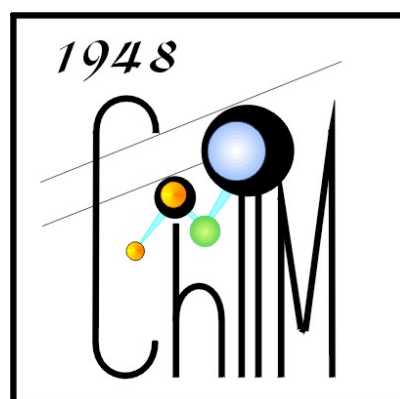


# FACULTY OF INDUSTRIAL CHEMISTRY AND ENVIRONMENTAL ENGINEERING



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**RESEARCH CENTRE  
PROTECTION AND DEPOLLUTION WATER ENGINEERING  
AND ENVIRONMENTAL ANALYSIS OF INDUSTRIAL  
PROCESS - P.D.W.E.E.A.I.P.**

**GENERAL PRESENTATION**

This research centre is a CNCSIS accredited, type C, research centre reapproved by CNCSIS in 12.09.2006, according to CNCSIS certificate nr. 28. The director of the Center is **Prof. PhD. eng. Rodica Pode**.

**MAIN ACTIVITIES**

The Centre accomplishes research and design in the following topics:

- Environmental analysis of industrial processes
- Drinking and industrial water treatment
- Wastewater treatment
- Process control equipments for research plants in chemical industry
- Control systems using computers for researching plants and low tonnage plants in chemical industry
- Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents
- Mathematical modeling and numerical simulation of environmental pollution and depollution processes
- Modeling, simulation and process control
- Heat transfer organic agents
- Unit processes
- Magnetic Fluids: Preparation, Characterization and Applications
- The Intensification of Transfer Processes
- Rheological characterization of the substances
- Studies and projects for thermo-technical installations of the silicates industry
- Electrochemical processes
- Obtaining and characterization of oxide compounds

**CONTACT**

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**RESEARCH FIELDS**

- **Environmental analysis of industrial processes**

*Keywords:* environmental, pollution, waste

- **Drinking and industrial water treatment**

*Keywords:* water treatment, drinking water, industrial water

- **Wastewater Treatment**

*Keywords:* waste water treatment, pollution

- **Process control equipments for research plants in chemical industry**

*Keywords:* measuring, control devices

- **Control systems using computers for researching plants and low tonnage plants in chemical industry**

*Keywords:* process control, research and low tonnage plants

- **Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents**

*Keywords:* Climate changes, pollution, risk, sustainable chemistry, modeling

- **Mathematical modeling and numerical simulation of environmental pollution and depollution processes**

*Keywords:* modeling, simulation, environmental protection

- **Modeling, simulation and process control**

*Keywords:* modeling, simulation, optimization, process control, absorption-desorption with chemical reaction

- **Oily compounds extraction from waste waters using magnetic fluids**

*Keywords:* extraction, magnetic fluid

- **Coordinative compounds with organic ligands**

*Keywords:* coordinative compounds, heterocyclic compounds, hydroxycarboxylic acids, pharmaceutical substances, pigments, dyes

- **Synthesis of nanocomposites with controlled magnetic, optic and catalytic properties**

*Keywords:* nanoparticles, sol-gel, silica, magnetic, catalytic, polyols

- **Homo-and heteropolynuclear compounds with organic ligands**

*Keywords:* organic ligand, polinuclear compound, magnetic materials, catalysts, pigments, ferrites, chromites

➤ **Physical Chemistry. Chemically Active Species Grafted on Polymer-Supports**

*Keywords:* catalysis, homogeneous catalysts, heterogeneous catalysts, polymer grafted catalysts, polymer-grafted reagents, polymer-support

➤ **Physical Chemistry. The obtaining and characterization of some oxide compounds**

*Keywords:* solid-state, oxide compounds, unconventional methods

➤ **Organic Electrochemistry**

*Keywords:* organic electro synthesis, organic electro reduction and oxidation

➤ **Electro catalysis**

*Keywords:* skeleton electrodes, thermal arc spraying, potentiometer sensors

➤ **Electroplating**

*Keywords:* copper, zinc, nickel electrodepositing, brighteners

➤ **Fuel Cells**

*Keywords:* fuel cells, skeleton electrodes, proton exchanges membrane, anion exchange membrane

➤ **Synthesis of ceramic materials through hydrosilicatic forerunners**

*Keywords:* ceramic, hydrosilicatic, synthesis

➤ **Semi conducting glasses. Fast ion-conducting glasses. Redox equilibrium in glasses. Low melting glasses for fusion type application**

*Keywords:* conducting, glasses, redox equilibrium, vitreous systems

➤ **Ceramic glazes. Synthesis and characterization of thermo resistant pigments**

*Keywords:* ceramic glazes, thermo resistant pigments, synthesis method

➤ **Chemistry and technology of building materials**

*Keywords:* cements, mineral binders

#### Researches in *WATER TREATMENT AND PURIFICATION*

The activity intensifying and diversifying of the industrial processes leads to the quality degradation of water sources, with important implications for water supplies. In this context it is important to research and to elaborate some treatment and purification technologies, more efficient and at low costs. The research activity was concerning with the majority of aspects involved by water chemistry and technology, as follows:

- physical and chemical characterization of water supplies and of wastewaters
- researches concerning water treatment for drinking and industrial purposes
- researches concerning the technologies of industrial and municipal wastewater treatment

Results of the research activity were published in journals of specialty and communicated at the national and international Symposia.

#### RESEARCH TEAM

Georgeta Burtica, Aurel Iovi, Petru Negrea, Rodica Pode, Ioan Ursoiu, Adina Negrea, Eugen Lungu, Marius Gheju, Florica Manea, Laura Coheci, Giannin Moșoarcă, Lavinia Lupa, Mihaela Ciopec.

#### Researches in *INORGANIC CHEMICAL TECHNOLOGY*

Different processes for obtaining of the new products, with superior qualities have been studied (chemical fertilizers with microelements, inorganic salts, etc.), for turning to good account of the native raw materials, industrial wastes and for the recovery of the useful compounds from wastewaters.

Researches in:

- mineral fertilizers: urea, ammonium nitrite, NP, NPK, fertilizers with microelements
- improving and modernizing of the technological processes
- Turning to good account of some native minerals zeolites for wastewaters treatment and for the obtaining and conditioning of the fertilizers with microelements.

The results of researches were applied in industry.

#### RESEARCH TEAM

Petru Negrea, Georgeta Burtică, Rodica Pode, Laura Coheci, Lavinia Lupa, Mihaela Ciopec

#### Researches in *PROCESS CONTROL EQUIPMENTS FOR RESEARCH PLANTS IN CHEMICAL INDUSTRY*

Some specific control equipments for research plants from chemical industry (measurement and control of small and micro gas and liquid flows, gas and liquid compositions, pressure) using as information support low pressure signals.

Elaboration, design and realization of a high performance reference models.

#### RESEARCH TEAM

Marcel Suta, Carmen Rusnac, Alina Brusturean

**Researches in CONTROL SYSTEMS USING COMPUTERS FOR RESEARCHING PLANTS AND LOW TONNAGE PLANTS IN CHEMICAL INDUSTRY**

Realization of some specific control equipments using computers and process interfaces for automation of laboratory, research and low tonnage plants from chemical industry.

Elaboration, projecting and realization of control equipments using computers, process interfaces and proper software programs.

**RESEARCH TEAM**

Marcel Suta, Carmen Rusnac, Alina Brusturean

**Researches in INTENSIVE METHODS FOR THE EXONERATION OF SOIL FROM RADIOACTIVE MINERALS EXPLOITATION AND PROCESSING AREAS IN THE CONDITION OF NATURAL DISASTERS OR ENTROPIC ACCIDENTS**

Chemical decontamination of soil in the presence of ultra-sounds

Mathematical models and methods regarding the transfer mechanism in solid-liquid heterogeneous systems for the selection of optimal hydrodynamic parameters

Implementation of interface equipment in measurement devices

**RESEARCH TEAM**

Carmen Rusnac, Gabriela Alina Brusturean, Dana Silaghi – Perju

**Researches in MATHEMATICAL MODELING AND NUMERICAL SIMULATION OF ENVIRONMENTAL POLLUTION AND DEPOLLUTION PROCESSES**

Mathematical modeling and numerical simulation of soil depollution processes

Elaboration of analytical and statistical models of air pollution phenomenon

Waste recycling process control and optimization

**RESEARCH TEAM**

Carmen Rusnac, Gabriela Alina Brusturean, Dana Silaghi Perju,

**Researches in MODELING, SIMULATION AND PROCESS CONTROL**

Modeling and simulation of chemical processes using programming languages and software in process engineering: MATLAB, HYSIS, Aspen Plus, Aspen Custom Modeler;

Apply chemical reactor analysis, process modeling, simulation and optimization to chemical and

petrochemical plants and find out solutions for industrial problems;

Modeling, simulation and process control of absorption-desorption with chemical reaction processes.

**RESEARCH TEAM**

Teodor Todinca, Carmen Rusnac, Alina Brusturean

**Researches in OILY COMPOUNDS EXTRACTION FROM WASTE WATERS USING MAGNETIC FLUIDS**

It was studied the oily fraction recovery (especially oil products) from waste waters using magnetic fluids. The process is strongly influenced by the magnetic field presence; both the oily fraction and the magnetic phase could be recovered;

**RESEARCH TEAM**

Andra Tamas

**Researches in THE PERFORMANCE OF THE COLUMNS WITH STRUCTURED PACKINGS**

The structured packing present a high efficiency by comparison with the random packing because of the very high specific surfaces. It was followed the knowledge of wettability degree influence in extraction or rectification processes. The aim of the future experiments is the increase of wettability degree through electrochemical or chemical activation

**RESEARCH TEAM**

Andra Tamas

**Researches in CONDITIONING MODELS OF SEWAGE SLUDGE**

The aim of this research consists in efficiency evaluation of chemical conditioning models by calculation of the sludge volume index (SVI), the specific resistance to filtration to improve sludge dewatering, as well as appropriation of a statistic mathematic model for the correlation of the obtained results.

**RESEARCH TEAM**

Vasile Pode, Andra Tamaş

**Researches in NANOCOMPOSITES WITH CONTROLLED MAGNETIC, OPTIC AND CATALYTIC PROPERTIES**

Nanocomposites of type ferrite and ferrite/SiO<sub>2</sub> were synthesized trough two original methods: the thermal decomposition of some heteropolynuclear complex compound (with hydroxocarboxylic anions as ligands) and a modified sol-gel methods.

The fine nature of the obtained nanoparticles gives to the synthesized nanocomposites special magnetic properties that can be used in potential applications. Studies have been made in order to establish the

dependence between the synthesis conditions, the dimensions of nanoparticles and their properties. Studies have been made for the synthesis of hybrid polyol-silica matrix, correlation between synthesis conditions and textural properties of the silica matrix, for its use as support for some catalysts. Studies are going to be made for the synthesis of metallic nanoparticles in silica matrix, with special properties and for the use of these materials as thin films for biological and environmental applications.

#### **RESEARCH TEAM**

Mircea Ștefănescu, Marcela Stoia

#### **Researches in HOMO - AND HETEROPOLYNUCLEAR COMPOUNDS WITH ORGANIC LIGANDS**

Synthesis and characterization of some inorganic compounds in order to obtain simple and mixed oxides with catalytic, pigmental and magnetic properties

A new synthesis method has been carried out in order to obtain some homo - and heteropolynuclear compounds with hydroxocarboxylic acid anions as ligands. The simple and mixed oxides with special properties have been obtained by thermal conversion of some complex compounds

#### **RESEARCH TEAM**

Mircea Niculescu, Mircea Ștefănescu, Marcela Stoia, Raluca Vodă, Ilie Julean

#### **Researches in PHYSICAL CHEMISTRY OF SOLIDS. OBTAINING AND CHARACTERISATION OF SOME OXIDE COMPOUNDS**

The properties of the oxide compounds formed by reactions in the solid state are significantly dependent on the synthesis method used, respectively on the initial state of the reactants.

For the obtaining of some oxide compounds, different synthesis methods have been used: a) the sol-gel method; b) thermal conversion of certain complex combinations; c) combustion synthesis; d) hydroxide co precipitation; e) annealing of salts and/or oxides mixtures. The reactivity of the systems was studied comparatively for the different synthesis methods used.

#### **RESEARCH TEAM**

Cornelia Păcurariu, Dumitru Becherescu, Ioan Lazău, Radu Ioan Lazau, Robert Ianos, Marius Jurca

#### **Researches in ORGANIC ELECTROCHEMISTRY**

Electrochemistry represents today a very convenient method for the synthesis of a variety of important organic compounds, which in many cases have been extended to an industrial scale.

Since 1982 theoretical and practical investigations have been made upon electrode processes of organic electrochemistry. The synthesis of quinine, hydroquinone, and ethylene glycol has been analyzed, especially in undivided electrochemical reactors. Studies upon mediated reduction and oxidation of organic compounds have been undertaken.

#### **RESEARCH TEAM**

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu

#### **Researches in ELECTROCATALYSIS**

Obtaining, characterization and application of the electrodes with catalytic activity.

Methods for the preparation of electrocatalytic films have been elaborated in our research team, based on the thermal decomposition of some complex compounds and through thermal arc spraying technique. These films have been characterized through scanning electron microscopy, X-ray diffraction and voltammetry. The practical applications refer to water electrolysis and to the synthesis of some organic compounds.

#### **RESEARCH TEAM**

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu

#### **Researches in ELECTROPLATING**

Obtaining and characterization of metal coatings

Studies regarding the influence of the nature of the galvanic additives upon the quality of the metal deposition have been made. Metal layers have been characterized by X-Ray diffraction, scanning electron microscopy and energy dispersive X-ray microanalysis. The practical applications refer to the replacement of the cyanide galvanic baths with non-toxic ones.

#### **RESEARCH TEAM**

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Radu Bănică

#### **Researches in FUEL CELLS**

The conventional energy systems are the main source of pollution on our planet. Considering the decreasing of the Earth's resources of hydrocarbons, it is necessary to improve an alternative energy conversion technology such as the fuel cells. This technology offers many attractive possibilities for reducing the air pollution, diminishing climate changes and preserving our natural resources. Widespread application of this technology is still prohibitive because materials used to make electrodes are expensive.

The aim of our research is the reducing of the  $H_2-O_2$  fuel cell costs by changing the Pt based electrodes with non-noble based electrode obtained using various methods (thermal decomposition, thermal spraying).

**RESEARCH TEAM**

Nicolae Vaszilcsin, Andrea Kellenberger, Mircea Dan, Narcis Duțeanu, Radu Bănică

**Researches in SYNTHESIS OF CERAMIC MATERIALS THROUGH HYDROSILICATE FORERUNNERS**

The use of hydrosilicatic forerunners from precipitate reactions to obtain at lower temperatures some high quality ceramic materials such as: wollastonite, enstatite, diopside, willemite, anortite, magnesium spinel and a multitude of oxidic pigments.

The studies in this field have been made at the "Politehnica" University of Timișoara since 1985. The researches have been materialized in a laboratory synthesis method of the materials involved. Verification of the behavior of some synthesized materials in industrial circumstances.

**RESEARCH TEAM**

Ioan Lazău, Dumitru Becherescu, Marius Jurca, Radu Lazău

**Researches in SEMICONDUCTING GLASSES. FAST ION CONDUCTING GLASSES. REDOX EQUILIBRIA IN GLASSES. LOW MELTING GLASSES FOR FUSION TYPE APPLICATION**

Studies regarding electrical conductivity in new molybdenum glass systems. Influence of different transitional ions upon conduction properties of glasses was studied. Synthesis and characterization of fast ion conducting glasses containing  $\text{Ag}^+$ ,  $\text{Li}^+$  and  $\text{Cu}^+$  ions. Glasses with optimal ion conductivity were design. New fast ion conducting glasses were obtained. The behavior of redox equilibrium  $\text{Mn}^{2+}/\text{Mn}^{3+}$  was studied in the following binary systems:  $\text{SiO}_2\text{-R}_2\text{O}$ ,  $\text{P}_2\text{O}_5\text{-R}_2\text{O}$  and  $\text{B}_2\text{O}_3\text{-R}_2\text{O}$ .

The influence of melting conditions (reducing-oxidizing) upon the presence of  $\text{Ti}^{4+}$  was studied, as well as its relationship with the iron present. The reciprocal influence of  $\text{Ti}^{4+}$  and other different ions usually present as impurities upon the color in industrial glasses was studied.

Design, synthesis and characterization of low melting glasses for fusion type applications was studied. The reciprocal influence fusion glass-support glass was investigated using microscopic techniques.

**RESEARCH TEAM**

Adina Lația, Cosmin Vancea

**Researches in CERAMIC GLAZES. SYNTHESIS AND CHARACTERIZATION OF THERMORESISTANT PIGMENTS**

The research field extends over the conventional and unconventional synthesis methods for thermoresistant pigments designed to the ceramic industry (ceramic glazes and enamels), characterization of the obtained pigments from the

point of view of crystallochemical structure and color. At the same time, the behavior of the synthesized pigments in the glass generating melt is being pursued.

**RESEARCH TEAM**

Ioan Lazau, Cornelia Păcurariu, Dumitru Becherescu, Radu Ioan Lazau, Robert Ianos

**RESEARCH PROJECTS**

**1. PN II ZEO-NANOSPP 71-056/2011:** *Synthesis of functionalized zeolite materials with doped titanium dioxide nanoparticules and testing in water potabilization pilot stations*

*Value:* 45000 LEI

*Director:* Prof. PhD.eng. Georgeta BURTICĂ

*Members:* Asist. Prof. PhD. eng. Florica MANEA  
PhD. eng. Daniela SONEA  
Eng. Cristina PROCA  
Eng. Adriana REMES

**FIELD DESCRIPTION**

Studies over the doped  $\text{TiO}_2$  nanocrystals getting through alternative methods, processing to the efficient solutions to get the modified zeolitic materials with  $\text{TiO}_2$  nanocrystals doped with metallic/nonmetallic ions, like the characteristics of source and drinking water and a dinking water decontamination

**ACTIVITIES AND RESULTS**

Studies of concordance on the  $\text{TiO}_2$  nano crystals doped with metallic/non-metallic ions trough RX diffraction, Electronic microscopy (TEM, AFM, SEM) - UV-VIS spectrometry. Preliminary researches of synthesis of zeolitic materials functionalised with  $\text{TiO}_2$  doped with non-metallic ions. Semination of the results on large scale, trough national and international communication and publishing.

**2. IDEI - 927/2011:** *Integrated concept about depollution of waters with arsenic content, through adsorption on oxides materials, followed by immobilization of the resulted waste in crystalline matrices*

*Value:* 175000 LEI

*Director:* Lect. PhD. eng. Adina NEGREA

*Members:* Prof. PhD. eng. Ioan LAZAU  
Assist. PhD. eng. Lavinia LUPA  
Lect. PhD. eng. Radu LAZAU  
C.S. PhD. eng. Mihaela CIOPEC  
Ph. student eng. Suba Mariana

**FIELD DESCRIPTION**

The project is connected to a main direction of the international researches, main field environment – sustainable development – global changing and brings fundamental elements in constitution of capable research teams for the competitions in european

programs. As part of this project the depollution of waters with arsenic content is intended, through adsorption on synthetic oxides materials. As adsorbent materials sludge with iron oxides content resulted from other processes will also be studied. The absolute novelty of this project consists in using the waste resulted after arsenic adsorption as auxiliary raw material in glasses manufacturing; this procedure assures not only the pollutant immobilisation in the crystalline matrix, but even the substitution of a classical raw material  $As_2O_3$  and the concomitant capitalization of the components resulted from adsorbent – in full agreement with the principles of the sustainable development.

#### ACTIVITIES AND RESULTS

The synthesis and characterisation of the oxide materials used as adsorbents (obtaining, chemical analysis, specific surface area, adsorption capacity, adsorption degree). There will be synthesized in laboratory a series of oxide materials based on iron or on silicates, which will be characterised together with the unconventional ones. Is anticipated new possibilities of the oxide composition and adsorbent structure optimisation, so that this can be used as auxiliary raw material in crystalline matrix obtaining. Testing – experimental determination of adsorption, as well as kinetic study.

**3. PN II- 72-171/2011, Micro porous sensors with polyaniline functionalised with pendant groups, innovative materials used in the identification and control of the Parkinson disease.**

Value: 30000 LEI

Director: Assoc. prof. Ph. eng. Andrea KELLENBERGER

Members: Prof. PhD. eng. Nicolae VASZILCSIN  
Assist. Ph. eng. Mircea Laurentiu DAN  
Assist. PhD. eng. Narcis DUTEANU  
PhD. eng. Radu BANICA  
Student Anuta NASUI  
Student Raluca NITOI  
Student Diana MIHART

#### FIELD DESCRIPTION

Electrochemical sensors based on polyaniline for the detection of dopamine in the Parkinson disease.

#### ACTIVITIES AND RESULTS

Reference materials study regarding the obtaining of the micro porous sensors with polyaniline functionalised with pendant groups.

**4. PN II- STEDIWAT- 32-125/2011: Technical-decisional support system for sustainable management of water.**

Value: 29500 LEI

Director: Assoc. prof. Ph. eng. Florica MANEA

Members: Prof. PhD. eng. Georgeta BURTICA  
PhD. eng. Daniela SONEA  
PhD. eng. Aniela POP  
Eng. Cristina PROCA  
Eng. Adriana REMES

#### FIELD DESCRIPTION

The development of some innovative technical support instruments, for monitoring, design and prediction which to be used for sustainable and incorporated management, at hydrographic basin level. Also, the development of the capacity of the collaboration, knowledge and communication transfer between universities and local/regional authorities of water resources management, users and other interest parts in the four studied basins (Prut., Banat, Arges-Vedea, Olt) with impact on the sustainable development at the local and regional level.

#### ACTIVITIES AND RESULTS

Research base with contain studies about: evaluation of the infrastructure and of the institutional capacity, management performance, organiser structure and communication channels, sources of pollution and sloop of the waste waters specific for users, hidromorphologic pressure, evolution of the water supply and request, normative for the prevention and full control of pollution, protected areas. In this step will be study, also: the facilities of treatment and purification, water price and the settlement regarding the quality, environment particularities (clime, geography, topography, water resources), field use, demographics data (actual state and tendency), ecological and hydro geological limited conditions. All these studies will be considered in the context of the national and international legislation.

**5. UEFISCDI-PN-II-RU-TE-3-0024/2011 – Innovative solutions in the field of large surface area ceramic nanopowder preparation via combustion synthesis.**

Value: 51099 RON

Director: Assist. Ph..D. eng. Robert IANOS  
Members: Lecturer Ph.D. eng. Radu LAZĂU  
PhD eng. Silvana BORCĂNESCU  
Student Roxana BĂBUŢĂ

#### FIELD DESCRIPTION

Preparation of ceramic powders with controlled properties under more advantageous conditions is a real challenge for the field of ceramics. One of the recently developed synthesis methods is the solution combustion synthesis, which in some cases yields the designed crystalline compounds directly from the combustion reaction, no further annealing being necessary.



**ACTIVITIES AND RESULTS**

Objective 1.- Management and communication: Conducting the public procurement procedures. / Preparation of intermediate and final progress reports. / Monitoring and internal control of the project implementation process. / Results processing and elaboration of scientific materials (articles, OSIM patent application, posters, presentations). / Results dissemination and attending international conferences. / Creating and updating a project web site.

**Objective 2.** Increasing the surface area of  $ZnAl_2O_4$  powders by removing the residual carbon via  $H_2O_2$  oxidation: elaboration of a literature review in the field of  $ZnAl_2O_4$  preparation. / Combustion synthesis of  $ZnAl_2O_4$  using an excess of triethylenetetramine. / Carbon removal by  $H_2O_2$  oxidation. / The influence of a moderator aid -  $Zn(CH_3COO)_2$  - on the  $ZnAl_2O_4$  characteristics. / Sample characterization (TG-DTA, XRD,  $S_{BET}$ , FT-IR, SEM).

**6. UEFISCDI-PNII-165/2011- Nano-enhanced electrochemical green technology for advanced integrated water treatment and quality control**

Value: 119102 RON

Director: Assoc. prof. Ph. eng. Manea Florica,

Members: Prof. PhD. eng. Poda Rodica,

PhD. eng. Pop Aniela,

PhD. eng. Remes Adriana,

PhD. eng. Motoc Sorina,

PhD. eng. Baciu Anamaria

**FIELD DESCRIPTION**

The objective of this project is to explore potential use of a new-proposed nano-enhanced electrochemical dual green technology based on nanostructured carbon electrode materials and electrochemical techniques to improve access to clean water.

WP1. Elaboration of new composite materials based on carbon nanotubes (CNT)/carbon nanofibres (CNF) in epoxy matrix as electrode materials for oxidation of POPs from water

Tasks:

1. Assessment of dispersion degree of CNT in different types of solvents and epoxy matrix
2. Synthesis of new CNT/CNF –epoxy composites
3. Synthesis of new composites - CNT/CNF modified with natural or synthetic zeolite doped with Ag/ Cu/  $TiO_2$  in epoxy matrix.

**ACTIVITIES AND RESULTS**

Series of composite materials using epoxy matrix with different compositions based on CNT/CNF and natural or synthetic zeolite doped with Ag/ Cu/  $TiO_2$  in epoxy matrix

**7. IDEI -647/2011 - Innovative technologies for the removal of hexavalent chromium from wastewaters by reuse of scrap iron**

Value: 190651 RON

Director: Lect. PhD. Eng Marius GHEJU

Members: Prof. PhD. Eng. Aurel IOVI

Prof. PhD. Eng. Rodica PODE

Assist. PhD. Eng. Laura COCHECI

C.S. PhD. Eng. Mihaela CIOPEC

**FIELD DESCRIPTION**

Long term column experiments for the assessment of Cr(VI) concentration (5-40 mg/L) influence on the efficiency of Cr(VI) reduction with scrap iron.

Batch experiments for the assessment of experimental parameters (NaOH dose, mixing time, mixing intensity, settling time, temperature) influence on the precipitation of species resulted from the reduction of Cr(VI).

**ACTIVITIES AND RESULTS**

The scrap iron reduction capacity recorded until the moment of Cr(VI) breakthrough followed the order: 5 mg/L > 10 mg/L > 20 mg/L > 40 mg/L.

The optimum conditions for the precipitation of cations resulted from the reduction of Cr(VI), were: NaOH dose: 500 mg/L, mixing time: 5 minutes, mixing intensity: 50 rpm, settling time: 30 minutes, solution temperature: 14°C.

**7. POSDRU – PERFORM-ERA - ID 57649/2010: Scientific performance by post-doctoral studies for integration in the European research area**

Value: 720000 RON

Director: Prof. PhD. Eng. Nicolae VASZILCSIN

Members: Prof. PhD. Eng. Corneliu DAVIDESCU

Prof. PhD. Eng. Aurel GONTEAN

**FIELD DESCRIPTION**

The project has as a main objective the building-up of a new generation of researchers, competitive in today's labor market by training in an integrated and interdisciplinary program. The targeted results are: sustainable improvement of a human resources and integration in the European area of the research and education.

**ACTIVITIES AND RESULTS**

Admittance of 15 post-doctoral researcher and starting of the research activities in the domain of the engineering sciences.

**8. POSDRU–MASTERMAT–SOP HRD 86/1.2/S / 58146 /2010: Development and implementation of master programs in the field of Micro and Nanomaterials**

*Value:* 684100 RON  
*Director:* Prof. PhD. Eng. Ioan LAZAU  
*Members:*  
 Prof. PhD. Eng. Cornelia PACURARIU  
 Prof. PhD. Eng. Corneliu DAVIDESCU  
 Prof. PhD. Eng. Petru NEGREA  
 Prof. PhD. Eng. Nicolae VASZILCSIN  
 Prof. PhD. Eng. Rodica PODE  
 Prof. PhD. Eng. Lucian RUSNAC  
 Assoc. prof. PhD. eng. Geza BANDUR  
 Assoc. prof. PhD. eng. Mihai MEDELEANU  
 Assoc. prof. PhD. eng. Andrea KELLENBERGER  
 Lect. PhD. eng. Adina NEGREA  
 Lect. PhD. eng. Adina LATIA  
 Lect. PhD. eng. Marius JURCA  
 Lect. PhD. eng. Radu LAZAU  
 Assist. PhD. Eng. Robert IANOS  
 Assist. PhD. Eng. Gerlinde RUSU  
 Financial expert Pandor Corina.

#### **FIELD DESCRIPTION**

Improving the learning opportunities for students via elaboration and implementation of innovative and flexible Bologna master programs, in accordance to the labour market needs and knowledge-based society.

#### **ACTIVITIES AND RESULTS**

Analysing the master programs in the approached field, from different European countries.  
 Forming activities of the teaching personnel from the partner universities.  
 Description of the master program by professional and cross- competences.

**9. FP7 – 211517- Integration of particulate abatement, removal of trace elements and tar reforming in one biomass steam gasification reactor yielding high purity syngas for efficient CHP and power plants (UNIQUE)**

*Value:* 20854,1 RON  
*Director:* Prof. PhD. Eng. Todinca Teodor  
*Members:* Lect. PhD. Eng. Gabriela Alina Dumitrel  
 Assist. Eng. Carmen Holotescu

#### **FIELD DESCRIPTION**

The main objective of the project was to develop an innovative technology for the production of syngas with the specifications required for use in fuel cells in a cost-effective way.

#### **ACTIVITIES AND RESULTS**

Set-up of a computational tool developed to help potential users to evaluate technical and economic advantages of the UNIQUE technology. A comprehensive simulation tool based on process flow sheet calculation was set up for describing the gasification process. The tool is on-line available

(via link through Unique homepage: [www.uniqueproject.eu](http://www.uniqueproject.eu)) with open access for potentially users.

**10. POSDRU/87/1.3/S/61839 -Looking to the Future - Teachers training to use computers in teaching chemistry**

*Value:* 9800 RON  
*Director:* Prof. PhD. Eng. Teodor TODINCA  
*Members:* Lect. PhD. Eng. Gabriela-Alina DUMITREL  
 Assist. PhD. Eng. Narcis DUTEANU

#### **FIELD DESCRIPTION**

Education and training as a tool of economic growth and development of knowledge-based society. Developing human resources from education and training.

#### **ACTIVITIES AND RESULTS**

Establishing contacts with school inspectorates from the West and Northwest regions of the country; Organization of conferences in order to highlighting the project; Identifying potential students and their preregistration.

**11. UEFISCDI-PNII-ID-PCE-3-0473/2011 – Eco-friendly design/synthesis of nanooxide: control of size, shape, morphology and functionalization of ZnO by polisaccharide assisted methodologies**

*Value:* 2000 RON  
*Director:* P.C. I. PhD. Oana Carp  
*Members:* Assist. PhD. Eng. Raluca Vodă  
 S.C. PhD. Eng. Diana Visinescu,  
 S.C. PhD. Eng. Greta Socoteanu,  
 S.C. PhD. Eng. Jose Calderon Moreno  
 S.C. PhD. Eng. Raluca Damian  
 S.C. PhD. Eng. Sanada Barjega

#### **FIELD DESCRIPTION**

A flexible *design* of oxide materials via biopolymers (like polysaccharides) is today an open research field that requires thorough investigations. Thus, we intend to develop in this project research suitable chemical procedures in order to tune the size, morphology, structure and functionalization of the oxides based materials, procedures that take advantage of polysaccharide various peculiarities like water-solubility, polyfunctionality, hydrophilicity, high chemical reactivity, chirality, chelation/coordination, gelling, assembling and adsorption abilities.

#### **ACTIVITIES AND RESULTS**

Precipitation synthetic protocols The precipitation protocols will be used for the *design/synthesis* of crystalline oxides/oxide-polysaccharide composites. As green suitable features of the methodology we can mention: the use of low cost and nontoxic reagents, simplicity, high-yield, water-based procedures

performed at room/low-temperature (<80°C) using unsophisticated equipment. The obtained oxides, are crystalline, nanosized and well dispersed.

**12. BS-ERA-NET-7-046/2011 – Hysufcel Hysulfcel-** Hydrogen Production From Black Sea Water By Sulfide-Driven Fuel Cell

Value: 90885.8 RON  
 Director: Prof. PhD.eng. Vaszilcsin Nicolae,  
 Members: Prof. PhD.eng. Serban Viorel-Aurel,  
 Assoc. Prof. PhD.eng. Kellenberger  
 Andrea,  
 Assoc. Prof. PhD.eng. Raduta Aurel,  
 Assoc. Prof. PhD.eng. Manea Florica,  
 Assoc. Prof. PhD.eng. Nicoara Mircea,  
 Assist. PhD. Duteanu Narcis,  
 Assist. PhD. student Eng. Dan Mircea  
 Eng. Serac Anuta

**FIELD DESCRIPTION**

The present project is directed to the simultaneous goals: first, remediation of the severe environmental situation in the Black Sea, to produce “carbon-free” energy in the form of hydrogen and to extract valuable compounds from the deep marine water. It is based on the opportunity to recover energy from the hydrogen sulfide in the Black Sea.

The thermodynamic analysis shows that the energy recovery of the latter is an energy alternative to the natural gas used in the coastal countries.

The successful accomplishment of the project goals requires the composition of various chemical and physico-chemical methods into an integrated technology. This technology will be based on the principles of environment remediation, energy saving, energy efficiency and storage of hydrogen for direct or further use. Very important feature of this technology is the utilization of the energy, conserved in the very hydrogen sulfide as well as of other compounds contained in the deep marine water (like methane) for the purpose of hydrogen production.

**ACTIVITIES AND RESULTS**

The proposed technology will consist of the following steps: pumping of the water from depths where the sulfide concentration is relatively high; enrichment of the pumped water to attain higher concentrations of sulfide and to enhance the next step: generation of electromotive force in a new designed fuel cell operating by catalytic sulfate oxidation by oxygen; sufficiently high and required for the very hydrogen production by electrolysis. Here other processes for water splitting, alternative to electrolysis will be tested too and the final decision on this step of the technology will be made after the comparison of their feasibility. The final step is hydrogen storage or its utilization as a

complementary energy source for electrolysis, used in another traditional fuel cell.

**PhD RESEARCH ACTIVITIES**

**1. Prof. PhD. eng. Aurel IOVI, PhD Supervisor in Chemical Engineering**

*PhD students:*

- Monica Ihoş: *Unconventional technologies of elimination from water of some specific pollutants*
- Daniela Micu: *The study of the toxic compounds elimination processes from rural waters sources*
- Adrian Gheorghe Rus: *The study of the obtaining processes of the active principles from medicinal plants and their characterizations*
- Ioan Macarie: *Contribution to the synthesis of some amino – organic – phosphoric with biological applied*
- Valeria Rus: *Studies regarding the sludge treatment from the local purification plant in the view of put in good use or elimination*
- Mihaela Maria: *Studies regarding the control and effect of the exposure to hard metals in the professional and unprofessional medium*

**2. Prof. PhD. eng. Georgeta BURTICĂ, PhD Supervisor in Chemical Engineering**

*PhD students:*

- Nicoleta Luminița Jurj: *Contributions regarding improvement of the municipal wastewater treatment technology for fall in with the European Normative*
- Damian Maria Teodora: *Studies regarding unconventional technologies elaboration for water treatment.*
- Tudur Teodora: *Studies regarding nitrites/nitrates removal from underground water*
- Baci Ana Maria: *Electromechanical methods for quatitative evaluation for water polutants*
- Motoc Sorina: *Electro oxidation process application in water treatment technologies*
- Amalia Corina Macarie: *Contributions at the eco-technologies elaboration for the metallic ions recovery from the used electrolyte*

**3. Prof. PhD. eng. Ioan LAZĂU, PhD Supervisor in Materials' Science and Engineering**

*PhD students:*

- Mariana Suba: *The use of the unconventional methods in synthesys of some mineralogic compounds and solid solution for ciment chemistry*
- Babuta Roxana: *Synthesis of oxide compounds via Pechini method*
- Ciobanu Cristina: *The role and action mechanism of additives in dry mortars*
- Vancea Cosmin Nicolae: *New immobilisation routes of industrial wastes in vitreous matrices*

➤ **4. Prof. PhD. eng. Nicolae VASZILCSIN, PhD Supervisor in Chemical Engineering**

*PhD students:*

- Mircea Dan: *Metal removal from residual water in electrochemical reactor with vibrating electrodes*
- Doru Buzatu: *Electro catalise based on niobium*
- Ștefan Dănică Novaconi: *Solar cells with TiO<sub>2</sub> and dyes*
- Vaduva Constantin Claudiu: *Corelation between the electronic structure of lever agents and double layer capacity*
- Iorga Mirela Ioana: *Metals removal from dilute solutions*
- Bobină Marian: *Correlations between the electronic structure and double layer capacitance of organic compounds and their ability to inhibit corrosion processes.*
- Crețu Raluca: *Catalytic effects in hydrogen evolution reaction*
- Novaconi Ștefan Dănică: *Development of nanostructured photoelectrochemical cells based on TiO<sub>2</sub> and dyes*
- Pop Nadia Loredana: *Synthesis and characterization of some perovskites*
- Rujan Dan Lucian: *Fractals theory in galvanotechnics*
- Văduva Constantin: *Relationships between electronic structure of organic compounds and their leveling effect in the cathodic deposition of metals*

➤ **5. Prof. PhD. eng. Delia PERJU, PhD supervisor in Chemical Engineering**

*PhD students:*

- Cicoare Eugeniu: *Contributions to the Implementation Possibilities of Low Pressure Equipments in Physical-Mechanical Test-Installations Used in the Chemical Technology of Leather*
- Clavac Bogdan: *Impact evaluation study on the environment induced by the refuse dumps derived from coke-chemical plants by means of mathematical modelling techniques*
- Crivineanu Marilena: *Study of heavy metal emission processes in running waters by mean of mathematical modelling methods*

**6. Prof. PhD Mircea ȘTEFĂNESCU, PhD Supervisor in Chemistry**

*PhD students:*

- Vlăzan Paulina: *Oxides nano materials used as environment sensors*
- Barbu Mirela: *The preparation and characterisation of some nanocomposites based on transitional metal chromites*
- Lungu Eugen: *VIS and UV photocatalytic oxidation in water treatment*

- Sorescu Simona Luminița: *Carboxylic complex combinations embedded in silica gels. Obtaining nanocomposites*

**7. Prof. PhD. Rodica PODE, PhD supervisor in Chemical Engineering**

*PhD students:*

- Ilinoiu Elida-Cristina: *Contributions to the development of hybrid advanced oxidation processes for the degradation of persistent organic pollutants*
- Colar Liliana Andreea: *Improvement of specific industrial effluents treatment technology by applying photocatalytic heterogenous processes*
- Jakab Agnes: *Hybrid oxidation processes used to remove refractory organic pollutants from wastewater*
- Ardelean Dorica Magdalena: *Sensors based composite materials with applications in water quality monitoring*
- Roșu Dan: *Contributions to the development of innovative inorganic materials with applications in residual effluents treatment*

**8. Prof. PhD Cornelia PACURARIU, PhD supervisor in Chemical Engineering**

- Tăculescu Alina Elena: *Powders with magnetic properties obtained by the combustion method*
- Mihoc Georgeta: *The use of some oxide and polymeric materials with tailored properties for the removal of some organic pollutants from wastewater*
- Pașka Oana: *Enzymatic biodegradation of some organic dyes from wastewater*

**PhD THESIS SUSTAINED**

1. Mirela-Nicoleta Calisevici - *Studies Regarding The Improvement And Optimization Of Drinking Waters Qualities Using Advanced Measurement Techniques And Mathematical Modeling*, PhD supervisor: prof. PhD. Eng. Delia Perju
2. PISOI Ilie: *Contributions regarding the improvements of the drinkable technologies of waters*, PhD supervisor: prof. PhD. Eng. Georgeta Burtică
3. Remes Adriana: *Use of some zeolite materials functionalized with TiO<sub>2</sub> nano crystals doped./undoped with metals/non-metals ions for wastewater treatment* PhD supervisor: prof. PhD. Eng. Georgeta Burtică
4. Ana Maria Dabici: *Nano particles type TiO<sub>2</sub> with photocatalytic activity*, PhD supervisor: prof. PhD. Eng. Nicolae Vaszilcsin
5. Tita Bogdan: *Contributions on the study of the compatibility and thermal stability of some drugs from NSAID class. Synthesis of their coordination*

compounds, PhD supervisor: prof. PhD. Eng. Mircea Ștefănescu

6. Popescu (Pintilie) Georgeta Sofia: *The evaluation of renal calculi composition by performing physico-chemical methods*, PhD supervisor: prof. PhD. Eng. Mircea Ștefănescu

## PUBLICATIONS

### BOOKS

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3. Mircea Ștefănescu, Marcela Stoia, Oana Ștefănescu, *The Sol-Gel Process: Uniformity, Polymers and Applications*, Chapter: *Nanocomposites with Controlled Properties Obtained by the Thermal Treatment of Some Tetraethyl Orthosilicate-Diols-Metal Nitrates Gels*, Nova Science Publisher New York, USA pp. 289-338
4. Adina Negrea Cristina Costache, *Chimia și protecția mediului*, Academiei Oamenilor de Știință din România (AOSR) Publisher, ISSN: 978-606-8371-06-1, pp. 109
5. Lazau Ioan, Ianos Robert, Pacurariu Cornelia, *Sinteza și procesarea micro și nanomaterialelor*, Politehnica Timisoara Publisher, ISSN: 978-606-554-409-3, pp. 265
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2. A. Negrea, M. Ciopec, L. Lupa, C. M. Davidescu, A. Popa, G. Ilia, P. Negrea, *Removal of As(V) by Fe(III) loaded XAD7 impregnated resin containing di(2-ethylhexyl) phosphoric acid DEHPA: Equilibrium, Kinetic, and Thermodynamic modeling studies*, Journal of Chemical and Engineering Data, 565, ISSN: 0021-9568, pp. 3830
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4. M. Ciopec, C. M. Davidescu, A. Negrea, L. Lupa, P. Negrea, A. Popa, C. Muntean, *Use of D2EHPA-impregnated XAD7 resin for the removal of Cd(II) and Zn(II) from aqueous solution*, Environmental Engineering and Management Journal, 10(10), ISSN: 1582-9596, pp. 1597
5. C. M. Davidescu, M. Ciopec, A. Negrea, A. Popa, L. Lupa, P. Negrea, C. Muntean, M. Motoc, *Use of di-(2-ethylhexyl)phosphoric acid (DEHPA) impregnated XAD7 copolymer resin for the removal of chromium (III) from water*, Revista de chimie, 62(7), ISSN:0034-7752, pp. 712
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  18. C. Lazau, C. Rațiu, C. Orha, R. Pode, F. Manea, *Photocatalytic activity of undoped and Ag-doped TiO<sub>2</sub>-supported zeolite for humic acid degradation and mineralization*, Materials Research Bulletin, 46, ISSN: 0025-5408, pp. 1916
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  24. A. Dabici, P. Sfirloaga, C. Lazau, C. Bandas, C. Misca, N. Vaszilcsin, *Effect Of Natural Zeolite Functionalized With Tio(2) For Enterococcus Faecalis Removal From Water*, Digest Journal Of Nanomaterials And Biostructures, 6(3), ISSN: 1842-3582, pp. 1325
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  26. C. Ratiu, F. Manea, C. Lazau, C. Orha, G. Burtica, I. Grozescu, J. Schoonman, *Photocatalytically-assisted electrochemical degradation of p-aminophenol in aqueous solutions using zeolite-supported TiO<sub>2</sub> catalyst*, Chemical Papers, 65(3), ISSN: 0366-6352, pp. 289
  27. M. Gheju, R. Pode, F. Manea, *Photocatalytically-assisted electrochemical degradation of p-aminophenol in aqueous solutions using zeolite-supported TiO<sub>2</sub> catalyst*, Hydrometallurgy, 108(1-2), ISSN: 0304386X, pp. 115
  28. I. Vlaicu, A. Pop, F. Manea, C. Radovan, *Degradation of humic acid from water by advanced electrochemical oxidation method*, Water Science and Technology: Water supply, 11(1), ISSN: 16069749 pp. 85
  29. A. Pop, C. Lazau, I. Grozescu, V. Tiponut, F. Manea, *Structural characterization and the sorption properties of the natural and synthetic zeolite*, Journal of Optoelectronics and Advanced Materials, 13(5), ISSN: 14544164, pp. 544
  30. A. Pop, E. Ilinoiu, F. Manea, G. Burtica, *Determination of organic pollutants from water by electrochemical methods*, Environmental Engineering and Management Journal, 10(1), ISSN: 1582-9596, pp. 75
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- Environmental Engineering and Management Journal, 10(10), ISSN: 1582-95961, pp.451
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  33. M. Stefanescu, M. Barbu, T. Vlase, P. Barvinschi, L. Barbu-Tudoran, M. Stoia, *Novel low temperature synthesis method for nanocrystalline zinc and magnesium chromites*, Thermochimica Acta, 526, ISSN: 0040-6031, 130
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  35. C. Orha, A. Pop, C. Lazau, P. Sfirloaga, I. Grozescu, V. Tiponut, F. Manea, *Structural and sorption properties of copper doped natural and synthetic zeolite*, Proceedings of the International Semiconductor Conference, CAS 2, ISSN: 978-161284171-7, pp. 299
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  38. M. Gheju, R. Pode, *Decontamination of Cr(VI) polluted wastewater by use of low cost industrial wastes*, World Academy of Science Engineering and Technology, 78(54), ISSN: 2010-376X, pp. 240
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  43. M. N. Calisevici, D. Perju, M.C. Lysandrou, G.A. Dumitrel, M. Glevitzky, *Determination of anion and cation contents in Cyprus drinking waters*
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  45. A. Negrea, M. Ciopec, C. Muntean, P. Negrea, L. Lupa, R. Lazau, *Studii comparative privind depoluarea apelor cu continut de As, prin adsorbție pe materiale oxidice*, Bul. AGIR, 2, ISSN:1224-7928, pp. 71
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**RESEARCH CENTRE  
CHEMISTRY AND CHEMICAL ENGINEERING OF  
ORGANIC, MACROMOLECULAR AND NATURAL  
COMPOUNDS – C.C.E.O.M.N**

**GENERAL PRESENTATION**

**Chemistry and Chemical Engineering of Organic, Macromolecular and Natural Compounds** (formerly Synthesis and Applications of Organic and Macromolecular Compounds - a research centre, type C, evaluated and approved by CNCISIS, created in 2002, in accordance with the CNCISIS certificate, nr. 47/4.12.2003) is a research center evaluated and approved by UPT research

staff in 2011. The director of the Centre is **Prof.dr.eng. Corneliu M. Davidescu**.

**MAIN ACTIVITIES**

The Center performs research activities in domains such as:

- BioNanoMaterials – obtaining, characterization and applications of the biocompounds and biosystems/cyclodextrins or liposomes nanoparticles

- Drug Design and Synthesis – molecular modeling, SAR, QSAR, virtual high throughput screening, docking, synthesis, analysis and applications of drugs
- Natural Food Flavours and Spices – isolation, purification, stabilization, conditioning, and characterization of natural extracts or compounds used as flavours and spices
- Perfumes and Cosmetics – obtaining, stabilization, characterization of natural biosystems with applications in perfumery and cosmetic industry
- New methods in organic synthesis
- Studies on structure-properties relationship using the topological model of organic molecules
- Structured packings and their applications in systems with chemical reaction
- Synthesis and characterization of PVC plasticizers
- Oligomers with functional groups
- Chemistry and technology of drugs and pesticides
- Process control equipments for research plants in chemical industry
- Control systems using computers for researching plants and low tonnage plants in chemical industry
- Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents
- Mathematical modeling and numerical simulation of environmental pollution and depollution processes
- Modeling, simulation and process control
- Heat transfer organic agents
- Unit processes
- The Intensification of Transfer Processes
- Rheological characterization of the substances

#### CONTACT

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#### RESEARCH FIELDS

##### ➤ **BioNanoMaterials**

*Keywords:* bioactive compounds, drugs, natural compounds, nanoparticles, nanocapsules, cyclodextrins, liposomes, scanning electron microscopy, SEM, transmission electron microscopy, TEM, thermogravimetry, TG, differential scanning calorimetry, DSC, preparative liquid chromatography

##### ➤ **Biocatalysis**

*Keywords:* industrial biotechnology, enzyme, hydrolase, lipase, protease, cellulase, enzyme immobilization, enzyme kinetics, ionic liquids, bioproducts, biomaterials, biopolymers, biofuels, optical resolution, enantiomer separation, lignocellulose.

##### ➤ **Drug Design and Synthesis**

*Keywords:* drugs, drug design, total synthesis, semi-synthesis, biosynthesis, quantitative structure-activity relationships, QSAR, virtual high throughput screening, VHTS, docking, gas chromatography, GC-MS, GC-FID, preparative liquid chromatography, high pressure liquid chromatography, HPLC

##### ➤ **Natural Food Flavours and Spices**

*Keywords:* flavor, flavour, aroma, food, odorant, spice, biosynthesis, biotechnology, extraction, natural food additives, gas chromatography, GC-MS, GC-FID, analytical high pressure liquid chromatography, HPLC, spectrometry, spectrofotometry, UV-Vis, sensory analysis, GC-O, GC-Sniffing, statistical multivariate analysis, PCA, HCA

##### ➤ **Perfumes and Cosmetics**

*Keywords:* perfumes, cosmetics, odorants, terpenoids, biosynthesis, biotechnology, extraction, toiletries, essential oils, volatile compounds, design of perfumes, gas chromatography, GC-MS, GC-FID, analytical high pressure liquid chromatography, HPLC, spectrometry, spectrofotometry, UV-Vis, olfactometry, GC-O, GC-Sniffing, statistical multivariate analysis, PCA

##### ➤ **New methods in organic synthesis**

*Keywords:* synthesis of organic compounds, carbonic acid derivatives, sterically hindered phenols with antioxidant activity, structure determination by NMR, biocatalysis of organic reactions

##### ➤ **Studies on structure-properties relationship using the topological model of organic molecules**

*Keywords:* topology, graphs, structure-properties relationship (SAR), size and shape of molecules, van der Waals volume and surface

##### ➤ **Structured packings and their applications in systems with chemical reaction**

*Keywords:* static mixers, motionless mixers

##### ➤ **Plasticizers for polymers**

*Keywords:* plasticizer, plasticizing

##### ➤ **Oligomers with functional groups**

*Keywords:* oligomer, functional group, reactive oligomers

##### ➤ **Chemistry and technology of drugs and pesticides**

*Keywords:* drug, pesticides, chemistry, technology, semi synthesis, agriculture

➤ **Process control equipments for research plants in chemical industry**

*Keywords:* measuring, control devices

➤ **Control systems using computers for researching plants and low tonnage plants in chemical industry**

*Keywords:* process control, research and low tonnage plants

➤ **Intensive methods for the exoneration of soil from radioactive minerals exploitation and processing areas in the condition of natural disasters or entropic accidents**

*Keywords:* climate changes, pollution, risk, sustainable chemistry, modeling

➤ **Mathematical modeling and numerical simulation of environmental pollution and depollution processes**

*Keywords:* modeling, simulation, environmental protection

➤ **The performance of columns with structured packings**

*Keywords:* wet ability, specific surface

#### Researches in *BIONANOMATERIALS*

Obtaining and analysis methods on the bioactive compounds and systems/cyclodextrins and liposomes micro/nanoparticles. The bioactive compounds used for nanoencapsulation are: drugs, natural compounds with biological activity (*e.g.* alkaloids, flavonoids, anthocyanins, fatty acids, and derivatives, volatile oils etc.), perfumes and cosmetics, natural food additives (*i.e.* natural flavors, natural colorants). This products have excellent properties in comparison with the starting materials: oxidative & thermal stability, protective properties against radiations, controlled release of the bioactive compounds, hydrosolubilization of hydrophobic biocompounds, masking of the unpleasant taste and odors, easily handling of the powdery bionanomaterials.

The methods used for obtaining of the bionanomaterials are: crystalize from solution, spray-drying, spray-chilling, fluidized bed, by mixing or melting, by ultrasonication. The main methods of separation-purification and analyses are: preparative liquid chromatography (preparative HPLC), scanning electron microscopy (SEM), transmission electron microscopy (TEM), thermogravimetry (TG), differential scanning calorimetry (DSC).

#### RESEARCH TEAM

Daniel Hădărugă, Geza Bandur, Gerlinde Rusu, Iulia Pinzaru, Volica Dămășa

#### Researches in *BIOCATALYSIS*

The biocatalysis research in Timișoara dates from 1981, when Prof. Radu Bacaloglu initiated the first

research group in this field from Romania. In the last years, the scientific interest of this group was focused on stabilization of enzymes through immobilization by sol-gel encapsulation in hybrid organic-inorganic matrices, synthesis of optically active intermediates and synthons by chemoenzymatic processes, utilization of ionic liquids in biocatalysis, valorization of lignocellulosic materials, and synthesis of new biopolymers and biomaterials from renewable resources. An important part of these activities were joint research works, accomplished in cooperation with groups from the University of Wageningen (The Netherlands), Pannon University of Veszprém (Hungary), University of Debrecen (Hungary), and Technical University of Graz (Austria).

#### RESEARCH TEAM

Francisc Peter, Cristina Paul, Livia Corîci, Ramona Croitoru, Mihaela Ungurean, Anca Ursoiu, Anamaria Todea

#### Researches in *DRUG DESIGN and SYNTHESIS*

Design of new compounds with potential drug properties and synthesis of hits. The methods used for drug design are: molecular modeling of the pharmacologically active compounds, qualitative and quantitative structure-activity relationship studies (SAR and QSAR), virtual high throughput screening (VHTS), molecular docking of the predicted drugs.

The hits selected by drug design are obtained by classical or advanced methods (total synthesis, semi-synthesis, biosynthesis), separated and analyzed by modern methods (preparative liquid chromatography – preparative HPLC, liquid and gas chromatography – HPLC and GC, <sup>1</sup>H- and <sup>13</sup>C-NMR, X ray diffraction, UV-VIS, IR, MS spectroscopy) and further evaluated as drugs.

#### RESEARCH TEAM

Daniel Hădărugă, Mihai Medeleanu, Geza Bandur, Gerlinde Rusu, Iulia Pinzaru, Volica Dămășa

#### Researches in *NATURAL FOOD FLAVOURS AND SPICES*

Developing new natural food flavours and spices with enhanced stability and bioactivity, more healthy and with functional properties. The obtaining of food flavours and spices (especially those from the romanian tradition) are realized by classical methods (non-aggressive, such as hydrodistillation, hydroalcoholic or supercritical fluid extraction etc.). The analysis of these biosystems are realized by chromatographic (GC, HPLC, GC-O, TLC), spectroscopic (FT-IR, UV-Vis, NMR), and sensorial methods. The protection and controlled release of the natural bioactive compounds are realized by micro/nanoencapsulation in natural bioavailable matrices (such as cyclodextrins and

liposomes), and the analysis of these nanoparticles/nanocapsules are realized by microscopic and thermal analyses (e.g. SEM, TEM, TG, DSC).

#### **RESEARCH TEAM**

Francisc Peter, Daniel Hădărugă, Mirabela Pădure, Geza Bandur, Gerlinde Rusu, Cristina Paul, Iulia Pînzaru, Volica Damșa

#### **Researches in PERFUMES AND COSMETICS**

Design and evaluation of new perfume and cosmetic formulations. The main ingredients from perfume or cosmetic formulations are obtained from natural resources (especially from the traditional herbs) by classical or modern methods (hydrodistillation, hydroalcoholic or supercritical fluid extraction, pervaporation etc.). The analysis of these biosystems are realized by gas chromatography (GC-FID, GC-MS, GC-Sniffing etc.), liquid chromatography (RP-HPLC-UV-Vis/MS) spectroscopic methods for bioactive compounds (FT-IR, UV-Vis, NMR), and sensory analysis. The protection and controlled release of the natural odorant compounds from natural bioactive systems are realized by micro/nanoencapsulation in natural bioavailable matrices (such as cyclodextrins and liposomes), and the analysis of these nanoparticles are realized by microscopic and thermal analyses (e.g. SEM, TEM, TG, DSC).

#### **RESEARCH TEAM**

Daniel Hădărugă, Mirabela Pădure, Gerlinde Rusu, Iulia Pînzaru, Volica Damșa

#### **Researches in NEW METHODS IN ORGANIC SYNTHESIS**

Synthesis of organic compounds (carbonic acid derivatives, phenolic antioxidants, amino acids and peptides) using new methods or reagents: single electron transfer reactions, triphosgene as a low toxic and easy to handle substitute of phosgene, isatoic anhydrides.

The chemistry of organic derivatives of carbonic acid is the traditional field of our Department, pioneered by Professor Giorgio Ostrogovich. Studies in the field of synthesis of chlorocarbonates, carbonyl chlorides, carbamates, carbonates, ureas, aryl cyanates, isocyanides and heterocyclic as well as kinetics and mechanisms of reactions of carbonic acid derivatives were performed. Since 1980 synthesis of phenolic antioxidants, studies of biocatalytic processes in organic synthesis and structure determination of organic compounds by NMR spectroscopy were also investigated.

#### **RESEARCH TEAM**

Carol Csunderlik, Mihai Medeleanu, Marius Milea

#### **Researches in STUDIES ON STRUCTURE-PROPERTIES RELATIONSHIP USING THE TOPOLOGICAL MODEL OF ORGANIC MOLECULES**

The topological model, as an application of graph theory in chemistry is a useful tool for quantification of molecular structure and has been largely used in the last years, due to its simplicity and good correlation results in studies concerning the shape and size of molecules and structure-properties relationship for many classes of compounds.

By applying the topological model to organic molecules, information's like the number of atoms and the connectivity's are compressed in numbers named topological indices. These can be correlated with physical and chemical properties and biological activities and are also used to describe the shape and size of molecules. Better correlation coefficients were obtained when certain heteroatom were included into topological model (halo derivatives, oxygen and sulphur derivatives, and local anesthetics). Van der Waals surface and volume of organic molecules were also performed using the Monte Carlo algorithm.

#### **RESEARCH TEAM**

Mihai Medeleanu, Daniel Hădărugă

#### **Researches in STRUCTURED PACKINGS AND THEIR APPLICATIONS IN SYSTEMS WITH CHEMICAL REACTION**

The structured packings (former name: static mixers or motionless mixers) increase the mixing efficiency in all flow regime, but any other device does not equalize their performances in the laminar flow regime. Their application in all types of reactive systems (homogeneous or heterogeneous) has started several years ago and is in a continuous expansion. Recently, catalysts supported on static mixers are commercially available.

Since 1986, different applications were developed (e.g. reactor for hydrogenation of fatty oils, CO<sub>2</sub> absorption in monoethanolamine solutions). Theoretical studies include: investigations concerning the mixing mechanism in columns equipped with Sulzer SMV type static mixers; influences of main parameters on the size and distribution of the droplets formed in column fitted with structured packings; analysis of gas holdup and solid distribution in three phase gas-liquid-solid reactors equipped with different motionless mixers in order to grow the liquid phase conversion in slurry bubble columns.

#### **RESEARCH TEAM**

Lucian Rusnac, Sabina Nițu, Carmen Rusnac

#### **Researches in PLASTICIZERS FOR POLYMERS**

The undertaken research aims to correlate the structure and the plasticizing properties, both

permanent and temporary of certain polymers, belonging to new series of chemical compounds.

More than 100 new substances have been synthesized, described and assessed. Within the same framework of activity, there has been a practical and theoretical concern for the problems of both permanent and temporary plasticizing of polar polymers, thus enabling the drawing of conclusions with a view to industrial applications and to new correlation of the structure and the plasticizing properties. The research is represented by more than 60 scientific papers and research agreements.

#### RESEARCH TEAM

Geza Bandur, Gerlinde Rusu

#### Researches in OLIGOMERS WITH FUNCTIONAL GROUPS

Synthesis and characterization of some low-molecular polymers of different structure, containing two or several functional groups capable of undergoing some subsequent chemical transformations

Synthesis, characterization and application of dimethacrylates as reactive plasticizers for poly(vinyl-chloride). Synthesis and characterization of functional oligomers under non-stoichiometric conditions with a total conversion ( $\alpha,\omega$ -dihydroxy-polyesters). Chemical modification of polyethylene oligomers.

#### RESEARCH TEAM

Geza Bandur, Gerlinde Rusu

#### Researches in PHYSICAL CHEMISTRY. CHEMICALLY ACTIVE SPECIES GRAFTED ON POLYMER-SUPPORTS

Preparation and investigation of chemically active species (catalysts, reagents, substrates, enzymes, polycationic biocides) grafted on polymer-supports (styrene-divinylbenzene copolymers, polyethylene glycol) acting as "hybrid-phase" systems. Studies on the structure-activity relationship. Synthesis and testing of multifunctional or multistep recyclable and reusable catalysts.

Since 1982 the research program in the field was focused on the synthesis of the new types of polymer ligand homologous of Schiff bases, hydrazones, oximes and azines by polymer-analogous reactions, synthesis of polymer-grafted tertiary heterocyclic amines acting as "hybrid-phase" biomimetic catalysts similar to chemotripsine and studies of the kinetics, mechanism and structure-activity relationship in a test reaction of activated esters hydrolysis. A new kinetic model of the nucleophile bimolecular substitution using phosphonium and/or ammonium salts grafted on polymer-supports as phase-transfer catalysts was proposed.

#### RESEARCH TEAM

Corneliu Davidescu, Erika Reisz, Radu Ardelean

#### RESEARCH PROJECTS

1. HURO 0901/274/2.2.2 (2011-2012): *Isolation, enantioselective synthesis and structure elucidation of heterocycles with potential pharmacological activity (HETEROCYCLES)*

Value: 33.500 euro (17.800 euro in 2011)

Director: Prof.dr.eng. Francisc PETER

Members: Lect.dr.eng. Vasile BERCEAN

Assist.dr.eng. Cristina PAUL

PhD Stud.eng. Ramona CROITORU

PhD Stud.eng. Anca URSOIU

PhD Stud.eng. Anamaria TODEA

#### FIELD DESCRIPTION

The project is developed in the Priority Axis 2 (Strengthen social and economic cohesion of the border area), Key Area of Intervention 2.2 (Promotion of cooperation in the field of R+D and innovation) and Action 2.2.2 (Delivery of joint research projects) of the Operational Programme. It allows dissemination of scientific knowledge, establishes personal contacts between scientists from the border area of the Romania and Hungary, and bring together the expertise and instrumentation of partners, to promote scientific cooperation.

In the framework of drug development and application, synthesis of heterocycles with potential pharmacological activity represents a major scientific topic. This project will provide new methods for synthesis and analysis of pharmaceutically active compounds. The main objectives of the project are:

- 1) HPLC-CD and HPLC-MS analysis of the flavanolignan components of *Silybum marianum*, which is the natural source of (+)-silybin, the active ingredient of the hepatoprotective drug Legalon (Madaus AG, Köln) used in the treatment of liver diseases. Identification of possible new drugs.
- 2) Enantioselective synthesis and pharmacological studies of the flavanolignan components of *Silybum marianum*.
- 3) Synthesis of optically active O- and O,N-heterocycles of potential pharmacological activity with enzyme-catalyzed kinetic resolution and organocatalysis.
- 4) Characterization of new compounds by MS and spectroscopic methods, determination of their absolute configuration by chiroptical methods.
- 5) Establishment of cross-border research network for efficient structure elucidation of synthetic and natural products with an emphasis on MS and coupled MS techniques and chiroptical methods.

2. PN2 PC 72152/1.10.2008: *Synthesis and investigation of biodegradable polymers based on polylactic acid, with applications in medicine (BIOPLAST)*

*Value:* 87602 RON (33347 RON / 2011)  
*Director:* Assoc.prof.dr.eng. Geza BANDUR  
*Members:* Prof.dr.eng. Francisc PETER  
 Assist.dr.eng. Gerlinde RUSU  
 PhD Stud. eng.  
 Sandor KAKASI-ZSURKA

#### FIELD DESCRIPTION

One of the main contemporary scientific challenges is discovery and manufacturing of new ecologically friendly, biodegradable and biocompatible polymers which could replace the existing polymeric materials.

Poly(lactic acid) is such a material, extensively studied for industrial and biomedical applications. Its biocompatibility is owed to lactic acid, the degradation products which can be metabolized.

The main objectives of this project are the synthesis and characterization of polymeric structures with new properties, based on racemic and/or enantiomerically pure (L-form) lactic acid. Polycondensation reactions of lactic acid monomers will be investigated by non-catalyzed reactions at 100-300°C, or in microwave conditions. Inclusion of other monomers like as diphenyl-methyl isocyanate and/or ethyleneglycols in the polymer chain will be also studied to obtain new copolymers with improved properties and extended applications.

Oligomer mixtures and multibloc copolymers will be characterized by specific methods as size-exclusion chromatography, magnetic resonance spectrometry, mass spectrometry, infrared spectroscopy, thermal analysis. The mechanistic and elastic properties of the new biopolymers will be also evaluated, compared to well-known polymeric materials (polyvinyl chloride, polyethylene, polyurethanes), as well as the degradation and biodegradation properties.

#### ACTIVITIES

- Survey of the recent scientific literature concerning biodegradable polymers holding ester linkages

3. P4 – Priority Domains Partnership, Research grant 52-145 (2008-2011), *Antioxidant and Hypoglycemia Food Supplements with Anthocyanidin Structure (SAHASA)*

*Value:* 200 000 RON (3 000 RON/2011)  
*Director:* Assoc. prof. dr. eng.  
 Mihai MEDELEANU  
*Members:* Assist. dr. eng. Valentin BADEA  
 Assist. eng. Zlatimir STANOIEV  
 PhD Student Eng. Iulia Păușescu

#### FIELD DESCRIPTION

This project is focused on the evaluation of potential antioxidant activity as well as hypoglycemia effects of compounds with

anthocyanidin structure obtained from natural extracts.

#### ACTIVITIES

- Identification and dosage of possible antioxidant activity and hypoglycemia effects components from inland plant species.
- Technology setup for biological active components extraction
- Physico-chemical methods for exactly identification of structures and compositions of biological active mixtures.
- *In vitro* testing of biological activity.

4. PN2 PC-62072 / 1.10.2008: *Hepatoprotecting nanoparticles with enhanced bioavailability (Nano-HEPAT)*

*Value:* 326 750 RON (78 039 RON/2011)  
*Director:* Lect.dr.eng. Daniel-Ioan HĂDĂRUGĂ  
*Members:* Assoc.prof.dr.eng. Geza N. BANDUR  
 Prof.dr.eng. Francisc PETER  
 Assoc.prof.dr.eng.Mihai MEDELEANU  
 Lect.dr.eng. Andra TAMAS  
 Teach.assist.dr.eng. Gerlinde RUSU  
 Teach.assist.dr.eng. Cristina PAUL (ZARCULA)  
 PhD Stud. eng. Iulia A. PÎNZARU  
 Tehn. Volica DAMȘA

#### FIELD DESCRIPTION

In this project, the obtaining (separation, purification), semi-synthesis, nanoencapsulation, analysis, and hepatoprotective evaluation of natural or modified biosystems or biocompounds from *Chelidonium*, *Berberis*, *Matricaria* species will be studied.

The obtaining of the hepatoprotective biosystems from *Chelidonium*, *Berberis*, *Matricaria* species will be realized by classical ethanol-water extraction, the extracts will be fractionated by preparative liquid chromatography, and evaluated from the hepatoprotective point of view. The extracts/fractions/natural compounds with the best activity will be used for the obtaining of cyclodextrin-like nanoparticles (or other encapsulation matrices). Furthermore, some active compounds will be chemically modified in order to increase the hepatoprotective activity and these compounds will be used for the obtaining of nanoparticles with enhanced bioavailability.

The analysis of the extracts/fractions/natural or modified compounds will be realized by GC (after derivatizing), HPLC, MS, NMR, FT-IR etc. The analysis of nanoparticles will be realized by microscopical methods (SEM, TEM, AFM), thermoanalytical methods (thermogravimetry, differential scanning calorimetry), X ray diffraction, EDAX etc.

## ACTIVITIES

- Literature survey on the obtaining and characterization of *Chelidonium*, *Berberis*, *Matricaria* extracts/main compounds, and on the obtaining and analysis of such bioactive compounds/cyclodextrin nanoparticles;
- Experimental design of the nanoencapsulation processes between bioactive compounds/cyclodextrins;
- Obtaining and characterization of the *Chelidonium*, *Berberis*, *Matricaria* extracts/fractions/bioactive compounds (with hepatoprotective activity);
- Obtaining and characterization of the bioactive compounds or extracts/cyclodextrin nanoparticles (with enhanced bioavailability on the hepatoprotection);
- Optimization of the nanoencapsulation processes.

**PhD RESEARCH ACTIVITIES**

1. Prof.dr. Carol CSUNDERLIK, PhD supervisor

*PhD students:*

- Palani Adil: *Thermal Decomposition of N-Carbamoyl Derivatives of Cyclic Imides*
- Paușescu Iulia Maria: *Doctoral School*
- Pinteă Benjamin Nicolae: *Doctoral School*

2. Prof.dr.eng. Alfa-Xenia LUPEA, PhD supervisor

*PhD students:*

- Grăvilă Corina: *Synthesis of substituted N-amides of aromates hydroxy-acids*
- Taloș Ioan (\*): *Synthesis and properties of some phosphonic acids and derivatives*

3. Prof.dr.eng. Corneliu-Mircea DAVIDESCU, PhD supervisor

*PhD students:*

- Kakasi-Zsurka Sandor: *New bioactive compounds by modification of polyhydroxyalkanoates*
- Croitoru Ramona: *Synthesis of carbohydrate oligomers and polymers by enzymatic catalysis*
- Răfăilă Madian: *Doctoral School*
- Ardelean Radu Ovidiu: *Doctoral School*
- Peli Beata Monika (căs. Cioplea): *Doctoral School*
- Urmosi Zoltan Gyula (\*): *Doctoral School*

4. Prof.dr.eng. Lucian RUSNAC, PhD supervisor

*PhD students:*

- Anghelescu Mihaela-Sorina: *Polymers from regenerable sources*

- Ștefan Liliana-Marinela: *Obtaining and characterization of some carbohydrates-based polymers*
- Dobren Flavius Andrei: *Modeling and simulation research of the carbon dioxide dispersion process in urban environment*
- Maris Ioan-Dorel: *Identification and analysis of industrial technological risks*
- Kiss Antonie Gabriel: *Contribution regarding the polyurethans*
- Schmidt Adreea Cristina: *Doctoral School*

5. Prof.dr.eng Liviu MIRCI, PhD supervisor

*PhD students:*

- Ismană Lidia Anița: *Doctoral School*

6. Prof.dr.eng Francisc PETER, PhD supervisor

*PhD students:*

- Ungureanu Mihaela: *Bioethanol from lignocellulosic sources (Doctoral School)*
- Ursoiu Anca: *Optically active compounds obtained by enzymatic catalysis (Doctoral School)*
- Fitigau Firuta: *Enzymatic modification of lignin and lignin compounds*
- Todea Anamaria: *Doctoral School*

**PhD THESIS SUSTAINED**

1. Mihai-Cosmin PASCARIU: *Carbohydrate based surfactants*; December 24, 2011; PhD supervisor: Prof. Dr. Eng. Lucian Mircea Rusnac
2. Valentina-Liliana BIRA: *Optimization of chip-based electrospray mass spectrometric methods for biomolecule analysis*; October 24, 2011; PhD supervisor: Prof. Dr. Eng. Lucian Mircea Rusnac
3. Iulia Andreea PÎNZARU: *Flavonoids and bioconjugates with biological activity: synthesis, analysis, and enhanced bioavailability by molecular encapsulation*; November 29, 2011; PhD supervisor: Prof. Dr. Eng. Francisc Peter
4. Carmen Manuela PLEȘA: *Juniperus extracts: obtaining and uses in pharmaceuticals, cosmetics, and food fields*; September 27, 2011; PhD supervisor: Prof. Dr. Eng. Alfa Xenia Lupea
5. Corina-Iuliana COSTESCU: *Stabilization of some bioactive compounds from Compositae family plants by nanoencapsulation in cyclodextrins*; October 10, 2011; PhD supervisor: Prof. Dr. Eng. Alfa Xenia Lupea
6. Corîci Livia Nicoleta: *Immobilization of protease alcalase for application in peptide synthesis*; December 20, 2011; PhD supervisor: Prof. Dr. Eng. Corneliu Mircea Davidescu

## PUBLICATIONS

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1. Diudea, M.; Medeleanu, M., *Hosoya vs. Wiener Polynomials*. In: *Distance in Molecular Graphs - Applications*, Gutman, I.; Furtula, B. (Eds.), University of Kragujevac, Serbia, 2011, ISBN: 978-86-6009-015-9, 28 pages
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