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 four years (8 semesters) with the total of 240 ECTS credit points.
Study offers 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;
- beeing 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

Doctoral study is carried out as a part-time study.

Admission to doctoral studies in Chemical Sciences is allowed under the following provisions:
- second cycle study programme;
- study programmes providing education for occupations regulated by Directives of the European Union, evaluated with at least 300 credits;
- undergraduate university programme from the previous system;
- 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);
- 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 UL FKKT Senate or another appointed body.
- 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 UL.
- mentor's agreement and short conceptual design of the research work.

List of potentional mentors is published on our faculty web site http://www.fkkt.uni-lj.si/sl/studij/bolonjski-studijski-program-3-stopnje/ under ”Seznam potencialnih mentorjev”

Information on the research work of the faculty is published on our web site http://www.fkkt.uni-lj.si/en/scientific-research/

Selection of candidates will be based on the following citeria:
- grade-point average for all exams and exercises completed (without diploma) on previous university studies or second-cycle Bologna programme (75%);
- 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 5 credit points obtained from obligatory subject, at least 5 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 at least by the UL FKKT Senate.

For progression to the fourth year of doctoral studies, the candidate should complete all the requirements from organised forms of study in the all previous years, and have the title of doctoral thesis approved by the UL Senate.

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 UL FKKT Senate. 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 UL and Criteria for Transitions Beetween Programmes adopted by the FKKT Senate, or by 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 FKKT which have been adopted by the Senate of FKKT.

The grading scale, as laid down by the Statute of UL, will be used for knowledge assessment.

9. Course description with anticipated lecturers

The doctoral programme in Chemical sciences lasts four years with the total of 240 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 180 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: 60 credit points from research work and
- 4th 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 at least by the UL FKKT Senate**, (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);
- **obligatory subject Academic writing**, 5 credit points**;**
- **elective subjects**, as listed below.

The structure of the programme with credit points is presented below.

1st year		***Contact hours***						***Individual student work***	***ECTS***	***Total hours***
		P	***S***	***SV***	***LV***	***TD***	***DO***			
1	Academic writing	30					90	30	5	150
2	Induction seminar						75	75	5	150
3	Mandatory participation at organised invited lectures						150	150	10	300
4	Professional training						75	75	5	150
5	* Compliance with the conditions (presentation of research hypothesis)						75	75	5	150
6	Ellective subject 1	i	i					75	5	150
7	Elective subject 2	i	i					75	5	150
8	Research work						300	300	20	600
	Total 1st year	**30+i**	**i**				**765**	**855**	**60**	**1800**

2nd year		***Contact hours***						***Individual student work***	***ECTS***	***Total hours***
		P	***S***	***SV***	***LV***	***TD***	***DO***			
9	Mandatory participation at organised invited lectures						150	150	10	300
10	* Compliance with the conditions (approval for the topic of doctoral dissertation)						75	75	5	150
11	Research work						675	675	45	1200
	Total 2nd year						**900**	**900**	**60**	**1800**

3rd year		***Contact hours***						***Individual student work***	***ECTS***	***Total hours***
		P	***S***	***SV***	***Total hours***	***TD***	***DO***			
12	Research work						900	900	60	1800
	Total 3rd year						**900**	**900**	**60**	**1800**

4th year		Contact hours						Individual student work	ECTS	Total hours
		P	S	SV	Total hours	TD	DO			
12	Research work						825	825	55	1650
13	* Compliance with the conditions (defence of the doctoral thesis)						75	75	5	150
	Total 4th year						**900**	**900**	**60**	**1800**
	Total all four years	**30+i**					**2465**	**3555**	**240**	**7200**

The programme offers 24 elective modules, each accounting for 5 credit points. In addition to this the candidate may, upon agreement with the mentor, take other electives for 5 credit points from other PhD programmes offered by of the UL and/or other universities from home or 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 principal lecturer responsible for preparing a uniform exam and the course director will coordinate the work.

List of subjects with lecturers:

Obligatory subject

1. Academic writing (Prof. Matija Strlič)

Elective subjects

1. Selected topics in inorganic chemistry (Prof. Iztok Turel)
2. Advanced methods in inorganic synthesis (Assist. Prof. Barbara Modec)
3. Modern diffraction techniques (Prof. Anton Meden)
4. Frontiers in analytical chemistry (Prof. Helena Prosen)
5. Approaches in modern analytical chemistry (Prof. Matevž Pompe)
6. Selected topics in experimental physical chemistry (Prof. Marija Bešter Rogač)
7. Theoretical methods in physical chemistry (Prof. Barbara Hribar Lee)
8. Selected topics in organic chemistry (Prof. Janez Košmrlj)
9. Selected topics in heterocyclic chemistry (Prof. Jurij Svete)
10. Study on mechanisms of organic transformations (Assoc. Prof. Janez Cerkovnik)
11. Modern NMR approaches in characterization of compounds (Prof. Janez Plavec)
12. Selected topics in biochemistry (Prof. Brigita Lenarčič)
13. Modern methods and techniques in biochemistry (Assoc. Prof. Marko Dolinar)
14. Contemporary computational methods in biochemistry (Assoc. Prof. Marko Novinec)
15. Biopharmaceuticals (Assist. Prof. Gregor Gunčar)
16. Selected topics in materials for new energy sources (Assist. Prof. Boštjan Genorio)
17. Selected topics in polymer engineering (Prof. Urška Šebenik)
18. Selected topics in separation processes (Assoc. Prof. Aleš Podgornik)
19. Selected topics in rheology and structure of compex fluids (Prof. Igor Plazl)
20. Selected topics in chemical reaction engineering (Prof. Matjaž Krajnc)
21. Selected topics in environmental engineering (Assoc. Prof. Andreja Žgajnar Gotvajn)
22. Selected topics in transport phenomena (Prof. Igor Plazl)
23. Selected topics in bioprocess engineering (Prof. Polona Žnidaršič Plazl)
24. Selected topics in materials engineering (Assoc. Prof. Marjan Marinšek)

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 subjects

Obligatory subject

ACADEMIC WRITING
Objectives of the course
The course represents an introduction to scientific writing related to the student's field of study and research. Student gets familiar with different kinds of scientific communications and develops skills needed for successful articulation of ideas and their dissemination.
Contents
Characteristics of effective academic writing (accuracy, clarity, conciseness, coherence, appropriateness). Stating the document purpose. Defining the problem of our written account. Adjusting the style to different audience types. Organization of the document. Document types (research reports, scientific papers, review papers, project proposals, oral presentations, thesis, CV, ...). How to write a scientific project. Oral presentations. Elements of technical documents.

Elective subjects

SELECTED TOPICS IN INORGANIC CHEMISTRY
Objectives of the course
Student acquires knowledge on selected chapters in inorganic chemistry, knows how to 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
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 (wood preservation; enzyme models, etc.), photosensitive ruthenium compounds used in Graetzel cells, fluorescence metal compounds and their application in analytics, gold compounds and nanotechnology, electrode materials.
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:
- coordination of metal ions on bulk polymers
- 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
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
Student selects (in agreement with the supervisor) those topics 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. 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
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
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.
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

Students extend their knowledge of novel instrumental 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

From the topics listed below the student selects (in agreement with the supervisor) those that are most related to their research work. The course coordinator, and the leader of the study programme provide the student's workload corresponding to 5 credits. If several lecturers cooperate on the course, the whole process is coordinated by course coordinator.

- Methodology and application of novel spectroscopic methods in analytical chemistry. Sample introduction problems in atomic spectrometry related to 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.
- Mass spectrometry in analytical chemistry: instrumentation, ionization techniques, mass spectra interpretation. Novel mass spectrometric techniques (MALDI, proton transfer mass spectrometry, desorption electrospray ionization - DESI).
- Hyphenated techniques GC-MS, HPLC-MS, HPLC-ICP-MS
- Electroanalytical 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

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

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.

- Sophisticated chemometric 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 inenvironment.
- 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

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

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 the 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 behavior 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

The purpose of statistical thermodynamics is to predict macroscopic properties of thermodynamic systems, using as input the knowledge about constituent atoms (or molecules) and forces between them. This knowledge makes it possible to interpret experiments on the molecular level.

Contents

From the topics listed below, the student selects (in agreement with his supervisor) those being of most relevance for his PhD Thesis. The number of chosen hours of study must carry 5 credits. The Lecturer coordinates the process, if more than one teacher is involved.

- *Potential theories*. Basic facts. Poisson−Boltzmann equation, modified Poisson−Boltzmann equation. Boundary conditions and solution of linearized and non-linearized equation in different symmetries.
- *Thermodynamic perturbation theory*.

Basics, Gibbs−Bogoliubov inequality. Barker−Henderson theory. Weeks–Chandler–Andersen theory. Wertheim's thermodynamic perturbation theory.

- *Distribution functions*. Ornstein−Zernike integral equation in different closures. Multipole expansion for molecular systems. Wertheim's integral equations for systems with highly directional forces.
- *Simulation methods*. Monte Carlo method in generalized ensemble. Use 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, multi-configuration interaction, coupled cluster method. Density functional theory (DFT): Kohn-Sham equations, Hohenberg-Kohn theorems, local approximations, non-local approximations. Methods of quantum dynamics and mechanics.
- *Chemical kinetics*. Rate of chemical reaction in solutions and effects of ionic reactants on the reaction rate. Catalysis.

SELECTED TOPICS IN ORGANIC CHEMISTRY

Objectives of the course

Advancing knowledge on selected topics and methods of organic chemistry, as a basis for practical problem solving in organic chemistry.

Contents

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. Mitsunobu reactions. Biochemical properties of diazenes. 'Click' chemistry: 1,2,3-triazole, triazolium salts, triazolylidenes, ligands and catalysis. (Prof. Janez Košmrlj)
- *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 vapors in solid state halogenations, diffusion membranes, micro reactors, continuous processes. New halogenation reagents, enantioselective halogenations, synthesis of halosubstituted chiral synthons. (Prof. Marjan Jereb).
- *Selected topics in selective synthesis*. The application of transition-metal catalysis in organic synthesis. The design of transition-metal catalysts. Catalysed cascade reactions. Selective formation of single end double C-C bonds via transition-metal catalysts. Coupling reactions: Suzuki, Heck, Negishi, Still, Sonogashira. Activation of inert C-H bonds. Selective functionalisation of C-H bonds driven by directing groups. The aplication of Ru-catalysts in selective formation of C(sp2)-C(sp2) and C(sp2)-C(sp3) bonds. The application of transition-metal alkylidene(carbene) complexes for C=C bond formation. Cross and ring-closing metathesis of alkene and alkyne substrates. The Formation of C-H bonds; asymmetric reduction of ketones. The synthesis and selectivity of 1,3-diketo-BF2 complexes. (Prof. Franc Požgan, Prof. Bogdan Štefane).

SELECTED TOPICS IN HETEROCYCLIC CHEMISTRY

Objectives of the course

Advancement of knowledge on selected topics and methods in organic and heterocyclic chemistry, which is basic for student ability to solve practical problems in the field of organic chemistry.

Contents

From the topics listed below the student selects (in agreement with the supervisor) those that are most relevant to his research work. The course- and the study-leader take care that the student's

workload corresponds to 5 credits. In case of multiple teachers, the performance is coordinated by the course leader.

- *Synthesis and application of heterocycles in stereoselective organocatalysis*. 5- and 6-membered heterocycles and their fused analogues as an important group of catalysts in stereoselective organocatalysis. Synthesis of N-heterocyclic carbenes (NHC's), proline derivatives, and imidazolidinones and their applications in stereoselective transformations combined with respective catalytic cycles/activation modes of substrates will be presented. (U. Grošelj)
- *Diels–Alder reaction as the fundamental method for the construction of new C–C bond in heterocyclic chemistry*. Use of alkenes (maleimides, maleic anhydride etc.) and alkynes as dienophiles as well as various heterocyclic systems (furans, thiophenes, 2H-pyran-2-ones, 2-pyridones, coumarins etc.) as dienes in Diels–Alder reactions. Synthesis of heterocyclic systems with the use of cycloadditions: (benzo)isoindoles, indoles, oxabicyclo[2.2.2]octenes, dianhydrides of bicyclo[2.2.2]oct-7-ene tetracarboxylic acids etc. and the issues of regio- and stereoselectivity of these transformations. Preparation of important compounds: derivatives of Taxol, Boscalid, Thalidomide etc. Improvement of such syntheses by the application of modern approaches: use of microwaves, high pressure (up to 18 kbar), water and other non-toxic solvents etc. (K. Kranjc)
- *Modern approaches in the synthesis of heterocyclic compounds.* Heterocyclizations, ring transformations, molecular rearrangements, regio- in stereoselective cyclizations, synthesis of saturated systems. Modular approach to the ring synthesis. Building blocks, modular approach to the ring synthesis, chemo- regio- and stereo-control. Synthesis of functionalized heterocycles. Combinatorial synthesis of heterocycles. Synthesis and transformations of alkyl 3-(dimethylamino)propenoates and related enaminones; from heterocycles to natural products. Reactions with nucleophiles and electrophiles, cycloadditions. Applications in the synthesis of heterocyclic systems, functionalized heterocycles, and natural products and their analogues. (J. Svete)

STUDY ON MECHANISMS OF ORGANIC TRANSFORMATIONS

Objectives of the course

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

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. Kinetc methods: kinetic principles of reactions in a solution, transition state, activation parameters and their interprettion, 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 (1O2) and triplet (3O2) 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. These informations can be obtained from kinetcs of photophysical and photochemical processes and can be applied in designing of molecular structures leading to the 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, 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 (lasers 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. The chemistry of stananes and related hydrides, redox processes, etc. Catalysis with “Umpolung”. Chemistry of the atmosphere.

MODERN NMR APPROACHES IN CHARACTERIZATION OF COMPOUNDS
Objectives of the course
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
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 BIOCHEMISTRY
Objectives of the course
Graduate students will gain an overview of scientific literature, they will be able to critically assess information and use it to plan and evaluate their own work.
They will be able to write an adequate grant proposal according to the funder’s instructions. They will be able to describe the background of research, formulate the concise set of hypotheses or specific aims, include the most advanced techniques and methods and combine all items into a coherent proposal.
Contents
Introduction to subject areas (lectures). The rest of the course will focus on structuring a research proposal addressing topics relevant to the student’s research in the field of biochemistry. Querying for appropriate funding calls.

MODERN METHODS AND TECHNIQUES IN BIOCHEMISTRY
Objectives of the course
Keeping up-to-date with new methods and techniques in the field of biochemistry and molecular biology. Critically assessing the advantages and shortcomings of the improvements and applicability of new methods.
Contents
- Introductions to subject areas (lectures).
- Technology developments in biochemistry (seminars).
- Suggestion for an introduction of a new method or for improving one of the methods used by the student in his/her research (individual assignment and seminar).

CONTEMPORARY COMPUTATIONAL METHODS IN BIOCHEMISTRY

Objectives of the course

Students will become familiar with contemporary compoutational methods for the analysis of biochemical data and will learn to use them in their own research work.

Contents

The course discusses contemporary methods and approaches used for computational analysis of proteins, nucleic acids, molecular evolution and biomolecular interactions. It focuses on bioinformatics methods for database analyses as well as computational methods for the analysis of experimental data. The major focus is on novel and advanced methods developed in the past several years and methods that are still under intensive development and are therefore not included in standard textbooks or undergraduate courses. Students will the theoretical background of these methods and learn to use them through individual project work.

BIOPHARMACEUTICALS

Objectives of the course

Overview of the field of biopharmaceuticals, their identification, development, production, optimization, mode of action and their use.

Contents

Introduction to biopharmaceuticals
Development of biopharmaceuticals
Therapeutic target protein and gene identification and bioinformatic methods for their analysis. Role of genomics, proteomics and metabolomics.
Biotechnology methods for large scale recombinant protein production
Therapeutic and clinical applications of biopharmaceuticals
Antibodies, growth and coagulation factors, cytokines, interferons, hormones, enzymes, DNA, RNA, vaccines and other biopharmaceuticals
3D structures of biopharmaceuticals
Biosimilars
Advance drug delivery
Gene and cell therapy
Clinical evaluation and regulation
Future of biopharmaceuticals
Project seminar: My Ph. D. research in context of biopharmaceuticals.

SELECTED TOPICS IN MATERIALS FOR NEW ENERGY SOURCES

Objectives of the course

Acquiring specialized knowledge in specific fields of materials for new energy sources. Studying scientific and professional literature in a specific field, critical evaluation of literature. These competences enable students to conduct research in a particular research field, to suggest research methods and to state its goals.

Contents

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.

<u>Materials for new energy converters</u>

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 its purity, temperature of operation 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 fuel cells, 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 the chemical energy into electrical energy).

Li 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).
- Chaeracteristics of advanced accumulators (lithium insertion batteries, Li air battery, polymer accumulators, lithium-sulphur accumulator).

Supercapacitors:
- Principle of operation of supercapacitor (solid-liquid interface, electrical double layer, thermodynamics and kinetics of 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 nonaqueous electrolytes).
- Characterization, properties and application of selected supercapacitors

Materials for environment protection (materials for lowering of emissions into environment, removal of VOC – volatile organic compounds), development of catalytic materials and systems, lifetime cycles and impact of different groups of materials on the environment).

A seminar from a selected topic of materials for new energy sources, which is based on scientific and professional literature review.

Elaboration of a project proposal for engineering of a specific material for new energy sources

SELECTED TOPICS IN POLYMER ENGINEERING

Objectives of the course

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

- a review of polymer engineering topics with emphasis on polymer reaction engineering and phenomenological treatment of viscoelasticity of polymer materials will be given by lectures;
- a seminar from a selected topic from polymer engineering, which is based on scientific and professional literature review;
- elaboration of a project proposal for a specific process design;

SELECTED TOPICS IN SEPARATION PROCESSES

Objectives of the course

Post-graduate students will upgrade their fundamental engineering knowledge of mass transfer, thermodynamics, mass-heat balances and separation unit operation, and implement it for analyses and design of complex separation processes involving several steps. Focus will be on pharmaceutical and biotechnological processes by discussing peculiarities of these systems and their transfer from laboratory to industrial scale and from batch to continuous operation mode.

Contents

- Separation unit operations in chemical, pharmaceutical and biotechnological processes;
- Mass and heat balances of metabolic processes;

- Thermodynamics of non-ideal liquid-liquid and liquid-solid systems;
- The role of research on laboratory and pilot scale unit - scale up criteria;
- Selected separation processes of pharmaceutical and biotechnological products:
  - crystallization and precipitation
  - ATPS extraction
  - gradient chromatography
  - preparative chromatography
  - continuous separation processes – simulated moving bed (SMB)
  - membrane processes
- Optimization of separation processes involving several steps;

SELECTED TOPICS IN RHEOLOGY AND STRUCTURE OF COMPEX FLUIDS

Objectives of the course

Objective of the course is to upgrade the existing knowledge in the field of complex fluid flows, microfluidics of multiphase flows, multiscale modeling concept, and to deepen understanding of experimental approaches to rheological characterization of structured fluids. Acquired knowledge enables the student independent research work in the field of complex fluid systems and rheological properties of complex fluids and semi-solids.

Students acquire the specific competences for ability to understand the basic principles, and to design and optimize the complex flow systems.

Contents

- The complex fluid systems: non-Newtonian, multiphase, turbulent, and/or chemically reacting flows at different length and time scales.
- Microfluidics: the advantages of using microsystems. The problems of modeling microsystems with two-phase flow: determination of viscous shear stress, slip at the wall, surface tension.
- Development and implementation of multiscale computation techniques. Single Droplet/Bubble Dynamics, Multiscale Transfer Phenomena.
- Non-conventional solvents: Ionic liquids (ILs), aqueous two-phase system (ATPS), eutectic mixtures.
- Experimental approaches to rheometry: the principles of measurement, measuring techniques and procedures for rheological characterization of complex liquids and semi-solid materials.

SELECTED TOPICS IN CHEMICAL REACTION ENGINEERING

Objectives of the course

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

Catalysis. Solid catalysts. 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 ENVIRONMENTAL ENGINEERING
Objectives of the course
Upgrading knowledge in environmental engineering, acquisition of skills for critical evaluation, selection and optimisation of processes and technologies. Assessing accomplished work in terms of the impacts on local and global environment; to solve actual environmental problems within economical, social and legislative limits.
Contents
From the topics listed below the student selects (in agreement with the supervisor) those that are mostly related to his research work.
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. Up-to-date trends in pollution prevention, solid waste management, Life Cycle Analyses (LCA), principles and methods of industrial ecology. Chemical, membrane and biochemical processes for protection, bioremediation and remediation of the environment (water, air, soil):
- Chemical Processes: Treatment of wastewaters and drinking waters using chemical methods. Electrocoagulation. Advanced oxidation processes (AOPs). Photo-catalytic oxidation. Fenton's oxidation. Ozonation. Electrochemical oxidation. Wet air oxidation. Supercritical water oxidation. Accoustic and hydrodynamic cavitation. Heterogenic catalysts for environmental protection. Catalytic wet oxidation. Kinetics and mechanisms of reactions. Processes and reactor systems. Application of AOPs for removal of micro-pollutants from aquatic (drinking and wastewaters) and atmospheric environments.
- Membrane Processes.
- Biochemical Processes: Up-to-date techniques for biological treatment of wastewaters, bioremediation.
Integrated process schemes: Connection of AOPs and biological processes.
Slovenian and international environmental legislation.

SELECTED TOPICS IN TRANSPORT PHENOMENA
Objectives of the course
Upgrading knowledge of fluid dynamics, heat and mass transfer.
Contents
- Complex fluids – origins of Non-Newtonian behavior;
- constitutive equations for Non-Newtonian fluids;
- boundary conditions at solid walls and fluid interfaces (the kinematic condition, thermal boundary conditions, the 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, the 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 Reyleigh-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 at large Reynolds number.

SELECTED TOPICS IN BIOPROCESS ENGINEERING

Objectives of the course

Deepening knowledge for an independent design and optimization of bioprocesses and technologies. Competences: comprehension of selected biotechnological processes and their engineering analysis, understanding of the significance of continuous process operation and implementation of micro-scale devices in biotechnology.

Contents

Selected topics in bioprocessing:
- specifics of submerged bioprocesses with filamentous microorganisms
- biotechnological production of enzymes and their applications
- continuous bioprocess operation.

Selected topics in biocatalytic processing:
- kinetic description of biocatalytic processes
- biotransformations in non-conventional media
- novel techniques for biocatalyst immobilization.

Miniaturization in biotechnology:
- microbioreactors
- enzymatic microreactors
- application of microstructured systems in downstream processing
- mathematical description of selected biocatalytic process/separation in a microfluidic device.

Integration of bioprocesses with separation processes.

SELECTED TOPICS IN MATERIALS ENGINEERING

Objectives of the course

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

At the beginning of school year 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, bioceramics and nanomaterials will be worked out as seminars.

- *Principles of materials design*:

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

- *Principles of materials selection for engineering design*:

When the material is designed for a specific application, a number of factors must be taken into account. Specific properties of materials with high relevance to the design of components and structures will be studied. Materials must be designed with recquired physical or mechanical properties, their fabrication should be 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, 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.