SPECIALISATION – MATERIALS CHEMISTRY (since academic year 2008/2009)

L – lectures; T – tutorial; S – seminar ; Lab – laboratories

C – credits are awarded based on continuous assessment ;

CE - credits are awarded based on continuous assessment and final exam

Course code	Course title	Teaching hours L	T	S	Lab	Total	Exam	ECTS
	SEMESTER I							
UMA-1	Physicochemistry of interfaces	30			30	60	CE	***5***
UMA-2	Theoretical chemistry	15	15			30	C	***2***
UMA-3	Crystallography	15			30	45	CE	***5***
UMA-4	Solid state chemistry	15	15			30	CE	***3***
UMA-5	Technology and properties of new polymers	30			30	60	C	***4***
UMA-6	Optical fibres technology	30		15	30	75	C	***5***
PFA	Elective courses					90	C	***6***
	Total	135	30	15	120	390	**3**	***30***

Course code	Course title	Teaching hours L	T	S	Lab	Total	Exam	ECTS
	SEMESTER II							
UMA-7	Theoretical chemistry	30			30	60	CE	***7***
UMA-8	Instrumental analysis	30			45	75	CE	***7***
UMA-9	Spectroscopy	15			30	45	C	***4***
PFA	Elective courses					90	CE	***6***
UMA-10	Specialization course	30		30	90	150	CE	***6***
	Total	105		30	195	420	**4**	***30***

Course code	Course title	Teaching hours					Exam	ECTS
		L	T	S	Lab	Total		
	SEMESTER III							
UMA-11	Monographic lecture	30				30	CE	**8**
UMA-12	Diploma seminar			30		30	C	***3***
UMA-13	Diploma project*				225	225	C	***16***
PFA	Elective courses					45	CE	***3***
	Total	30		30	225	330	**2**	***30***

*- 15 h/student

Course code	Course title	Teaching hours					Exam	ECTS
		L	T	S	Lab	Total		
	SEMESTER IV							
UMA-12	Diploma seminar			30		30	C	***5***
UMA-13	Diploma project*				225	225	C	***25***
	Total			30	225	255		***30***

*- 15 h/student

Elective courses

Course code	Course title	Teaching hours L	T	S	Lab	Total	Exam	ECTS
	SEMESTER I-II							
PFA-1	Trace analysis; activation analysis and radiochemical methods; chromatographic methods in trace analysis	30			30	60	C/ CE	***4***
PFA-2	Modern diffraction methods in crystalline state investigations	30			30	60	CE	***4***
PFA-3	Adsorbents and catalysts	30			30	60	CE	***4***
	SEMESTER I-III							
PFA-4	Physical adsorption on solid surfaces – theoretical bases and applications	15				15	C/CE	***1***
PFA-5	An outline of green chemistry	15				15	C/CE	***1***
PFA-6	Introduction to heterogeneous catalysis		30			30	C/CE	***2***
	Total	120	30		90	240		

Chemistry – description of courses

Course title: **Physicochemistry of interfaces**

Course code: **UMA-1**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I**

Number of credits: **5**

Name of lecturer: **prof. Emilian Chibowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The introduction with basic contents concerning delivered during the course.

Prerequisites: received credits for laboratory and seminar on physical chemistry, passed exam on physical chemistry.

Course contents: *Introduction:* characteristic of interfacial phenomena, capillarity, surface and interface free energy, surface enthalpy and entropy. *Surface of liquids:* surface tension, Young-Laplace's equation, Kelvin's equation, methods of surface tension determination, components of surface tension, temperature dependence of surface tension, the liquid density and surface tension, parachor, surface tension of solutions, Szyszkowski equation, Traube's rule. *Surface of solids*: surface free energy and its components, methods for the energy determination, contact angle and Young's equation, wetting of the solid surface by a liquid - spreading, immersional and adhesional, interfacial solid/liquid free energy, Lifshitz-van der Waals and Lewis acid-base interactions. *Films on liquid surface*: methods of investigation, film pressure, classification - gaseous, liquid and solid films, structure of the films, duplex films, black films, Langmuir-Bludgett's films, bilayers and vesicles. *Adsorption from solution on liquid surface:* Gibbs adsorption and surface excess, Guggenheim-Adam's reduced surface excess, various definitions of surface excess and interrelationship, Gibbs adsorption equation and Gibbs adsorption isotherm, the adsorbed films and their structure, Gibbs monolayers, two-dimensional film and its gas law. *Adsorption at solid/gas interface:* description of the phenomenon, physical and chemical adsorption, Henry's equation, Freundlich's isotherm, theory and adsorption isotherm of Langmuir, potential field theory of Polanyi, Dubinin-Raduschkievich equation, BET theory and adsorption isotherm, types of the adsorption isotherms, capillary condensation, preparation and structure of adsorbents, classification of adsorbents. *Adsorption at solid/liquid interface:* Description of the process, adsorption isotherm equation, surface excess and apparent adsorption, the isotherm types, ion exchange process, ion exchangers and their types. *Colloidal systems:* characteristic of colloidal systems and their occurring, methods of preparation, properties of colloidal systems, electric charge of colloids, stability of the systems, DLVO theory of stability.

Recommended reading:

1. A.W. Adamson, *Physical Chemistry of Surfaces*, 5th edition, Interscience Publ., New York, 1990.

2. J. Ościk, *Adsorption*, *PWN*, Warszawa, 1982.

3. P.W. Atkins, *Physical chemistry, 4th Ed.*, Oxford University Press, 1992.

4. C.J. van Oss, *Acid-base interfacial interactions in aqueous media,* Colloids and Surfaces A: **78** (1993) 1-49.

5. (Th.F. Tadros Ed.) *Colloid Stability. The role of surface forces – Part II*, V.2., Wiley, 2007.

Teaching methods: **lectures (30 h), laboratories (30 h)**

Assessment methods: **written final exam, partial tests during laboratories classes, credit for the lab exercises.**

Language of instruction: **English**

Course title: **Theoretical Chemistry**

Course code: **UMA-2 and 7**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I and II**

Number of credits: **9**

Name of lecturer: **prof. Władysław Rudziński and prof. Krzysztof Woliński**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to teach the current methods of computational chemistry and their applications to important chemistry problems. This includes most popular quantum chemistry and statistical thermodynamics methods.

Prerequisites: Fundamentals of linear algebra, mathematical statistics and basic calculus as well as the elementary knowledge of quantum chemistry.

Course contents: One Electron Approximation and the Hartree-Fock method, Electron Correlation, Post Hartree-Fock Methods (Moller-Plasset MP2, Configuration Interaction CI, density functional theory DFT) Geometry Optimization, Simulation of the IR and NMR spectrum.

Statistical-mechanical Ensembles and Thermodynamics (ensembles and postulates, canonical ensemble, canonical ensemble and thermodynamics, grand canonical ensemble), Systems Composed of Independent Molecules, Ideal Monatomic Gas, Monatomic Crystals, Classical Statistical Mechanics.

Recommended reading:

1. A. Szabo, N. S. Ostlund, *Modern quantum chemistry, introduction to advanced electronic structure theory,*

McGraw-Hill, 1989.

2. D.B. Cook , *Handbook of computational chemistry*, Oxford University Press, Oxford, 1998.

3. T.L. Hill, *An introduction to statistical thermodynamics*, Courier Dover Publications, 1986.

Teaching methods: **lectures (45 h), tutorials (15), laboratories (30 h)**

Assessment methods: **exam**

Language of instruction: **English**

Course title: **Crystallography**

Course code: **UMA-3**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I**

Number of credits: **5**

Name of lecturer: **prof. Stanisław Pikus**

Objectives of the course (preferably expressed in terms of learning outcomes and competences: description of the molecular and crystal solid phase symmetry as a introduction for crystallochemistry and spectroscopy.

Prerequisites: Knowledge of fundamental concepts of geometry and mathematics.

Course contents: (lecture) Concepts of crystallinity, definition of ideal crystal, stereography projection, symmetry operations, symmetry elements, point groups, crystal systems, molecular symmetry, morphology of crystals, Miller indices. Crystal lattice, unit cell, symmetry elements of lattices, Bravais lattices, space groups, coordination number, coordination polyhedra. Crystal Chemistry: chemical bond; atomic, ionic, covalent and non-covalent interactions. Close packed structures; structural holes, structure of metals, ionic crystals, covalent crystals, molecular crystals, structure of chosen crystal compounds used as cosmetics.

Isotypes, Isomorphism, Polymorphism. X-ray diffraction, Bragg's and Laue Laws. Intensity of diffracted beams. Diffraction methods: The Laue method, Rotation method, DSH method.

(laboratory work) Description of the symmetry of molecules and crystal forms (symmetry elements, point groups, crystal systems, steroegraphic projection of crystal forms symmetry). Lattice symmetry, symmetry elements of lattices. Crystal Chemistry: description of the crystal structure, interpretation of the structural data. Powder X-ray diffraction, DSH method, identification of crystalline phase. Determination of unit cell for cubic crystalline phase.

Recommended reading:

1. C. Giacovazzo *et al.*, *Fundamentals of crystallography*, Oxford University Press, 1992.

2. W. Borchardt-Ott, *Crystallography*, Springer-Verlag, 1995.

3. M.J. Buerger, *Elementary crystallography: an introduction to the fundamental geometrical features of crystals*,

Chapman & Hall,1956.

Teaching method: **lecture (15h), laboratories (30h)**

Assessment methods: **exam**

Language of instruction: **English**

Course title: **Solid-state chemistry**

Course code: **UMA-4**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I**

Number of credits: **3**

Name of lecturer: **prof. Anna Deryło-Marczewska**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

acquaintance of students with the basics of solid-state chemistry useful in various applications in science and technology.

Prerequisites: advanced level of general chemistry and physical chemistry.

Course contents: Chemical bonds in solids. Structure of solids: basics of electron structure of solid state, crystals, amorphous solids – glasses, polymers. Defects of solid structure: point, line, planar and bulk defects, effect of dopants on physicochemical properties of solids, equilibrium states of defects. Surfaces of solids: structure and properties of surface layers, surface energy, phenomena occurring at solid/solid interface. Phase equilibria and transitions of solids: phase rule, phase diagrams, phase transitions, thermodynamics of mixing, deviations from equilibrium, processes of nucleation and crystallization. Reactions in solid phase: reaction types, processes of diffusion and their mechanisms, mechanism and kinetics of oxidation, processes of sintering, decomposition of solids, mechanism and kinetics of reactions between solids.

(*laboratory*) Synthesis of mesoporous silica materials. Estimation of total heterogeneity of solid surfaces. Photovoltaic cells – preparation and investigation of properties. Studies of the surface properties of mesoporous solids by means of different thermogravimetric and microgravimetric methods.

Recommended reading:

1. J. Dereń, J. Haber, R. Pampuch, Chemia ciała stałego, PWN, Warszawa, 1997.

2. J. Łaskawiec, Fizykochemia powierzchni ciała stałego, Wydawnictwo Politechniki Śląskiej, Gliwice, 2000.

3. N.B. Hannay, Chemia ciała stałego, PWN, Warszawa, 1972.

4. H. Schmalzried, Reakcje w stanie stałym, PWN, Warszawa, 1978.

5. Praca zbiorowa, Fizyka i chemia ciała stałego, Ossolineum, Wrocław, 1987.

Teaching methods: **lectures (15 h), laboratories (15 h)**

Assessment methods: **exam**

Language of instruction: **English**

Course title: **Technology and Properties of New Polymers**

Course code: **UMA-5**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I**

Number of credits: **4**

Name of lecturer: **prof. Barbara Gawdzik / dr Małgorzata Maciejewska**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to present information about world tendencies in polymer chemistry. Attention will be specially focused on technologies and applications of new polymers.

Prerequisites: Knowledge from organic and macromolecular chemistry.

Course contents: Polymers of high thermal resistance: polyimides, poly(bismaleimides), poly(amidoimides), poly(etherimides), aromatic poly(sulfones) and poly(sulfides), aromatic heterocyclic polymers: poly(benzimidazoles), poly(benzoxazoles), poly(hydantoines), poly(quinoxalines). Polymers of high chemical stabilities: epoxy resins, epoxyacrylic and epoxymethacrylic resins. Fire resistant polymers: polymers containing halogen or nitrogen atoms, role of antypirenes. Liquid crystal-polymers: thermotropic liquid crystal-polymers, liotropic polymers. Biodegradable polymers: aliphatic poly(esters), poly(hydroxyacids), poly(hydroxyesters), poly(lactides) and poly(lactones). Polymers applications in medicine and pharmacy.

Recommended reading:

1. J. Brandrup, E.H. Immergut, E.A. Grulke, *Polymer handbook,* Hoboken 1999.

2. T. Borsali, *Advanced polymeric materials*, Viley-VCH, London 2007.

Teaching methods: **lectures (30 h), laboratories (30 h)**

Assessment methods: **credit** (**final colloquium)**

Language of instruction: **English**

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*Course title***: Optical Fibres Technology**

Course code: **UMA-6**

Type of course: **obligatory**

Level of course: **advanced**

Year of study: **1st year of 2nd stage**

*Semester***: I**

Number of credits: **5**

Name of lecturer: **dr Jan Wójcik**

Objective of the courses (preferably expressed in terms of learning outcomes and competences):

The main goal is to teach the fabrication methods of optical fibres. Also, the basic properties of the different kinds of optical fibres will be done.

Prerequisities: Fundamentals of optics, theory of solids state including glasses.

Course contents: The technical, social and economical reasons of introduction of optical fibres technology. The basics of optical fibres operation, constructional materials, classification of optical fibres according to materials, length of transmission. Definitions of the basic parameters: attenuation, dispersion, numerical aperture, mechanical strength, optical and structural parameters. Spectral attenuation, components of spectral attenuation, attenuation caused by different materials. Theoretical limit of attenuation. Optical purity of materials. Cleanness of laboratory.

Rods and crucible methods of optical fibres fabrication. Construction and operation of fibre drawing tower. MCVD, OVD VAD PCVD and PMCVD methods of preform fabrication from fused silica glasses. Raw materials purification. Kinds of optical fibres, technology and properties of quartz optical fibres: fibres for telecommunication (GI., SM), special (SMPM, SH), thick-core fibres, . Hydrogen effect, resistance to radiation. Optical fibres for optical amplifiers and sensors. Optical fibres made with multicomponent glasses, polymers and non-oxide glasses – fabrication methods, properties applications, technical and economical importance.

Technology and kinds of optical cables. Mechanical strength and life-time of optical fibres.

Seminar: Optical cables. Glass technology. Glass fibres technology. Optical glasses. Technical and laboratory glasses. Fused silica glasses. Planar and strip waveguides. Elements of optical fibres technique. Optical amplifier.

Laboratory: PCS optical fibres, fibre drawing, fibre structure, spectral attenuation, numerical aperture, far-field mode distribution. Multimode fibres, MCVD method, spectral attenuation, determination of attenuation components, bending attenuation. Singlemode fibres, their technology, characteristics, cut-off wavelength, mode-field diameter, spectral attenuation, attenuation as a fiber length function, reflectometry, connectors attenuation, fibres splicing. Optical fibre cables, cables structure, measurements of cables parameters, causes of attenuation increase, battery effect. Mechanical strength of fibres, test machine, histograms, Weibull distribution, proof-test, fibres life-time.

Recommended reading: The literature will be given at the first lecture.

Teaching methods: **Lectures (30h), seminar (15h), laboratory (30h)**

Assessment method: **credit**

Language of instruction: **English**

Course title: **Instrumental analysis**

Course code: **UMA-8**

Type of course: **obligatory**

Level of course: **basic**

Year of study: **1st year of the 2nd stage**

Semester: **II**

Number of credits: **7**

Name of lecturer: **prof. Andrzej L. Dawidowicz, assist. prof. Małgorzata Grabarczyk**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The aim of the subject is to acquaint the students with most important instrumental analytical methods with regard to the spectroscopic and electrochemical ones. By the end of course student should known the fundaments of chromatographic process and should be able to: optimize the chromatographic separation of complex mixtures, chose the most proper chromatographic equipment for chromatographic analysis, understand the problems of chromatographic separation.

Prerequisites: Basic knowledge concerning physical and analytical chemistry.

Course contents: The characterization of chromatographic process; types of chromatography; fundamental chromatographic definitions and chromatographic nomenclature. Resolution and efficiency of chromatographic separation; kinetic theory of concentration zone spreading; the influence of selectivity and efficiency on resolution of chromatographic system. Stationary phases for GC and LC; Columns for GC and LC; Mobile phases for GC and LC. Equipment for GC and HPLC. Qualitative and quantitative analysis by chromatography. Optimization of chromatographic process. Chromatographic separation of non-ionic samples in normal phase and reversed phase systems. Separation of ionic samples in RP systems; Ion pair chromatography. Ion exchange chromatography. Chromatographic separation of macromolecules.

Methods of environmental samples acquiring and problems relative to their proper preparation for the determination with instrumental methods, selection of the proper mineralization method. Division of the instrumental methods into spectroscopic and electrochemical ones with discussion of the basic chemical principles that they are based on.

<u>*Absorptive spectroscopic methods*</u>. *UV VIS spectrophotometry*. Principles of absorption: Beer`s law, additivity law. Blank solution - its selection and purpose. Quantitative analysis methods in spectrophotometry – standard curve method, spectrophotometric titration method. Error in determination. The range of the determined substances. Advantages of the UV VIS spectrophotometry. *Atomic absorptive spectrometry (AAS).* Principle of the measurement. Qualitative and quantitative range. Diagram of the AAS spectrophotometer. Sources of radiation (cavity cathode lamps, electrodeless lamps). Atomizers. Physical, chemical and spectral interferences and methods of their elimination. Sample preparation for the flame and flameless AAS analysis.

<u>*Emission spectroscopic methods*</u>. *Flame photometry*. Explaining of the terms: resonance potential and ionization potential. Connection of the radiation intensity and the analyzed substance concentration. Diagram of the apparatus. Interferences in the flame photometry methods. Range of the determined

elements. *Spectrography.* Analytical range. Advantages and disadvantages of spectrography. *Atomic emission spectrometry (AES) with special regard to inductively coupled plasma method (ICP-AES).* Qualitative and quantitative range. Diagrams of the apparatus. Interferences in the ICP method (physical, chemical and spectral) and methods of their elimination. Costs of hardware and working costs.

Fluorescence spectroscopic methods. *Atomic fluorescence method.* Principle of measurement.

X-ray fluorescence method. Diagram of apparatus. Qualitative and quantitative range. Types of the analyzed samples. Preparation of sample for the analysis. *Spectrofluorometry.* Diagram of apparatus. Comparison of the analytical range of spectrofluorometry and spectrophotometry. Relations between excitating radiation and the fluorescent one.

Electrochemical methods. Electrolysis. Principles of electrolysis The aim of using electrolysis at the controlled potential. The application of electrolysis. *Coulometry.* Potentiostatic coulometry – the principle of measurement. Amperostatic coulomatric titration – the principle of measurement. Advantages of the amperostatic coulomatric titration. Examples of the generation of reagent and its application in the quantitative determinations. *Potentiometry.* Nernst and Nikolski`s equation. Division and characteristics of electrodes with special regard to ion-selective electrodes. Methods of determination – calibration curve and standard additions methods. *Polarography and voltammetry.* Polarographic currents (diffusive, kinetic, catalytic, capacitance, residual). Characteristics and comparison of the alternating current, differential pulse and square wave polarography. Methods of elimination of the capacitance current. Ilkovic`s equation. Advantages and disadvantages of the mercury drop electrode. The role and selection of the supporting electrolyte. The influence of oxygen and methods of its removing. Practical application in qualitative and quantitative analysis.

Voltammetry and voltammetry with preconcentration. Stages of the voltammetric process with preconcentration – exemplary electrode reactions in the course of the individual measurement step. Types of the electrodes in use. Interferences in the voltammetry with preconcentration method and exemplary means of their elimination.

Laboratory: Practical estimation of chromatographic values from exemplary chromatograms. Optimization of column parameters in GC. HPLC and its application for quantitative analysis. Thin layer chromatography. Mass spectrometry detection in gas chromatography. The influence of mobile phase composition on chromatographic separation in HPLC. Gradient elution in chromatography. Optimization of UV-Vis detection.

Recommended reading:

1. Lecture notes.

2. C.F. Poole, The essence of chromatography, 1st Ed., Elsevier Science, 2002.

3. N.A. Parris, Instrumental liquid chromatography, Journal of chromatographic library, Vol. 27, Elsevier, Amsterdam,

1984.

4. D.A. Skoog, D.M. West, F. Holler, Fundamentals of analytical chemistry, Sounders College Publishing, New York,

1988.

Teaching methods: **Lectures (30h), laboratories (45h)**

Assessment methods: **credits and exam**

Language of instruction: **English**

Course title: **Spectroscopy**

Course code: **UMA-9**

Type of course: **obligatory**

Level of course: **basic**

Year of study: **1st year of the 2nd stage**

Semester: **II**

Number of credits: **4**

Name of lecturers: **prof. Andrzej Patrykiejew and dr Piotr Borowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to teach the interpretation of the IR, Raman, NMR, and MS spectra as well as the basic experimental aspects of molecular spectroscopy.

Prerequisites: Fundamentals of physics, quantum chemistry and organic chemistry.

Course contents: Interaction of a matter and electromagnetic radiation, theoretical and experimental fundamentals of molecular spectroscopy. Vibrational (IR and Raman) spectra: (i) one-dimensional harmonic oscillator and its spectrum, (ii) anharmonicity, (iii) vibrations of polyatomic molecules (force fields, normal modes, group vibrations), (iv) IR spectroscopy (apparatus, methodology, interpretation of spectra), (v) scattering of the electromagnetic radiation, Raman spectroscopy (apparatus, methodology, interpretation of spectra). NMR spectra: (i) interaction between the magnetic field and the nuclei (the Zeeman effect), (ii) shielding of the nuclei (chemical equivalence), (iii) NMR spectroscopy (apparatus, methodology), (iv) ^{1}H NMR spectroscopy (homo-, enantio-, diastereo-, and heterotopic protons, spin-spin coupling, magnetic equivalence, interpretation of spectra), (v) ^{13}C NMR spectroscopy (decoupling techniques, DEPT techniques, interpretation of spectra). MS spectra: (i) MS spectrometry (sample ionization methods, analyzers, methodology), (ii) fragmentation, (iii) interpretation of spectra. Other techniques: (i) rotational spectroscopy, (ii) electron spectroscopy, (iii) ESR spectroscopy, (iv) photoelectron spectroscopy.

Recommended reading:

1. R.M. Silverstein, G.C. Bassler, and T.C. Morrill, *Spectrometric Identification of Organic Compounds*, John Wiley &

Sons, Inc., 1991.

2. P.W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.

3. P.W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press, Oxford, 1983.

4. L.M. Harwood and T.D.W. Claridge, I*ntroduction to Organic Spectroscopy*, Oxford Science Publications,

Oxford 1996.

Teaching methods: **lectures (15 h), laboratories (30 h)**

Assessment methods: **credit**

Language of instruction: **English**

Elective courses

Course title: **Trace analysis; activation analysis and radiochemical methods; chromatographic methods in trace analysis**

Course code: **PFA-1**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I or II**

Number of credits: **4**

Name of lecturer: **prof. Andrzej Dawidowicz, prof. Władysław Janusz, and prof. Mieczysław Korolczuk**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

Students should: optimize the chromatographic separation of complex mixtures in the context of trace analysis; apply the most important experimental techniques allowing for analytical procedure of traces by chromatography; chose the most proper chromatographic equipment for trace analysis; understand the problems of trace analysis.

Student should be able to: demonstrate an understanding of the basics nuclear spectroscopy analysis; demonstrate an understanding and apply basic radioisotope method of analysis; show a basic level of competency in the practical skills, problem solving, data processing and analysis associated with the field of radioisotope method of analysis.

Moreover, student ought to know: the basic scheme of trace analysis, basic knowledge concerning preparation of samples for trace analysis, how to chose the appropriate method to resolve the problem of analysis of samples with complex matrix, interferences in most commonly used method in trace analysis and their elimination.

Prerequisites: Basic knowledge concerning chromatography, instrumental analysis and physical chemistry. Completion of radiochemistry course. Basic knowledge about instrumental methods of analysis.

Course contents: Chromatographic methods in trace analysis. Sensitivity optimization (injection of large volume sample, effect of column efficiency, effect of column diameter, effect of particle size). Importance of detection in chromatographic trace analysis. Detectors for GC and HPLC. Peak height vs. peak area in quantitative analysis of traces. The most important concepts in trace analysis – LOD, LOQ, baseline noise, signal to noise ratio, operation and dynamic linearity, detector sensitivity, detector time constant, etc. Sample derivatization for chromatographic analysis of trace. Derivatization for GC analysis, derivatization for HPLC analysis. Post-column derivatization. Sample preparation procedures for chromatographic trace analysis.

Activation analysis and radiochemical methods. Nuclear radiation spectrometry. Activation Analysis - fundamentals, equipment, applications advantage and drawbacks. Neutron activation analysis. Cyclic neutron activation analysis. Charge particle activation analysis. Photon activation analysis. Method analysis based on the adsorption and scattering of nuclear radiation. Photon Induced X-ray Emission. Particle Induced Gamma-ray Emission. Rutherford backscattering. Radiometric titration.

Isotope dilution analysis - Fundamentals, methods, applications advantages and drawbacks. Direct isotope dilution analysis. Reverse isotope dilution analysis. Derivative IDA. Substechiometric IDA,

Trace analysis. Scheme of trace analysis. Parameters influencing on the results of trace analysis. Purification of reagents used in trace analysis. Subboiling distillation, isothermal distillation, crystallization, prolonged electrolysis, cementation and sublimation. The methods of separation used in trace analysis. Detection methods: AAS, ICP OES, ISP MS and electrochemical methods. Preparation of samples to mentioned detection methods. Elimination of interferences.

Recommended reading:

1. J.R. Dean, *Methods for environmental trace analysis*, John Willey and Sons, Chichester, 2003.

2. P.R. Loconto, *Trace environmental quantitative analysis, principles, techniques and application*,

   Marcel Dekker, Inc. New York, 2006.

3. S. Ahuja, *Trace and ultratrace analysis by HPLC*, John Wiley and Sons, New York, 1992.

4. P.J. Schoenmakers, *Optimization of chromatographic selectivity*, Elsevier Science, Amsterdam, 1986.

5. C.F. Poole, *The essence of chromatography*, Elsevier Science; Amsterdam, 2002.

6. J. Tolgyessy, T. Braun, M. Kyrs, Isotope dilution analysis, Akademiai Kiado, Budapest 1972.

7. G. Gilmore, Practical gamma-ray spectrometry. J. Wiley & Sons, New York 1995

8. W.D. Ehmann, D.E. Vance, Radiochemistry and nuclear methods of analysis, J. Wiley & Sons, New York 1991.

9. A.G. Howard, P.J. Statham, *Inorganic trace analysis: philosophy and practice*, Wiley, Chichester, 1993.

10. E. Prichard, G.M. MacKay, J. Points (Eds.), *Trace analysis: a structured approach obtaining reliable results*,

    Thomas Graham House, Cambridge, 1996.

Teaching methods: **lectures (30 h), laboratories (30 h)**

Assessment methods: **credits and final exam**

Language of instruction: **English**

Course title: **Modern diffraction methods in crystalline state investigations**

Course code: **PFA-2**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st year of the 2nd stage**

Semester: **I or II**

Number of credits: **4**

Name of lecturer: **prof. Stanisław Pikus**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to teach the current modern X-ray diffraction methods and their applications to characterization of crystalline state.

Prerequisites: Fundamentals of crystallography.

Course contents: The production and properties of X-rays. The geometry of diffraction on crystals. Intensity of diffraction beams, scattering by electron, atoms, crystals. Modern X-ray diffraction qualitative analysis. Diffraction databases. Special databases for minerals, semiconductor, poisons, metalorganic compounds. Methods for searching of X-ray diffraction databases. Basics of X-ray diffraction quantitative analysis. Standard X-ray diffraction methods for quantitative phase analysis. Rietveld refinement – special use for quantitative analysis. Crystallite size determination. Preferred orientation(texture). Unit cell lattice parameters precision refinement. X-ray diffraction methods for estimating of degree of crystallinity (polymers, biomaterials). Small angle X-ray scattering (SAXS) method. Basics of SAXS. Using of SAXS method for characterization of porous material – specific area, size of pores, fractal dimension, etc.

(*laboratory*) X-ray diffraction qualitative analysis (phase identification) – computer program XRAYAN for X-ray diffraction pattern treatment (smoothing, peak searching), match pattern, database services. Quantitative analysis – direct comparison method for two phase system, internal standard method for two and more phase system. Quantitative analysis by Rietved analysis – initial structure file, analysis of two phase materials. Measurement of degree of crystallinity for polymers. Appointment degree of texture and preferred direction for biomaterials and polymers. Precision determination of lattice constants for chosen samples.

Recommended reading:

1. C. Giacovazzo *et al.*, *Fundamentals of Crystallography*, Oxford University Press, 1992.

2. W. Borchardt-Ott, *Crystallography*, Springer- Verlag, 1995.

3. M.J. Buerger, *Elementary Crystallography*, John Wiley & Sons, Inc.,1956.

4. R. Jenkins, R.L. Snyder, *Introduction to X-ray Powder Diffractometry*, John Wiley & Sons, Inc., 1996.

5. H.P. Klug and L.E. Alexander, *X-ray diffraction procedures for polycrystalline and amorphous materials*,

John Wiley & Sons, Inc., 1974.

6. R.A. Young, *The Rietveld Method*, Oxford University Press, 1995.

Teaching methods: **lectures (30 h), laboratories (30 h)**

Assessment methods: **credit and exam**

Language of instruction: **English**

Course title: **Adsorbents and catalysts**

Course code: **PFA-3**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st or second year of the 2nd stage**

Semester: **I or II**

Number of credits: **4**

Name of lecturer: **prof. Jacek Goworek, prof. Janusz Ryczkowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to deliver practical examples of adsorption and catalysis applications in practices.

Prerequisites: Fundamentals of physical chemistry, chemical technology and base knowledge of spectroscopic methods.

Course contents: Definition of the adsorption, the thermodynamical description , free energy at the interfaces (Gibbs equation). Adsorption isotherms for the gas-phase; determination and the Langmuir model. Theory and BET equation. The potential of the adsorption. Adsorption from solutions. Kinds of adsorbents and their physicochemical characterization (with the regard of spectroscopic methods).

The catalysis and catalysts. Models of the reacting molecules. The energy-part of the third body in chemical reactions. The formal kinetics of heterogeneous catalytic reactions – mono- and bimolecular reactions. Mechanisms of the catalytic bimolecular reactions. Stages limiting rate of the catalytic reactions. Experimental kinetic equations of the catalytic reactions. Active centers on the catalysts' surface and catalytic activity. Geometrical, energetic and electronic aspects of of the heterogeneous catalysis phenomena. The classification of heterogeneous catalysts and the characterization of main catalysts groups. Preparation of heterogeneous catalysts - basic stages, methods of preparation, unit and process operations for catalysts precursors transformation into the final form (drying, calcination, reduction). The modern approach for catalysts design.

Recommended reading:

1. M. Bowker, The basis and application of heterogeneous catalysis, Oxford Univ. Press, 1998.

2. J.M. Thomas, W.J. Thomas, Principles and practice of heterogeneous catalysis, VCH Weinheim, 1996.

3. G.C. Bond, Heterogeneous catalysis (2nd edition), Oxford Univ. Press, 1987.

4. J.M. Campbell, Catalysis at Surfaces, Chapman and Hall, London 1988.

Teaching methods: **lectures (30 h), laboratories (30 h)**

Assessment methods: **credits and final exam**

Language of instruction: **English**

Course title: **Physical adsorption on solid surfaces – theoretical bases and applications**

Course code: **PFA-4**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st or second year of the 2nd stage**

Semester: **I, II or III**

Number of credits: **1**

Name of lecturer: **prof. Andrzej Dąbrowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

An aim of the lecture is the introduction to the adsorption processes, with particular reference to the theoretical description using various models of the solid surface. After the short discussion of historical aspects of the development of the knowledge about the physical adsorption, will be introduced the thermodynamical description of the adsorption of gases, their mixtures and liquid solutions on heterogeneous solid surfaces, and also the indispensable knowledge about the kinetics the adsorption and the molecular modeling of adsorption processes. Finally, examples of the practical application of the adsorption, both in the industry and in the environmental protection will be presented.

Prerequisites: the average advanced level of English language, passed exams: physical chemistry and the statistical thermodynamics.

Course contents: Introduction with the historical aspects. The adsorption on heterogeneous surfaces; adsorption of: individual components, gas and liquid mixtures. The fractal theory of the adsorption. Elements of the kinetics of the adsorption process. Bases of the molecular modeling of adsorption processes. Adsorbents – division, preparation methods, and their characteristic. Chosen examples of the adsorption processes applications in the: industry, environmental protection. Short review of the literature connected with the lecture content.

Recommended reading:

1. J. Ościk, *Adsorption*, Ellis Horwood, Chichester, PWN, Warszawa, 1975.

2. M. Jaroniec, R. Madey, *Physical Adsorption on Heterogeneous Solids*, Elsevier, Amsterdam, 1988.

3. A. Dąbrowski, M. Jaroniec, *Adv. Colloid Interface Sci*., **27** (1987) 211.

4. A. Dąbrowski, M. Jaroniec, *Adv. Colloid Interface Sci*., **31** (1990) 155.

5. A. Dąbrowski, Adsorption – from Theory to Practice, *Adv. Collid Interface Sci*., **93** (2001) 135.

6. A. Dąbrowski (Ed.), *Adsorption and its Applications in Industry and Environmental Protection*, Elsevier, Amsterdam, 1998, vol. 120A, 120B.

Teaching methods: **lectures (15 h)**

Assessment methods: **credit or exam**

Language of instruction: **English**

Course title: **An outline of green chemistry**

Course code: **PFA-5**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st or second year of the 2nd stage**

Semester: **I, II or III**

Number of credits: **1**

Name of lecturer: **prof. Janusz Ryczkowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The main goal is to deliver the current knowledge of various aspects in broad area of green chemistry.

Prerequisites: Fundamentals of physical chemistry, chemical technology and elementary knowledge of spectroscopy methods.

Course contents: Atom economy – principles and examples. Selected solutions in area of homogeneous and heterogeneous catalysis as well as biocatalysis. The use of catalytic systems for pollution abatement with the special emphasis on destruction of volatile organic compounds, reduction of carbon and nitrogen oxides emissions. Examples of technologies improvement will be given, too.

Recommended reading:

1. R.A. Sheldon, I. Arends, U. Hanefeld, Green chemistry and catalysis, Wiley-VCH, Weinheim, 2007.

2. R.M. Heck, R.J. Farrauto, S.T. Gulati, Catalytic air pollution control, John Wiley & Sons, Inc., New York, 2002.

3. Green catalysis (R.H. Crabtree, Ed.), Vol. 1-3, Wiley-VCH, Weinheim, 2009.

Teaching methods: **lectures (15 h)**

Assessment methods: **credit** (Power point presentation or poster) **or exam**

Language of instruction: **English**

Course title: **Introduction to heterogeneous catalysis**

Course code: **PFA-6**

Type of course: **elective**

Level of course: **advanced**

Year of study: **1st or second year of the 2nd stage**

Semester: **I, II or III**

Number of credits: **2**

Name of lecturer: **prof. Janusz Ryczkowski**

Objectives of the course (preferably expressed in terms of learning outcomes and competences):

The introduction of students with the basic nomenclature concerning the heterogeneous catalysis, occurring in English-speaking elaborations. Training the students how to write their theoretical chapter of the master thesis, as well as short speeches and presentations in English.

Prerequisites: English knowledge at the average advanced level, passed an exam in chemical technology, the skill of using selected components of the MS Office pack.

Course contents: The basic nomenclature, the preparation of catalysts, the characterization of supports and catalysts, industrial examples of catalytic reactions, catalysts deactivation, application of physicochemical methods for the catalysts characterization. The detailed course contents will be established with the students according to their interest.

Recommended reading: All available manuals and specialistic scientific periodicals in English, and also internet resources of the Main Faculty Library of UMCS.

Teaching methods: **tutorials (30 h)**

Assessment methods: **credit** (on the ground of a prepared poster or PowerPoint presentation as well as a 6-page elaboration in English, in the form of a camera-ready text for a perspective publication) **or exam**.

Language of instruction: **English**