guest lectures, colloquia				respective			
,				.,	semester, ca. 40		
Prerequisites				•			
Admission to	Master Cour	se Program: Ba	asic knowledge of	general, inorg	anic, and analytical		
chemistry, run		incage on mate	ind synthesis and	properties.			
Learning outco	mes						
The put	rpose of this :	module is to far	niliarize students v	vith important เ	out selected		
example	es of advance	d materials and	issues relating to t	heir advantages	, disadvantages and		
limitati	ons		-	-	-		
Guiding	g the student	s to get an overv	view of various inte	rdisciplinary re	search topics		
ranging	g from materi	als synthesis to	their properties an	d applications	-		
• The mo	dule will pro	vide a knowledg	e basis and orienta	tion for the stu	dents to choose		
from th	e various ele	ctive courses off	ered within the Fo	cal Point Functi	onal Materials;		
student	s communica	ate and discuss	with active scientis	ts (e.g. ''colloqu	ia'', guest lectures).		
Content							
A series	s of topics in	the field of Fun	ctional Materials ar	e covered by th	is overarching		
module	. The team te	eaching covers to	opics that bridge ch	emistry and pr	ocessing of		
materia	ls for techno	logical application	ons with an empha	sis on solid stat	e materials		
Fxampl	es are drawn	from industrial	practice in semico	nductor manuf	acturing protective		
coating	s energy gen	eration and stor	age to emerging to	echnologies suc	h as hatteries		
sensors	electronic d	evices antifouli	ng coatings etc	cerinologies suc	ii as batteries,		
<ul> <li>The det</li> </ul>	ailed content	s of this module	will be composed	from selected r	esearch areas		
current	ly including t	be following:	e will be composed	fioni sciected i	cscarcii arcas		
Son	niconductor	electronic and o	ntoelectronic mate	rials: processing	a and application		
	soporous mat	terials for cataly	sis and sensors	riais. processing	g and application		
> Pro	tective coatin		sis and sensors				
> Mat	terials for ene	ergy conversion	and electrochemic:	al sensing			
Teaching meth	ods						
Lecture with se	minars						
Mode of assess	ment						
End-of-term wr	ritten exam						
Requirement for	or the award	of credit points					
Passing the wri	itten examina	tion					
Module applica							
Chemistry (Ma	ster)						
Weight of the mark for the final score							
Weighted accor	Weight of the fillar to CDs						
Module coordin	nator and lect	uror(s)					
Aniana Davi A	vel Rosenhal	unci (s) n Eardi Schütt	Kristing Techulik				
Further informer	ation		i, ivitsuita 18011011K				
r ui uier iiiiorm	ativii						



In-depth prac	ctical: Solid	State and Ma	terial Synthe	sis			
Module	Credits	Workload	Term	Frequency	Duration		
5 3	7 5 CP	225 h	$1^{st}$ to $3^{rd}$	WS and SoS	6 Weeks		
5.5	7.5 GI		Sem.		o weeks		
Courses		I	Contact	Self-Study	Group size		
Analytical	Methods	in Inorganic	hours	65 h	Individual		
Chemistry	(Lab practical	)	160 h				
	V I	,					
Prerequisites							
Basic Understa	nding of gene	ral chemistry, i	norganic and n	naterials chemistry	and analytical		
methods	0 0	·	C		·		
Learning outco	mes						
After successfu	l completion	of this practical,	the students				
	F	<b>F</b>					
- will be	able to indepe	ndently apply o	r transfer mate	rials synthesis skil	ls and methods to		
other so	cientific conte	xts which may l	be connected w	ith or dependent of	n materials		
chemis	try.	,		1			
- Hands-	on experience	in performing	selected mater	ial synthesis via sol	id state, vapor phase		
or wet o	chemical route	es frequently us	ed in inorganio	c materials chemist	try		
- A pract	ical understar	ding of materia	als synthesis an	d material analysis	3		
- Analyze	e and professi	onally report / c	locument analy	vtical data			
Content	*	· · · · ·					
In this lab prac	tical, the stude	ents will furthe	r develop the ex	xperimental skills a	t an advanced level		
and introduces	modern mate	rials processing	g techniques clo	osely related to the	various research		
areas of the scie	entific supervi	sor (guided by	PhD or Postdoo	c). The student will	be trained in		
critical thinking	g and evaluat	ion of obtained	data related to	challenges in mate	rials synthesis and		
characterisation	n. After compl	etion of the mo	dule, the stude	nt will be able to ir	ndependently apply		
or transfer thes	e skills and m	ethods to other	scientific cont	exts which may be	connected with or		
dependent on r	naterials chen	nistry.					
Teaching meth	ods						
Lab practical							
Mode of assess	ment						
Written report,	typically in th	e form of a scie	entific publicati	on and oral presen	tation		
Requirement for	or the award o	f credit points					
Active participa	Active participation in lab work, successful completion of written report and oral presentation						
Module applicability							
Master Chemis	Master Chemistry						
Weight of the mark for the final score							
Weighted according to CP							
Module coordin	nator and lectu	urer(s)					
Ulf-Peter Apfel	, Lars Borchai	dt, Anjana Dev	i				
Further information							



Research Prac	tical: Functi	onal Material	5				
Module	Credits	Workload	Term	Frequency	Duration		
5.4	15 CP	450 h	3 <sup>rd</sup> Sem.	WS and SoS	3 Months		
Courses			Contact	Self-Study	Group size		
Functional	l Materials		hours	130 h	Individual		
(Lab practi	cal)		320 h				
	,						
Prerequisites	1				1		
Advanced Und	erstanding of	Materials Che	mistry, includii	ng synthesis and an	alytical methods		
Learning outco	mes						
After successfu	l completion	of this practica	l, the students	have	. 1		
- advance	ed expertise i	n materials che	emistry, includi	ng synthesis, analy	tical or		
comput	tational meth	ods as applicat	ble to the projec	t			
- a good	practical und	erstanding of r	naterials chemi	stry			
The students of	ro ablo to						
select s	uitable mater	inl systems to	ddress a given	nrohlem			
- select s	uitable math	al systems to a	oir research to	solve the given prol	hlem		
	their researc	h under super	vision of a men	tor	DICIII		
- cxccuic	ionally analy	re and docume	nt their data ac	cording to the estab	lished scholarly		
standar	ds in materia	ls chemistry		cording to the estat	senorariy		
Content	us in materie	ils chemistry					
The research p	ractical will b	e performed as	part of an ong	oing research proie	ct. forming by itself		
a small indeper	ident project	Content will i	nclude a literati	ure search, identific	ration, and		
application of s	uitable meth	ods (e.g., mater	rials synthesis.	analytical technique	es), and independent		
execution of the	e work, in clo	se interaction v	with the superv	isor / mentor. The	research topic will		
be in the scient	ific project of	f the supervisor	· ·	1	1		
Teaching meth	ods						
Lab practical							
Mode of assess	ment						
Written report,	typically in t	he form of a pr	oject proposal c	or manuscript and o	oral presentation		
Requirement for	or the award o	of credit points					
Active participa	ition in lab w	ork, successful	completion of	written report and o	oral presentation		
Module applica	Module applicability						
Master Chemistry, master of engineering							
Weight of the n	Weight of the mark for the final score						
Weighted according to CP							
Module coordin	Module coordinator and lecturer(s)						
Ulf-Peter Apfel	Ulf-Peter Apfel, Lars Borchardt, Anjana Devi						
Further inform	ation						



# Organische und Bioorganische Chemie

Enzyme Catalysis In Organic Chemistry: White Biotechnology							
Module	Credits	Workload	Term	Frequency	Duration		
6.1	5 CP	120 h	semester 1-3	Every 2 <sup>nd</sup>	1 semester		
				summer			
				semester			
Courses			Contact hours	Self-Study	Group size		
Enzyme Cataly	vsis In Organi	c Chemistry:	3 SWS	100 h	20 students		
White Biotech	nology						
Prerequisites							
Knowledge of b	asic organic c	hemistry and b	iochemistry				
Learning outco	mes						
Student	ts will gain a l	proad overview	of biotechnolog	y in chemical synthe	esis, with		
particul	lar emphasis o	on enzyme engi	ineering method	ds and strategies.			
Teaching meth	ods						
Offered as hybr	rid lecture (lec	ture hall / Zooi	m) with support	ing materials provid	led via moodle.		
Mode of assess	ment						
Oral exam							
Requirement for	or the award o	f credit points					
Passing the ora	l exam						
Module applica	bility						
Elective Lecture	e I-VI						
Weight of the n	nark for the fi	nal score					
Weighted acco	Weighted according to CPs						
Module coordin	nator and lectu	arer(s)					
Frank Schulz							
Further inform	ation						
Textbooks: K. Faber, Biotransformations in Organic Chemistry, M. T. Reetz: Directed Evolution							
of Selective Enz	of Selective Enzymes: Catalysts for Organic Chemistry and Biotechnology						



Metabolomi	cs for the c	liscovery of	new natural	products and	biomarkers		
Module	Credits	Workload	Term	Frequency	Duration		
6.2	5 CP	120 h	semester 1-3	1/year	1 semester		
<b>Courses</b> Metabolomics for the discovery of new natural products and biomarkers		Contact hours 3 SWS	<b>Self-Study</b> 100 h	Group size 20 students			
Prerequisites Knowledge of b	asic analytica	l and organic cl	hemistry, basic l	biochemistry			
Learning outcom	mes						
Student	ts acquire a br	oad overview u	ipon instrument	al analytics for th	e identification of		
natural	products and	biomarkers for	r various disease	es.			
Teaching metho	ods						
Offered as hybr	id lecture (lec	ture hall / Zoo	m) with support	ing materials pro	vided via moodle.		
Mode of assess	ment						
Oral exam							
Requirement for	or the award o	f credit points					
Passing the ora	l exam						
Module applica	bility						
Elective Lecture	e I-VI						
Weight of the n	nark for the fi	nal score					
Weighted accor	Weighted according to CPs						
Module coordin	nator and lectu	urer(s)					
Frank Schulz							
Further inform	ation						
The lecture will publications.	The lecture will be based on review articles, selected book chapter and current primary research publications.						



Organofluorine	Chemistry				
Module	Credits	Workload	Term	Frequency	Duration
6.3	5 CP	120 h	2 Sem	each SoS	1 Semester
	Contact hours	120 11	2. 5011.	Self-Study	Croup size
a) Lecture	2 + 1 SWS			75 h	20 Students
b) Exercises	2115005			75 11	20 Students
Prorequisites					
None Ideally knowled	dge of basic method	s for organic t	ransformati	ons	
Loarning outcomes	age of busic method	5 for organic i	runsiormuti		
Studenta will acquire	broad avamian of	rganofluorin	- chomistry	After complet	ion of the course
students will know all	fundamental approx	ches toward th	e synthesis	of organofluor	ine compounds and will
be able to independent	tly devise synthetic i	coutes and solv	ve correspoi	of organoliuo nding problem	s Students will also be
able to interpret the so	ometimes unusual re	eactivity of org	anofluorine	components a	and to analyze the
influence of fluorine s	substituents in organ	nic molecules.	In addition	to textbook kn	owledge, current
publications in the field	ld will also repeated	y be included	in the lectu	re.	
Content	History of organ	ofluorine cher	nistry, Sou	rces of fluorine	5
Content	, ,				
Synthesis of	- fundamental fl	uorine reagent	ts	_	
organofluorine	- direct (per)fluo	rination, electi	rochemical	fluorination	
compounds	- nucleophilic an	d "electrophili	ic" fluorinat	tion	
_	- synthesis of flu	oroarenes			
	- conversion of f	unctional grou	ips		
Properties and	- C-F bond: fund:	amentals			
structures of	- steric effects				
organofluorine	- physic-chemical	l properties			
compounds	- Bent's rule and	special fluorin	ne effect		
1	- dipol interaction	ns, intramolec	ular interac	tions	
	- analytics: 19F-N	MR			
	- acidities				
	- fluorine substit	uents as pi-doi	nors		
Reactivity of	- fundamental co	nsiderations			
organofluorine	- perfluorocarbor	is and substitu	ited perfluo	rocarbons, fluc	prinated alkanes
compounds	- per- and polyflu	oroolefins			
	- fluoroarenes: Sl	NAr and ortho	metalation		
	- C-F activation a	nd polyfluoroa	arenes in cro	oss-coupling re	eactions (C-H activation)
	- fluorinated eno	ethers and ar	lalogues		
Applications	- fluorous biphas	e catalysis			
	- pharmaceutic	als			
Teaching methods	-				
Blackboard and Powe	erpoint, online video	os, discussion (	of recent res	search papers	
Mode of assessment	t			* *	
Written exam (90 m	in)				
Requirement for the	e award of credit p	oints			
Passing of final writte	en examination				
Module applicability	7				
Master of Science Ch	emistry				
Weight of the mark	for the final score				
according to credit po	ints				
Module coordinator	and lecturer(s)				
S. Huber					
Further information	1				

Master of Science Chemistry (M. Sc. Chemistry)



Supramol	ecular Cl	nemistrv					
Module	Credits	Workload	Term	Frequency	Duration		
6.4	5 CP	120 h	1./3. Sem.	each WS	1 Semester		
Courses			Contact hours	Self-Study	Group size		
a) Lecture			2 + 1 SWS	75 h	20 Students		
b) Exercises							
Prerequisites	5						
None. Ideally:	knowledge (	of basic methods fo	r organic transforma	tions.			
Learning outcomes Students will acquire a broad overview of supramolecular chemistry. After completion of the course, students will be aware of all relevant concepts in supramolecular chemistry and will be able to identify them independently. Participants will also study all relevant noncovalent interactions, including their electronic origin, their manipulation and their limitations. On the basis of the most common structural motifs, cation binders, anion binders and neutral molecule binders will be discussed. Students will be aware of the fundamentals of self-assembly as well as of its most important applications. Finally, participants will be able to interpret the use of non-covalent interactions in organocatalysis. In addition to textbook knowledge, current publications in the field will also repeatedly be included in the lecture.							
Content	De	finition. history					
Concepts	- Lo	ck & key, induced fit	- binding cor	nstants			
	- CO	operativity / chelate e	ffect - preorganiz	ation / complement	arity, selectivity		
Noncovalent	- io1	n pairing, ion-dipole,	dipole-dipole				
Interactions	- hy	- hydrogen bonding, halogen bonding, further closed-shell interactions					
	- Ca	- cation-D, DD/DD , anion-DD interactions					
Fundamontal	- va.	h-dilution synthesis		ophoble effect, effet	,p)		
Techniques	- ter	- template synthesis					
Cation Bindin	ng - cro	own ethers, lariat ethe	ers				
	- cry	ptands, Spherands					
Anion Bindin	• ca	ognition by electrost	atics				
	- rec	cognition by electrost	atics and hydrogen bon	ding			
	- ree	cognition by hydroger	n bonding - recogniti	on by Lewis acids, c	ore motifs		
Neutral Guest	t - reo	cognition by hydrogen	n bonding obic offect				
Self-Assembly	- rev	taxanes - caten	anes, knots - ca	psules			
Applications i	n - 10'	octions in confined sr	$\frac{1}{2}$	ncovalent organoca	talveie		
Catalysis	- se	f-replication, noncov	alent catalyst assembly.	"classical" supramo	olecular catalysis		
		r reprication, noncov	aront cataryst association,	chabblear Supraine	siccular catalysis		
Teaching me	ethods						
Blackboard a	nd Powerpo	int, online videos, a	liscussion of recent re	esearch papers			
Mode of asse	essment						
Written exan	1 (90 min)						
Requiremen	Requirement for the award of credit points						
Passing of fin	al written es	camination					
Module appl	ICability	4					
Waster of Sch	ence Chemis	try					
weight of the	e mark ior	me mai score					
Module coor	dinator and	lecturer(s)					
S. Huber	umator allu						
Further info	rmation						



Organic Synthesis I: Stoechiometric Organometallics							
Module	Credits	Workload	Term	Frequency	Duration		
6.5	5 CP	120 h	semester 1-3	every semester	1 semester		
Courses			Contact	Self-Study	Group size		
Organic Synthes	sis II: Stoechior	netric	hours	100 h	20 students		
Organometallics	3		3 SWS				
Prerequisites							
Knowledge of ba	sic organic read	tions.					
Learning outcom	nes	1 .	1	C . 1.	. 11.		
Student	ts acquire a br	oad overview u	pon application	s of stoechiometric o	organometallic		
reagent	s, focussing o	n selectivities c	onnected with v	arious metals.			
Content	. 11	.1 . 1	1		. 11.		
HSAB-concept in	i organometalli	c synthesis; endo	cyclic restriction	test; DOM reactions, o	organometallic		
reagents based of	n litnium, mag	nesium, zink, tita	anium, boron and	i copper; stereoselectiv	e reactions with		
Teaching method	lagents.						
Offered as e-learn	ning module: L	ink: http://www.	ruhr-uni-bochum		ungen html		
Mode of assessm	ent						
Oral exam							
Requirement for	the award of cr	edit points					
Passing the oral	exam						
Module applicab	ility						
Elective Lecture I	I-VI						
Weight of the ma	ark for the final	score					
Weighted accord	Weighted according to CPs						
Module coordinator and lecturer(s)							
Further informat	tion						

#### FAKULTÄT FÜR CHEMIE UND BIOCHEMIE Master of Science Chemistry (M. Sc. Chemistry)



Organic Synthesis II: Catalytic Organometallics							
Module	Credits	Workload	Term	Frequency	Duration		
6.6	5 CP	120 h	semester 1-3	every semester	1 semester		
Courses			Contact hours	Self-Study	Group size		
Organic Synthe	sis II: Catalyti	с	3 SWS	100 h	20 students		
Organometallic	S						
Prerequisites							
Knowledge of ba	asic organic rea	actions.					
Learning outco	omes						
Students acquire	e a broad overv	view upon applica	tions for homoger	neous transition met	al catalysis.		
Content							
Key steps in cata	lytic cycles; H	Ieckreaction and	other Pd-catalyzed	domino processes,	catalytic activities of		
Au-, Co-, Cu-, Fe	e-, Mn-, Ni-, Rl	n <mark>-, Ru- and Lant</mark> h	anoid-complexes.				
Teaching metho	ds						
Offered as e-lean	ming module;	Link: http://www	ruhr-uni-bochun/	n.de/oc2/dyker/Vorl	esungen.html		
Mode of assessm	nent						
Oral exam							
Requirement for	r the award of	credit points					
Passing the oral	exam						
Module applicat	oility						
Elective Lecture I-VI							
Weight of the mark for the final score							
Weighted according to CPs							
Module coordinator and lecturer(s)							
Gerald Dyker							
Further information							



Organic Synthesis III: Designing Organic Syntheses							
Module Credits	Workload	Term	Frequency	Duration			
6.7 5 CP	150 h	semester 1-3	every semester	1 semester			
<b>Courses</b> Organic Synthesis III: Desig	ning Organic	Contact hours 3 SWS	Self-Study 100 h	Group size 20 students			
Syntheses							
<b>Prerequisites</b> Knowledge of basic organic re	eactions.						
Learning outcomes							
Knowledge of the ret	ron concept						
Ability to identify stra	ategic bonds						
• Ability to develop a sy	nthesis plan for ta	arget molecules w	ith medium complex	ity.			
Content	•	0	•				
Key expressions of retrosynth	esis: strategic bond	ds, synthon, synth	etic equivalent, retro	n, bidirectional			
synthesis, linear and konverge	ent synthesis plan.	Typical structura	l units in retrosynthe	tic analysis such as			
1,n-dicarbonyl compounds an	d hetarenes; exerc	ises in developing	strategies for synthe	sis of target			
molecules.							
Teaching methods							
Offered as e-learning module	Link: http://www	ruhr-uni-bochum	1.de/oc2/dyker/Vorle	sungen.html			
Mode of assessment							
Oral exam	1						
Requirement for the award of	credit points						
Modulo applicability							
Floctive Locture LVL							
Weight of the mark for the final score							
Weighted according to CPs							
Module coordinator and lecturer(s)							
Gerald Dyker							
Further information							



Companyly						
Concepts of		r Chemistry	1: Physical C			
Module		Workload	1 3 Sem	W/S	1 Somostor	
6.8	J CP	130 11	1., J. Sciii.		1 Semester	
Courses			Contact	Self-Study	Group size	
a) Lecture			hours	105 h	30 Students	
D) Exercises			a)2 SWS / 30 h b)1 SWS / 14 h			
Prerequisites						
Learning outco	mes					
<ul> <li>Studen of phys evaluat reaction experin</li> <li>Studen of phys present (15 min</li> <li>Content</li> <li>The conditional of physical</li> </ul>	ts acquire ad sical organic of ion of proper n surfaces. mental metho ts learn to reasical organic t the essential n + 5 min dis valent chemic con-covalent	vanced knowled chemistry such ties of experime The main foc ds. ad and understa chemistry, how ls of the publica cussion). cal bond (prope chemical bor	dge on the theor as bond models ental interest, in cus lies on th nd advanced sel v to summarize tion in an oral p rties, experimen nd (van der	ry and techniques s, thermochemist particular the the e interplay betw ected scientific pu- the publication resentation using tal methods) Waals complexe	s of the basic concepts try, and the theoretical cory of potential energy ween theoretical and ublications in the topic in an abstract, and to g presentation software	
- Therm	ochemistry (r	properties. Bens	son's additivity 1	ules)		
- Potenti	al energy s	urfaces (intern	al coordinates,	Born Oppenhe	eimer approximation,	
station	ary points, re	eaction coordinate	ates, Marcus th	eory, Curtin Han	nmett principle, More	
O'Ferra	al-Jencks diag	grams, reactivity	y and selectivity,	tunneling)		
- Force f	ield calculatio	ons (MM2)				
- Linear	free energy re	elations				
- Experir	nental techni	iques (matrix is	olation)			
Teaching meth	ods					
Lecture, semin	ar based teac	hing with active	e participation o	f the student		
Mode of assess	ment					
30 min end-of-term oral exam or 2-hour end-of-term written exam						
Requirement f	or the award	of credit points				
Successful oral presentation, passing the exam						
Module applicability						
Weight of the 1	mark for the f	final score				
Module coordi	Module coordinator and lecturer(s): W. Sander					
Further inform	nation					



Modern Org	ganotrans	ition metal c	atalysis		
Module	Credits	Workload	Term	Frequency	Duration
6.9	5 CP	150 h	2./4. Sem.	nur SS	1 Semester
<b>Courses</b> a) lecture b) exercise		-	Contact hours 2+1 SWS	Self-Study 100 h	<b>Group size</b> 10 students
Prerequisites					
-					
Learning outco <ul> <li>student</li> <li>and the</li> </ul>	mes s aquire kno ir mechanis	owledge on the tic principles	theory of transi	tion metal catalys	ed coupling reactions
Content					
Cross-c	oupling read	ctions and their	elementary cata	lytic steps	
<ul> <li>Catalyti</li> </ul>	c activation	of C-O bonds,	C-C bonds and	d C-H bonds: me	chanistic approaches,
selected	l examples, s	synthetic applic	ations.		
<ul> <li>Catalyti</li> </ul>	c functional	ization of alken	es.		
Teaching meth	ods				
b) lecture b	) exercise				
Mode of assess	ment				
Drai exam (30 m	in) after the r	nodule			
Passing the evan	אנט אווע מאמוע א	of credit points	1		
Module applicability					
M Sc. Chemistry					
Weight of the mark for the final score					
Module coordinator and lecturer(s) Prof. Dr. Lukas Gooßen					
Further inform	ation	, <i>i</i>			

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In-depth Pra	In-depth Practical: Organocatalysis							
Module	Credits	Workload	Term	Frequency	Duration			
6.10	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester			
<b>Courses</b> In-depth Pract	ical: Organoo	catalysis	Contact hours 9 SWS	<b>Self-Study</b> 105 h	<b>Group size</b> Max 3 students			
Prerequisites								
Learning outcom Student of Supra- Student practica Student collabor	mes ts acquire ad amolecular ( ts learn to w l ts learn scier cation while	vanced knowled Chemistry rite a detailed l ntific work unde carrying out o	lge on the theor ab report on the er the guidance experiments, ge	y and techniques of e topic and experim of teaching assistan eneral knowledge o	the basic concepts ental results of the ts, teamworking in of software and of			
necessa <b>Content</b>	ry lab equip	ment.						
- Studen gas con develop Compo spectro catalyst	ts will most aditions. Thi bed within th unds will t scopy. Bind performance	ly perform vari is comprises lit ne group. They be characterize ing constants ce will be judge	ious organic sy terature-known will also test ne d by the usual will be obtaine ed by obtaining	ntheses, including protocols and unp ew approaches to sy means, including ed via NMR and T reaction kinetics of	ones under inert- published methods withetic problems. g NMR and mass TC titrations, and n model reactions.			
Teaching metho	ods		, 0					
Practical under	guidance of	research assiste	ent					
Mode of assess Active participa by teaching ass	<b>ment</b> tion in pract istant.	ical, feedback d	uring the experi	ments, feedback on	written lab reports			
Requirement for	or the award	of credit points						
All experimets a	are complete	d successfully a	nd written up sa	atisfactorily in a lab	report			
Module applica	bility							
Weight of the n	nark for the	final score						
Module coordin	nator and lec	turer(s)						
S. Huber								
Further inform	Further information							



In-depth Pra	actical: Sup	ramolecular	r Chemistry		
Module	Credits	Workload	Term	Frequency	Duration
6.11	8 CP	240 h	1., 2. Sem.	Every semester	1 Semester
Courses			Contact	Self-Study	Group size
In-depth Pract	ical: Supramo	lecular	hours	105 h	Max 3
Chemistry	-		9 SWS		Studierende
Prerequisites					
Learning outco	mes				
• Student	ts acquire adv	anced knowled	ge on the theor	y and techniques of	the basic concepts
of Supr	amolecular C	hemistry		-	-
• Student	ts learn to wr	ite a detailed la	b report on the	topic and experime	ental results of the
practica	ıl				
• Student	ts learn scient	ific work unde	r the guidance o	of teaching assistant	ts, teamworking in
collabo	ration while	carrying out e	xperiments, ge	neral knowledge o	f software and of
necessa	ry lab equipm	ient.			
Content					
- Studen	ts will mostly	y perform vari	ous organic syı	ntheses, including	ones under inert-
gas con	ditions. This	comprises lite	erature-known	protocols and unp	ublished methods
develop	ped within the	e group. They	will also test ne	w approaches to sy	nthetic problems.
Compo	ounds will be	e characterized	l by the usual	means, including	NMR and mass
spectro	scopy. Bindi	ng constants v	will be obtaine	d via NMR and I	FC titrations, and
catalyst	performance	e will be judged	d by obtaining i	reaction kinetics or	model reactions.
Teaching meth	ods				
Practical under	guidance of r	esearch assista	nt		
Mode of assess	ment	1 6 11 1 1		C 11 1	
Active participa	tion in practic	cal, feedback du	iring the experii	nents, feedback on	written lab reports
by teaching ass	istant.	<u> </u>			
Requirement fo	or the award o	f credit points	1		
All experiments	s are complete	a successfully	and written up s	satisfactorily in a lat	report
модше аррпса	Dility				
Weight of the n	nark for the fi	nal score			
Module coordin	nator and lectu	arer(s)			
S. Huber					
Further information					



Module 6.12       Credits 8 CP       Workload 240 h       Term semester 1-3       Frequency every semester       Duration 8 weeks         Courses       Contact hours       Self-Study 40 h       Group size 2 students         Prerequisites       Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics       Group size 2 students         Learning outcomes       •       Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography       •         Interpreting observations of own scientific results       •       •         Content       Synthesis of target molecules within the context of a current research project.       •         Practical lab course within research projects       •       •         Mode of assessment       •       Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol       •         Module applicability       •       •       •         n-depth Practical I-III       •       •       •         Module coordinator and lecturer(s) Gerald Dyker       •       •       •	In-depth Practical: Metal-Organic Chemical Synthesis								
8 CP       240 h       semester 1-3       every semester       8 weeks         Courses       In-depth Practical: Metal-Organic Chemical Synthesis       Contact hours 25 SWS       Self-Study 40 h       Group size 2 students         Prerequisites       Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics       January 100 (1998)         Learning outcomes       •       Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography       •         •       Interpreting observations and results       •       •         •       Writing presentations of own scientific results       •       •         Content       •       Synthesis of target molecules within the context of a current research project.       •         Practical lab course within research projects       •       •       •       •         Mode of assessment       •       •       •       •       •       •         Requirement for the award of credit points       •	Module 6.12	Credits	Workload	Term	Frequency Duration				
Courses In-depth Practical: Metal-Organic Chemical SynthesisContact hours 25 SWSSelf-Study 40 hGroup size 2 studentsPrerequisites Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic OrganometallicsInterpretion 2 studentsInterpretion 2 studentsLearning outcomes Ike Kugelrohr distillation and medium pressure automatic chromatographyInterpreting observations and results 9 Writing presentations of own scientific resultsSelf-Study 40 hSelf-Study 2 studentsContent Synthesis of target molecules within the context of a current research project.Teaching methods 9 Practical lab course within research projectsForget and the protocol and of the performance in the labRequirement for the award of credit points Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocolModule applicability In-depth Practical 1:11Weight of the mark for the final score Weighted according to CPs Module coordinator and lecturer(s) Gerald DykerModule applicability		8 CP	240 h	semester 1-3	every semester	8 weeks			
In-depth Practical: Metal-Organic Chemical Synthesis       hours 25 SWS       40 h       2 students         Prerequisites       Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics       Participation         Learning outcomes       •       Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography       •         •       Interpreting observations and results       •         •       Writing presentations of own scientific results         Content       Synthesis of target molecules within the context of a current research project.         Synthesis of target molecules within research projects       Mode of assessment         Rating of the protocol and of the performance in the lab       Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol       Module applicability         In-depth Practical I-III       Weight of the mark for the final score       Weighted according to CPs         Module coordinator and lecturer(s) Gerald Dyker       Gerald Dyker       Further information	Courses	•		Contact	Self-Study	Group size			
Synthesis       25 SWS         Prerequisites       Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics         Learning outcomes       • Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography         • Interpreting observations and results       • Writing presentations of own scientific results         Content       Synthesis of target molecules within the context of a current research project.         Teaching methods       • Practical lab course within research projects         Mode of assessment       Rating of the protocol and of the performance in the lab         Requirement for the award of credit points       Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol         Module applicability       In-depth Practical I-III         Weight of the mark for the final score       Weighted according to CPs         Module coordinator and lecturer(s)       Gerald Dyker         Further information       Event	In-depth Practic	al: Metal-Organ	nic Chemical	hours	40 h	2 students			
Prerequisites         Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics         Learning outcomes         • Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography         • Interpreting observations and results         • Writing presentations of own scientific results         Content         Synthesis of target molecules within the context of a current research project.         Teaching methods         Practical lab course within research projects         Mode of assessment         Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol         Module applicability In-depth Practical I-III         Weight of the mark for the final score Weighted according to CPs         Module coordinator and lecturer(s) Gerald Dyker         Further information	Synthesis			25 SWS					
Prerequisites         Knowledge of basic methods for organic transformations. Recommendation: successful participation in lectures Stoechiometric Organometallics and Catalytic Organometallics         Learning outcomes         • Performing preparative experiments, including organometallics and special techniques like Kugelrohr distillation and medium pressure automatic chromatography         • Interpreting observations and results         • Writing presentations of own scientific results         Content         Synthesis of target molecules within the context of a current research project.         Teaching methods         Practical lab course within research projects         Mode of assessment         Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weighted according to CPs         Module coordinator and lecturer(s)         Gerald Dyker         Further information									
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Gerald Dyker Further information	Module coordin	nator and lectu	urer(s)						
Further information	Gerald Dyker								
	Further inform	ation							

Module	Credits	Workload	Term	Frequency	Duration
6.13	8 CP	240 h	semester 1-3	1/year	8 weeks
<b>Courses</b> In-Depth Practic Natural Product	cal: "Semi-Synt s"	hesis Of	Contact hours 25 SWS	Self-Study 40 h	<b>Group size</b> 2 students
<b>Prerequisites</b> Knowledge of bas in practicals: O	sic methods for C F.	organic transfo	rmations. Recom	mendation: success	ful participation
<ul> <li>Learning outcom</li> <li>Perform or relate</li> <li>Interprese</li> <li>Writing</li> </ul>	mes ning preparati ed synthesis ta eting observat presentation	ve experiment argets ions and result s of own scient	s towards the sy ts ific results	nthesis of natural p	roducts derivatives
<b>Content</b> Synthesis of targe	et molecules wi	thin the context	of a current resea	urch project.	
Teaching methe	ods urse within re	search projects	,		
Mode of assess	ment	search projects	,		
Rating of the pr	otocol and of	the performan	ce in the lab		
Requirement for Active participation experimental rest	or the award o on in practical, ults in the grou	<b>f credit points</b> feedback during p, submitting a	g the experiments, satisfactory protoc	, written lab report, pr col	esentation of the
Module applica In-depth Practica	<b>bility</b> 1 I-III	<u> </u>	* ±		
Weight of the mark for the final score					
Module coordinator and lecturer(s)					
Frank Schulz					
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In-Depth Practical: "Natural Products Chemistry and Biochemistry"							
Module	Credits	Workload	Term	Frequency	Duration		
6.14	8 CP	240 h	semester 1-3	1/year	8 weeks		
Courses			Contact	Self-Study	Group size		
In-Depth Practic	al: "Natural Pr	oducts	hours	40 h	2 students		
Chemistry and I	Biochemistry "		25 SWS				
Prerequisites			:	ملية المنامية المنتقا ما	a sea i atoma		
Knowledge of bas	sic methods fro	om organic chem	istry or biochemi	stry and analytical ch	emistry		
Learning outcom	mes			C . 1 1 .			
HPLC a	ind mass spec	trometry for th	e identification	of natural products			
• Statistic	al data interp	retation in the l	ramework of m	letabolomics			
Interpre	eting observat	ions and result	S 1				
Writing	presentation	s of own scient	ific results				
Content	11				. 1		
Biosynthesis, iso	lation and char	acterization of ta	rget molecules w	ithin the context of a	current research		
Teaching meth	ods						
Practical lab con	arse within re	search projects					
Mode of assess	ment	1 /					
Rating of the pr	otocol and of	the performan	ce in the lab				
Requirement for	or the award o	f credit points					
Active participati	on in practical,	feedback during	the experiments,	written lab report, p	resentation of the		
experimental rest	ults in the grou	ıp, submitting a s	satisfactory proto	col			
Module applica	bility						
In-depth Practica	<u>1 I-III</u>						
Weight of the n	Weight of the mark for the final score						
Weighted according to CPs							
Module coordin	hator and lectu	urer(s)					
Frank Schulz	Frank Schulz						
Further inform	ation						



Module 6.15Credits 8 CPWorkload 240 hTerm semester 1-3Frequency 1/yearDuration 8 weeksCourses In-Depth Practical: "Fermentation of Natural Products"Contact hours 2 S SWSSelf-Study 40 hGroup size 2 studentsPrerequisites Knowledge of basic methods from organic chemistry or biochemistry40 h2 studentsLearning outcomes • • • Interpreting observations and resultsFermentation of natural products from fermentation broths or harvested cells •	In-Depth Practical: "Fermentation of Natural Products"							
6.158 CP240 hsemester 1-31/year8 weeksCourses In-Depth Practical: "Fermentation of Natural Products"Contact hours 2 S WSSelf-Study 40 hGroup size 2 studentsPrerequisites Knowledge of basic methods from organic chemistry or biochemistry2 studentsPrerequisites Knowledge of basic methods from organic chemistry or biochemistryLearning outcomes•Fermentation of microorganisms•Interpreting observations and results•Writing presentation of colspan="4">of own scientific resultsContent Biosynthesis, isolation and characterization of target molecules within the context of a current research project.Teaching methodsPractical lab course within research projectsMode of assessment Rading of the protocol and of the performance in the labRequirement for the award of credit points Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocolModule applicability In-depth Practical I-IIIWeight of the mark for the final score Weighted according to CPsModule coordinator and lecturer(s) Frank SchulzFurther information	Module	Credits	Workload	Term	Frequency	Duration		
Courses       Contact       Self-Study       Group size         In-Depth Practical: "Fermentation of Natural Products"       25 SWS       40 h       2 students         Prerequisites       Knowledge of basic methods from organic chemistry or biochemistry       40 h       2 students         Learning outcomes       Fermentation of microorganisms       Isolation of natural products from fermentation broths or harvested cells       1 solation of natural products from fermentation broths or harvested cells         Interpreting observations and results       Writing presentations of own scientific results       Content         Biosynthesis, isolation and characterization of target molecules within the context of a current research project.       Teaching methods         Practical lab course within research projects       Mode of assessment       Rating of the protocol and of the performance in the lab         Requirement for the award of credit points       Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol       Module applicability         In-depth Practical I-III       Weight of the mark for the final score       Weight of the mark for the final score         Weighted according to CPs       Module coordinator and lecturer(s)       Frank Schulz       Further information	6.15	8 CP	240 h	semester 1-3	1/year	8 weeks		
In-Depth Practical: "Fermentation of Natural Products"       hours 25 SWS       40 h       2 students         Prerequisites Knowledge of basic methods from organic chemistry or biochemistry       2       students         Itearning outcomes       •       •       Fermentation of microorganisms         •       Isolation of natural products from fermentation broths or harvested cells       •         •       Interpreting observations and results       •         •       Writing presentations of own scientific results         Content       Biosynthesis, isolation and characterization of target molecules within the context of a current research project.         Teaching methods       •       •         Practical lab course within research projects       •         Mode of assessment       •       Rating of the protocol and of the performance in the lab         Requirement for the award of credit points       •       ×         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol       •         Module applicability       •       •       •         In-depth Practical 1-III       •       •       •         Weight of the mark for the final score       •       •       •         Weighted according to CPs	Courses			Contact	Self-Study	Group size		
Products       25 SWS         Prerequisites       Knowledge of basic methods from organic chemistry or biochemistry         Learning outcomes       •         •       Fermentation of microorganisms         •       Isolation of natural products from fermentation broths or harvested cells         •       Interpreting observations and results         •       Writing presentations of own scientific results         Content       Biosynthesis, isolation and characterization of target molecules within the context of a current research project.         Teaching methods       Practical lab course within research projects         Mode of assessment       Rating of the protocol and of the performance in the lab         Requirement for the award of credit points       Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability       In-depth Practical I-III         Weight of the mark for the final score       Weighted according to CPs         Module coordinator and lecturer(s)       Frank Schulz         Frank Schulz       Further information	In-Depth Practic	cal: "Fermentat	ion of Natural	hours	40 h	2 students		
Prerequisites         Knowledge of basic methods from organic chemistry or biochemistry         Learning outcomes         • Fermentation of microorganisms         • Isolation of natural products from fermentation broths or harvested cells         • Interpreting observations and results         • Writing presentations of own scientific results         Content         Biosynthesis, isolation and characterization of target molecules within the context of a current research project.         Teaching methods         Practical lab course within research projects         Mode of assessment         Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information	Products"			25 SWS				
Prerequisites         Knowledge of basic methods from organic chemistry or biochemistry         Learning outcomes         • Fermentation of microorganisms         • Isolation of natural products from fermentation broths or harvested cells         • Interpreting observations and results         • Writing presentations of own scientific results         Content         Biosynthesis, isolation and characterization of target molecules within the context of a current research project.         Teaching methods         Practical lab course within research projects         Mode of assessment         Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information								
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<ul> <li>Fermentation of microorganisms</li> <li>Isolation of natural products from fermentation broths or harvested cells</li> <li>Interpreting observations and results</li> <li>Writing presentations of own scientific results</li> </ul> Content Biosynthesis, isolation and characterization of target molecules within the context of a current research project. Teaching methods Practical lab course within research projects Mode of assessment Rating of the protocol and of the performance in the lab Requirement for the award of credit points Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol Module applicability In-depth Practical I-III Weight of the mark for the final score Weighted according to CPs Module coordinator and lecturer(s) Frank Schulz	Learning outco	mos	in organic chem	istry of Diochenni	Sily			
<ul> <li>Formeritation of mitriologamisms</li> <li>Isolation of natural products from fermentation broths or harvested cells</li> <li>Interpreting observations and results</li> <li>Writing presentations of own scientific results</li> <li>Content</li> <li>Biosynthesis, isolation and characterization of target molecules within the context of a current research project.</li> <li>Teaching methods</li> <li>Practical lab course within research projects</li> <li>Mode of assessment</li> <li>Rating of the protocol and of the performance in the lab</li> <li>Requirement for the award of credit points</li> <li>Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol</li> <li>Module applicability         <ul> <li>In-depth Practical I-III</li> <li>Weight of the mark for the final score</li> <li>Weighted according to CPs</li> <li>Module coordinator and lecturer(s)</li> <li>Frank Schulz</li> </ul> </li> </ul>	Eermer	ines	oorganisms					
<ul> <li>Interpreting observations and results</li> <li>Writing presentations of own scientific results</li> <li>Content</li> <li>Biosynthesis, isolation and characterization of target molecules within the context of a current research project.</li> <li>Teaching methods</li> <li>Practical lab course within research projects</li> <li>Mode of assessment</li> <li>Rating of the protocol and of the performance in the lab</li> <li>Requirement for the award of credit points</li> <li>Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol</li> <li>Module applicability</li> <li>In-depth Practical I-III</li> <li>Weight of the mark for the final score</li> <li>Weighted according to CPs</li> <li>Module coordinator and lecturer(s)</li> <li>Frank Schulz</li> <li>Further information</li> </ul>	<ul> <li>Isolatio</li> </ul>	n of natural n	roducts from fe	rmentation bro	ths or harvested cell	c		
<ul> <li>Writing presentations and results</li> <li>Writing presentations of own scientific results</li> <li>Content</li> <li>Biosynthesis, isolation and characterization of target molecules within the context of a current research project.</li> <li>Teaching methods</li> <li>Practical lab course within research projects</li> <li>Mode of assessment</li> <li>Rating of the protocol and of the performance in the lab</li> <li>Requirement for the award of credit points</li> <li>Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol</li> <li>Module applicability</li> <li>In-depth Practical I-III</li> <li>Weight of the mark for the final score</li> <li>Weighted according to CPs</li> <li>Module coordinator and lecturer(s)</li> <li>Frank Schulz</li> <li>Further information</li> </ul>	Interpre	eting observat	ions and result	s		5		
Content         Biosynthesis, isolation and characterization of target molecules within the context of a current research project.         Teaching methods         Practical lab course within research projects         Mode of assessment         Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information	Writing	presentation	s of own scienti	fic results				
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Mode of assessmentRating of the protocol and of the performance in the labRequirement for the award of credit pointsActive participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocolModule applicability In-depth Practical I-IIIWeight of the mark for the final score Weighted according to CPsModule coordinator and lecturer(s) Frank SchulzFurther information	Practical lab con	urse within re	search projects					
Rating of the protocol and of the performance in the lab         Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information	Mode of assess	ment						
Requirement for the award of credit points         Active participation in practical, feedback during the experiments, written lab report, presentation of the experimental results in the group, submitting a satisfactory protocol         Module applicability         In-depth Practical I-III         Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information	Rating of the p	rotocol and of	the performance	ce in the lab				
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In-depth Practical I-III Weight of the mark for the final score Weighted according to CPs Module coordinator and lecturer(s) Frank Schulz Further information	experimental res	uits in the grou	p, submitting a s	satisfactory protoc	201			
Weight of the mark for the final score         Weighted according to CPs         Module coordinator and lecturer(s)         Frank Schulz         Further information	In-depth Practica	J LIII						
Weighted according to CPs Module coordinator and lecturer(s) Frank Schulz Further information	Weight of the n	Weight of the mark for the final score						
Module coordinator and lecturer(s) Frank Schulz Further information	Weighted according to CPs							
Frank Schulz Further information	Module coordinator and lecturer(s)							
Further information	Frank Schulz	Frank Schulz						
	Further inform	Further information						



In depth pr	actical Or	·oanotransit	ion metal cat	alvsis"		
Module	Credits	Workload	Term	Frequency	Duration	
6.16	8 CP	240 h	2./4. Sem.	By appoitment	1 Semester	
<b>Courses</b> a) practical			Contact hours 9 SWS	<b>Self-Study</b> 100 h	<b>Group size</b> 3 students	
Prerequisites						
Learning outco • student techniq	o <b>mes</b> ts acquire exj jues of analys	perience in prac sis and spectros	ctical organic an scopical method	d metal-organic labv s	work and associated	
<ul> <li>Synthes</li> <li>Handli</li> <li>Hands-</li> <li>Mechan</li> <li>study o</li> </ul>	ses in the fie ng of air sen on work with nism evaluat f catalytic pro	ld of organome sitive compoun h analytical me ion by e. g. deu ocesses	tallic chemistry ds thods such as G teration experin	; C, GC-MS, NMR nents		
<b>Teaching meth</b> c) Practice	ods al lab course					
<b>Mode of assessment</b> active participation in practical, feedback during and on the experiments, feedback on written lab reports						
<b>Requirement for the award of credit points</b>						
Module applica	ability		juuro			
M. Sc. Chemistry						
Weight of the mark for the final score						
Module coordinator and lecturer(s) Prof. Dr. Lukas Gooßen						
Further inform	ation					



## Physical Chemistry

Module	<b>Credits</b>	Workload	<b>Term</b> 2. Semester	Frequency SS	Duration
<b>Courses</b> a) Biophysical	Chemistry I	150 11	Contact hours 4 SWS, 60 h	Self-Study 90 h	Group size 30 Students
Prerequisites			·		
Knowledge in	basic Physica	l Chemistry.			
Learning outco	omes				
<ul> <li>Acquire focus on</li> <li>Understant</li> <li>Analyze</li> <li>Develop</li> <li>Utilize d</li> </ul>	advanced kn structure det and their app and screen re presentation igital techniq	owledge in exp ermining meth lications, advan elevant literatur skills in front c ues to prepare	perimental techn nods. ntages, and disad es independently of an audience and conduct a pr	iques in biophys vantages of the n y resentation	sical chemistry with a nethods
Content					
Advanced Biop Protein s Molecula Computa X-ray dif Calorime Fluoresc Super-re	physical techn structures ar interaction ational approa fraction etry technique ence theory, I solution mice	iques: s aches es FRET roscopy			
Teaching meth	ods				
Lecture (2 SWS	S, 30 h), Exerc	cise (1 SWS, 15	h), Seminar (1 S	SWS, 15 h).	
Participation in Written exame Requirement f	n all seminars of 60 mins. <b>or the award</b>	s and presentat of credit points	ion about an assi	igned publication	1.
Pass both parts Module applics	s: presentatio ability	n (50%) and wr	ritten exam (50%	).	
M.Sc. Chemist Weight of the	ry, M.Sc. Bio mark for the f	chemistry. f <b>inal score</b>			
Weighted acco	rding to CPs.				
Module coordi	nator and lec	turer(s)			
Moune coordi	nutor und rec				
Lecturers from	Physical Che	emistry departr	nents.		

#### FAKULTÄT FÜR CHEMIE UND BIOCHEMIE

Master of Science Chemistry (M. Sc. Chemistry)



Biophysical	Chemistr	y II			
Module 7.2	Credits 5 CP	Workload 150 h	Term 3. Semester	Frequency WS	Duration 1 Semester
<b>Courses</b> a) Biophysical	Chemistry I	I	Contact hours 4 SWS, 60 h	<b>Self-Study</b> 90 h	Group size 30 Students
Prerequisites			·		
Knowledge in	basic Physica	l Chemistry.			
Learning outco	omes				
thermod on select Understa Analyze Develop Utilize d	ynamics of p ed examples and their app and screen re presentation igital technic	proteins and me lications, advan elevant literatur skills in front c jues to prepare	embranes, and o stages, and disad es independently of an audience and conduct a pr	on protein reaction vantages of the r y resentation	on and function based nethods
<ul> <li>Microcal</li> <li>Fluoresc</li> <li>Advance</li> <li>Fourier t</li> <li>Attenuat</li> <li>Vibration</li> <li>Scanning</li> </ul>	orimetry in p ence-based n d fluorescend ransform sp ed total refle- nal spectrosco g probe micr	nques. protein characte nethods in prote ce microscopy ectroscopy ction (ATR) spe opy in biomolec oscopy (SPM) in	rization ein interactions ctroscopy cular solvation n biochemistry		
Teaching meth	nods				
Lecture (2 SWS	S, 30 h), Exer	cise (1 SWS, 15	h), Seminar (1 S	SWS, 15 h).	
Mode of assess	sment				
Participation in Written exam	n all seminar of 60 mins.	s and presentat	ion about an ass	igned publication	1.
Requirement f	or the award	of credit points		,	
Pass both parts Module applica	s: presentatio ability	n (50%) and wr	itten exam (50%	).	
M.Sc. Chemist	ry, M.Sc. Bio	chemistry.			
Weight of the	mark for the	final score			
Weighted acco	rding to CPs				
		urer(s)			
Further inform	nation	emistry departr	nents.		



Concepts of	Spectroso	rony 1			
Module	Credits	Workload	Term	Frequency	Duration
7.3	5 CP	150 h	1. Semester	Each WS	1 Semester
Courses			Contact hours	Self-Study	Group size
a) Lectures			a) 2 SWS	105 h	a+b) 20 - 50
b) Exercises			b) I SWS		
Prerequisites Pagic knowlodd	no in guantu	n chomistry a	untum machani	ca apostrogeopie	tochniquog and the
necessary math	ematical for	malism		cs, specifoscopic	. teeninques and the
Learning outco	mes				
After successfu	l completion	of the module	/course, students	will be able to:	
<ul> <li>Obtain the second second</li></ul>	neoretical an	d practical kno	wledge of mode	rn linear and no	onlinear spectroscopic
methods	(time- and	frequency-don	nain) which allo	ow for the eluc	idation of molecular
structure	and dynami	cs in different e	environments		
<ul> <li>Understa</li> </ul>	ind applicati	ions of laser s	pectroscopic tec	hniques from t	he THz to the VUV
waveleng	th region to	the study of mo	lecules and their	interactions	
Content					
1. Electrom	agnetic radia	ation, molecular	structure, light-	matter interactio	n
2. Optical a	nd spectrosc	opic elements			
3. Line broa	idening mec	hanisms, specti	al bandwidth, Fo	ourier transform	ation
4. Molecula	r symmetry,	point groups, r	nolecular symme	etry groups	
5. Rotationa	al spectrosco	py: linear, symr	netric, spherical,	and asymmetric	rigid rotor molecules,
rotationa	l infrared, m	illimeter, micro	wave and Rama	n spectra	1 1
6. Vibration	al spectrosco	opy: diatomic a	nd polyatomic m	olecules, infrare	d and Raman spectra,
VIDration 7 Electroni	al selection r	ules, normal m	ode analysis	moloculog olo	stronic and vibronic
7. Election	rules Franc	ly. Gondon trans	alla polyatollic	molecules, ele	ve processes (internal
conversio	n intersyste	em crossing) ci	rve crossings an	d conical interse	ctions
8 Laser bas	sics populati	on inversion ar	nd gain medium	s cavity modes	properties of coherent
radiation	. specific lase	er systems	ia guili illearaili.	s, cuvity models,	properties of concretie
9. Introduc	tion to nonli	near spectrosco	DV		
Teaching meth	ods	1	17		
Active participa	tion during	lectures and exe	ercises with prob	lems for self-stu	dying, Q&A and
discussion sess	ions with pr	esentations give	en by the particip	ants, Moodle co	urse with online
material	-	-			
Mode of assess	ment				
2-hour end-of-t	erm written	exam on the co	ntent of the lectu	res	
Requirement for	or the award	of credit points			
Passing the wr	itten examin	ation			
Module applica	bility				
M.Sc. Chemist	ry; M.Sc. iM	OS; M.Sc. Laser	s and Photonics		
Weight of the r	nark for the	tinal score			
Weighted accor	raing to CPs				
Module coordi	nator and lec	turer(s)			
P. Petersen	Dhave - 1 Cl				
Lecturers from	Physical Ch	emistry departn	nents		
Further inform	ation				



Concepts	of Spectros	conv 2				
Module	Credits	Workload	Term	Frequency	Duration	
7.4	5 CP	150 h	2. Semester	Each SuSe	1 Semester	
Courses			Contact hours	Self-Study	Group size	
a) Lectures			a) 2 SWS	105 h	a+b) 20 - 50	
b) Exercises			b) 1 SWS			
Prerequisite Advanced kr such as prov	s nowledge in qu rided by the mo	antum chemistr dules Concepts	y, quantum mec of Spectroscopy	hanics and spect 1 and Dynamics	roscopic techniques, and Simulation.	
Learning ou	tcomes					
After succes <ul> <li>Obtain spectr</li> <li>of che</li> <li>Develo</li> <li>Utilize</li> </ul>	sful completion n theoretical an oscopic and mic mical and biocl op presentation e digital technic	n of the module, nd practical kno croscopic techni nemical samples skills in front c jues to prepare a	/course, students owledge of nonl ques to investiga s of an audience and conduct a pr	s will be able to: inear optics imp te structure, dyna esentation	ortant for non-linear mics and interactions	
Content						
11.Non-li 12.Non-li resolu	inear spectrosco inear microscop tion microscop ethods	ppy techniques: py techniques: ( y, Multi-photon	SFG, SHG, Time Confocal microsc microscopy met	e-resolved spectro opy, Fluorescenc hods, Scanning r	oscopy e microscopy, Super- nethods.	
reaching m						
Active partic discussion s material.	essions with pr	lectures and exe resentations give	ercises with prob en by the particip	lems for self-stuc ants, Moodle cou	lying, Q&A and ırse with online	
Mode of ass	essment					
20 - 40 min lectures	end-of-term ora	ll exam or 2-hou	ır end-of-term wi	ritten exam on the	e content of the	
Requiremen	it for the award	of credit points				
Passing the	written examin	ation				
Module app	licability					
M.Sc. Chem	istry; M.Sc. iM	OS; M.Sc. Laser	s and Photonics			
Weight of th	e mark for the	final score				
Weighted ac	cording to CPs					
iMOS: CP-w	eighted average	e of the exam (5	CP) and the lab	report (4 CP) gra	des according to the	
examination	examination regulations					
Module coor	rdinator and leo	cturer(s)				
P. Petersen						
Lecturers fro	Lecturers from Physical Chemistry departments					
Further info	Further information					

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75	Credits	Workload	Term	Frequency	Duration	
1.5	5 CP	150 h	1. Semester	WS	1 Semester	
Courses			Contact hours	Self-Study	Group size	
a) Compact cou	rse "Laser and	l Optics"	6 SWS, 75 h	75 h	12 Students	
Prerequisites						
Knowledge in l	oasic Physica	l Chemistry and	d Physics.			
Learning outco	mes					
<ul> <li>After successful completion of the module/course, students will be able to:</li> <li>Acquire advanced knowledge in laser and optics</li> <li>Analyze and evaluate the experimental results</li> <li>Write reports with theories, experiments, and discussion of results</li> <li>Analyze and screen relevant literatures independently</li> <li>Develop skills in handling lab setups, measurements</li> <li>Develop presentation skills in front of an audience</li> <li>Utilize digital techniques to prepare and conduct a presentation</li> </ul>						
Content		uo noni, propur				
Lectures and exercises on topics: laser, polarization, Fourier transformation, spectroscopy, basic optics, Gaussian optics, nonlinear optics. Lab work, handling, and measurements of experimental systems: beam alignment, interferometer, polarization, spectrometer. <b>Teaching methods</b> Lecture (2 SWS, 25 h), Exercise (0,5 SWS, 5 h), Seminar (0,5 SWS, 5 h), Lab work (3 SWS, 40 h).						
Lecture (2 SWS Compact cours	5, 25 h), Exer e in two wee	cise (0,5 SWS, 5 k (Mo-Fr) and o	5 h), Seminar (0,5 me seminar dav i	5 SWS, 5 h), Lab	work (3 SWS, 40 h). week	
Lecture (2 SWS Compact cours <b>Mode of assess</b>	5, 25 h), Exer e in two wee <b>ment</b>	cise (0,5 SWS, 5 k (Mo-Fr) and o	i h), Seminar (0,5 ne seminar day i	5 SWS, 5 h), Lab n the following	work (3 SWS, 40 h). week.	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an	5, 25 h), Exer <u>e in two wee</u> <b>ment</b> ation during ad report abo	cise (0,5 SWS, 5 <u>k (Mo-Fr) and o</u> lectures, exercis put the lab work	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta	5 SWS, 5 h), Lab <u>n the following</u> lab work. al results.	work (3 SWS, 40 h). week.	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for	5, 25 h), Exer <u>e in two wee</u> <b>ment</b> ntion during nd report abo or the award	cise (0,5 SWS, 5 <u>k (Mo-Fr) and o</u> lectures, exercis <u>out the lab work</u> <b>of credit points</b>	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta	SWS, 5 h), Lab n the following lab work. al results.	work (3 SWS, 40 h). week.	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results.	5, 25 h), Exer <u>e in two wee</u> <b>ment</b> ation during ad report abo or the award or the award	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis <u>out the lab work</u> of credit points on (50%) and rep	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. d experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica	5, 25 h), Exer <u>e in two wee</u> <b>ment</b> ation during ad report abo or the award :: presentation ability	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis out the lab work of credit points on (50%) and rep	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. l experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica	5, 25 h), Exer e in two wee ment ation during nd report abo or the award cor the award cor the award cor the award cor the award cor the award	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis out the lab work of credit points on (50%) and rep	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about O Chemistry.	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. l experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica M.Sc. Chemist Weight of the r	5, 25 h), Exer e in two wee ment ation during nd report abo or the award c presentatio bility ry, M.Sc. Bio nark for the	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis out the lab work of credit points on (50%) and rep ochemistry, PhD final score	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about OChemistry.	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. l experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica M.Sc. Chemist Weight of the r	5, 25 h), Exer e in two wee ment ation during nd report abo or the award cor the award :: presentation ability ry, M.Sc. Bio nark for the rding to CPs	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis out the lab work of credit points on (50%) and rep ochemistry, PhD final score	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about OChemistry.	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. l experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica M.Sc. Chemist Weight of the r Weighted accord Module coordin	5, 25 h), Exer e in two wee ment ation during nd report abo or the award cor the cor the c	cise (0,5 SWS, 5 <u>k (Mo-Fr) and o</u> lectures, exercis <u>out the lab work</u> <b>of credit points</b> on (50%) and rep ochemistry, PhD <b>final score</b> 	5 h), Seminar (0,5 one seminar day i ces, seminar, and and experimenta port (50%) about O Chemistry.	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week. d experimental	
Lecture (2 SWS Compact cours Mode of assess Active participa Presentation an Requirement for Pass both parts results. Module applica M.Sc. Chemist Weight of the r Weighted account Module coordin M. Havenith-N	5, 25 h), Exer e in two wee ment ation during nd report abo or the award c presentation ibility ry, M.Sc. Bio nark for the rding to CPs nator and leo ewen, P. Pet	cise (0,5 SWS, 5 k (Mo-Fr) and o lectures, exercis out the lab work of credit points on (50%) and rep ochemistry, PhD final score	5 h), Seminar (0,5 one seminar day i ses, seminar, and and experimenta port (50%) about 9 Chemistry.	5 SWS, 5 h), Lab n the following lab work. al results. the lab work and	work (3 SWS, 40 h). week.	

Master of Science Chemistry (M. Sc. Chemistry)



Compost Cou	urse "Seenn	ing Droho Mi	orocoopu"				
Module	Credits	Workload	Term	Frequency	Duration		
7.6	5 CP	150 h	1., 3. Sem	WS	3 weeks		
Courses	0.01	10011	Contact hours	Self-Study	Group size		
Compact Cour	se "Scanning	Probe	a) 18 h	65 h	15 Students		
Microscopy"	0		b) 32 h				
			c) 5 h				
Prerequisites							
Knowledge in b	basic Physical	Chemistry.					
<ul> <li>Knowledge in basic Physical Chemistry.</li> <li>Learning outcomes</li> <li>After participating in the scanning probe microscopy (SPM) compact course the students <ul> <li>are familiar with the basics of scanning probe microscopy.</li> <li>are familiar with the functionality of different SPM techniques.</li> <li>have an overview of applications of scanning probe microscopy.</li> </ul> </li> <li>After participating in the SPM compact course the students are able to <ul> <li>process and analyze SPM data in a proper way.</li> <li>perform AFM and STM measurements with commercial microscope systems.</li> <li>recognize imaging artifacts in SPM images.</li> <li>present results of an individual experimental SPM project (12 hours) in a short talk.</li> </ul> </li> <li>Content <ul> <li>Quantum mechanical tunneling effect; basics of scanning tunneling microscopy (STM) and atomic force microscopy (AFM); functionality of different SPM imaging techniques; image processing and imaging artifacts; preparation of STM tips; spectroscopic measurements with an STM; STM and AFM measurements of oxides and biological samples; sample preparation in ultra high vacuum: digression scanning electron microscopy (SFM): combined SEM/STM</li> </ul></li></ul>							
Teaching meth	ods						
(a) lecture (b) p	ractical exerci	ses (c) seminar					
Mode of assess	ment						
Oral exam		C 11					
Requirement fo	or the award o	r credit points					
Passing the ora	l exam bility						
M Sc. Chemist	ionity m						
Weight of the n	nark for the fi	nal score					
Weighted accor	Weight of the mark for the man score						
Module coordin	nator and lect	urer(s)					
Lecturers from	Physical Cher	mistry departm	ents.				
Further inform	ation						
The registration for the SPM compact course is necessary.							



In-denth n	ractical· I a	ser snectroso	onv in cluste	rs liquids an	d interfaces			
Madula	Credita	Workload	Term	Frequency	Duration			
Module		WORKIOAD	1 & 2  Sem	W/S SS				
/./	o Cr	240 11			1 Semester			
a) In-depth pr	actical: Laser sp	ectroscopy in	8 SWS, 120 h	Self-Study 120 h	Group size			
clusters, liquid	clusters, liquids and interfaces							
Prerequisites								
Knowledge in l	oasic Physical C	Chemistry.						
Learning outo	comes							
After successfu	l completion of	f the module/cou	rse, students will t	be able to:				
<ul> <li>Acquire</li> </ul>	advanced know	ledge in laser saf	ety issues and lase	er spectroscopic te	chniques			
<ul> <li>Carry ou</li> </ul>	it supervised la	ser experiments c	on molecular cluste	ers, on liquids, or o	on interfaces			
<ul> <li>Obtain g</li> </ul>	general knowled	lge of necessary l	ab equipment					
<ul> <li>Visualiz</li> </ul>	e and present r	esults orally and i	in written form	c 1 . 1				
Write re	ports with theo	ries, experiments	, and discussion o	t results in adequa	ite manner			
Utilize d	ligital technique	es to analyze and	evaluate the data a	ind for graphical p	oresentation			
<ul> <li>Develop</li> </ul>	teamwork skill	s and collaboratio	on while carrying o	out hands on expe	riments			
Content								
In this practic	al, an experin	nent chosen from	m the research fi	elds available in	the Havenith's group			
will be carried	l out. The stud	dent summarize	es his findings in	dependently in a	a written report.			
Included topi	cs:		C	1	-			
1. Laser safety	: laser classes	, risks, and prot	tection measures					
2. Selection of	f experimenta	l methods:						
<ul> <li>Spectro</li> </ul>	scopy in heliu	Im nanodroplets	5					
• THz sp	ectroscopy of	liquid and solid	phases using a I	Fourier transform	n spectrometer			
• THz tir	ne-domain sp	ectroscopy	1 0		1			
2 0 1	с. ·	17						
3. Selection of	t topics							
• Vacuun	n techniques	1 / 1.		•				
Dealing	g with ultracol	d gases (e.g. liqi	uid helium and r	utrogen)				
Leak de	tection							
<ul> <li>Mass sp</li> </ul>	pectrometry							
<ul> <li>Laser te</li> </ul>	chnology: OP	O, diode laser, o	or femto second	laser				
<ul> <li>Genera</li> </ul>	tion of THz ra	diation						
<ul> <li>Wavelet</li> </ul>	ngth depende	nt: appropriate o	detector element	S				
<ul> <li>Phase s</li> </ul>	ensitive signa	l detection (lock	-in techniques, r	nodulation techr	niques)			
Teaching met	hods							
Hands-on lab	course (8 hou	urs per week per	module).					
Mode of asses	ssment							
Active partici	pation in pract	tical, feedback d	uring and on the	e experiments, fe	edback on written lab			
reports by tea	ching assistan	its.		·				
Requirement	for the award	of credit points						
All experimer	its are comple	ted successfully	and written up	satisfactorily in a	lab report.			
Module appli	cability			in u	······································			
M.Sc. Chemis	stry.							
Weight of the	mark for the	final score						
Weighted acc	ording to CPs							
Module coord	linator and lec	turer(s)						
M. Havenith-	Newen, G. Scl	hwaab.						
Further infor	mation							



In-depth Practical: Nanoscale surface characterization							
Module	Credits	Workload	Term	Frequency	Duration		
7.8	8 CP	240 h	1.to 3. Sem	Every semester	5 weeks		
Courses			Contact hours	Self-Study	Group size		
In-depth Pract	ical: Nanoscal	e surface	up to 40 h	40 h	1 Student		
characterizatio	n		per week				
Prerequisites							
Physical Chemi	stry I to IV.						
Learning outcom	mes						
Students acquir	e a knowledg	e about differei	nt methods used i	n physical chemis	try and their		
applications							
Content				1 1.00			
scanning probe	methods, ph	otoelectron spe	ctroscopy, low en	ergy electron diffra	action, electron		
energy loss spe	ctroscopy						
Teaching metho	ods						
practical							
Mode of assess	ment						
Report							
Requirement fo	or the award o	f credit points					
Performing exp	eriments and	the report					
Module applica	bility						
M.Sc. Chemistr	у						
Weight of the n	nark for the fi	nal score					
Weighted accor	ding to CPs.						
Module coordin	nator and lectu	ırer(s)					
Lecturers from	Physical Chei	nistry departm	ents.				
Further inform	ation						
possible start in	dependent of	lecture schedu	le; length in week	ks depends on avai	lability of student		
during week							



In-depth Pr	actical: Flu	orescence n	nicroscopy and	1 spectroscopy		
Module	Credits	Workload	Term	Frequency	Duration	
7.9	8 CP	240 h	1.to 3. Sem	Every semester	6 weeks half time or equivalent	
Courses In depth practic and spectroscop	al Fluorescenc y	e microscopy	Contact hours 8 h	<b>Self-Study</b> 120 h	<b>Group size</b> 1 Student	
Prerequisites						
Knowledge of t	oasic spectros	copy principles				
Learning outco	mes					
<ul> <li>After successful completion of the module/course, students will have: <ul> <li>Acquired advanced knowledge in fluorescence-based methods</li> <li>Carried out supervised microscopy and spectroscopy experiments of fluorescent samples</li> <li>Obtained general knowledge on different types of fluorophores and spectral ranges (visible, near infrared)</li> <li>Analyzed data (spectra/images) with standard software and Python-based scripts</li> <li>Written reports and interpreted data with respect to the current literature</li> </ul> </li> <li>Learned to discuss with group members and assess the scientific advance or limitations of experimental approaches and results</li> </ul> Content <ul> <li>Laser safety; Principles of fluorescence spectroscopy and microscopy; preparation of fluorescent samples; chemical modification of fluorophores; image and spectral image processing techniques. </li> </ul>						
Hands on lab c	ourse of curr	ent research toj	pics			
Mode of assess Written lab rep	ment ort					
Requirement for	or the award	of credit points				
Active participa	ation in lab co	ourse and succe	ssful summary of	the lab course res	ults.	
Module applica	bility					
M.Sc. Chemist	ry	<b>N</b> 1				
Weight of the r	nark for the f	inal score				
Weighted accor	rding to CPs.					
Module coordin	nator and lect	urer(s)				
S. Kruss	ation					





In-depth Pr	actical: Nar	omaterials	and Biointerf	aces		
Module	Credits	Workload	Term	Frequency	Duration	
7.10	8 CP	240 h	1.to 3. Sem	Every semester	6 weeks half time or equivalent	
<b>Courses</b> In depth practic Biointerfaces	al Nanomateria	lls and	Contact hours 8 h	Self-Study 120 h	<b>Group size</b> 1 Student	
Prerequisites			•		•	
Knowledge of c	hemical conju	agation technic	lues and basic spe	ectroscopy		
Learning outco	mes					
<ul> <li>After successful completion of the module/course, students will have:</li> <li>Acquired advanced knowledge in synthesis and assembly of fluorescent nanomaterials</li> <li>Prepared nanomaterials and modified their surface using biofunctionalization techniques</li> <li>Carried out microscopy or spectroscopy experiments with these samples</li> <li>Obtained general knowledge on the interplay between surface chemistry and photophysics</li> <li>Analyzed data (spectra/images) with standard software and Python-based scripts</li> <li>Written reports and interpreted data with respect to the current literature</li> <li>Learned to discuss with group members and assess the scientific advance or limitations of experimental approaches and results</li> <li>Content</li> <li>Preparation of fluorescent nanomaterials; optical characterization techniques (absorption spectroscopy), fluorescence spectroscopy, Raman spectroscopy); surface chemistry approaches;</li> </ul>						
Teaching meth	ods					
Hands on lab c	ourse of curre	ent research top	pics			
Written lab rep	ment ort					
Requirement fo	or the award o	f credit points				
Active participa	tion in lab co	urse and succe	ssful summary of	the lab course res	ults.	
Module applica	bility					
M.Sc. Chemist	ry					
Weight of the n	nark tor the fi	nal score				
Weighted accor	ding to CPs.					
	hator and lect	urer(s)				
S. Kruss	ation					



In-depth practical: Chemical Microscopy of Surfaces and Biomaterials							
Module	Credits	Workload	Term	Frequency	Duration		
7.11	8 CP	240 h	1., 2. Sem	Every semester	6 weeks half time or equivalent		
Courses			Contact hours	Self-Study	Group size		
In-depth Pract	ical: I - III		8 h	120 h	~ 1-3 Students		
Prerequisites							
Knowledge of b	asic spectros	copic and data e	evaluation technic	lues.			
Learning outco Students acquir microscopic tec	<b>mes</b> re knowledge hniques and l	on how to prep how to analyse	are samples, how the image and sp	to investigate ther ectral data acquire	n with Raman d.		
Content Laser safety; Pr samples; data a processing tech	inciples of con cquisition tec miques.	nfocal Raman n hniques; estima	nicroscopy; prepa ates of data qualit	ration of chemical y; image and spect	and/or biological ral image		
Teaching meth	ods						
hands on lab co	ourse						
Mode of assess	ment						
Written lab rep	ort	<u> </u>					
Requirement fo	or the award o	f credit points					
Active participa	tion in lab co	urse and succes	ssful summary of	the lab course resu	ults.		
Module applica	bility						
M.Sc. Chemistr	ry						
Weight of the n	nark for the fi	nal score					
Weighted accor	ding to CPs.						
Module coordin	nator and lect	urer(s)					
Lecturers from	Physical Cher	mistry departm	ents.				
Further inform	ation						



Research Pra	actical in the	e Focal Point	Programme "F	Physical Chemis	stry"			
Module	Credits	Workload	Term	Frequency	Duration			
7.12	15 CP	450 h	3. Sem	Every semester	1 semester			
Courses			Contact hours	Self-Study	Group size			
Research Prac	tical in the Fo	cal Point	15 h	120 h	1 Student			
Programme								
Prerequisites	Prerequisites							
"Practical Scien chemistry	"Practical Science and Communication", In-depth practical I–III, basic knowledge of physical chemistry							
Learning outco	mes							
The student wi Physical Chemi the student will to design, impl	ll be introduce istry research l acquire adva ement, perfor	ed to and traine groups. Initiall nced scientific m, and analyze	ed in the scientific y under the guida knowledge and w a research projec	e methods applied in ance of experienced ill learn the skills r et related to the cur	in one of the l research staff, necessary in order rrent research of			
the groups. The software needed	e student will d for analysis	become acquai and simulation	nted with the exp , learn how to sea	erimental techniqu arch the scientific l	ies and/or the iterature for			
previous work in the co	relevant for th	e project, and a ent research	icquire the ability	to summarize and	discuss the			
Content	unchi or curr	ent rescuren.						
The student will groups. These of	ll participate i comprise spec	n an experimer ctroscopy, micro	nt from the resear oscopy, biophysic	ch areas of the Phy al chemistry, photo	ysical Chemistry ochemistry,			
processes at su	rfaces and int	erfaces, calorin	netric methods, so	olvation, nanoclust	ers, mass			
spectrometry, v	acuum techn	iques, structura	l properties and o	lynamics, developi	ment of scientific			
apparatus, sign	al demodulat	ion, advanced d	ata evaluation tec	hniques, lab safety	v, laser safety, and			
more specialize	ed physicoche	mical topics.						
The student wi	ll also take pa	rt in the meetin	igs of the research	n group on a regula	ar basis and			
actively contrib	ute to the disc	cussion of the p	roject.					
The student su	mmarizes the	findings indep	endently in a wri	tten report and/or	will present the			
results in a sem	ninar talk.							
Teaching meth	ods							
Hands-on lab c simulation	ourse, active j	participation in	experimental dat	a acquisition and/o	or analysis &			
Mode of assess	ment							
written lab repo	ort and/or sen	ninar talk						
Requirement for	or the award o	of credit points						
all experiments in a lab report a	and/or simu and/or presen	lations are com ted in an adequ	pleted successful ate manner in a s	ly; they are written seminar talk.	up satisfactorily			
Module applica	bility							
Master of Scier	ice Chemistry	7						
Weight of the n	nark for the fi	nal score						
Weighted accor	ding to CPs.							
Module coordin	nator and lect	urer(s)						
Lecturers from	Physical Che	mistry departm	ents.					
Further inform	ation	flocture ashad	lo. longth in mest	a dononda on origi	lability of atudant			
possible start if	idependent of	i iecture schedu	ne, iengtri in weel	ks depends on avai	ladinity of student			
during week								



### Industrial Chemistry

Heterogeneous Catalysis							
Module	Credits	Workload	Term	Frequency	Duration		
81	5 CP	150 h	1. Sem.	only WS	1 Semester		
Courses			Contact hours	Self-Study	Group size		
Heterogeneous	Catalysis		a) 2 SWS	105 h	All students choosing		
			b) 1 SWS		Industrial Chemistry		
Prerequisites							
Solid knowledge	of basics in In	dustrial Chemist	rv. Physical Chem	nistry. Inorganic (	Chemistry, and Organic		
Chemistry			-,,,~				
Learning outco	mes						
Students	a get insight in	to the scientific h	asis of heterogen	eous catalysis wi	th emphasis on the		
element	ary steps of cat	alvtic reactions of	on relations betwe	en catalyst struct	ure and reactive		
propertie	es between pre	enarction routes	and obtained stru	ctures and on th	e interdisciplinary		
approac	in catalyst i	research. They ar	e introduced to th	e most importan	t characterization		
methods	s for heterogen	eous catalysts an	d get an overview	over the most im	portant technical		
applicati	ons of heterog	eneous catalysis.	The course enabl	es students to ori	ent themselves in the		
multifac	eted field of in	dustrial heteroge	neous catalysis ar	nd creates the bas	is for own scientific		
activities	s in catalysis re	search.	,,				
<ul> <li>Soft skil</li> </ul>	ls: interactive r	presentation to ar	n experienced aud	ience, taking not	es during lectures.		
unsolici	ted follow-up o	f module conten	ts, unsolicited cor	sultation of relev	ant literature		
Content	I		,				
1. Elementary st	eps of heterog	eneous catalvsis ·	- chemisorption: e	energetics, adsorr	otion sites and surface		
phases; surfac	ce reaction, sur	face reaction dyr	namics	8			
2. Relations bety	ween structure	and reactivity of	catalytic surfaces	- spatial structure	e: anisotropy of surface		
structures and	d properties in	metal and non-n	netal catalysts, ens	semble effects an	d their use, electronic		
structure - vol	cano relations	and their basis, l	igand effects				
3. Promotors an	d poisons in ca	atalysis - chemica	l and structure pr	omoters and me	chanisms of their		
function, pror	noting selectiv	ity and stability,	basics of poisonin	ig effects			
4. Supported cat	alysts - introdu	iction to texture j	properties, structu	ire and properties	s of important supports,		
surface chem	istry of typical	supports, interac	tions between sup	pported compone	nts and supports		
5. Preparation a	nd activation o	f catalysts - basis	steps in the prepa	aration of solid m	aterials from the		
viewpoint of o	atalysis, additi	on of active comp	ponents to suppor	ts, shaping of cat	talyst pellets, thermal		
aftertreatmen	t, activation of	catalyst precurso	ors				
6. Important cat	alyst types and	their application	ı - metal catalysts	(including bifund	ctional catalysis),		
catalysis with	redox oxides, i	ndustrial acid cat	talysis, environme	ental catalysis			
7. Characterizat	ion of heteroge	eneous catalysts -	laboratory reactor	rs for reactivity cl	naracterization, texture		
characterizati	on by physisor	ption and chemis	sorption techniqu	es, thermoanalyti	ical (temperature-		
programmed)	methods, stru	ctural analysis by	y XRD, by X-ray a	bsorption, surfac	e analysis by XPS, ISS,		
vibrational sp	ectroscopy, opt	tical and scannin	g probe microsco	py, miscellaneous	s techniques (incl.		
Mößbauer-, E	PR-, NMR- and	d UV-vis spectros	scopy)				
Teaching method	ds						
a) Lecture; b) Exe	ercises						
Mode of assessm	ient						
30 min end-of-ter	rm oral exam						
Requirement for	the award of c	realt points					
Modulo applicab							
Master of Chemi	stry focal poin	t Industrial Cher	nistry				
Weight of the m	ark for the fine		y				
Weighted accord	ing to CPg						
Module coordina	tor and lecture	or(s)					
B. Mei M Muhl	er	-(3)					
Further inform	ation						

All lectures, additional contents of exercises, summaries of student lectures are distributed via *moodle*.



Module 8.2Credits 5 CPWorkload 180 hTerm 1. Sem.Frequency only WSDuration 1 Semester					
8.25 CP180 h1. Sem.only WS1 Semester					
Courses Contact hours Self-Study Croup size					
Industrial Chemistry II: Chemical Reaction (a) 2 SWS (105 h) (105 h)	ina				
Engineering					
Dramonicitar	uy				
Solid knowledge of basics in Industrial Chemistry and Physical Chemistry					
Learning outcomes					
• Students acquire advanced knowledge about reactors used in chemical industry. They can app mathematical models to describe ideal reactors und will know reasons of deviations from idea behavior and know basic models for description of non-ideal reactors. In addition, students ca	ly l n				
apply thermodynamic and kinetic tools in the analysis of reactions and are able to evaluate					
consequences of transport limitations on overall reaction rates and are able to select appropria	te				
counteractive measures.					
• Soft skills: interactive presentation to an experienced audience, taking notes during lectures,					
unsolicited follow-up of module contents, unsolicited consultation of relevant literature					
<b>Content</b>					
<ol> <li>Basics of chemical reaction engineering: terms and definitions</li> <li>Stoichiometry and thermodynamics: stoichiometric balance and chemical conversion, calcula</li> </ol>	ion				
2. Stochonerty and merinodynamics, stochonerte balance and chemical conversion, calcula of reaction enthalpy under reaction conditions, chemical equilibrium, definition of equilibrium.	n 1011				
constants in diluted and concentrated systems. Michaelis, Menten, Kinetik	11				
3 Kinetics of chemical reactions: volume-constant reactions in ideal reactors, kinetics of multipl	ρ				
homogeneous reactions (first Damköhler number, polymerization, Michaelis-Menten-kinetic	3)				
kinetics of heterogeneous reactions (catalysis steps Langmuir isotherm competitive adsorpt	on				
monomolecular and bimolecular reactions. Langmuir-Hinshelwood Elev-Rideal Hougen-	011,				
Watson rate laws. Bodenstein principle, rate-limiting step, most abundant surface intermedia	e.				
mass transport in heterogeneous reactions	/				
4. Combination of mass and heat transfer: kinetics of heterogeneous reactions limited by surfac	ć				
reaction or transfer processes, reaction through liquid/liquid interface, effectiveness factors,					
consecutive model in heterogeneous catalysis (second Damköhler number) and in reaction					
through liquid/liquid interface, parallel approach in heterogeneous reactions (Thiele modulus	) and				
in reactions through liquid/liquid interface (Hatta number), especially for catalytic reactions					
(generalized Thiele modulus, criteria for limitation of mass transfer - Weisz modulus, mass					
transfer and overall kinetics, combining of reaction and heat transfer - Prater number)					
5. Reactors in chemical industry (overview): ideal reactors (types, calculation of conversion, resid	ence				
time distribution, cascade of CSTRs, complex reactions in CSTR, PFR, selectivity, non-isother	mal				
reactions, instability), non-ideal reactors (residence time distribution, dispersion model, CSTI	ls-in-				
series model, segregation, time of mixing, influence of segregation on kinetics)					
6. Modelling of real reactors, selectivity in parallel and consecutive reaction networks					
7. Non-steady state reactor operation: transition behavior of a CSTR, transient experiments					
Teaching methods					
a) Lecture; b) Exercises					
Mode of assessment					
30 min end-of-term oral exam					
Requirement for the award of credit points					
Passing the oral exam					
Module applicability					
Waster of Chemistry, focal point industrial Chemistry					
Weighted according to CDg					
Medule coordinator and lecturor(c)					
Muller B Mei					
Further information					
All documents are provided via moodle					

#### FAKULTÄT FÜR CHEMIE UND BIOCHEMIE

Master of Science Chemistry (M. Sc. Chemistry)



Modern Mic	rokinetics						
Module	Credits	Workload	Term	Frequency	Duration		
8.3	5 CP	150 h	2. Sem.	only SoS	1 Semester		
Courses Modern Microk	inetics		Contact hours a) 2 SWS b) 1 SWS	<b>Self-Study</b> 105 h	Group size All students choosing Industrial Chemistry		
Prerequisites				I			
Solid knowledg	e of basics in	Chemical React	ion Engineering,	Industrial Cher	nistry and Physical		
Chemistry							
<ul> <li>By mea modern describe problen</li> <li>Soft ski lectures literatu</li> </ul>	<ul> <li>Learning outcomes</li> <li>By means of examples students acquire advanced knowledge on basics and application of modern simulation tools used in chemical engineering. The kinetics of a reaction is described based on elementary steps. After the course students are able to solve basic problems of chemical reaction engineering using MATLAB.</li> <li>Soft skills: interactive presentation to an experienced audience, taking notes during lectures, unsolicited follow-up of module contents, unsolicited consultation of relevant</li> </ul>						
Content							
<ol> <li>Modelin modelin statistic prograr</li> <li>Microki algorith</li> <li>Reactor models of kinet</li> <li>numeri equatio</li> <li>overviev introdu</li> </ol>	<ul> <li>Content</li> <li>8. Modeling a chemical reaction using elementary steps: introduction of microkinetic modeling, description of adsorption, desorption and reaction on a molecular basis, statistical thermodynamics, estimation of kinetic parameters, modeling of temperature-programmed experiments, simulation of SSITKA experiments</li> <li>9. Microkinetic models: determination of kinetic parameters, Levenberg-Marquardt algorithm, examples</li> <li>10. Reactor models: adiabatic packed-bed reactors, heterogeneous and pseudo-homogeneous models, consideration of non-steady reactor states, model selection, programs of estimation of kinetic constants</li> <li>11. numerical tools for solution of non-linear algebraic equations and non-linear differential equations: boundary and initial value problems, one- and multiple-step procedure</li> <li>12. overview of commercial software and routines in numerical/statistical libraries, introduction to MATLAB</li> </ul>						
a) Lecture: b) E	vercises using	MATLAB					
Mode of assess	ment	,					
30 min end-of-t	erm oral exam	n					
Requirement for	or the award o	f credit points					
Passing the ora	l exam	*					
Module applica	bility						
Master of Chen	nistry, focal po	oint Industrial (	Chemistry				
Weight of the n	nark for the fi	nal score					
Weighted accor	ding to CPs						
Module coordin	nator and lectu	urer(s)					
M. Muhler, B. I	Mei						
Further inform	ation						
All documents	All documents are provided via <i>moodle</i>						

Master of Science Chemistry (M. Sc. Chemistry)



Processes in Chemical Production - Past, Present and Future					
Module	Credits	Workload	Term	Frequency	Duration
84	5 CP	150 h	2. Sem.	only SoS	1 Semester
Courses			Contact	Self-Study	Group size
Processes in C	Themical Prod	uction - Past.	hours	105 h	All students
Present and Fi	uture	action rubt,	a) 2 SWS	103 11	choosing
			b) 1 SWS		Industrial
			-,		Chemistry
Prerequisites					
Solid knowledg	e of basics in	Industrial Cher	nistry Inorgani	c Chemistry Organ	ic Chemistry and
Physical Chem	istrv		instry, morgani	e Gileinisti), organ	ie Gheinistry, und
Learning/Cours	e Objectives:				
Students will a	cauire knowle	dge on importa	nt processes in	chemical production	and on the
network of raw	materials and	l product flows	in a national ec	onomy into which th	lese are
integrated The	v are to appre	ciate the influe	nces of access to	raw materials inclu	ding renewables
technological st	tandard and re	ogional conditio	ons on the struct	ture of the chemical	industry and to
know importan	it final produc	ts of chemical r	production and	typical quality charac	teristics targeted
in the production	on process. Th	nev get insight i	n important ma	inagement aspects it	n the chemical
industry, in par	ticular related	l to the assessm	ent and innova	tion of production p	rocesses.
Content				r - F F	
1. Raw ma	aterials for inc	lustrial organic	chemistry in pa	st, present and futu	re
2. Oil refi	ning, processe	es and actual tre	ends	, <b>F</b>	
3. Produc	tion and use c	of synthesis gas	and of hydroge	n; production and us	se of olefins;
oxidatio	on processes i	n chemical indu	ustry; synthesis,	properties and tech	nology of polymer
materia	ls			1 1	
4. Basic p	rocesses of in	organic chemic	al technology (ii	ncl. fertilizers)	
5. Industr	rial use of rene	ewables, presen	ce and perspect	ive	
6. Busines	ss-manageme	nt aspects of a c	hemists' job in	industry	
7. Criteria	for the evaluation of the eval	ation of chemic	al production p	rocesses, methodolo	gy for the design
of new	chemical proc	luction process	es		
Teaching meth	ods				
a) Lecture; b) E	xercises				
Mode of assess	ment				
30 min end-of-	term oral exar	n			
Requirement for	or the award o	f credit points			
Passing the ora	ll exam				
Module applica	bility				
Master of Cher	nistry, focal po	oint Industrial (	Chemistry		
Weight of the r	nark for the fi	nal score			
Weighted accor	rding to CPs				
Module coordin	nator and lecture	urer(s)			
B. Mei, H. Zan	thott, A. Wolf	, M. Muhler			
Further inform	ation		1	. 1	
All lectures and additional contents of exercises are distributed via <i>moodle</i> .					


Module	Credits	Workload	Term	Frequency	Duration
8.5	8 CP	240 h	1. Sem.	only WS	1 Semester
Courses			Contact hours	Self-Study	Group size
Characterizatio	on of Heterogen	eous Catalysts	a) 8 SWS	105 h	Max. 12
	C	·	b) 1 SWS		participants
Prerequisites Solid knowled Chemistry, an	ge of basics in d in Industrial	Heterogeneous ( Chemistry	Catalysis, Chemic	cal Reaction Eng	ineering, Physical
Learning/Cour	se Objectives:				
Practical exper related data tro critical assessm of the results f training in rep	elence with im eatment metho nent of the po for catalyst reso porting, presen	portant characte ods and approac tential of the tec earch, tation and publ	erization technic ches to data inter chniques, the ac ic discussion of	ques for heterog rpretation, curacy of the da the results.	geneous catalysts, the ta and the significance
Content					
Practical expen	riments using				
<ul> <li>nitrog</li> <li>therm</li> <li>X-ray j</li> <li>FTIR s</li> <li>Raman</li> <li>UV-Vi</li> <li>X-ray o</li> <li>and virtual exp</li> <li>X-ray a</li> <li>and ot</li> </ul>	en physisorptio ogravimetry, photoelectron s spectroscopy, n spectroscopy s spectroscopy diffraction, periments (trea absorption spe her methods	on, spectroscopy, , , atment of measu ctroscopy	ured data only) i	n	
are offered. 4	selected experi	ments are perfo	ormed by groups	s of 2 students.	
Teaching met	hods				
a) Practical; b)	Seminar				
Mode of asses	sment	1 C . 1	1) - to -1. 1' 1'	· · · · ·	
SU min end-of	-term presenta	tion of the resu	ints including dis	scussion	
Requirement	for the award of	of credit points			
Successful exp	erimental per	formance, 4 acc	epted protocols,	and successful	oral presentation
Module applic	ability		C1		
Waster of Che	mistry, focal p	oint industrial	Cnemistry		
Weight of the	mark for the f	mai score			
weighted acco	ing to CPS	11808(3)			
	mator and lect	urer(s)			
D. WICI, WI. WIL	nation				
All required d	nation	as foty in atmissi	ong ara diatribu	tod via moodla	
An required de	ocuments incl.	. Safety mistructi	ions are distribu	icu via mooule.	

# FAKULTÄT FÜR CHEMIE UND BIOCHEMIE

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Master of Science Chemistry (M. Sc. Chemistry)



In-depth Practical: Industrial Catalysis								
Module	Credits	Workload	Term	Frequency	Duration			
8.6	8 CP	240 h	12. Sem.	WS and SoS	1 Semester			
Courses			Contact hours	Self-Study	Group size			
Industrial Catalysis a) 8 SWS 105 h Max. 4								
	b) 1 SWS participants							
Prerequisites								
Solid knowledg	e of basics in	Chemical React	ion Engineering,	Heterogeneous Cata	lysis and in			
Industrial Cher	nistry							
Learning/Cours	e Objectives:							
Students plan,	perform and e	evaluate experir	nents in the fiel	d of fundamental r	esearch under the			
supervision of a	an experience	d scientist. The	y receive a detai	led introduction int	to selected			
scientific metho	ods used in m	odern research	in the field of h	eterogeneous catal	ysis.			
Soft skills: team	nwork and col	laboration whil	e carrying out e	xperiments, graphi	cal presentation of			
practical results	s, general kno	wledge about o	perating system	s, software and con	nputing, scientific			
writing skills								
Content								
Scientif	fic collaboration	on in a team wo	orking on a selec	ted problem of het	erogeneous			
catalysis	S							
Detailed	d introduction	to the scientifi	c methods appl	ied in fundamental	research			
Literatu	ire search and	evaluation of t	he scientific tas	KS	_			
Plannin	ng, performing	g and evaluating	g of the experim	ents under the sup	ervision of an			
experier	nced scientist							
Written	report and or	al presentation	of the theoretic	al basics and obtain	ned results			
Teaching meth	ods							
a) Practical; b) S	Seminar							
Mode of assess	ment	· · · · · ·	1. • 1 1• 1•	•				
50 min end-of-t	erm presenta	tion of the resu	its including dis	scussion				
Requirement io	or the award o	r credit points		d				
Successful expe	rimental peri	ormance, accep	oted protocol, ar	id successful oral p	resentation			
Module applica	Dility	int Induction (	The operation					
Waster of the n	nistry, iocar po		Shennsuy					
Weighted accor	ding to CPg	liai score						
Module coordir	ung to CI s	1ror(s)						
M Muhler R	Mei	1101(5)						
Further inform	ation							
All required do	cuments incl	safety instructi	ons are distribu	ted via moodle				
All required documents incl. safety instructions are distributed via <i>moodle</i> .								



# In-depth Practical: Reaction Engineering of Heterogeneously Catalyzed Reactions

iteactions	Reactions							
Module	Credits	Workload	Term	Frequency	Duration			
8.7	8 CP	240 h	1. Sem.	only WS	1 Semester			
Courses			Contact hours	Self-Study	Group size			
Reaction Engineering of Heterogeneously			a) 8 SWS	105 h	Max. 8			
Catalyzed Reactions			b) 1 SWS		participants			

#### Prerequisites

Solid knowledge of basics in *Chemical Reaction Engineering, Heterogeneous Catalysis, Physical Chemistry,* and in Industrial Chemistry

# Learning/Course Objectives:

Advanced knowledge in basic fields of chemical reaction engineering, which are important for heterogeneously catalyzed reactions: ignition/quenching behavior and stability, reaction limitation by external and internal mass transfer, influence of mixing on conversion. After the course students are familiar with procedures used for the analysis of kinetics of heterogeneously catalyzed reactions (operation of a challenging flow set-up with on-line analysis, test for transfer limitations, collection of kinetic data, data processing).

Soft skills: teamwork and collaboration while carrying out experiments, graphical presentation of practical results, general knowledge about operating flow systems, software and computing

# Content

In-depth kinetic experiment (one experiment per group of two students):

- steam reforming of methane
- photocatalytic degradation of methylene blue
- isothermal and transient biochar oxidation
- further experiments depending on availability

Investigation of the kinetics of a complex heterogeneously catalyzed reaction (calibration of the experimental set-up, testing the analytical detection of reaction products, standard tests of external and internal mass transfer limitations, measurement of concentration/time dependences, evaluation of practical results concerning the reaction mechanism, calculation of kinetic parameters)

Basic experiments (for each group of two students):

- nitrite reduction
- polytropic tank reactor
- residence time distribution and conversion calculation

Studying ignition/quenching behavior and instabilities (oscillations) exemplified with an exothermic reaction (decomposition of hydrogen peroxide); influence of internal mass transfer (pore diffusion, Thiele modulus) on the overall reaction rate in a three-phase system (nitrite reduction); experimental determination of residence time behavior and conversion of different reactors (CSTR, PFR, CSTRs-inseries) depending on mixing; data evaluation using different models for ideal and non-ideal reactors (dispersion, CSTRs-in-series and segregation model, calculation of Bodenstein and Damköhler number).

#### Teaching methods

a) Practical; b) Seminar

# Mode of assessment

50 min end-of-term presentation of the results including discussion

# Requirement for the award of credit points

Successful experimental performance, accepted protocols (1+3), and successful oral presentation

Module applicability

Master of Chemistry, focal point Industrial Chemistry

Weight of the mark for the final score

Weighted according to CPs

Module coordinator and lecturer(s)

M. Muhler, B. Mei

# Further information

All required documents incl. safety instructions are distributed via *moodle*.



# Theoretical Chemistry

Computational Chemistry I: Structure and Dynamics of Molecules							
Module	Credits	Workload	Term	Frequency	Duration		
9.1	5 CP	150 h	1., 3. Sem	WS	1 Semester		
Courses	I	1	Contact	Self-Study	Group size		
a) Lectures			hours	75 h	~ 10 students		
b) Exercises			a) (2 SWS)				
			b) (1 SWS)				
Prerequisites							
Admission to the	ne Master Co	urse Program					
Learning outcom	mes						
Students acquin	re a broad ove	erview upon co	mputational tecl	nniques applied i	n drug design		
Content							
Forcefields, Qu	antum chem	ical methods (s	emiempiric, ab	initio, DFT, TDD	FT), Protein		
structures, Mol	ecular dynam	nics, Monte Car	lo, Free Energy	Calculations			
Teaching meth	ods						
a) Lecture (2 ho	ours per week	)					
b) Computer ex	ercises (1 ho	ur per week or	block course)				
Mode of assess	ment						
Oral examination	on						
Requirement for	or the award o	of credit points					
Passing the oral	examination						
Module applica	bility						
M.Sc. Chemistr	<u>ry</u>						
Weight of the n	hark for the fi	inal score					
Weighted accor	ding to CPs						
Module coordir	nator and lect	urer					
M. Schindler							
Further inform	ation						



Computatio	nal Chemi	stry II: Qua	intitative Stru	cture-Activity	y Relations in			
Drug Design								
Module	Credits	Workload	Term	Frequency	Duration			
9.2	5 CP	150 h	2., 4. Sem	SS	1 Semester			
Courses Contact Self-Study Group size								
a) Lectures			hours	75 h	~ 10 students			
b) Exercises			a) (2 SWS)					
			b) (1 SWS)					
Prerequisites								
Knowledge acq	uired in Com	putational Che	emistry I					
Learning outco	mes							
Students acquir	re a broad ove	erview upon co	mputational tecl	nniques applied i	n drug design			
Content								
Classical QSAR	ls in rational	drug design: M	ILR, PCR (Hans	ch, Free-Wilson,	LFER), Partial least			
squares, Advan	ces methods:	3D-QSAR(Co	MFA, WAVE3D)	, ANN, SVM, Fu	zzy Logic, Protein			
modeling, Desi	gn of experin	nents						
Teaching meth	ods							
a) Lecture (2 ho	ours per week	)						
b) Computer ex	ercises (1 ho	ur per week or	block course)					
Mode of assess	ment							
Oral examination	on	<u> </u>						
Requirement for	or the award o	of credit points						
Passing the oral	examination							
Module applica	Dility							
M.SC. Chemisti	ry norde for the f							
Weight of the f	ding to CDg	inal score						
Modulo coordia	unig io Crs	11404						
Module coordin	lator and lect	uler						
Further inform	ation							
	auvii							



Theoretical					
Module	Credits	Workload	1 erm	Frequency	Duration
9.3	5 CP	150 h	1. or 3. Sem.	Each WiSe	1 Semester
Courses			Contact hours	Self-Study	Group size
a) Lectures			a)+b)	a) 30 h	10 – 20 Students
b) Exercises			2+1 SWS	b) 75 h	
Prerequisites					
Undergraduate	level knowledg	ge in classical mee	chanics, statistical	mechanics and tin	ne-
independent no	n-relativistic qu	uantum mechani	CS		
Learning outcor	nes				
Students acquir	e advanced kno	owledge of the th	eory and computat	tional techniques o	of statistical mechanics
and (bio)molecu	lar dynamics s	simulations in the	e realm of (bio)mo	lecular systems su	ch as (bio)molecules,
clusters, liquids	solids and su	rfaces. In addition	n, analysis method	s to extract observation	ables of experimental
interest, such as	various specti	roscopic, scatterir	ng, and diffraction	techniques, are pr	esented such that the
students can juc	lge both their s	strengths and wea	aknesses with the t	focus on topical pr	oblems in Theoretical
Chemistry with	a focus on Sol	vation Science.		1 1	
Content					
Essentials of clas	ssical and statis	stical mechanics:	Formulations acco	ording to Newton, I	Lagrange and Hamilton,
corresponding of	equations of n	notion, conservat	tion laws/conserve	ed quantities, Noe	ther theorem, Liouville
theorem, ensen	nbles, distribu	tion functions, f	first and second i	moments of distri	ibutions, connection to
averages and fl	uctuations of	observables, corr	elation functions	in space and time	e, van Hove correlation
function, pair a	nd radial corre	elation function	with connection to	o x-ray diffraction	and neutron scattering
experiments, dy	namic and stat	tic structure facto	rs.	·	Ũ
Potential energy	surfaces: Vale	ence force fields,	pair potentials, ma	ny-body effects, en	mpirical versus ab initio
parameterizatio	ns, characteriz	ation of stationary	y points, connectio	n between propert	ies of hypersurfaces and
chemical concep	ots, adiabatic cl	hemical reactions	3.		
Molecular dyna	mics: Basic i	dea of classical	molecular dynam	ics, deriving inte	grators via "pedestrian
approach" and	via Liouville	formalism, erg	godicity, extended	phase space/La	grangian methods for
thermostatting	and barostattii	ng, finite system	size effects, bour	dary conditions, o	convergence criteria for
dynamical comp	outer simulatio	ons, realizing vario	ous ensembles in t	erms of simulatior	n algorithms, holonomic
constraints, deri	ving molecula	r dynamics from	the time-depender	nt Schroedinger ec	juation, time-dependent
self-consistent f	ield dynamics	, ab initio molect	ular dynamics equ	ations of motion	according to Ehrenfest,
Born-Oppenheir	mer and Car-P	arrinello, includi	ng nuclear quantu	m effects via path	integral simulations.
Teaching metho	ds				
Lecture and exe	cises with pro	blems for self-stu	dying, Q&A and d	liscussion sessions	with presentations
given by the par	ticipants, digit	al material provid	led via TheoChem	Cloud.	
Mode of assessm	nent				
Written or oral e	end-of-semeste	er exam			
Requirement for	r the award of	credit points			
Passing the end	-of-semester ex	xam			
Module applical					
	oility				
M.Sc. Chemistr	oility y and M.Sc. Bi	ochemistry (Foca	l Point Program "I	Biomolecular Cher	nistry")
M.Sc. Chemistr Weight of the m	oility y and M.Sc. Bi ark for the fin	ochemistry (Foca al score	l Point Program "I	Biomolecular Cher	nistry")
M.Sc. Chemistry Weight of the m According to CF	oility y and M.Sc. Bi ark for the fin	ochemistry (Foca <b>al score</b>	l Point Program "l	Biomolecular Cher	nistry")
M.Sc. Chemistr Weight of the m According to CF Module coordin	pility y and M.Sc. Bi ark for the fin ator and lectur	ochemistry (Foca al score rer(s)	l Point Program "I	Biomolecular Cher	nistry")
M.Sc. Chemistr Weight of the m According to CF Module coordin D. Marx	pility y and M.Sc. Bi ark for the fin ator and lectur	ochemistry (Foca al score rer(s)	l Point Program "I	Biomolecular Cher	nistry")
M.Sc. Chemistr Weight of the m According to CF Module coordin D. Marx Further information	v and M.Sc. Bi ark for the fin ator and lectur	ochemistry (Foca al score rer(s)	l Point Program "I	Biomolecular Cher	nistry")
M.Sc. Chemistry Weight of the m According to CF Module coordin D. Marx Further informa Module can be i	v and M.Sc. Bi ark for the fin ator and lectur tion ntegrated CP-1	ochemistry (Foca al score rer(s) relevant in M.Sc.	l Point Program "I Biochemistry with	Biomolecular Cher	nistry") Program "Biomolecular



9.4	ule	Workload 150 h	5 CP	ints	Available in 1	semester	<b>Frequency</b> Each WiSe	1 Semester
1	Teaching methodsHours per weekContact timeSelf-studya) Lecturea) 2 h45 h105 h							<b>Self-study</b> 105 h
2	Learn Stude simul to pro and th be int the m limita	ning objectives ents acquire ac lation method oteins to biolo he underlying troduced and i nolecular or ev ations of the re	dvanced kno s for studyir gical interfac thermodyna it will be disc ren atomic le	wledge ng bion ces. Th amic p cussed evel. A	e of both experin nolecular syster e focus will be o roperties and p how simulation particular objec	nental techn ns, ranging f on structure- tinciples. A r 1s can be use tive is to pro	iques as well a from the solvat dynamics-func number of selec ed to interpret vide insights in	s molecular ion of small solutes ition relationships cted techniques will the experiments at ito the merits and
3	Soft s intera conte literat	kills active presenta nts, independ ture	ation in fron ent revision	t of an of mo	audience, ident dule contents, i	ification and ndependent	l recording of p consultation of	rincipal lecture the relevant
4	Prere Admi	quisite(s) ission to the M	laster Cours	se Prog	ram			
5	Evalu active	ation of the le participation	arning proce during lectu	ess ures, in	teractive preser	ntation of ho	mework during	g exercises
6	Mode 30-45	e of examination min end-of-te	on erm oral exa	m or 2	-hour end-of-ter	m written ex	kam	
7	Requi Passi	irements for a ng the end-of-	cquiring cre term exam	edit poi	nts			
8	Signi Weig	ficance for ove hted according	erall grade g to CPs					
9	Modu Fund energ Biolog Waals Molee bound Förste spont diagra meas Bindi isothe	Ile contents amentals: Energy gical (macro)r s, hydrophobio cular models: dary condition er resonance of ameous vs. inco ams, quantum urements), or ng: Isotherma erm), statistica	ergy landscap rmal energy nolecules: S c effect. Diel Degrees of f ns, ingredien energy trans luced emiss n yields), FR ientation of al titration ca l mechanics	pe, Bol , soft v. tructur ectric j freedor ts and <b>fer</b> : Ba ion, tra ET (en transit alorime s (cano	tzmann ensem s. hard degrees e and relevant i properties of wa n, sampling (M parameterization sic principles of ansition dipoles ergy transfer effion dipoles, FR etry (basic prince pical/grand car	ble, hierarch of freedom, nteractions, ter, polariza olecular Dyn on of force fi fluorescenc moments, ra ficiency, Förs ET from MD iple, descrip	y of timescales fluctuations, en H-bonds, elect bility. namics, Monte elds. Water mo e (Einstein coe diative lifetime ster radius, dis simulations. tion of the app uric-isothermal	(Frauenfelder), ntropy. rostatics, van-der- Carlo), spatial odels. fficients, s, Jablonsky tance



# Theoretical Chemistry III: Electronic and Molecular Structure Theory (Chemistry)

(Cilcillistry)					
Module	Credits	Workload	Term	Frequency	Duration
9.5	5 CP	150 h	2. or 4. Sem.	Each Sose	1 Semester
Courses			Contact	Self-Study	Group size
a) Lectures			hours	a) 30 h	10-20 Students
b) Exercises			a+b) 3 SWS	b) 75 h	
				-	

# Prerequisites

Learning outcomes

After completing this course students will basic knowledge of modern wavefunction-based computational electronic and molecular structure methods and how these methods can be applied to solve typical problems in structure determination, spectroscopy, and the investigation of mechanisms and energetics of chemical reactions. Furthermore they will know how to judge the accuracy and reliability of such methods.

### Content

a+b) The course starts with basic principles for quantum mechanical many-particle systems and how their wavefunctions can be described in compact ways and then discusses a variety of modern wavefunction methods and their application:

- Pauli princple and Slater determinants
- Particle number representation (second quantization)
- Hartree-Fock and Multiconfigurational Self-Consistent Field methods
- Single- and Multiconfigurational Configuration Interaction methods
- Single- and Multireference Perturbation Theory
- Coupled-Cluster Methods
- Explicitly Correlated F12 Methods
- Response Theory approach to excitation energies and spectra
- Basis set convergence and basis set extrapolation
- Thermochemistry protocols

# **Teaching methods**

Lecture and exercises with problems for self-studying,Q&A and discussion sessions with presentations given by the participants, Moodle course with online material.

#### Mode of assessment

submission and grading of the solution sheets for the hands-on problems and a final oral end-of-semester exam

Requirements for the award of credit points

Passing the oral end-of-semester exam

Module applicability

M.Sc. Chemistry

Weight of the mark for the final score

According to CP

# Module coordinator and lecturer(s)

C. Haettig

Further information

Master of Science Chemistry (M. Sc. Chemistry)



Atomistic S	imulations	with Mach	ine Learning		
Module 9.6	Credits	Workload	Term	Frequency	Duration
11204410 710	5 CP	150 h	1-4 (tba)	annually	1 Semester
Courses	5 61	10011	Contact hours	Self-Study	Group size
a) Lectures (2 S	WS)		a) 30 hours	105 h	10-20 students
b) Exercises (1 S	SWS)		b) 15 hours		
Prerequisites A	, Admission to tł	ne Master Cour	se Program		
Learning outcom	ies				
After the success	ful participatio	n in the modul	e		
a) the students w	vill have obtaine	ed knowledge al	bout		
<ul> <li>different</li> </ul>	t machine learr	ning algorithms	:		
<ul> <li>suitable</li> </ul>	input descripto	ors/feature vect	ors for machine lea	arning	
<ul> <li>differen</li> </ul>	t generations of	f machine learn	ing potentials		
<ul> <li>the cons</li> </ul>	struction of ma	chine learning i	nteratomic potenti	ials	
• the com	bination of ma	chine learning ]	potentials with sim	ulation tools of th	eoretical chemistry
b) the students w	vill have obtaine	ed practical skil	ls in		
• training	and validating	neural network	, potentials		
<ul> <li>choosing</li> </ul>	g reference stru	actures by active	elearning		
<ul> <li>applying</li> </ul>	g neural networ	k potentials in	molecular dynamio	CS	
• managin	ng workflows fo	or machine lear	ning potentials wit	h python and jupy	vter notebooks
Contont			01		
a) The lecture wi	ll focus on the	use of machine	learning for atomi	istic simulations i	a chemistry and
materials science	ii iocus oli tile	use of machine	Icarining for atomi	istic simulations in	ii chennistry and
materials science	- learning algor	rithms like new	ural networks Cau	ssion processes	upport vector machines
and othe	rs	intillis like lieu		ssian processes, s	support vector machines
<ul> <li>mandate</li> </ul>	ry properties	of input descri	ntors various form	ns of atom-center	ed symmetry functions
Coulom	b matrix, smoo	th overlap of at	omic positions, ato	mic cluster expan	sion. etc.
<ul> <li>different</li> </ul>	t forms of re	epresenting th	e potential energ	ev using atomic	energy contributions.
electrost	atics, dispersio	n interactions.	long-range charge	transfer, magnetis	sm
<ul> <li>training</li> </ul>	algorithms for	parameter opti	mization	, 0	
<ul> <li>validatio</li> </ul>	n methods for	machine learni	ng potentials, extra	apolation, interpol	ation errors, uncertainty
quantific	cation		01	1 1	
<ul> <li>combina</li> </ul>	tion of machin	e learning pote	ntials with molecu	lar dynamics and	Monte Carlo
b) In the comput	er exercises pra	actical experient	ce in the construct	ion, validation and	l use of neural network
potentials will be	gained				
<ul> <li>setting ι</li> </ul>	ıp working env	ironments and	computational fram	neworks	
<ul> <li>selection</li> </ul>	n of suitable tra	ining structure	s		
<ul> <li>training</li> </ul>	different gener	rations of high-	dimensional neura	l network potentia	als
<ul> <li>validation</li> </ul>	on and applicab	ility of machine	e learning potential	ls	
<ul> <li>running</li> </ul>	, molecular dyn	amics simulati	ons using neural n	etwork potentials	
Teaching metho	ds				
a) Lecture (2 hou	rs per week) l	o) Computer exe	ercises (1 hour per	week or block cou	irse)
Mode of assessm	nent				
a) 30-45 min end	l-of-term oral ex	kam or 2-hour e	end-of-term written	exam b) compu	ter exercises
Requirement for	the award of c	redit points			
a) passing the en	d-ot-term exam	n b) active part	1c1pation in the exe	ercises and reports	5
Module applicab	ility	-1 <b>1</b>			
M.Sc. Chemistry	and M.Sc. Bio	chemistry			
The final score a	arresponde to t	he score of the	evam		
Module coording	itor and lecture	r	Challi		
J. Behler		-			
Further information	tion				
Some knowledge	e in Python, ele	ctronic structur	e calculations and	/or molecular dyna	amics is recommended



Theoretical	Spectrosco	opy (Chemi	stry)						
Module	Credits	Workload	Term	Frequency	Duration				
0.7	5 CP	150 h	2. or 4. Sem.	Each SoSe	1 Semester				
			Contact hours	Self-Study	Croup size				
a) Lectures b)	a) Loctures b) Exercises a b) Exerci								
Prerequisites	LACICISCS		a+0/2+15W5	105 11	10 – 20 Students				
Undergraduate l	evel knowledge	e in classical me	- chanics, statistical	mechanics and tir	ne-				
independent nor	n-relativistic ou	iantum mechan	ics as well as advar	nced knowledge at	the level of the				
"Dynamics and	"Dynamics and Simulation" M.Sc. lecture								
Learning outcon	nes								
Students unders	tand and are a	ble to explain th	eoretical approach	es relving on time-	dependent methods to				
compute observa	ables which are	e obtained exper	rimentally using sp	ectroscopic, scatter	ring, and diffraction				
techniques. They	y are able to as	sess the scope a	nd limitations of s	uch methods in the	e context of Solvation				
Science with a fo	, ocus on (bio)m	olecular conden	used phase systems	, in particular aque	eous solutions and soft				
matter.	× ,		± ,	* *					
Content									
Review of stand	lard molecular	spectroscopy:	Approximate deco	oupling of time-in	dependent Schrödinger				
equation in ter	ms of transla	tional, rotation	al, vibrational an	d electronic contr	ributions, ro-vibrational				
spectroscopy of	diatomics base	d on rigid rotor	harmonic oscillat	or approximation,	selection rules, vibronic				
effects in the	Frank-Condor	n approximatio	on, Frank-Condon	principle applie	d to the solvation of				
chromophores, 1	normal mode a	nalysis of vibra	tions of polyatomic	molecules					
Time-dependence	e in quantum	n mechanics:	Time-dependent S	chrödinger equati	on and its wavepacket				
solutions, prope	erties of free p	article and Ga	ussian wavepacket	s, quantum/classic	cal correspondence and				
Enrentest theore	em, time-evolut	tion operator for	rmalism and Dysoi	n equation, Schrödi	inger versus Heisenberg				
Versus Dirac pic	tures of quant	ima denomics,	time-aependent va	ariational principle	e (Dirac-Frenkel IDVP),				
extension Cause	sentials of the t	t propagation r	naturee (IDH) me	nger)					
Time-dependent	nerturbation t	theory for spect	roscopy: Formalisi	n and applications	to important schematic				
models linear T	DVP in Dirac p	icture first-and	l second-order diag	rams virtual states	and transitions Fermi's				
Golden Rule	b v i m b nuc p	icture, mot une	becond order diag	fullib, filtual states					
Molecular system	ns in the radia	ation field for s	pectroscopy: Trans	ition probability, a	bsorption cross section,				
dipole approxim	ation, transitio	n dipole, semic	lassical approach t	o molecule-radiatio	on field coupling, basics				
of the quantizati	on of the radia	tion/electromag	netic field for spor	ntaneous emission,	multi-photon processes				
and non-linear s	spectroscopy, F	Raman scatterin	g process, transfo	rmation of spectro	scopy formulated in the				
static Schröding	er picture to th	e dynamic Heis	enberg picture (Ku	bo-Gordon formali	sm to compute spectra),				
time-autocorrela	tion functions	and spectral l	ine shape functio	n, time-domain ve	ersus frequency-domain				
spectroscopy									
Neutron scatteri	ng and x-ray di	ffraction: van F	Iove formalism, fir	st Born approxima	tion, dynamic and static				
structure factor,	scattering leng	th and form fac	tors, coherent and	incoherent scatteri	ng, van Hove correlation				
Torching mathe	e structural dyn	lamics of liquid	s, pair correlation f	unctions, radial dis	stribution functions				
Lecture and over	us	lems for solf at	udving O&A and	discussion engine	with presentations				
given by the part	ticinants digita	ul material provi	ided via TheoCherr	n Cloud	s with presentations				
Mode of assessn	nent			i Cloud.					
Written or oral e	nd-of-semester	r exam							
Requirement for	the award of c	redit points							
Passing the end-	of-semester ex	am							
Module applicab	oility								
M.Sc. Chemistry	and M.Sc. Bio	chemistry (Foc	al Point Program "	Biomolecular Cher	mistry")				
Weight of the m	ark for the fina	l score	<b>¥</b>						
According to CP									
Module coordina	ator and lecture	er(s)							
D. Marx									
Further informa	tion				_				
Module can be in	ntegrated CP-r	elevant in M.Sc	. Biochemistry witl	nin the Focal Point	Program				
"Biomolecular C	hemistry"								
					82				

Γ



Industrial C	omputatio	nal Chemist	ry I: Fundan	nentals	
Module	Credits	Workload	Term	Frequency	Duration
9.8	5 CP	150 h	3. Sem	WS	1 Semester
Courses	I		Contact hours	Self-Study	Group size
a) Lectures			a) (2 SWS)	100 h	~ 10 students
b) Exercises			b) (1 SWS)		
Prerequisites					
Learning outcom	mes				
Students acquir	re working kn	owledge on the	techniques of c	omputational chem	istry in the realm
of (bio)molecul	ar systems su	ch as small dru	g-like molecules	s and proteins. Besid	des calculated and
experimentally	determined n	10lecular prope	rties of small m	olecules, valuable so	ources of
information are	e published X-	ray stuctures of	f enzyme-substr	ate complexes or tra	ansition metal
complexes, the	critical evalua	tion of which is	s mandatory bef	ore they can be uses	s in rational drug
and catalysis de	esign.				
Content					
Essentials of cla	assical and sta	tistical mechan	ics: formulation	is according to New	ton, Lagrange and
Hamilton, corre	esponding equ	uations of motion	on, conservatior	n laws/conserved qu	antities,
ensembles			1		
Born-Oppenhei	mer approxin	nation, potentia	l energy surface	es i c	0.11
Computational	methods for 1	nolecular geom	ietries and prop	erties: valence force	fields, semi-
empirical, ab in	utio (Hartree-	Fock and beyon	id) and density f	unctional methods,	incorporation of
solvent effects l	by continuum	approaches, co	nceptual DFT d	erived properties lik	te
electronegativit	y, hardness, F	ukui functions	and reactivity d	escriptors	. 1 . D . C
Experimental p	rotein-substra	ite complexes, 2	C-ray structures	from the protein da	tabase. Basics of
protein strucure	e prediction: L	bioinformatics t	ools necessary i	or constructing 3D-	structure models
of relevant but i	unknown pro	terns from expe	ochogi	wones by normology	modelling.
bagic ideag and	tochniquog of	f MC and MD	acties.	different engembles	long rango
forces and hour	adam conditio	mc and MD,	in protein hor	nology modelling a	od
thermodynamic	cycles for Fr	e Energy colou	lations	noiogy modeling a	liu
Teaching meth	ode	ce Lifergy careu	liations.		
a) Lecture (2 ho	urs per week)				
b) Computer ex	ercises (1 hor	ır per week or b	lock course)		
Mode of assess	ment	i per week of b	ioen coursej		
30 - 45 min end	l-of-term oral	exam or 2-hour	end-of-term wr	itten exam	
Requirement fo	or the award o	f credit points			
Passing the exam		r crean points			
Module applica	bility				
M.Sc. Chemistr	íV.				
Weight of the n	nark for the fi	nal score			
Weighted accor	ding to CPs				
Module coordin	nator and lectu	ırer			
R. Franke					
Further inform	ation				

Γ



Industrial Co	mputationa	al Chemistry	II: Application	s in Process D	Development					
Module	Credits	Workload	Term	Frequency	Duration					
9,9	5 CP	150 h	3. Sem	WS	1 Semester					
Courses			Contact hours	Self-Study	Group size					
a) Lectures			a) (2 SWS)	100 h	~ 20 students					
b) Exercises	b) Exercises b) (1 SWS)									
Prerequisites										
Trerequisites										
Learning outcom	mes									
Students becom	ne aquainted v	with various the	eoretical tools use	ed within project	s for process					
development.										
Essential contri	butions of co	mputational ch	emistry are in the	e field of chemica	al and physical					
properties of co	mplex system	ns, in developm	ent and understa	nding of reaction	n mechanism, and					
in microkinetic	modelling.									
Important issue	es in industria	al research are t	the timelines of p	rojects. These ar	nd the inherent					
limitations of m	nethods deter	mine the miles	tone plans of ind	ustrial computati	ional chemistry					
projects.										
Content										
- Short overview	v of the chem	ical business.								
- Introduction in	nto innovatio	n management	and new product	t development in	chemical industry.					
- Short overview	v of project m	anagement.								
- A recapitulation	on of mixed p	hase thermody	namics with focu	s on gases and li	quids is given.					
- Group contrib	ution method	ls commonly us	sed in process syt	hesis are briefly	introduced.					
- The semiempi	rical COSMC	<b>)-RS</b> approach i	s derived and its	use and limitatio	ons are illustrated.					
- Gibbs ensemb	le Monte Car	lo and molecul	ar dynamics metl	nods using empi	rical force fields for					
calculation of in	ndustrial relev	ant phase diag	rams are illustrat	ed.						
- Calculations of	f thermodyna	imical propertie	es of gas-phase re	actions with emp	phasis of highly					
accurate ab initi	io methods ar	re reviewed.								
- Generic aspect	ts of catalysis	are recapitulate	ed.							
- Short overview	v of importan	t homogeneous	sly catalysed react	ions in chemical	industry is given.					
- The formulation	on of the syste	em of different	ial equations desc	cribing the micro	okinetics of a					
catalytic cycle ba	ased on the C	hristiansen for	malism is introdu	ıced.						
- Selected exam	ples of compu	utational chemi	stry research pro	jects on homoge	neous catalysis are					
discussed.										
Teaching metho	ods									
a) Lecture (2 ho	urs per week)	)								
b) Computer ex	ercises (1 hou	ır per week or l	olock course)							
Mode of assessi	ment	- 1	1 6 .							
30 - 45 min end	-of-term oral	exam or 2-hour	r end-of-term writ	tten exam						
Requirement fo	or the award o	of credit points								
Passing the exam	l 1 •1•.									
Module applica	Dility									
M.Sc. Chemistr	<u>y</u>	1								
Weight of the m	hark for the fi	nal score								
Weighted accor	aing to CPs									
Module coordin	ator and lect	urer								
R. Franke										
Further information	ation									



Scientific Programming Methods for Chemists						
Module	Credits	Workload	Term	Frequency	Duration	
9.10	5 CP	150 h	2. or 4. Sem.	only in SoS	1 Semester	
Courses			Contact	Self-Study	Group size	
a) Lecture "Sci	ientific Progra	imming	hours	a) 30 h	10-20 Students	
Methods for C	Chemists"		3 SWS	b) 75 h		
b) Exercises for Methods for C	or Scientific Pi Themists	rogramming				
Prerequisites						
None						
Learning outco	omes					
After successfu	l completion	of the module s	tudents will:			
•	have basic kn	lowledge progra	mming concept	ts of modern progra	mming languages	
•	know how to	structure code a	and how to test	and validate source	code	
•	be able to tur	n scientific moo	lelling problem	s into programmabl	le algorithms	
have so	me experienc	e on how to use	e code libraries t	o solve standard ma	athematical	
probler	ns and to visu	alize scientific	data			
The lecture use	og Duthon og o	n evample of a	modern object o	riented programmi	ng language to	
introduce stud	ents to:	ii example of a	inodern object-c	filemed programmi	ing language to	
elemen	itary data type	s (integers floa	ts strings etc.)	and their represent:	ation in computers	
control	structures (lo	ons conditions	functions etc.)		dion in computers	
<ul> <li>basics of</li> </ul>	of object orien	itation (classes	inheritance etc.			
• comple	ex data types (1	ists tunles dict	ionaries etc.)	•)		
<ul> <li>reading</li> </ul>	and writing	data from/to file	etc.)			
<ul> <li>math li</li> </ul>	braries (num	ov. scipy, blas, l	anack)			
<ul> <li>visualiz</li> </ul>	zation of data	with matplotlib	apueny			
<ul> <li>solving</li> </ul>	differential e	quations numer	rically on grids			
<ul> <li>solving</li> </ul>	algebraic pro	blems (linear eo	mations. SVD.	eigenvalue problem	s)	
Teaching meth	ods		1	<u>0</u>	- <u> </u>	
Lecture, Hands-	on coding proje	ects for self-study	ing on own laptor	os with online suppor	t by teaching	
assistants via a c	hat work space	, Q&A and discus	ssion sessions, M	oodle course with onli	ine material.	
Mode of assess	ment					
submission an	d grading of t	he solution shee	ets for the hands	s-on problems and a	a final written or	
oral end-of-semester exam						
Requirements for the award of credit points						
successful written or oral end-of-semester exam						
Module applicability						
Master of Science in Chemistry and Master's program Molecular Sciences – Spectroscopy and						
Weight of the mark for the final score						
by CP						
Module coordinator and lecturer(s)						
R. Schmid, C. H	aettig	× 7				
Further information						

Module	Credits	Workload	Term	Frequency	Duration	
9 11	9 CP	270 h	2. Semester	Each SuS	1 Semester	
			Contact hours	Self-Study	Group size	
a) Lectures			a+b 3 SWS	a) 30 h	10-20 Students	
h) Exercises			(15) 5 SWS	b) 75 h	10 20 Students	
c) Integrated co	mputer practi	cal	C/ 5 5 W 5	c) 75 h		
Proroquigitog	inputer pruet	cui		C/7511		
rielequisites						
a+b) After compl computational el typical problems energetics of che such methods. c) They will be fa electronic structu electronic and m <b>Content</b> a+b) The course wavefunctions ca methods and the	leting this cou- lectronic and in structure of mical reaction umiliar with se- ure methods to olecular struct starts with ba- an be describe- ir application	urse students wil molecular struct determination, sy ns. Furthermore oftware for electr to practical probl ture calculations sic principles for ed in compact wa	l have basic knowle ure methods and h pectroscopy, and th , they will know ho conic structure calc ems and how to an s. r quantum mechar ays and then discus	edge of modern wa now these methods ne investigation of ow to judge the acc ulations, know how nalyze, visualize an nical many-particle sses a variety of mo	avefunction-based can be applied to solve mechanisms and uracy and reliability of w apply modern d present results of systems and how their odern wavefunction	
<ul> <li>Particle</li> <li>Hartree</li> <li>Single- a</li> <li>Single- a</li> <li>Coupled</li> <li>Explicitle</li> <li>Response</li> <li>Basis see</li> <li>Thermodynamics</li> </ul>	number repre- Fock and Mu and Multicon and Multirefe l-Cluster Metl y Correlated I se Theory app t convergence chemistry pre-	esentation (secon ilticonfigurational figurational Con rence Perturbati hods F12 Methods proach to excitation e and basis set exprocols	na quantization) al Self-Consistent I figuration Interact on Theory on energies and sp ttrapolation	Field methods ion methods ectra		
c) Application of between conform electronically exc energies.	electronic str ners, barriers tited states, op	for interconversion of the second sec	to determine mole ion, vibrational spe V-Vis), accurate rea	cular structures, e ectra (IR and Rama action energies and	nergy differences n), characterization of l intermolecular binding	
Teaching metho	ds	ula	a lf ata de tra o Q			
a+D) Lectures an	u exercises wi	tripports Marsh	self-studying, Q&A	A and discussion so	essions with	
c) Commutations give	en by the par	ticipants, Moodl	e course with onlin	ie material.	lab with different	
oftware package	i iiaiius-oii pi	ojecis io de solve	a on own taptops	anu/or a computer	iao witti utiterefit	
Mode of assessm	ent		a sessions and part	any as sen-study.		
+b) submission	and orading	of the solution of	heets for the everci	ses and a final ora	l end-of-semester evan	
a+u) submission and grading of the solution sneets for the exercises and a final oral end-of-semester exam						
Requirements for	r the award o	f credit points				
c) successful acc	entance of the	reports for the	computational han	de-on projects and		
y successive the	oral end of a	mester even	computational nam	us-on projects and		
atuj passilig ille	ility					
M Sc iMOS and	MSc Cham	stry				
Woight of the are	wi.sc. Citerill					
weight of the ma	aik for the fin	ai score				
LEADER TO I II						
Modulo coordina	tor and last	ror(a)				
Module coordina	tor and lectu	rer(s)				



# In-depth Practical in Theoretical Chemistry

1			/				
(up to three st	ich modules in '	Theoretical Chem	nistry during winte	r semester 1 and sum	1mer semester 2)		
Module	Credits	Workload	Term	Frequency	Duration		
9.12	8 CP	240 h	1.+2. Sem.	Every semester	1 Semester		
Courses	·	·	Contact hours	Self-Study	Group size		
Computer lab course 9 SWS 105 h 5-10 studen					5-10 students		
Prerequisites							
Methodological and computational working knowledge in Theoretical Chemistry at the level of the B.Sc. Chemistry degree at RUB subject to specialization in Theoretical Chemistry							
Learning outcomes							
Advanced kn order to unde	owledge of the erstand the prop	use of computat perties of (bio)m	tional methods em olecular systems i	ployed in state-of-th n the broadest sense	e-art research in e, critical		

order to understand the properties of (bio)molecular systems in the broadest sense, critical assessment of the scope and limitations of various approaches/approximations in theoretical and computational (bio)chemistry, visualization and presentation of results, gaining first insights into simple programming. Team working and collaboration while carrying out virtual experiments, general knowledge of operating systems, software and computing close to the level of state-of-the-art research in Theoretical Chemistry, presentation of the research results close to the level of scientific publications in Theoretical Chemistry

# Content

This computer practical is composed of several independent compact courses which are devoted to specific topics. Some examples are provided here, but the specific options are subject to the preferences of the students and adjustments depending on advances in Theoretical Chemistry:

Module on classical molecular dynamics and molecular modeling: Simulating structure and dynamics of selected (bio)molecular condensed phase systems at finite temperature and subject to periodic boundary conditions, such as molecular liquids and solutions, critical evaluation and/or generation of interatomic potentials.

Module on electronic structure and spectroscopy: Computing electronic properties, response properties and spectra of selected molecules, clusters, and complexes using wavefunction-based methods or density functional theory (DFT).

Module on molecular structure and reactions: Computing accurate equilibrium structure with various quantum chemistry methods, searching reaction pathways and transition states, accurate calculations of reaction and activation enthalpies.

Module of solid state and surface calculations: Computation of two and three-dimensional periodic structures including crystal surfaces with vacancies, adatoms, admolecules, thermodynamic description of condensed matter.

# **Teaching methods**

Hands-on computer course with integrated seminar (9 hours per week per module): These blocked courses take place during either the first or second half of a given semester and might take place embedded within the research groups or in our Virtual Lab "Theoreticum" both subject to very intense supervision by experienced teaching assistants. The virtual experiments must be introduced ("motivation"), presented in terms of tables, graphs, text and critically discussed ("results and discussion") as well as summarized ("abstract") and concluded ("conclusions and outlook") in a practical report that notably also includes an concise introduction into the corresponding methodological and computational underpinnings ("methods and computational details") all with pertinent references, thus overall mimicking a short scientific publication.

# Mode of assessment

The virtual experiments must be completed successfully and written up satisfactorily in terms of a practical report as outlined above.

Requirement for the award of credit points

# FAKULTÄT FÜR CHEMIE UND BIOCHEMIE

Master of Science Chemistry (M. Sc. Chemistry)



Acceptance of the practical report based on the formal criteria outlined above.

# Module applicability

M.Sc. Chemistry and M.Sc. Biochemistry (Focal Point Program "Biomolecular Chemistry")

Weight of the mark for the final score

According to CP

# Module coordinator and lecturer(s)

J. Behler, C. Hättig, D. Marx, L. Schäfer

Further information

Module can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program "Biomolecular Chemistry"

Master of Science Chemistry (M. Sc. Chemistry)



Focal-point	Focal-point Research Practical in Theoretical Chemistry						
Module Credits Workload			Term	Frequency	Duration		
9 1 3	15 CP	450 h	3. Sem.	Each WiSe	1 Semester		
			Contact	Self-Study	Group size		
Computational	research prac	tical	hours	225 h	5 - 10 Students		
Compatitional	researen piac	licui	15 SWS				
			19 5 10 5				
Prerequisites			I	I	I		
Methodological a	nd computation	al working knowl	edge in Theoretica	al Chemistry at the leve	l of the B.Sc.		
Chemistry degree	at RUB subject	t to specialization	in Theoretical Ch	emistry			
Learning outcom	mes						
Planning of a self-	-contained resea	arch project, adva	nced knowledge o	f the use of computatio	nal methods		
employed in state	-of-the-art resea	arch in order to un	derstand the prope	erties of (bio)molecular	systems in the most		
general sense, crit	tical assessment	of the scope and	limitations of vari	ous approaches/approx	imations in		
theoretical and co	mputational (bi	o)chemistry in the	e broadest sense, v	isualization, written an	d oral presentation		
of results, simple	programming ta	asks, critical evalu	ation of the releva	ant scientific literature,	writing of a practical		
report that mimicl	ks state-of-the-a	rt scientific public	cations. Team wor	king and collaboration	while carrying out		
virtual experiment	ts, general knov	vledge of operatin	g systems, softwa	re and computing close	e to the level of		
state-of-the-art	research in Th	neoretical Cherr	iistry, presentatio	n of the research result	s close to the level of		
scientific publicat	ions in Theoret	ical Chemistry.					
Content							
This research com	nputer practical	can be devoted to	a topic that is cov	ered by one of the rese	arch groups in the		
field of Theoretica	al Chemistry at	RUB. The specifi	c topic can be in s	ubjects such as comput	ational inorganic		
chemistry, bioche	mistry, organic	chemistry, physic	al chemistry, solv	ation science, surface s	cience, or materials		
science. The corre	esponding resea	rch groups can be	found on the hom	lepage of the Fakultaet	as well as the		
research fields tha	at are currently of	covered by these g	groups in their con	temporary scientific re	search. A critical		
Tagahing math		report which shot	nd minic a typica	r scientific publication.			
Teaching metho	ous	tradically taleas al	a within a smaaif	ia maaaanah amayon uuhan	a the student is		
hosted together w	ith other group	members. This wi	ice within a specific and the specific a	mwork and collaboration	e the student is		
the group but poss	sibly also involv	ving experimental	groups depending	on the topic. There wi	11 be close contact to		
the group member	rs as well as wit	the group leader	r and/or an experie	enced coworker. The la	tter provide		
feedback during a	nd on the virtua	al experiments as y	well as feedback of	on the written lab report	supervised by		
teaching assistant	s In The virtual	experiments mus	t be introduced ("	motivation") presented	in terms of tables		
graphs, text and c	ritically discuss	ed ("results and d	iscussion") as wel	l as summarized ("abst	ract") and concluded		
("conclusions and	outlook") in a	practical report th	at notably also inc	ludes an concise introd	uction into the		
corresponding me	thodological an	d computational u	underpinnings ("m	ethods and computation	nal details") all with		
pertinent reference	es, thus overall	mimicking a shor	t scientific publica	ation.	,		
Mode of assess	ment						
The virtual experi	ments must be	completed success	sfully and written	up satisfactorily in tern	ns of a practical		
report as outlined	above.						
Requirement for	or the award o	f credit points					
Acceptance of the practical report based on the formal criteria outlined above.							
Module applicability							
M.Sc. Chemistry and M.Sc. Biochemistry (Focal Point Program "Biomolecular Chemistry")							
Weight of the mark for the final score							
According to CP							
Module coordin	nator and lectu	urer(s)					
J. Behler, C. Hättig, D. Marx, L. Schäfer							
Further inform	ation						
Module can be integrated CP-relevant in M.Sc. Biochemistry within the Focal Point Program "Biomolecular							
Chemistry"							



Introduction	n to Comp	utational Ch	emistry				
Module	Credits	Workload	Term	Frequency	Duration		
10.1	4 CP	120 h	x. Sem.	Every WS	1 Semester		
Courses			Contact	Self-Study	Group size		
a) Lecture (2h	per week)		hours	5h per week	about 10-15		
b) Hands on ex	xercises (HoF	) with a 1h	3 SWS	(including HoE)	students		
0&A session r	per week (onli	ine)	0010	(	Storaciitis		
Prerequisites	1	-1					
None							
Learning outco	mes						
Students who h	nave finished	this course will					
have ba	sic knowledge	e about modern	computational	chemistry methods,	ranging from force		
field m	odels over d	ensity function	al theory to w	vave function based	post-Hartree-Fock		
electror	nic structure r	methods.					
be able	to apply such	methods for ro	outine applicati	ons in their future so	cientific work.		
are able	e to understa	nd and assess t	he quality of co	omputational chemis	stry applications in		
publica	tions and oth	er scientific stu	dies.				
Content							
Within this mo	dule basic co	ncepts in comp	utational chem	istry are discussed. T	The following		
methods to con	npute a poten	tial energy surf	ace of a chemic	cal system are discus	sed:		
Force F	ield methods	and parameter	ized models				
<ul> <li>Density</li> </ul>	/ Functional T	Theory (DFT) ba	ased methods				
Post Ha	artree-Fock m	ethods to inclu	de electron cor	relation			
The following o	concepts and i	methods are tre	ated in the mo	dule:			
Optimiz	zing structure	es and transition	n states				
Basic co	oncepts of Mo	olecular Dynam	ics simulations	5			
Periodi	c Boundary C	conditions for c	rystalline syster	ns			
Exchan	ge and Correl	lation Function	al in DFT				
Basis se	ets for the rep	resentation of e	electronic wave	functions (and densi	ities)		
Frequence	<ul> <li>Frequency analysis, vibrational spectra and calculation of thermochemical data</li> </ul>						
Workin	g with comp	utational chemi	strv codes (on l	LINUX environment	s)		
Using r	nodern GUIs	for performing	g computations		· · · · ·		
Teaching meth	ods						
Lecture Hands	on exercises	on own lanton	(BYOD) for dif	ferent methods duri	ng the semester		
O&A sessions (	(online) by sti	ident assistants	and support fr	om student assistant	ts by a specific		
messaging serv	er to ask que	stions Content	is provide via a	Moodle course	is by a specific		
Mode of assessment							
Oral examination based on results from Hands on Exercises							
Requirement for the award of credit points							
Passing of oral exam							
Module applica	Module applicability						
Master of Science in Chemistry, IMOS							
Weight of the mark for the final score: by CP							
Module coordinator and lecturer(s): Prof. Dr. Christof Hättig, Prof. Dr. Christian Merten, Prof.							
Dr. Rochus Schmid							
Further inform	Further information						



From top-level science to top-level business							
Module	Credits	Workload	Term	Frequency	Duration		
10.2	5 CP	125 h	x. Sem.	Only WS	1 Semester		
Courses			Contact	Self-Study	Group size		
a) Seminar			hours	<b>90</b> h	30 Students		
b) Lecture			3 SWS				

# Prerequisites

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The module is intended for students from the 5th semester onwards in the Bachelor's and Master's degree in addition to doctoral students, but without exclusion criteria. Previous knowledge, especially in business administration or corporate law, is explicitly not required.

# Learning outcomes

After successful completion of the module

- students develop business ideas using different creativity techniques
- design their ideas using different prototyping methods
- understand how to define target groups
- select appropriate methods for customer interviews
- students master the presentation technique of pitching

#### Content

The module pursues the overarching goal of sensitising students and doctoral students of chemistry and related, similarly basic science degree programmes to a possible business start-up. To this end, the students are not only provided with basic knowledge on how to start a business, but also with tools to first develop an idea of a business model that suits their specific professional and/or methodological skills and to identify ways to master the transfer from science to practice. Personal experience reports by successful founders, who all have a strong background in basic research at the RUB, additionally provide vivid practical reports as "role models" in personal contributions. In addition to these practical reports, the participants benefit from the involvement of experts from different disciplines, such as customer interviews or pitching, who convey content in an application-oriented manner and enable the students to apply it independently. International external experts also help the participants to broaden their horizons.

# Teaching methods

Seminar-based teaching, group work, digital teaching formats.

# Mode of assessment

On the last day of the course, there is a 10-minute presentation of an individual business idea in group work using the creative techniques learned for business model generation. In addition, students are required to submit an individual guideline-based short reflection on the learned content one week later.

# Requirement for the award of credit points

Successful final presentation as well as timely submission of the guideline-based reflection.

# Module applicability

# Weight of the mark for the final score

The decisive assessment criterion is the group presentation of the business idea. The guiding questionbased reflection has an individual effect with tendencies of one mark level.

# Module coordinator and lecturer(s)

K. Tschulik, A. Beyer, F. Lehmann

# Further information

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Master of Science Chemistry (M. Sc. Chemistry)



Master Thesis							
Module	Credits	Workload	Term	Frequency	Duration		
11	30 CP	900 h	4. Sem.	Any time	1 Semester		
Courses Master Thesis			Contact	Self-Study	Group size		
			nours				
Prerequisites					I		
"Practical Science	e and Communi	cation" and Foc	al-Point Practical	l			
Learning outco	mes						
The Master Thes	is is the writte	n presentation of	f an experiment	al study on a chemic	al subject, including the		
interpretation of	the experiment	al data and the	evaluation with	in the scientific conte	ext. Within 6 months of		
working time the	participants sh	ould prove their	ability to apply	modern methods for s	solving or investigating a		
scientific problem	n self-reliently i	n the field of che	emistry.				
Content							
Literature survey	in a scientific re	esearch group					
Literature survey for a scientific project							
Planing, performi	ng, analyzing a	nd evaluating sc	ientific experime	ents			
Presentation of sc	eientific results		••••••••••••••••••••••••••••••••••••••				
Teaching meth	ods						
Coaching							
Mode of assess	ment						
Requirement for	or the award o	of credit points					
Master Thesis accepted as sufficient or better by two lecturers							
Module applicability							
Weight of the mark for the final score							
According to CP							
Module coordinator and lecturer(s)							
All lecturers affiliated with the study program for M. Sc. Chemistry							
Further information							