Content overview of lectures and lab courses from master's program Chemistry and Molecular Sciences (90 ECTS)

CURRENTLY OFFERED LECTURES

Ab-initio Computational Chemistry
3 ECTS, 2V
• Calculation of all properties of molecules and molecule ions • Wave functions and operators for many electron systems • Self consistent field calculations • Selected examples and practical work

Advanced Medicinal Chemistry
1.5 ECTS, 1V
This lecture series illustrates the modern drug discovery process from target identification to the selection of drug candidates for clinical testing. While the course reiterates key concepts and methodologies of traditional medicinal chemistry and pharmacology, several practical examples serve to highlight the advantages of a target-centric approach with a particular emphasis on 3D structural information.

Advanced NMR
2 ECTS, 1V+0.5Ü
The advanced NMR course is aimed at the students who are already familiar with using NMR on a day-to-day basis, but who wish to deepen their understanding of how NMR experiments work and the theory behind them. It will be assumed that the students are familiar with interpreting 1D & 2D spectra. Similarly, familiarity with the nuclear Overhauser effect (NOE) will be assumed. The course is divided in chapters, each chapter being associated with exercises, if needed. Chapter I covers the Quantum mechanics for NMR Spectroscopy, chapter II will introduce the notion of product operators, that represents the core of the lecture. In chapter III, 2D NMR will be discussed. in chpater IV, the concept of gradients and phase cycling will be discussed, followed by the chapter V on relaxation and NOE effect As such, this course is intended to students with a strong interest and a solid NMR background.

Advanced Solid State Chemistry and Spectroscopy
1.5 ECTS, 1V
The development of a chemical compound towards an optimized material is discussed, mainly on examples of solid state, light emitting materials. Beginning at the synthesis (e.g., starting materials, reaction conditions, purity) the process involves many more steps of optimization (e.g., doping, length scale (nm powder to cm sized crystal) and combination with other materials) towards a real (commercial) product. The chemical aspects are combined with optical spectroscopy and other methods of characterization. In the basic course the principles of e.g., light absorption, emission, energy migration, broad band and line emitters, f-f, f-d, d-d transitions are discussed. **The advanced course** includes more detailed discussions of e.g., scintillators, persistent phosphors, upconversion phosphors, and LEDs.

Applied Electrochemistry
1.5 ECTS, 1V

• Basic electrochemical thermodynamics
  o One electrode systems: derivation of the Nernst equation
  o Two electrode systems: definition of measurable quantities
  o Electrodes of the first kind
  o Electrodes of the second kind
• Basic electrochemical kinetics
• Electrochemical methods
• Electrochemistry and technology of electroplating
• Electrochemistry and technology of fuel cells and batteries (energy conversion)
• Organic electrochemistry (synthesis)

Applied Mass Spectrometry
1.5 ECTS, 1V
Mass spectrometry Demonstration of non-classical instrumentation and applications of modern mass spectrometry: • Stepping out of the lab: Miniature and portable mass spectrometry. • Ambient ionization techniques. • Mass spectrometry in the clinical and forensic sciences: Analysis of drugs, their metabolites, and illicit substances. • Mass spectrometry in arts and archeology. • Extreme mass spectrometry: Exploring the current of an analytical technique.

Applied NMR Spectroscopy
1.5 ECTS, 1V
NMR Spectroscopy • Basic Principles • Two-dimensional NMR spectroscopy • The Nuclear Overhauser effect • Diffusion NMR experiments • Processing of NMR spectra • Description of NMR experiments: the vector model

Applied Optical Spectroscopy in Chemical Biology
1.5 ECTS, 1V
• Introduction to chromophores and principles of photophysics • UV-vis absorption spectroscopy • Fluorescence spectroscopy • Circular dichroism (CD) spectroscopy • Linear dichroism (LD) spectroscopy • Practical demonstration of spectroscopic instruments

Atmospheric and Aerosol Chemistry
3 ECTS, 2V
• Why Atmos. Chemistry • A flavor about the main problems • General circulation, transport in the atmosphere • Spectroscopy, Photochemistry • Kinetics • Introduction Waste incineration (KVA), Introduction to aerosols • Excursion: Visit of KVA • Aerosols • Aerosol dynamics, Organic aerosols, Cloud droplets • Student presentations about current topics in Atmospheric Chemistry • 11. Clouds and aqueous chemistry

Basic Medicinal Chemistry
1.5 ECTS, 1V
What is medicinal chemistry? • The drug discovery process • Drug-Target interactions • Enzyme inhibitors • Drugs interacting with DNA • Drug metabolism • The prodrug concept

Basic Solid State Chemistry and Spectroscopy
1.5 ECTS, 1V
The development of a chemical compound towards an optimized material is discussed, mainly on examples of solid state, light emitting materials. Beginning at the synthesis (e.g., starting materials, reaction conditions, purity) the process involves many more steps of optimization (e.g., doping, length scale (nm powder to cm sized crystal) and combination with other materials) towards a real (commercial) product. The chemical aspects are combined with optical spectroscopy and other methods of characterization. **In the basic course** the principles of e.g., light absorption, emission, energy migration, broad band and line emitters, f-f, f-d, d-d transitions are discussed. The advanced course includes more detailed discussions of e.g., scintillators, persistent phosphors, upconversion phosphors, and LEDs.

Chemical Crystallography
3 ECTS, 2V
The course gives an introduction to the basics of three dimensional crystal structures, of microscopic and X-ray diffraction techniques and of crystal structure solution and refinement. The course is mandatory for the laboratory of crystal structure determination. **Symmetry in 3 dimension** • 1, 2 and 3-dimensional lattice types • Symmetry operators • Plane groups and space groups

Optical microscopy

- Refraction of light
- Optical indicatrix
- Birefringence
- Basics of optical microscopy

X-ray diffraction

- Electromagnetic radiation
- Scattering of radiation
- Bragg law, Laue conditions and Ewald sphere
- Diffraction techniques
- Crystal structure solution
- Structure refinements
- Applications to material science and life science
- Large scale facilities / Synchrotron X-ray diffraction
- X-ray powder diffraction

Chemical Biology
3 EC TS, 2V
Chemical biology is the application of chemical synthesis to the study of biological problems, and conversely the application of biological tools to chemical problems. The course takes a look at recent primary literature in chemical biology from selected authors. Two publications will be critically analyzed each week in a workshop format.

Chemical Modifications of Proteins
1.5 ECTS, 1V
• Introduction • Classic mutagenesis/unnatural amino acid mutagenesis • Total/semisynthesis of proteins • Chemical modification of nucleophilic amino acids • SAM-mediated modifications • Protein tag-mediated modifications • Metabolic labelling • Click chemistry • Cu-free click chemistry • Staudinger ligations • Other bioorthogonal reactions • Photoaffinity probes • Multimodular probes • Catch & release affinity probes

Clinical Chemistry and Laboratory Medicine – An Introduction
1.5 ECTS, 1V
• Laboratory medicine and clinical chemistry(next to haematology, immunology, microbiology and medical genetics) • Career opportunities in laboratory medicine? • knowledge and understanding of clinical chemistry in the areas of laboratory investigation of medical conditions • understanding of pre-analytical, analytical and post-analytical issues • critically discuss the interpretation of the laboratory results.

Crystal Structure Determination (Lab course)
4 ECTS, 16P
This laboratory is a practical course on X-ray single crystal diffraction analysis and crystal structure determination. The labory is divided into experimental and computational parts: • Experimental part: o selection of crystals under polarized light microscope o mounting crystals for X-ray diffraction o data collection • Computational part: o determination of unit cell parameters from precession photographs o determination of Laue classes and space groups o crystal structure solution o crystal structure refinement o analysis of the molecular geometries and the crystal packing structure correlation analysis

Environmental Radionuclides and Nuclear Dating
1.5 ECTS, 1V
• Introduction/Basics • Cosmogenic radionuclides I • Cosmogenic radionuclides II • Natural decay chains I • Natural decay chains II • Nuclear energy • Nuclear accidents • Nuclear weapons • Radiation exposure • Biological radiation effects • Dating I • Dating II • Exercises

Enzyme Mechanisms and Enzyme Models
3 ECTS, 2V
• Introduction • Chemical and enzymatic catalysis • Hydrolysis of amide bonds: Mechanism of Proteases • Enzymes for Carbon-Carbon bond formation

- Triosephosphate isomerase (TIM) – enzyme perfection
- Mechanism of enzymes requiring cofactors
- Enzyme models 1
- Mechanism of enzymes in the Shikimic acid pathway
- Radicals in enzyme catalysis
- Enzyme models 2
- Halogenases and dehalogenases
- Reaction catalyzed by orotidine 5'-monophosphate decarboxylase

Forensic Chemistry and Toxicology

3 ECTS, 2V

- Fundamentals in Forensic Toxicology, Pharmacologic Concepts
- Criminal and Accidental Poisoning (Medico-Legal Cases)
- Hemp Production, Cannabinoids, Analyses and Pharmacology
- Cocaine, Pharmacology, Analyses and Toxicology
- Amphetamine, Methamphetamine, Methylenedioxymethamphetamine (MDMA) and other Designer Drugs, Research Chemicals, Doping
- Ethyl Alcohol, Gammabutyrolactone (GBL), Gamm hydroxybutyrate (GHB), Pharmacology, Effects on the Body
- Opioids, Heroin, Methadone, Buprenorphine, Fentanyl…
- Hallucinogens, LSD, Mescaline, Psilocybin…
- Driving under the Influence of Ethyl Alcohol, Illicit and Therapeutic Drugs

Fragrance Chemistry

1.5 ECTS, 1V

The lecture provides a journey into the molecular world of scents from the chemical secrets behind Chanel N°5 to structure–odor relationships, industrial processes, and total synthesis of terpenoids. Each subunit is centered on one odorant family and highlights a certain class of chemical reactions, illustrated by prominent perfumery examples.

- Historical Introduction (Perkin • Fischer • Fougère • vanillin • aromatic aldehydes)
- Coco Chanel: Fatty Aldehydes and Raldeïnes (Darzens • aliphatic aldehydes • ionones • irone • maltol)
- From Ionones to Iso E Super and back (Diels–Alder • Iso E Super • Georgywood • Wender • Corey)
- Muguet: Essential but Essenceless (hydroxycitronellal • Enders • Oppolzer • muguet rules • Cope)
- The Sense of Smell (Heck • code of olfaction • Amoore • Rupe • mercaptanes)
- Rose and Rose Ketones (citronellol • rose oxide • Schenk photooxygenation • damascones)
- Metallic-green Pineapples and Leafy Cassis (Dynascone • Sonogashira • undecatriene • theaspiranes)
- Monoterpenes: Isoprene from Head to Tail (terpineol • ketenes • Komppa • pyrolyses • Carroll • (–)-menthol)
- Sesquiterpenes: Cedar, Vetiver and Patchouli (cedrol • khusimone • patchoulol • spirovetivenones • ketols)
- Jasmine: Benzyl Acetate vs. Hedione (Benzyl derivatives • Hedione • jasmon(ate) • Paradisone • Boelens rule)
- Steroids and Sandalwood (Timberol • Suzuki • santalols • isocamphene • campholenal)
- Musks of Nature – Macrocycles (Ruzicka • Carothers • Wilke • Eschenmoser–Ohloff • Dale nomenclature)
- Nitro, Polycyclic and Linear Musks (Carpenter • Galaxolide • horseshoe folding • dienone musks)
- "Marines": Calone 1951, Ambergris and Ketals (Dieckmann • ambreine • Ambrox • Cetalox • amberketals)

Heterocyclic Chemistry
3 ECTS, 2V
1. Starting with simple organic reactions and mechanisms, and comparing the carbocyclic (benzene and derivatives) chemistry, students will learn how to use that knowledge in heterocyclic compounds. 2. By understanding the mechanism of reactions, students will learn to synthesise tailor-made heterocyclic molecules. 3. Main topic is material science and surface chemistry. Students will get familiar with such applications. 4. Students will learn how to synthesize and the functionalisation of their desired molecules, 5-membered (pyrrol, furane, thiophene and related annulated compounds, e.g. indole) and 6-memebered (monoazines: pyridine, pyrimidine, pyridazine, pyrazine and the annulated ones such as quiinoline, isoquinoline, as well as multi-N-containing azines) aromatic heterocyles.

Introduction to Radiopharmaceutical Chemistry
1.5 ECTS, 1V
The lecture will give an overview from radionuclide production to their application in patients. The production of medically relevant radionuclides in cyclotrons, nuclear reactors, and with radionuclide generator systems as well as the synthesis and the preclinical evaluation of newly designed radiopharmaceuticals will be discussed. Translational aspects like GMP (good manufacturing practice) or other pharmaceuticals requirements and the application of radiolabelled pharmaceuticals for diagnosis and therapy of patients will be a further topic of the lecture.

Introduction to the Physics & Chemistry of Surfaces
3 ECTS, 2V
This lecture aims at introducing students to the fundamentals of modern surface physics and chemistry, both emphasising the role surfaces play in the general context of solid state physics & chemistry and demonstrating the importance of surfaces and interfaces in modern nanometre scale science. • Basics of Surface Science • Structure of Solids and Surfaces • Surface Analysis • Surface Electronic Properties

Mass Spectrometry (Lab course)
4 ECTS, 16P
Hands-on training in an analytical laboratory. The course covers modern techniques for sequencing of biopolymers and quantification of small molecules: • High-resolution electrospray tandem mass spectrometry of oligonucleotides • Peptide sequencing by MALDI-TOF-MS/MS • Quantification of drugs by multiple reaction monitoring

Modern Methods in Chemical Information
1.5 ECTS, 1V
• Introduction: Organization of Chemical Information • Planning the Course: Information Sources Case Studies: • Organic Compounds • Coordination Compounds • Inorganic Compounds • Substructure and Data Search • Preparation and Reactions This core program is modified/augmented according to the interests of the participants, with topics like Synthesis Planning, Patents, Topic (Keyword) Searching, Author Searching, Sequences of Biopolymers, Polymers, etc.

Neurochemistry
3 ECTS, 2V
• The cellular foundations of nervous system function • Synaptic transmission • Intracellular signaling • Acetylcholine – the transmitter which made history • Glutamate is exciting! • GABA – the brake in the brain • Modulating neurotransmitters • Atypical signaling in the nervous system • Food for thought (energy metabolism in the brain) • Long-term synaptic changes. The biochemistry of learning and memory • Neurodegenerative diseases (Parkinson's, Alzheimer's) • The biochemistry of schizophrenia • Pain and sensory perception

Nuclear- / Radiochemistry
3 ECTS, 2V
• Superheavy Elements: Chemistry and Physics - Stability & Production of Transactinides - Accelerators, Targets and Separators - Relativistic Effects - Experimental Methods to Investigate Transactinide Elements - Gas adsorption chromatography – Theory - Gas phase chemical properties of Transactinides • Energy for the Future: the Nuclear Option • CO_2, energy and our climate • Nuclear energy: basics, reactor types, nuclear energy worldwide • Concerns: the reactor accidents of Tschernobyl and Fukushima • Concerns: nuclear waste

Nucleic Acid Analaogues
1.5 ECTS, 1V
General aspects of DNA synthesis • Solid phase DNA synthesis • Solid phase RNA synthesis • Nucleic acid structure • Modifications • Natural modifications in DNA and RNA • α-DNA and α-RNA • Hexose nucleic acids • Design Principles • HNA • Bicyclo DNA (bcDNA) • Molecular Beacons • Principles to inhibit protein function • siRNA, miRNA mechanisms • ODN analaogues • tcDNA • Applications with tcTNA • Functional nucleic acids • Properties of unmodified functional nucleic acids • Properties of modified functional nucleic acids • Nucleoside triphosphates

Principles of Materials Science
3 ECTS, 2V
This master lecture presents an introduction to tensorial properties of materials, namely dielectrics. Theoretical models allowing a design of polar materials are discussed along with crystal growth methods.

Principles of Nucleic Acids
1.5 ECTS, 1V
• The Chemical Structure of Nucleic Acids • The Double Helix • Alternative Secondary and Tertiary DNA and RNA Structures • Intercalation • Chemical Synthesis of Nucleic Acids • On-line Demo - how to find and visualize nucleic acids structures

Process Chemistry
1.5 ECTS, 1V
The Process Chemistry course will be divided in two main parts, to be delivered in parallel. The first part will introduce, in general terms, the specific considerations for the synthesis of fine chemicals / elaborated active ingredients (AI) on Scale. Dedicated chapters will be (i) Process Safety ; (ii) Selection of synthetic routes, reagents and solvents on scale ; (iii) Practical considerations for

operating range, addition, mixing, quenching, extraction and purification. The second part, equal in weight with the first, will consist in real case studies from Pharmaceutical companies, where medicinal chemistry routes towards elaborated AI (marketed or abandoned candidates) were transformed into manufacturing routes. Those examples were chosen from recent literature to exemplify best the principles taught in the general section. They may also consist of single reaction optimizations, solving specific issues observed during scale up.
During the whole course, emphasis will be put on the deep understanding of the mechanisms of organic reactions shown, allowing for information driven optimization. Else, when chemical hypotheses fail to deliver optimally safe, manufacturing processes, Optimal Design of Experiments and multivariate analysis will be shortly introduced.

Radicals in Organic Synthesis (former Advanced Synthesis)

3 ECTS, 2V

- Introduction
- Tin hydride
- Substitute to tin hydride
- Tin mediated allylation and vinylation
- Atom-transfers
- Barton-decarboxylation
- Deoxygenation
- Xanthates
- Cyclizations
- Rearrangements
- CH-activation
- Homolytic aromatic substitution
- Alkoxyl radicals
- S-Radicals
- Sulfonyl radicals
- Phosphorous radicals
- Boron
- Oxidative Non-chain
- Reductive Non-chain
- Diastereoselectivity
- Enantioselectivity
- Organocatalysis
- Photoredox cazalysis

Scientific Writing

2 ECTS, 1.5V

This is a writing course in academic English at B2/C1 level in the Common European Framework. It is designed to help bio/chemistry students to

- become more familiar with different kinds of writing and writing strategies;
- increase the scope and accuracy of their written English, so that they can write texts in English with reasonable self-confidence
- improve their knowledge of English grammar, vocabulary and style.

Classes are planned to consist of the following activities: text analysis, practice exercises, correction activities, and writing practice.

Solid State Chemistry – Theoretical and Experimental Structural Investigations
3 ECTS, 2V
Part 1 • Thermodynamics in solids • Calorimetric techniques • Techniques to determine Solid state structures • Reaction in solid states • Optical / Electronic / Mechanical properties of materials Part 2 • DFT / Solids • Molecular Dynamics & Phase Transitions • Crystal Properties • Forces • Statistical Mechanics

Statistical Mechanics and Thermodynamic
3 ECTS, 2V
This lecture provides some bases on the theories linking microscopic to macroscopic description of matter. • Dynamical systems. • Microcanonical Ensemble • Canonical Ensemble • Grand-canonical Ensemble • Quantum-statistical mechanics • Molecular partition functions

Summer Course at Paul Scherrer Institute
4 ECTS, 2 months
Individual projects

Surface Electrochemistry
3 ECTS, 2V
The lecture course represents an introduction into basic concepts and applications of Surface Electrochemistry. We will discuss properties of electrolytes, electrodes and of the interface based on theoretical concepts and experimental investigations. Classical approaches will be combined with structure sensitive techniques, such as scanning tunneling microscopy, infrared and Raman spectroscopy as well as surface X-ray scattering. The in-class sessions will be accompanied by a lab-based tutorial on metal single crystal preparation and electrochemistry. • Introduction • Electrolytes (PCIV) • Electrochemical Double Layer • The Electrode Surface • (Single) Electrodes and Electrode Preparation • Cyclic Voltammetry – The „Spectroscopy“ of the Electrochemist • The Electrochemical Experiment (Lab Demonstration) • Concepts of Specific Adsorption

- Specific Adsorption – Molecules
- Scanning Tunneling Microscopy (STM)
- Atomic Force Microscopy (AFM)
- Vibrational Spectroscopy at Solid/Liquid Interfaces I (Infrared)
- Vibrational Spectroscopy at Solid/Liquid Interfaces II (Raman)
- Surface X-ray Scattering
- Project Work (Blocks 8 to 14)

Synthesis of Natural Products (former Biosynthesis and Synthesis of Natural Products)
3 ECTS, 2V
• Secondary Metabolites - The construction mechanisms • The Acetate Pathway • The Shikimate Pathway • The Mevalonate and Deoxyxylulose Phosphate Pathways: Terpenoids and Stereoids • Alkaloids

Therapeutic Proteins and Peptides
3 ECTS, 2V
An increasing proportion of drugs are so-called “biologics”, or agents of biological origin. The vast majority of biologics are recombinant proteins such as antibodies, insulins, growth hormones, etc. Peptides from natural or synthetic origin also play a major role as therapeutics, such as somatostatin, daptomycin, or lantibiotics. The course reviews important concepts and examples of therapeutic proteins and peptides, including also a brief discussion of gene and stem cells therapy.

Transporter Biology + Chemistry
3 ECTS, 2V
• Introduction on membrane transport / TransCure + Human diseases caused by ion channel dysfunction - Channelopathies • Mechanisms of transmembrane ion transport • ATP-binding cassette (ABC) transporters: Physiological functions, structures, mechanisms • Structure and mechanisms of ligand and voltage sensing in potassium channels • Structure and function of amino acid transporters • ATP-binding cassette (ABC) transporters: clinical significance • Physiological role of sodium/proton exchangers • Transporters and cancer: it works both ways • Vesicular transporters as potential targets in brain pathologies • The Swiss Kidney Project on Genes in Hypertension (SKIPOGH) • Role of transporters in drug disposition • Drug discovery in the area of transporter modulators • Natural products as leads in drug discovery • Bioorthogonal chemistry and other chemical tools to study transmembrane proteins

Legend:

V = Lecture
Ü = Exercises
P = Lab course hours
G = Lecture and exercises mixed
(e.g. 3V = 3 lecture hours per week)

1 ECTS credit point correponds to 25-30 working hours (lecture/lab course + homework).

LECTURES OFFERED IN PREVIOUS YEARS

Chromatographic Analysis
1.5 ECTS, 1V
• Trace Analysis • Qualitative Analysis • Quantitative Analysis • Integration • Sample Preparation • Quality Management

Environmental Chemistry
3 ECTS, 2V
• Introduction/ Atmosphere 1 • Atmosphere 2: Stratospheric ozone • Atmosphere 3: Tropospheric ozone, aerosols • Lithosphere: rocks, soils, weathering • Hydrosphere: hydrological cycle, hydrochemistry, marine geochemistry • Natural cycles of nitrogen, phosphorus, sulfur, acid rain • Cycles of Si, Fe, Al, Ca/Mg, Na/K, heavy metals • Ecotoxicology: Emissions, damage of ecosystems, POPs, CFCs, Xenobiotics, waste • Water pollution • Green chemistry • Radionuclides in the environment: Radioactivity, tracing of environmental processes • Carbon cycle, energy and climate • Analytical instrumentation • Stable isotopes in the environment

HPLC – From Theory to Instruments to Separations
1.5 ECTS, 1V
• **Theory**: Chromatography, resolution, peak capacity, reduced parameters • **Instrument**: Pumps, injectors, columns, detectors, capillaries, coupling with spectroscopy • **Phases**: Eluents (mobile phases), stationary phases • **Separation modes**: Adsorption, reversed-phase, bonded phases, ion exchange, size-exclusion chromatography, separation of enantiomers • **Separation strategies**: Isocratic vs. gradient

Laser Spectroscopy
3 ECTS, 2V
• Introduction: General principles (Basic principles of lasers, two-level and multilevel systems, three-level systems, four-level systems) • Optical resonators • Frequency selection and frequency tuning

Materials Characterization
1.5 ECTS, 1V
Materials science particularly aims at studying processing-structure-property relationships in materials, with a special attention to ”microstructure,” i.e., how materials are constructed on the microscopic and sub-microscopic (even nanometer) level, and how this affects their properties. This course aims at introducing the student to materials science and making him/her aware of the challenging opportunities this field offers to chemists. By a selection of case-studies, the student will become acquainted with synchrotron and imaging techniques, well-suited for the study of materials. Particular emphasis will be given to concepts important (but not limited) to materials, such as ”multiscale” properties and material heterogeneity, non-destructive, non-invasive and in-situ analysis, as well as representativity of the analysis (appropriate measurement scale, adequate statistics, issues with beam-induced damages). The student is also expected to learn good practices in material analysis (and science in general), i.e. how to choose analytical techniques relevant to the scientific question, sample the material adequately, perform a minimally invasive measurement and assess the robustness of the analysis.

Materials for Future Energy Technologies
3 ECTS, 2V
A lecture/master course on the chemistry of materials for energy conversion technologies: Topics will include the development, synthesis and characterization of functional materials for the better utilisation of renewable energy sources by understanding structure-composition-property-relations, e.g. of materials applied in improved solar cells, geothermal heat converters, thermoelectric converters, as well as in energy storage materials such as battery materials or hydrogen storage materials.

Measurement Uncertainty in Chemical Analysis
1.5 ECTS, 1V
• Introduction • Uncertainty of volumetric operations • Uncertainty of weighing operations • Uncertainty of the purity of chemicals • Uncertainty of molecular weights • Uncertainty of recovery • Uncertainty of calibration functions • Useful tools • Detailed example: Uncertainty of an analytical method

Methods for Molecular Simulations
3 ECTS, 2V
The aim of this course is to present to students the state-of-the-art in molecular modeling research. Critical assessments of different methodologies, with direct comparisons, and description of their strengths and pitfalls are done. A pool of possible subjects is presented to students (i.e., from excited state calculations, to protein folding, enzyme reactions etc). According to the specific interest of the students, the subjects of the course are decided at its beginning. The number of frontal lectures is limited to the minimum necessary to introduce basic concepts. The rest of the course is based on reading, presenting and discussing selected research papers on the various subjects of interest by the students. The course is addressed also to non-specialist students, i.e., students with a strong experimental profile. Possible topics of the course are: • Excited states dynamics • Density Functional Theory for intermolecular forces • Enhanced sampling techniques for exploration of the conformational-space • Simulations of chemical reactions and activated processes • Enzymatic catalysis • Protein folding • Protein-ligand interactions • Large-scale simulations

Nuclear and Radiochemistry (Lab course)
4 ECTS, 16P
• Thermochromatography (University of Bern) • Isotope exchange with radiotracers (University of Bern) • Neutron activation analysis (University of Basel) • Ion beam analysis (ETH) • Radiochemistry in atmospheric science (PSI)