DOCTORAL PROGRAMME IN CHEMICAL SCIENCES
UNIVERSITY OF LJUBLJANA, FACULTY OF CHEMISTRY AND CHEMICAL TECHNOLOGY

Programme description:

1. Basic data on the programme:

- The doctoral programme in Chemical sciences lasts three years (6 semesters) with the total of 180 ECTS credit points.
- There are three streams: *Chemistry, Biochemistry* and *Chemical Engineering*.
- Academic title conferred is *doktor/doktorica znanosti* (female holders).

2. Basic programme goals with general competencies

The principle **objectives** of doctoral programme in Chemical Sciences is to qualify professionals seeking employment in research-oriented institutions, assuming leader positions, in chemical and chemistry-related industries as well as public services, or for continuing their research careers in academic environment.

After completing the programme, graduates will acquire the following **competencies and skills**:

- Being able to critically analyse, evaluate and synthesize complex ideas;
- Communicate expert knowledge to colleagues, other expert groups, and to the broader public;
- Being able to promote advancements in science and technology at the academic and applicative level in a knowledge-based society.

3. Admission requirements and selection criteria in cases of limited enrolment

Admission requirements:
1. Admission to doctoral studies in Chemical Sciences is allowed under the following provisions:

a) completed second-cycle study programme
b) completed uniform master's programme, if assigned with 300 credit points
c) Completed undergraduate university programme from the previous system
d) Completed master's programme from the previous system (60 credit points will be assigned for study obligations, pending on the approval of the FKKT Senate, or another appointed body.)
e) Completed specialization with previous completion of a three-year higher professional programme. The candidate may be required to take a bridging programme in the total of 10 to 60 credit points, pending on the decision of the FKKT Senate or another appointed body.
f) Completed study programme from other domestic or foreign universities, according to the requirements which apply to students studying in Slovenia. The equivalence of previously obtained education abroad must be officially recognised according to the provisions of Art. 121 of the Statute of the University of Ljubljana.

Admission is limited to 40 regular and and part-time students. Mentor's agreement is required for admisssion to the programme.

Selection of candidates will be based on the following citeria:
1. grade-point average for all exams and exercises completed (without diploma) on previous university studies or second-cycle Bologna programme (75%).
2. grade obtained for diploma or master thesis from the second-cycle university studies (25%).
In case of limited access candidates will be ranked by the principle of total points collected.

4. Recognition of previously acquired knowledge and skills

Knowledge and skills, previously acquired by formal, informal or experiential learning will be assessed according to the provisions of Art. 9 of the Criteria for accreditation of study programmes in case the enrolment quota is exceeded. Recognition of previously acquired knowledge and skills must be approved by the FKKT Senate or another appointed body.
The following criteria will be taken into account:
– professional specialisation,
– diploma from another higher education institution,
– previous research work,
– scientific publications, and
– professional training.

5. Course progression requirements

For progression to the second year of studies the candidate must collect minimum 45 credit points, with at least 10 credit points obtained from elective subjects, and a positive grade for the presentation of research hypothesis for doctoral dissertation.

For progression to the third year of doctoral studies, the candidate should complete all the requirements from organised forms of study in the first and the second year, and have the title of doctoral thesis approved.

6. Conditions for the completion of studies

The doctoral study programme is completed after the candidate has fulfilled all obligations from the study programme and submitted and successfully defended his/her doctoral dissertation according to the Rules on Doctoral Dissertations, adopted by the Senate of the Faculty of Chemistry and Chemical Technology, University of Ljubljana. Prior to the approval of the thesis by the Senate, the candidate must publish the research results from his/her doctoral work in a relevant international scientific journal.

7. Transitions between programmes

Transition means termination of studies in another programme and continuing studies in the doctoral programme of Chemical Sciences. Transition does not apply to enrolments in the first year. Transitions are approved according to the provisions of the Statute of University of Ljubljana and Criteria for Transitions Between Programmes adopted by the Senate of FKKT, or by another officially body appointed by the Senate.

8. Assessment methods

Methods of knowledge assessment are defined in course descriptions of particular subjects. The assessment procedures are laid down by the Rules on Examinations of the Faculty of Chemistry and Chemical Technology which have been adopted by the Senate of FKKT.
The grading scale, as laid down by the Statute of the University of Ljubljana, will be used for knowledge assessment.

9. Course description with anticipated lecturers

The doctoral programme in Chemical sciences lasts three years with the total of 180 ECTS credit points. The programme complies with the provisions of Art. 36 and 37 of the Higher Education Act, and the Criteria for accreditation of higher education institutions and study programmes, which was adopted by the Council of RS for Higher Education. Course units have been weighted according to the European Credit Transfer System (ECTS) which provides for the recognition of studies abroad and exchange of students within the countries which have adopted the ECTS system.

One credit point is equal to 30 hours of student workload.

The study stream and the area of the doctoral thesis are determined by the subject of the student's research work, which also determines the selection of elective subjects and the content of other forms of study.

The study programme consists of various organised study units with the total of 60 credit points, while the remaining 120 credit points can be achieved by individual research work and doctoral dissertation. Allocation of credit points by years is the following:

- 1st year: 40 credit points obtained from organised forms of study and 20 credit points from research work,
- 2nd year: 15 credit points obtained from organised forms of study and 45 credit points from research work
- 3rd year: 5 credit points obtained from organised forms of study and 55 credit points from research work.

Organised forms of study are:

- **Public presentation of the research hypothesis of the doctoral thesis** (5 credit points) which must be completed before the enrolment in the second year;
- **Approval of the title of doctoral dissertation**, (5 credit points). The title must be approved prior to the enrolment in the 3rd year;
- **Writing and defending the doctoral thesis**, (5 credit points);
- **Mandatory participation at lectures with invited speakers**: the candidate must attend ten organised lectures per year. The topics are thematically balanced and selected to complement the research areas of students, taking into

consideration the level of demand which should be suited to all three areas of study, and active student participation (setting questions and participating in discussions). For five lectures out of ten (the selection being approved by the mentor), first and second year students will need to prepare a report about the lectures attended and supplement the report with relevant literature review, and relate the topic to their own research. The reports will be reviewed and approved by the mentor. Participation at 10 lectures and preparation of 5 reports in academic year (in the first and the second years of study) will be assigned with 10 credit points per year (total 20 credit points for two years for active participation at lectures and 10 credit points for preparing reports with literature review). In this way students will be updated with recent developments in various research fields, and by preparing the report broaden their knowledge by reflecting the problems to their own field of research;

- **induction seminar**: (5 credit points). The seminar will be organised within the mentor's research group. The purpose of the seminar is to **introduce students to complex experimental work**, provide the necessary theoretical backgrounds and implement methods of characterisation on their own samples, as well as introducing other activities necessary for starting up doctoral research;
- **professional training** (max. 5 credit points) for work in another research team (5 credit points equal to one month of work). This may also include theoretical studies of research methods and techniques according to individually designed programme, and/or participation at summer schools (number of credit points as determined by the school) and/or pedagogical work (number credit points corresponding the scope of pedagogical work);

- **elective subjects**, as listed below.

Table below presents the structure of the programme with credit points.

Module-contents	**1st year**	**2nd year**	**3rd year**	**Total**
Research work	20 ECTS	45 ECTS	55 ECTS	**120 ECTS**
Compliance with the conditions *	5 ECTS	5 ECTS	5 ECTS	**15 ECTS**
Mandatory participation at organised invited lectures	10 ECTS	10 ECTS		**20 ECTS**
Induction seminar	5 ECTS			**5 ECTS**
Professional training	5 ECTS			**5 ECTS**
Elective subjects	15 ECTS			**15 ECTS**
Total	**60 ECTS**	**60 ECTS**	**60 ECTS**	**180 ECTS**

* Compliance with the conditions encompasses: public presentation of research hypothesis for doctoral dissertation before enrolment in the 2nd year, obtaining approval for the topic of doctoral dissertation before enrolment in the 3rd year, and submission and defence of the doctoral thesis.

The programme offers 23 elective modules, each accounting for 5 credit points. In addition to this the candidate may, upon agreement with the mentor, take other electives, offered by other

MSc and PhD programmes of the University of Ljubljana and/or other universities home and abroad.
Elective subjects offered by FKKT are listed below. They have been selected and designed in view of the latest scientific achievements in a particular area and adapted to the needs of students (also catering for the needs of other students taking electives at FKKT). Subjects are organised as modules with a large number of lecturers available who will be able to cater for any number of students enrolled. The work will be coordinated by the principal lecturer, responsible for preparing a uniform exam, and the course director.

List of elective subjects with lecturers:
Selected topics in inorganic chemistry (Prof. Dr. Peter Bukovec)
Advanced methods in inorganic synthesis (Prof. Dr. Alojz Demšar)
Modern diffraction techniques (Prof. Dr. Ivan Leban)
Frontiers in analytical chemistry (Prof. Dr. Boris Pihlar)
Approaches in modern analytical chemistry (Prof. Dr. Marjan Veber)
Selected topics in experimental physical chemistry (Prof. Dr. Gorazd Vesnaver)
Theoretical methods in physical chemistry (Prof. Dr. Vojko Vlachy)
Selected topics in organic chemistry (Prof. Dr. Slovenko Polanc)
Selected topics in heterocyclic chemistry (Prof. Dr. Jurij Svete)
Study on mechanisms of organic transformations (Prof. Dr. Boris Šket)
Selected topics in biochemistry (Prof. Dr. Brigita Lenarčič)
Modern methods and techniques in biochemistry (Assist. Prof. Marko Dolinar)
Modern NMR approaches in characterisation of compounds (Prof. Dr. Janez Plavec)
Selected topics in chemical reaction engineering (Prof. Dr. Janez Levec)
Selected topics in transport phenomena (Prof. Dr. Igor Plazl)
Selected topics in separation processes (Prof. Dr. Janvit Golob)
Selected topics in environmental engineering (Prof. Dr. Jana Zagorc-Končan)
Advanced processes and methods in biotechnology (Prof. Dr. Marin Berovič)
Selected topics in polymer engineering (Prof. Dr. Matjaž Krajnc)
Mechanics of polymer materials (Prof. Dr. Matjaž Krajnc)
Selected topics in materials engineering (Prof. Dr. Stane Pejovnik)
Selected topics in materials for new energy sources and environmental protection (Prof. Dr. Jadran Maček)
Risk analyses in transportation of chemicals (Prof. Dr. Stojan Petelin)

10. Possibilities of elective subjects and mobility

The proposed study programme provides mobility of students and teachers. Students will be able to take elective subjects in a foreign institution, while teachers will be exchanged as invited lecturers. There will be other possibilities of cooperation through research work: students will be able to carry out part of their research in foreign institutions.
The procedure of recognition of credit points, acquired at other institutions, must be approved by the FKKT Senate or another appointed body.

11. Description of elective subjects

SELECTED TOPICS IN INORGANIC CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Student acquires knowledge on selected chapters in inorganic chemistry, knows how plan strategies for syntheses and is able to interpret the relationships between the structure, properties and potential application of selected types of compounds; knows how to apply various experimental methods to resolve problems associated with selected types of compounds.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Preparation of compounds with practical use.* Systematic review of synthetic principles used for the preparation of compounds and methods for their characterization. In-depth review of selected, up-to-date examples of practical applications: metal complexes as model compounds, photosensitive ruthenium compounds used in Graetzel cells, fluorescence metal compounds and their application in analytics, gold compounds and nanotechnology. Review of some most successful metal catalyst also used in industrial processes (Noyori, Grubbs, Heck, etc.). Mechanisms of action.
- *Biologically active complexes.* Review of selected compounds with confirmed biological activity already in clinical use, or have entered clinical trials. Design and synthesis of novel biologically active coordination compounds. Design will be based on the knowledge derived from the approved drugs (with known mechanisms of action) or from modern principles about functioning of biological systems. Novel strategies and methods will be used in the process. Through these procedures the student will acquire the knowledge for independent work in the field of biologically active compounds.
- *Metal complexes with macromolecules.* Metal complexes with macromolecules have great potentials for application. In general, two approaches for the synthesis of macromolecular metal complexes are known: a) coordination of metal ions on bulk polymers and b) preparation of a metal complex with monomeric unit followed by polymerization and formation of a polymer with metal ion bonded to the polymeric chain. Synthesis of metal complexes with macromolecules, characterization and structural properties of the macromolecular metal complexes, applications in biomedicine.
- *Organometallic compounds*. Planning of the syntheses of organometallic compounds, experimental techniques of the syntheses, characterization of the products. Dynamic NMR spectroscopy as a tool for the study of dynamic behaviour of molecules: background, determination of thermodynamic and kinetic parameters and mechanism of dynamic process. The use of dynamic NMR spectroscopy for studying the reaction mechanism catalyzed by organometallic catalysts.
- *Metals in the environment*. Distribution of metals and their compounds in the environment, essential and toxic metal compounds, geochemical and anthropogenic sources of metals, importance of metals for living beings. Reactions and circulation of

metals in environment (solubility of metal compounds; ligands for metals in the environment; origin, reactions and stability of coordination compounds; precipitation, adsorption, chemisorption, ionic exchange, redox reaction and fractionation of metals in ecosystems). Pollution of the environment with metal compounds (toxicity, limit values, legislation). Connection of mentioned topics with actual environmental problems. Remediation of soil and water, stabilisation of wastes (evaluation of the state of contamination with metals, principles and suitable methods of rehabilitation).

ADVANCED METHODS IN INORGANIC SYNTHESIS

Objectives of the course and intended learning outcomes (competences). Students acquire knowledge of advanced synthetic methods, reagents and techniques for the preparation of inorganic, coordination, organometallic and metallo-organic compounds, and for the preparation of compounds in the form of nanoparticles, thin films, porous material and other useful forms of matter. Particular attention will be given to the most promising methods.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Reactions:* outline of the important reactions and their mechanisms and reagents for the preparation of inorganic, coordination, organometallic and metalloid-organic compounds. Detailed study of some important research achievements that have opened new possibilities in the field.
- *Advanced synthetic techniques*, such as syntheses in the controlled atmosphere, solvothermal synthesis, sol- gel synthesis, sonochemical synthesis, thermal decomposition of precursors of inorganic compounds.

MODERN DIFFRACTION TECHNIQUES

Objectives of the course and intended learning outcomes (competences). Students acquire fundamentals in theory and practical applications of various novel advanced techniques of diffraction analysis for different aspects of characterization of solid state compounds.

Contents (syllabus outline). With mentor's agreement students chose among the techniques, which are closest to their respective research area. The course coordinator and the program coordinator make sure that the total workload of students does not exceed 5 ECTS. Should there be more lecturers involved in the implementation of the course; the course will be coordinated by the course coordinator.
Refreshing/revising student's knowledge of the diffraction of X-rays, neutrons and electrons on a solid state material.
Application of advanced single crystal techniques (electron density, anomalous dispersion, absolute configuration, use of a larger number of wavelengths in the vicinity of absorption edge, structure analysis of twinned crystals).

Application of advanced techniques on polycrystalline and amorphous materials (structure determination, Rietveld method for structure, microstructure and quantitative phase analysis, combination of neutron and X-ray diffraction, total scattering and pair-distribution-function (local order of crystalline and amorphous compounds), diffraction of nano-materials).

FRONTIERS IN ANALYTICAL CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Students extend their knowledge of novel analytical techniques (Theoretical basis and practical applications), which they have acquired at the master's level and raise their knowledge and skills to the level required for academic research and for solving complex professional problems in industry.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

Methodology and application of spectroscopic methods in analytical chemistry. Sample introduction problems in atomic spectroscopy related with gas, liquid and solid samples. Laser ablation in elemental analysis. The application of atomic spectrometry (ICP-OES, ICP-MS) for characterization of materials, environmental and biological samples.

- Novel mass spectrometric techniques (MALDI, proton transfer mass spectrometry, desorption electrospray ionization - DESI).
- Principles and application of modern separation techniques (electroseparation techniques, capillary electrophoresis, micelar chromatography, supercritical extractions).
- Theoretical and practical aspects of multidimensional chromatographic techniques.
- Electro analytical techniques (voltammetry and stripping techniques, their applications in analysis of inorganic and organic components, trace analysis, studies of metal-ligand interactions, characterization of biological systems and analysis of materials, and environmental analysis.
- Electrochemical sensors. Principles, application in equilibria studies, microelectrodes, chemically modified electriodes, micoelectrodes for flow systems, ultramicroelectrodes. Hyphenated techniques: spectroelectrochemistry (EC-UV-Vis, EC-IR, EC-MS, SEM, EC-STM, EC-AFM).

APPROACHES IN MODERN ANALYTICAL CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Students extend knowledge of analytical chemistry which they have acquired at the master's level and raise their knowledge and skills to the level required for academic research and solving complex professional problems in industry. They develop abilities for proper selection of analytical methods and for solving demanding research or technological problems.

Students will enhance their knowledge of the application of numerical methods and modelling in analytical chemistry.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- Numerical methods in analytical chemistry.
- Speciation in chemical analysis, sample preparation and selection of a proper detection technique.
- Miniaturisation in analytical chemistry: lab-on-a-chip concept, micro total analytical system (mTAS), micromachining techniques for mTAS and integration of detection into microfluidics devices, macro-to-micro interfaces for microfluidics devices.
- Analytical methods in food control; separation and characterization of food constituents.
- Approaches in studying transformation and binding of anthropogenic pollutants in environment.
- Analytical problems in atmospheric chemistry, characterization of aerosols and modelling.
- Importance of modern analytical methods in biomedicine, biology, environmental protection, protection of cultural heritage and industry.

SELECTED TOPICS IN EXPERIMENTAL PHYSICAL CHEMISTRY

Objectives of the course and intended learning outcomes (competences). During the learning process students acquire high-level knowledge from a narrow focused scientific field. With the experience they gain they will be able to carry out research autonomously in a chosen research field.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Solutions of biologically important macromolecules.*

Thermodynamics and kinetics of biopolymers in aqueous solutions. Model analysis of thermodynamic and kinetic quantities measured by spectroscopic and calorimetric techniques in correlation with structure and function of biological macromolecules.

- *Structural investigation of nano-systems by small angle x-ray scattering.*

General scattering theory. Model calculations: Spherical, rod-like and flat particles. Experimental setup. Data treatment and evaluation. Practical applications.

- *Investigation of ergodic and non-ergodic systems by SLS and various DLS methods.*

General theory of light scattering. Specific properties of auto-correlation, 3D, echo, and multi-speckle DLS experimental systems. Practical applications.

- *Thermodynamics of the association processes in solutions.*

Ion association in electrolyte solutions. Thermodynamic of micelle formation of ionic and non-ionic surfactants (isothermal titration calorimetry, isothermal titration conductometry, Philips's criterion, pseudo-phase separation model, equilibrium model, degree of ionization of the micelles.

- *Complex colloid systems.*

Associating systems: surfactants, polymers and polyelectrolytes, and mixed polymer-surfactant systems. Intermolecular association and gelation. Phase behaviour and structures. Experimental techniques for studying associating systems.

- *Aqueous solutions of polyelectrolytes.*

Principles of synthesis and analytics of polyelectrolytes samples. Basic characterization of polyelectrolytes: determination of solubility curves, ionization constants, titration curves. Model analysis of measured thermodynamic and transport properties of polyelectrolytes in correlation with the polyelectrolyte structure.

THEORETICAL METHODS IN PHYSICAL CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Student will acquire deeper knowledge of physical chemistry and develop scientific approach to problem-solving. This will enable the candidates to pursue their individual research in physical and related areas of chemistry.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Potential methods*.

Basic facts. Poisson−Boltzmann equation, modified Poisson−Boltzmann equation. Boundary conditions and solution of linearized and nonlinearized equation in different symmetries.

- *Thermodynamic perturbation theory*.

Basics, Gibbs−Bogoljubov inequality. Barker−Henderson theory. Weeks–Chandler–Andersen theory. Wertheim perturbation theory.

- *Distribution functions*.

Ornstein−Zernik integral equation in different closures. Multipole expansion for molecular systems. Wertheim integral equations for systems with highly directional forces.

- *Simulation methods.*

Monte Carlo method in generalized ensemble. Usage of impulse potential for modelling of attractive colloids. Molecular dynamics. Force fields. Molecular docking. Simulation of biomolecules.

- *Systems in external fields.*

Density functional theory.

- *Quantum chemistry methods.*

Periodical systems: Bloch functions, Hartree-Fock method for periodical systems. Correlation in electron motion: correlation energy, method of configuration interaction, multiconfiguration interaction, coupled cluster method. Density functional theory (DFT): Kohn-Sham equations, Hohenberg-Kohn theorems, approximation of local density, approximation of non-local density. Methods of quantum dynamics and mechanics.

- *Chemical kinetics.*

Rate of chemical reactions in solutions and effects of ionic reactants on the reaction rate. Catalysis.

SELECTED TOPICS IN ORGANIC CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Advancing knowledge on selected topics and methods of organic chemistry, as a basis for practical problem solving in organic chemistry.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Diazenes in organic synthesis.*

Synthesis of diazenes. Reactions with alkenes and arenes. Halogen migration. Intramolecular reactions. Reactions with carbonyl compounds. Synthesis of imidazoles, 1,2,4-triazoles, and 1,3,4-oxadiazoles. Chemo selective oxidations of thiols in selenols; electrochemical properties of diazenes. Applications of diazenes in 'click' chemistry and in cycloaddition reactions. Mitsunobu reactions. Biochemical properties of diazenes. (Prof. Janez Košmrlj, Prof. Slovenko Polanc)

- *Modern methods for halogenation of organic molecules.*

Halosubstituted organic molecules in (biological) chemistry, biologically active halosubstituted molecules, biohalogenation, influence of fluorine atom on biological activity. Sustainability and ecologically acceptable halogenation methods. Modern halogenation methods: solvent-free conditions, halogenation in water, solvent vapours in solid state halogenations, diffusion membranes, micro reactors, continuous processes. New halogenation reagents, enantioselective halogenations, synthesis of halosubstituted chiral synthons. (Prof.Marko Zupan, Assist. Prof.Marjan Jereb).

- *Selected topics in selective synthesis.*

Selective synthesis, protecting groups. Stereoselective synthesis, asymmetric induction. Catalysis in selective synthesis. Microwave-assisted selective synthesis, solvent-free reactions. High-pressure synthesis (>10 kbar), solvent effects, chemo-, regio- and stereoselectivity, examples. Cycloadditions and other transformations of 2*H*-pyran-2-ones: synthesis and transformations of bicyclo[2.2.2]octene derivatives, α,β-didehydro-α-amino acids, polisubstituted anilines and related compounds, indoles. Synthesis and reactivity of 1,3-diketo-BF_2 complexes. Formation of a C-C bond via catalytic activation of inert C-H bond. Metal-carbene complexes in formation of a C=C double bond. (Prof. Marijan Kočevar, Assist. Prof. Bogdan Štefane).

- *Molecular probes for structural and functional imaging.*

Overview of modern methods for structural and functional imaging (MRI, confocal microscopy, positron emission tomography (PET)...). Synthesis and characterization of fluorescent and radiolabelled molecular probes. Selected examples: probes for monitoring changes in central nervous system. (Prof. Andrej Petrič)

SELECTED TOPICS IN HETEROCYCLIC CHEMISTRY

Objectives of the course and intended learning outcomes (competences). Advancement of knowledge on selected topics and methods in organic chemistry, which is basic for student ability to solve practical problems in organic chemistry.

Contents (syllabus outline).

- *Heterocyclizations.*

Cyclosubstitutions, cyclocondensations, cycloadditions, pericyclic reactions, ring transformations, molecular rearrangements, regio- in stereoselective heterocyclizations, stereoselective and asymmetric synthesis of (partially) saturated systems.

- *Modular approach to ring synthesis.*

Building blocks, heterocyclization methods, modular approach to the strategy of ring synthesis, chemo- regio- and stereo-control.

- *Synthesis and transformations of alkyl 3-(dimethylamino)propenoates and related enaminones; from heterocycles to natural products.*

Synthesis and structure of alkyl 3-(dimethylamino) propenoates and related enaminones from acyclic and cyclic precursors with active methylene group. Typical reactivity: reactions with nucleophiles and electrophiles, cycloadditions. Transformations: synthesis of heteroaryl amino acids, synthesis of heterocyclic systems: aziridines, pyrroles, oxazoles, isoxazoles, pyrazoles, imidazoles, 1,2,4-oxadiazoles, 1,2,3-triazoles, pyranones, pyridines, pyridazines, pyrimidines, pyrazines and their fused analogues. Synthesis of natural products and their analogues, e.g. indole alkaloids such as aplysinopsins, meridianins, dipodazines, triprostatines and others.

- *Synthesis of functionalized heterocycles.*

Synthesis via ring functionalization, synthesis via heterocyclization of functionalized building blocks (precursors).

- *Combinatorial synthesis of heterocycles.*

STUDY ON MECHANISMS OF ORGANIC TRANSFORMATIONS

Objectives of the course and intended learning outcomes (competences). Advancement of knowledge on selected topics and methods of organic chemistry, which is a basis for student ability to solve practical problems in organic chemistry.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

- *Survey of methods for studying organic reaction mechanisms.*

Non-kinetic methods: identification of products, reactive intermediates, chemical and physical methods (spectroscopic methods: NMR, ESR, UV/VIS, IR) for detection and characterization of intermediates, isotopic labelling, stereochemistry and mechanism. Kinetic methods: kinetic principles of reactions in a solution, transition state, activation parameters and their interpretation, Hammond's postulate, reactivity-selectivity principle, kinetic isotope effect, structure-reactivity correlation, linear free energy relationships and transition state. Empiric correlation between solvent effect and reaction rate.

- *Organic reaction mechanism studies with emphasis on oxidations with peroxides and ozone.*

Synthesis, physical properties, and reactivity of important organic peroxides. Mechanism of oxygen transfer in (non)catalyzed oxidations of organic molecules with peroxides. Oxidations with singlet ($^1O_2$) and triplet ($^3O_2$) oxygen and ozone. Peroxides in biological systems. Chemistry of hydrogen trioxide (HOOOH) and its organic and organometallic hydrotrioxide (ROOOH) derivatives.

- *Organic photochemistry*.

Formation and behaviour of molecules in excited state is important for understanding of photochemical reactions. This information can be obtained from kinetics of photophysical and photochemical processes and can be applied in designing molecular structures leading to a desired final product of photochemical processes. a) Photophysical processes: photon absorption, singlet and triplet states. Photon emission (fluorescence, phosphorescence, chemiluminiscence). Selection rules for transitions (intersystem crossing, internal conversion) Franck-Condon principle. b) Experimental techniques: "time resolved" spectroscopy which enables monitoring of short-term excited states and intermediates on nano- in femtosecond scale. Determination of quantum yield of emission phenomena and photochemical processes. Discrimination between different types of excited states with specific inhibitors. c) Photochemical processes: typical chromophores and their reactivity. The use of photochemical processes in organic synthesis.

- *The chemistry of radicals.*

a) Structure and reactivity of radicals. Experimental techniques in reactivity studies, kinetic and "time resolved" spectroscopic methods (laser flash photolysis on nanosecond scale, etc.), electron spin resonance. Electronic effects in radical reactions. Computational methods (DFT) radical reaction energy studies.

b) The use of radical processes in organic synthesis. Chemistry of stananes and related hydrides, redox processes, etc. Catalysis with “Umpolung”.

SELECTED TOPICS IN BIOCHEMISTRY

Objectives of the course and intended learning outcomes (competences). Graduates will gain an overview of literature, they will be able to critically assess information and use it in planning and assessment of their own work. Students will also know how to search for information, write a description of research background according to instructions in tender documentation and propose a research project within the scope of the broader area of biochemistry.

Contents (syllabus outline).

- Introductions to subject areas (lectures)
- Seminar on current literature
- In-depth analysis of biochemistry news which appear in the media
- Discussion of a selected disease from the aspect of biochemistry
- Preparation of a research project in the field of biochemistry

MODERN METHODS AND TECHNIQUES IN BIOCHEMISTRY

Objectives of the course and intended learning outcomes (competences). Keeping up-to-date with new methods and techniques developed on biochemistry and critically assess the advantages and shortcomings of the improvements and applicability of new methods.

Contents (syllabus outline).

- Introductions to subject areas (lectures)
- Technology developments in biochemistry (seminars)
- Suggestions for introducing a new method or for improving one of the methods used by other students in their research

MODERN NMR APPROACHES IN CHARACTERIZATION OF COMPOUNDS

Objectives of the course and intended learning outcomes (competences). Introducing students with up-to-date techniques of nuclear magnetic resonance, both theoretically and practically. Students will be able to apply knowledge in solving scientific problems (preferably) associated with the student's own research work.

Contents (syllabus outline). Nuclear spin, NMR experiment, relaxation, composite pulses, heteronuclear decoupling, spin lock, selective excitation, gradient pulses, diffusion, processing and interpretation of NMR spectra, heteronuclear experiments, spectral editing, polarisation transfer, multidimensional NMR experiments, correlations through bonds and through space, spectral assignment, NMR restraint molecular modelling, equilibrium and dynamic properties of molecules, solid state NMR, polymorphism and solvation.
Contents and the program of the course will be individually adjusted as per requests and scientific interests of individual students. The course can be tailor-made to the level which will allow students to independently use NMR spectroscopy in later studies of organic, inorganic, pharmaceutical, biochemical and other samples in solid as well as in liquid states.

SELECTED TOPICS IN CHEMICAL REACTION ENGINEERING

Objectives of the course and intended learning outcomes (competences). Students gain deeper insight into the interaction between transport phenomena and kinetics of chemical reactions taking place on solid catalysts. These knowledge help them to: (i) quantitatively interpret the experimental kinetic data obtained in a multiphase reactor and (ii) optimally design and operate multiphase reactors such as frequently employed in pharmaceutical and related industry. Students are qualified to select the most appropriate reactor for achieving the highest selectivity and production of the desired products as well as to use their knowledge critically in order to solve more complex engineering problems for process intensification.

Contents (syllabus outline).

Catalysis. Solid catalysts. Catalyst synthesis. Characterization (physical methods, temperature programed techniques, transient methods). *In-situ* characterization of catalyst surface properties. Reaction rate theory. Surface reactivity. Models of chemisorption. Mechanisms and kinetics of heterogeneous catalyzed reaction. Catalytic oxidation and reduction (hydrogenation) reactions. Asymmetric heterogeneous catalysis. Heterogeneously catalyzed reactions in supercritical fluids and ionic liquids. Multifunctional catalysts. Catalyst deactivaion. Environmental catalysis. Application in petrochemical and pharmaceutical industry.

Multiphase reactors: single reactions. The role of mass and heat transfer at the surface reactions and within the porous catalyst. Model reactors for studying mass transfer with chemical reactions in heterogeneous systems: gas-liquid, liquid-liquid, fluid-solid. Measurement techniques for mass transfer coefficients in multiphase reactors.

Multiphase reactors: multiple reactions. Simultaneous mass transfer of two reactants with independent and dependent parallel reactions. Simultaneous mass transfer with consecutive reactions. Mass transfer with mixed parallel and consecutive reactions.

Heat effects in multiphase reators. Gas-liquid reactors. Bubble column and agitated reactors. Gas-solid reactors. Gas-liquid-solid reactors.

SELECTED TOPICS IN TRANSPORT PHENOMENA

Objectives of the course and intended learning outcomes (competences). Upgrading knowledge in fluid dynamics, heat and mass transfer.

Contents (syllabus outline).

- complex fluids – origins of Non-Newtonian behaviour;
- constitutive equations for Non-Newtonian fluids;
- boundary conditions at solid walls and fluid interfaces (kinematic condition, thermal boundary conditions, dynamic boundary condition);
- unidirectional and one-dimensional flow and heat transfer processes;
- introduction to asymptotic approximations (the effect of viscous dissipation on a simple shear flow, motion of a fluid through a slightly curved tube – the Dean problem, diffusion in a sphere with fast reaction – singular perturbation theory, bubble dynamics in a quiescent flow – the Rayleigh-Plesset equation;
- films with a free surface;
- creeping flow - general properties and solutions for 2D and axisymmetric problems;
- creeping flow - 3D problems;
- convection effects and heat transfer for viscous flows;
- boundary layer theory for laminar flows;
- heat and mass transfer in high Reynolds numbers.

SELECTED TOPICS IN SEPARATION PROCESSES

Objectives of the course and intended learning outcomes (competences). Post-graduate students will improve on their fundamental engineering knowledge pertaining to the mass transfer, thermodynamics and mass-heat balances, and apply them into the analyses and the design of complex separation processes. They will study the role of separation processes in the process and product engineering, and be engaged into research-development assignments regarding the transfer of separation techniques from the laboratory to the pilot-plant and industrial capacities.

Contents (syllabus outline).

- Reaction and separation processes in the process and product engineering;
- Mass and heat balances of complex processes;
- Thermodynamics of non-ideal systems;
- Mass transfer in two-phase complex systems;
- Methods for the calculation of separation time as the basis for the equipment dimensioning and model development for the separation time as well as the study of separation time on parametric sensitivity;
- Knowledge development on the level of product, equipment, and process in the analysis and design of separators;
- the role of research on laboratory and pilot scale unit as the basis for separation process development.

SELECTED TOPICS IN ENVIRONMENTAL ENGINEERING

Objectives of the course and intended learning outcomes (competences). Upgrading and deepening knowledge in environmental engineering as a prerequisite for successful solving of various environmental problems; acquiring skills for critical evaluation of the technologies already applied, being able to select, design and assess the possible improvements from various aspects; being able to assess his/hers own work in terms of the impacts on local and global environment; being able to address ethical issues in decision making; being able to critically approach different scientific and social problems.

Contents (syllabus outline). From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work. The course coordinator, who is in charge of the course, and the leader of the study take care that the student's workload corresponds to 5 credits. If more persons are taking the study programme, the whole process is coordinated by course coordinator.

Up-to-date techniques for qualification and quantification of hazardous substances: micro-pollutants (endocrine disrupters, biocides, PAH, PCB). *In vitro* and *In vivo* methods for detection and quantification of micro-pollutants. Advanced methods for identification and removal of hazardous substances from wastewaters: TIE – Toxicity Identification Evaluation and TRE – Toxicity Reduction Evaluation.

Chemical, membrane and biochemical processes for the protection and remediation of environment:

- Chemical Processes: Treatment of wastewaters and drinking waters using chemical methods. Advanced oxidation processes (AOPs). Photo-catalytic oxidation. Fenton's oxidation. Ozonation. Electrochemical oxidation. Wet air oxidation. Supercritical water oxidation. Heterogeneous catalysts for environmental protection. Catalytic wet oxidation. Catalytic denitrification. Kinetics and mechanisms of reactions. Multiphase reactor systems. Trickle bed reactor. Monolith reactors. Catalytic membrane contactor. Integrated process schemes: coupling of AOPs and biological processes. Application of AOPs for the removal of micro-pollutants from aquatic (drinking and wastewaters) and atmospheric environments.
- Membrane Processes.
- Biochemical Processes: Bioremediation using fungi. Bio-augmentation. Bioremediation of disperse pollution. Decolourization and degradation of organic dyes. Important process parameters. Degradation mechanisms, pathways and products. The role of enzymes in degradation of organic dyes. Micro-remediation bioreactors. Comparison to alternative technologies. Conclusions and perspectives: Micro-remediation of micro-pollutants using white rot fungi.

ADVANCED PROCESSES AND METHODS IN BIOTECHNOLOGY

Objectives of the course and intended learning outcomes (competences). Deepening knowledge in biotechnology methods needed for independent research in the field of analysis, optimization and design of new environmentally and human-acceptable bioprocesses and technologies.
Competences: Ability for solving various engineering tasks and problems in bioprocesses and technologies, using basic engineering principles and the latest technologies and engineering tools.

Contents (syllabus outline).

- Biotransformations in microreactors; biotransformations in non-conventional media (ionic liquids, organic solvents); biotransformations in pulp and paper industry.
- Miniaturization of bioprocesses: micro devices in biotechnology; advances and deficiencies of reactions and processes in microreactors; application of microsystems in down-stream processes, integrated lab-on-chip devices; analytical devices in microsystems (micro total analysis systems - μTAS): application for on-line bioprocess monitoring; enzyme microreactors.
- Morphology of filamentous fungi in submerged cultivations as a bioprocess parameter; mechanisms of submerged growth of filamentous fungi; morphological characterization (image analysis, rheological properties of broth); mycelial morphology and metabolite production; bioprocess design and control considering morphological characteristics.
- Biosynthesis of Basidiomycetes pharmaceutically active compounds : comprehensive methods for active biomass cultivation; production of intra and extracellular active compounds (polysaccharides, terpenoides, proteins and proteoglycans), strategy of extraction, isolation and purification of various active compounds; testing of immunostimulatory and therapeutic action of isolates on animal and human cell lines; medical application of various pharmaceutically active compounds.

- Bioprocess engineering of anaerobic fermentation processes: microbial scale-up and control criteria; the role and the influence of integrated factors on microbial scale-up and control criteria (influence of heath shocks, galvanic and magnetic field, combined methods and synergistic actions).

SELECTED TOPICS IN POLYMER ENGINEERING

Objectives of the course and intended learning outcomes (competences). Deepening knowledge in specific fields of polymer engineering science. Studying scientific and professional literature in a specific field, critical evaluation of literature; being able to propose the content of a research project, to suggest research methods and to state its goals.

Contents (syllabus outline).

- lectures, giving a review of polymer engineering topics
- seminar from a selected topic in polymer engineering, based on scientific and professional literature review
- elaboration of a project proposal for a specific process design
- elaboration of a project proposal for a specific product design

MECHANICS OF POLYMER MATERIALS

Objectives of the course and intended learning outcomes (competences). Deepening knowledge on the mechanics of polymer materials on macroscopic level and relations between mechanical behaviour and material structure and deformation mechanisms. Acquiring knowledge about modern techniques used for determination of the properties of polymer materials, interpreting results and modelling of viscoelastic behaviour.

Contents (syllabus outline). Phenomenological treatment of viscoelasticity of polymer materials. Modern techniques for measuring (dynamic) mechanical properties of polymers. Molecular mechanisms and mathematical description of continuum mechanics. Time-temperature correspondence. Transitions and relaxations in polymers. Elasticity in rubbery networks. Modelling of mechanical properties of polymer composites. Case study.

SELECTED TOPICS IN MATERIALS ENGINEERING

Objectives of the course and intended learning outcomes (competences). Basic chemistry and materials engineering data are given to understand correlations between the structure and properties of materials. Advanced knowledge on selected topics is presented as a basis of student's ability to solve scientific and engineering problems.

Contents (syllabus outline).
At the beginning of school year the student and course coordinator select specific topics from the course content, relevant for dissertation with the total of 5 ECTS. Course coordinator is responsible for appropriate organization of the course in case there are more than two lecturers on the programme.

- *Materials properties.*

The emphasis is on the underlying relationship and deeper understanding of the microstructure-composition-synthesis-processing relationships. Tensile test and the information that can be derived from it, elastic and plastic deformation, concept of slip, dislocations and their role in plastic deformation, Schmidt's law, creep, kinetics of phase transformations, strengthening mechanisms and hardness will be studied. Additional knowledge needed to understand electrical, magnetic and optical properties of materials, bio ceramics and nanomaterials will be acquired through seminars.

- *Principles of materials design.*

Seminars will be prepared as specific case studies for: steels and alloys, aluminium, ceramics, glass, polymer composites, continuous ceramic fibre composites, metal matrix composites, advanced ceramic materials (LTCC, FGM)

- *Principles of materials selection for engineering design.*

When a material is designed for a specific application, a number of factors must be taken into account. Therefore, specific properties of materials with high relevance to the design of components and structures will be studied. Materials must be designed with required physical or mechanical properties, their fabrication should simple and cost effective. Methodology for materials selection, including the selection criteria, and specific tools for selection of corrosion resistant materials functioning under specific conditions will be presented. Monitoring the processes for manufacturing will be studied: synthesis and analysis of composition and properties of materials, specific methods for powder preparation and characterization, shaping, drying, sintering; processes for property improvement and design: thermal, chemical and mechanical treatments. All processes will be studied on micro and nano levels. Special case studies of the use of contemporary physical and chemical synthetic routes will be elaborated by the students in seminar form.

SELECTED TOPICS IN MATERIALS FOR NEW ENERGY SOURCES AND ENVIRONMENTAL PROTECTION

Objectives of the course and intended learning outcomes (competences). Acquiring specialized knowledge in this field. These competences enable students to conduct research in a particular research field.

Contents (syllabus outline). Together with mentor the student chooses the course contents with the total of 5 credits among the topics listed below. If there is more than one lecturer on the course, the course coordinator takes care of the implementation of the program.

Materials for new energy converters

- *Hydrogen Technology: Technologies for hydrogen production* (processing of hydrocarbons – steam reforming, water gas shift reaction, electrolytic processes, thermo-chemical dissociation of water, conversion of biomass to hydrogen). *Storage and distribution of hydrogen* (pressurized systems, cryogenic systems, storage of hydrogen in hydride form , CNT etc.: distribution of hydrogen, safety of hydrogen technologies).
- *Fuel cells: Types of fuel cells and principles of their operation* (fuel sources and fuel purity, operating temperature of a FC, materials used in the construction of a cell, charge transfer). *Materials for electrolyte, electrodes and interconnect* (prerequisites for characteristics of the materials in fuel cells, electrocatalysts). *Operation of a fuel, yield of energy conversion and environmental impact* (activation, ohmic, concentration and other polarization losses, fuel cell systems and their infrastructure, yield of fuel cells, cogeneration of heat in fuel cells, environmental impact in direct conversion of chemical into electrical energy).
- *Lithium ion and other batteries: Principles of operation of classical and new insertial batteries and accumulators* (charge storage on surfaces/interfaces and in bulk, homogeneous insertion and insertion via phase transformation, influence of kinetic and thermodynamic properties). *Materials for anodes, electrolytes and cathodes* (graphite-based materials, lithium alloys, oxides and sulphides, sulphur cathode, air electrodes, liquid polymeric and mixed electrolytes, electrolytes based on ionic liquids). C*haracteristics of advanced accumulators* **(**lithium insertion batteries, Li air battery, polymer accumulators, lithium-sulphur accumulator).
- *Supercapacitors: Preparation principle of a supercapacitor* (solid-liquid interface, electrical double layer, thermodynamics and kinetics of a typical supercapacitor, influence of porosity, surface groups, difference between electrostatic and chemical charge storage on surfaces). *Materials for anode, electrolyte, and cathode* (graphitic materials, aqueous and non-aqueous electrolytes). *Characterization, properties and application of selected supercapacitors.*

Materials for environmental protection (materials for reducing emissions in environment, elimination of VOC – volatile organic compounds), development of catalytic materials and systems, lifetime cycles and impact of different groups of materials on the environment).

RISK ANALYSES IN TRANSPORTATION OF CHEMICALS

Objectives of the course and intended learning outcomes (competences). Predicting and controlling risks in transportation of hazardous substances.
Understanding transportation quantitative risk analyses for hazardous substances, how to communicate risk study objectives to an experienced risk analyst, and how to make a reasonably detailed calculation based on available risk data.

Contents (syllabus outline).

- Definitions of basic risk analysis terms
- Sources of data specific to accident rate, probabilistic distribution of accident force magnitude, and conditional probability of container failure. Databases for accident rate and frequency, accident force types and magnitudes, container failure probability, and release amounts. Quantification of risk reduction for modifying container design.
- Methodologies for accident scenario development, frequency and consequence analysis, and risk presentation.
- Mathematical formulations for quantitative risk analysis in transportation
- Methodologies for risk analyses and data uncertainties.
- Fault tree for different types of transportation risk analyses
- Steps of the QRA from preliminary hazards analysis to risk reduction alternatives.
- Example of a quantitative risk analysis for various transportation tapes: pipeline, truck, rail, fright transport vessels, naval vessels, etc.