Project title:

Multifunctional nanostructured silicone materials

Acronym:

NANOSIMAT

Contract 52/2006

Person in charge: Dr. Maria Cazacu

Partners

Main contractor:

"Petru Poni" Institute of Macromolecular Chemistry Iasi, Romania

Project coordinator: Dr. Maria Cazacu

Partner P1

"Gh. Asachi" Technical University Iasi, Romania–UTI

Prof. Dr. Silvia Curteanu

Partner P2

"Al. I. Cuza" University Iasi, Romania– UAIC

Prof. Dr. Felicia Iacomi

Partner P3

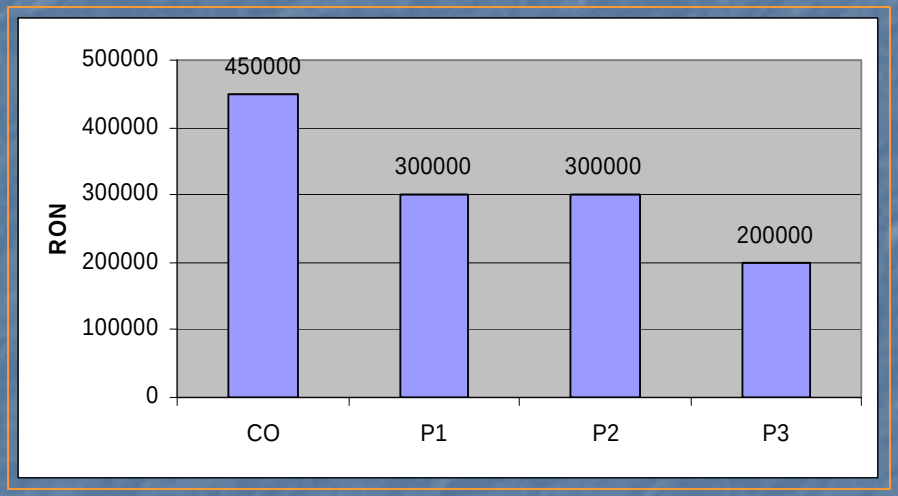
Research & Development National Institute for Electrical Engineering – INCDIE ICPE-CA

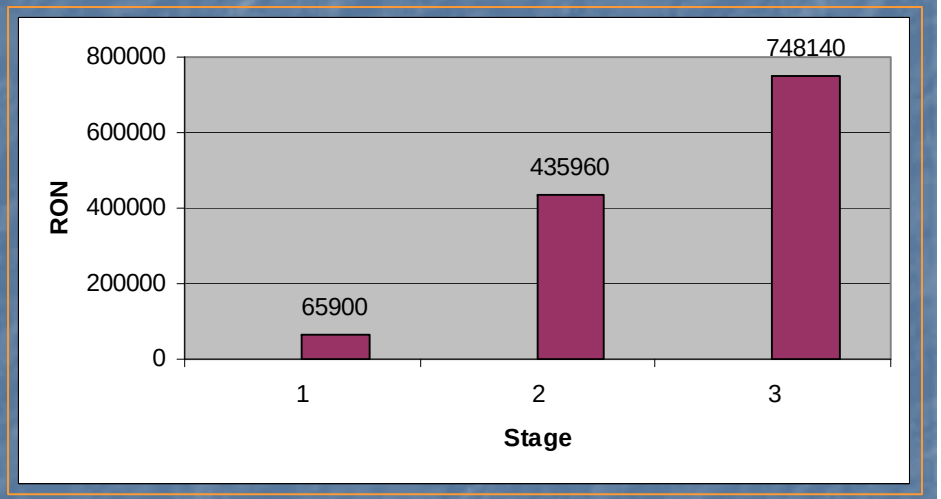
Dr. Petru Budrugeac

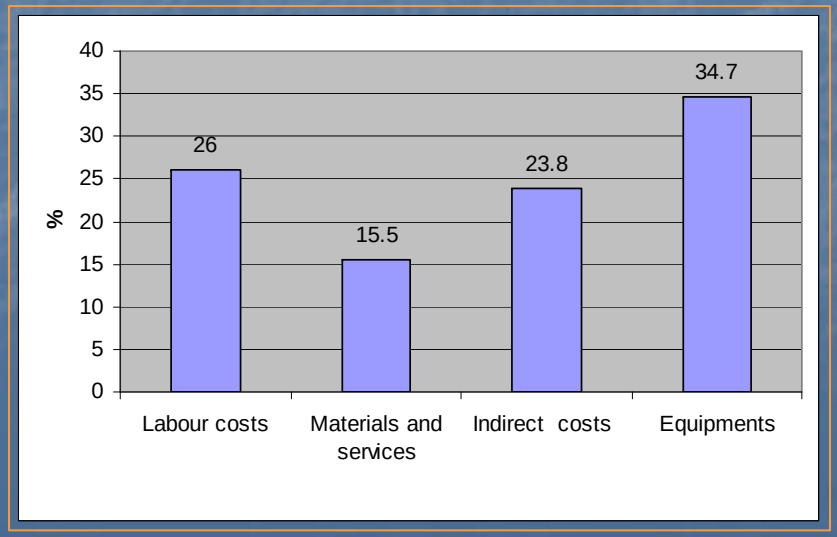
Project funding and costs plan

Total budget: 1 250 000 lei

Cofunding: -







General Objectives

1. Development of the *research activity* in a specialized area, that of the silicon based polymers, by optimum concentration and capitalization of the scientific potential, in order to reach the excellency level recognized by international standards.
2. Development of *new siloxane polymers* and materials on their basis, having new properties, through a new approach, using the instruments of artificial intelligence.
3. Valorization of the new synthesized products by *evaluating their properties*.
4. Integration of education and research by paralel aproach of both scientific and human resource formation - specialization elements.
5. Development of required *research infrastructure*.
6. Formation and development of a *research network* based on the experience and complementarity of competences, which to affords the enlargement of researches and to prepare the participation to the FP7.

Specific Objectives

1. Developments in the field of organo-siloxane copolymers capable of structuration by phase separation
2. New liquid crystalline (LC) polymers containing siloxane segments.
3. Polysiloxanes modified with polar or complexing groups
4. Polymeric structures containing siloxane segments and complexed metal units.
5. Siloxane/metal complexes nanocomposites by sol-gel technique .
6. Techniques of artificial intelligence with applications to the silicon based polymeric materials.

Project`s targets

New compounds and materials

Improved preparation techniques, new approaches to characterization and properties evaluation.

Models and techniques for optimization and classification

Human resources training

Improvement of the infrastructure

Scientific articles in ISI journals

Strengthening of the group having a competitive research area able to develop new national and international projects.

Phase I (1.08-20.11.2006): ***Developments in the field of organo-siloxane copolymers capable of structuration by phase separation.***

Achieved objectives:

1. Evaluation of the state and tendencies of the researches in the approached field by the project

2. Preparation of organo-siloxane copolymers with different internal functionalities

3. Investigation of the properties of synthesized copolymers

4. Literature survey on techniques of artificial intelligence used in polymerization processes engineering

Phase II (21.11.2006 – 30.05.2007) : *New liquid crystalline (LC) polymers containing siloxane segments*

Achieved objectives:

1. **Developments in synthesis and applications of polymeric liquid crystals**
2. **Preparation of new organo-siloxane copolymers with liquid crystal properties**
3. **Artificial intelligence techniques applied on the silicon-based polymeric materials instruments in processes based on silicon polymers**
4. **Classification algorithms used in the properties prediction**

Phase III (1.06.2007-15.10.2007) : ***Polysiloxanes modified with polar or complexing groups***

Achieved objectives:

1. Preparation of siloxanes modified with polar or complexing groups

2. Study of the properties of polar groups modified polysiloxanes

3. Evaluation of applicative potential of polar groups modified polysiloxanes

4. Modelling of the process to obtain polymeric nanoparticles stabilized with silicone surfactants by using neuronal networks

5. Study of the properties of siloxanes modified with complexing groups

Phase IV (*6.10.2007-30.05.2008*) : *Polymeric structures containing siloxane segments and complexed metal units*

Achieved objectives:

1. Preparation of new polymers containing siloxane segments and complexed metal units

2. Study of the properties of siloxane polymers with complexed metal units in the main chain

3. Modelling of the metal complexed by siloxane ligands process

Phase V (1.06.2008-31.11.2008) : *Siloxane- metal complexes nanocomposites by sol-gel technique*

Achieved objectives:

1. Preparation of silica xerogels doped with metal complexes

2. Evaluation of multiple properties by different techniques

3. Genetic algorithms – artificial inteligence instruments used in the processes optimization

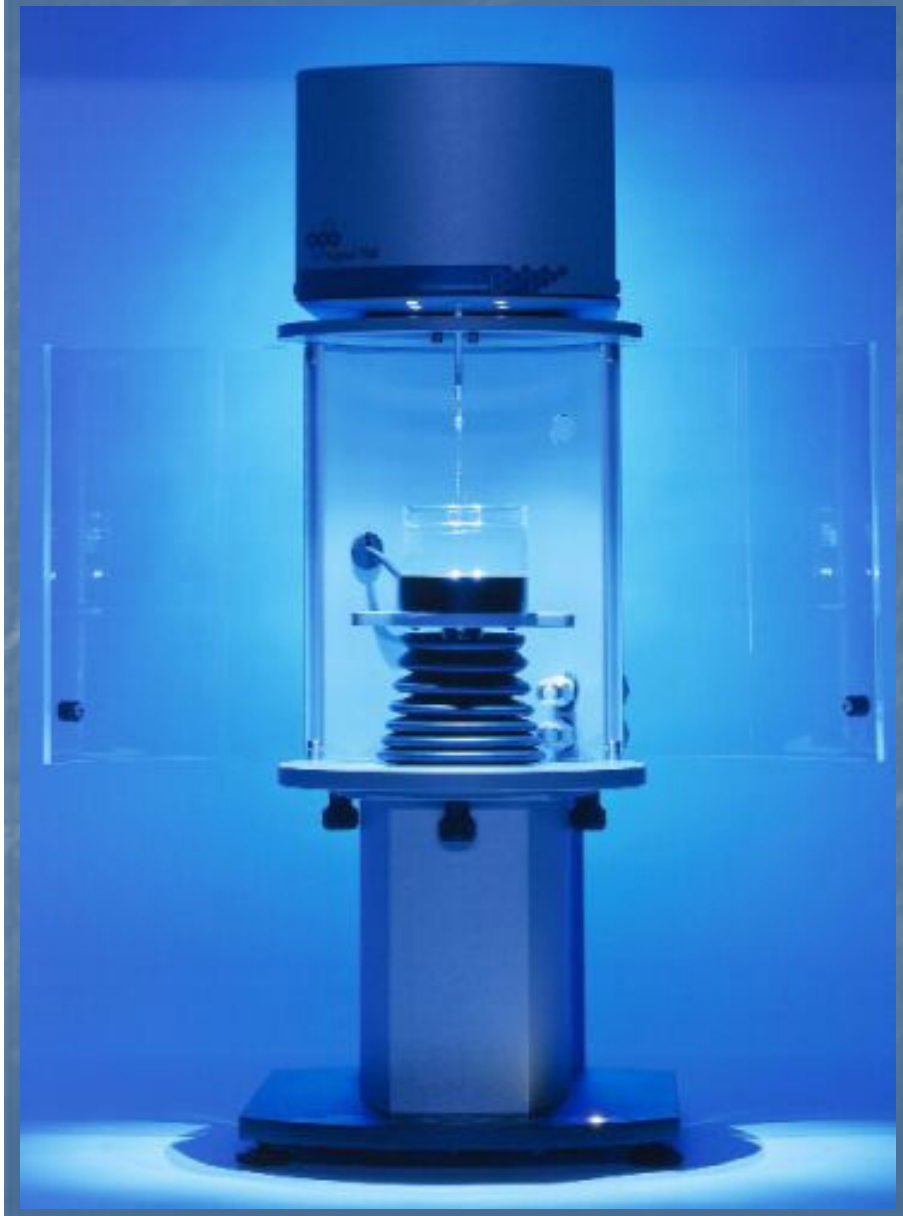
Compound types synthesized and studied in the project framework

1. Siloxane-organic copolymers able to structurate by phase separation
2. Liquid crystal polymers containing siloxane sequences
3. Polysiloxanes modified with polar or complexing groups
4. Siloxane/metal complexes nanocomposites by sol-gel technique

Acquisited equipments

1. Sigma 700 KSV Tensiometer (CO)
2. Dynamic Vapor Sorption Analyser (CO)
3. Compact Microwave Electron Spin Resonance Spectrometer (P2)

Sigma700 Tensiometer



Specifications

Measuring range 0.001 to 2000 mN/m

Resolution (standard probe) 0.001 mN/m

Maximum load 210 g

Weighing resolution 0.01 mg

Force resolution 0.1 µN

Contact Angle range 0-180°

Contact Angle resolution 0.01°

Calibration and locking Automatic

Stage speed 0.01-500 mm/min (others by reques

Stage positioning resolution 0.015 µm

Computer interface USB (RS232 as option)

Temperature range -10 to 80°C

Stainless steel water jacket -10 to 150°C

Electrically heated jacket room temp. to 250°C

Measurements 240 x 330 x 620 mm (D x W x H)

Software modules ST/IT Software

DCA Software

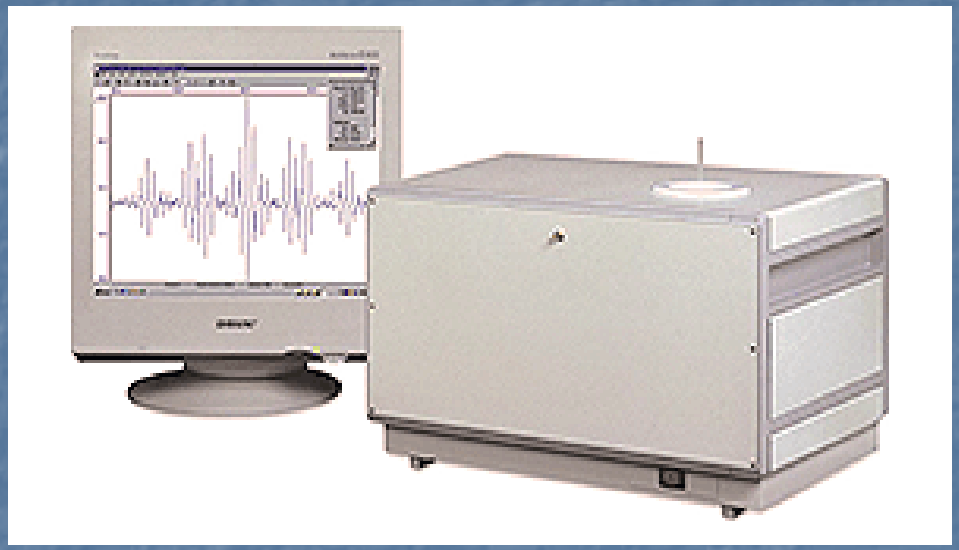
CMC Software

Density Software

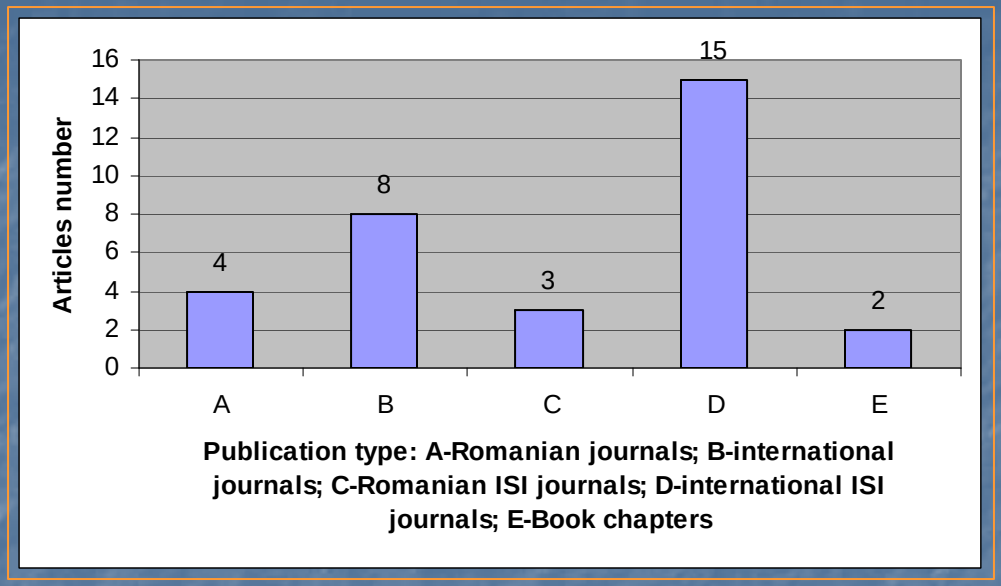
Powder Wettability and Sedimentation Software

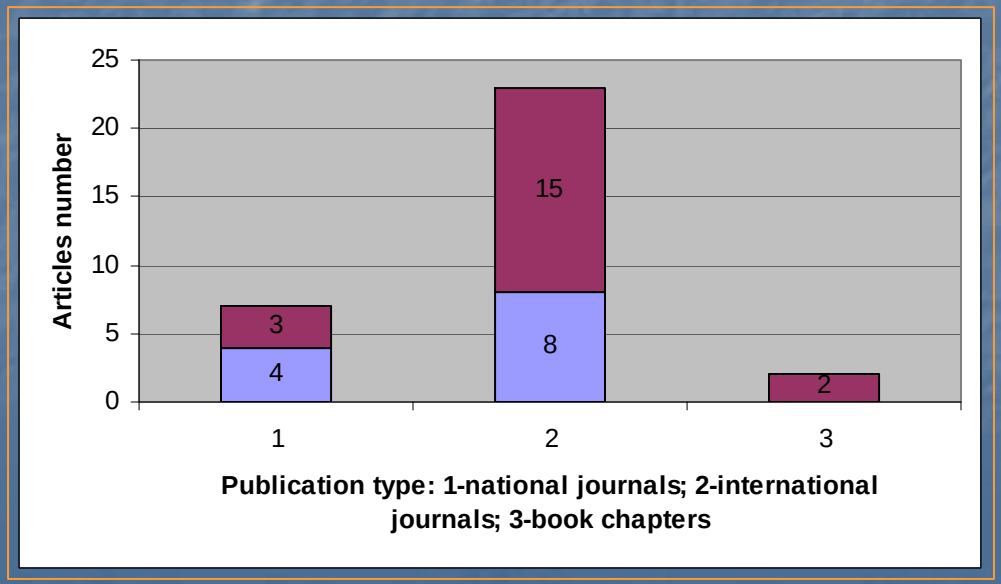
Dynamic Vapor Sorption Analyser

Compact Microwave Electron Spin Resonance Spectrometer



The project's results dissemination





Articles published in international peer reviewed scientific journals:

1. G. I. Rusu, A. Airinei, C. Baban, G. G. Rusu, D. Mardare, M. Rusu, Studies on the electronic transport and optical properties of some new chelate modified polysulfones in thin films, *J. Appl. Polym. Sci.,* 99(1), 100, 2006.
2. S. Bronnikov, C. Racles¸ A. Nasonov, M. Cazacu, Kinetics of the nematic ordered phase growth during a temperature quench of an isotropic siloxane-azomethine polymer, *Liq. Cryst.*, 33(9), 1015–1019, 2006.
3. C. Racles, V. Cozan, I. Sajo, Influence of Chemical Structure on Processing and Thermotropic Properties of Poly(siloxane-azomethine)s, *High Perform. Polym.* 19 (5), 541-552, 2007
4. P. Budrugeac, E. Segal, Applicability of the Kissinger equation in thermal analysis: revisited, *J. Therm. Anal. Calorim.*- 88 (3), 703-707, 2007.
5. P. Budrugeac, The Kissinger law and the IKP method for evaluating the non-isothermal kinetic parameters, *J. Therm. Anal. Calorim.*, 89 (1), 143-151, 2007.
6. G. Rusu, E. Rusu, L. Leontie, G. I. Rusu, Electrical DC Conduction Mechanism in Some Newly Synthesized Nylon 6/12 Copolymers, *J. Polym. Sci. Part B: Polym. Phys.*, 45, 794–799, 2007.
7. P. Budrugeac, C. Racles, V. Cozan, M. Cazacu, Thermal and thermo-oxidative stabilities of some poly(siloxane-azomethine)s, *J. Therm. Anal. Calorim.*, 92(1), 263–269, 2008.
8. M. Cazacu, A. Vlad, G. Munteanu, A. Airinei, Multifunctional materials based on polyazomethines derived from 2,5-dihydroxy-1,4-benzoquinone and siloxane diamines, *J. Polym. Sci. Part A: Polym. Chem.* 46(5): 1862-1872, 2008
9. S. Curteanu, M. Cazacu, Neural Networks and Genetic Algorithms Used for Modeling and Optimization of the Siloxane-Siloxane Copolymers Synthesis, *J. Macromol. Sci., Part A: Pure Appl. Chem.* 45(1), 23-36, 2008
9. M. Purica, F. Iacomi, C. Baban, P. Prepelita, N. Apetroaei, D. Mardare, D. Luca, Investigation of structural properties of ITO Thin films deposited on different substrates, *Thin Solid Films*, 515, 8674-8678 ,2007.
10. M. Alexandru, M. Cristea, M. Cazacu, A. Ioanid, B. C. Simionescu, Composite materials based on polydimethylsiloxane and *in situ* generated silica by using the sol-gel technique, *Polym. Compos, Published Online: Jun 20 2008 10:29AM DOI: 10.1002/pc.20608*
11.A. Vlad, M. Cazacu, G. Munteanu, A. Airinei, P. Budrugeac, Polyazomethines Derived from Polynuclear Dihydroxyquinones and Siloxane Diamines, *Eur. Poly. J. 44: 2668-26777 (2008)*
12. M. Alexandru, M. Cazacu, F. Iacomi, S. Vlad Polydimethylsiloxane-silica composites. Influence of the silica on the morphology and the surface, thermal, mechanical properties, *High Performance Polymers first published on October 13, 2008 doi:10.1177/0954008308094327*

Articles published in Romanian peer reviewed scientific journals:

1. P. Prepelita, C. Baban, F. Iacomi, The study of influence of Al and Sn doping on the optical and electrical properties of ZnO thin films, *J. Optoelectron. Adv. Mater.* 9(7) 2166 –2169, 2007.
2. A. Nistor, C.G. Piuleac, M. Cazacu, S. Curteanu, Neural network modeling of the equilibrium anionic polymerization of cyclic siloxane, *Mater. Plast., 45(1), 67-73,2008.*

Publications in Conference Proceedings and other journals

1. C. Racles, M. Cazacu, Siloxane-containing liquid-crystalline supramolecular polymers with tailored mesophase range, *Volumul: Second Bilateral Symposium „Functional Polymers", Berlin, 2-8 October 2006- CD*
2. M. Cazacu, A. Vlad, C. Racles, M. Alexandru, M. Marcu, Multifunctional siloxane-based polymeric structures containing metals, *Volumul: Second Bilateral Symposium „Functional Polymers", Berlin, 2-8 October 2006 – CD*
3. S. Curteanu, M. Cazacu, Neural networks based prediction and optimization applied to siloxane-siloxane copolymers synthesis, *Lecture Series on Computer and Computational Sciences, Volume 6, pp. 120-123, ISBN 90 04 15542 2, 2006*
4. M. Cazacu, A. Vlad, C. Racles, M. Alexandru, Condensation Polymers of the Metallocenes and Siloxane Derivatives, *Volumul: European Polymer Congress*, Portoroz, 2007
5. C. Racles, S. Curteanu, V. Cozan, M. Cazacu, Thermotropic poly(siloxane-Schiff bases): synthesis of new polymers and predictions of lc properties based on neural network, *Volumul: European Polymer Congress*, Portoroz, 2007
6. A. Vlad, M. Cazacu, A. Airinei, A new lanthanum complex encapsulated in silica network by sol-gel technique, *Volumul: A 5–a Conferinta Nationala "DIRECTII NOI DE CERCETARE IN STIINTA MATERIALELOR", ARM* – 5, 5-7 Septembrie, 2007, Sibiu, Romania, p. 399-341.
7. G. Lisa, C. Lisa, S. Curteanu, Application of feed-forward neural networks in prediction of excess molar volumes from experimental refractive index, *Proceedings of the Applied Sciences Symposium*, Bacău, p. 163-168, 2007.
8. C. Lisa, S. Curteanu, Neural network based predictions for the liquid crystal properties of organic compounds, *Proceeding 17th European Symposium on Computer Aided process Engineering*, ESCAPE 17, 27-30 mai, Bucuresti, 2007.
9. C. Lisa, S. Curteanu, G. Lisa, D. Apreutesei, Neural networks used to predict the relationship between liquid crystalline behaviour and chemical structures, *Bulletin of the Transilvania University of B*raşov, vol.3, 521-526, 2007
10. M. Alexandru, M. Cristea, C. Racles, M. Cazacu, Amphiphile networks reinforced with in situ generated silica, *Annual Meeting of the Polymer Processing S*ociety, PPS-24, Salerno (Italy), 15 - 19 June 2008.
11. M. Cazacu, A. Vlad, A. Airinei, C. Racles and M. Alexandru, Silica encapsulating lanthanum complexes by sol-gel technique, *Annual Meeting of the Polymer Processing Society*, PPS-24, Salerno (Italy), 15 - 19 June 2008.
12. S. Curteanu, M. Cazacu, N. Curteanu, Functional silica xerogel. modeling of the metal ions retaining process, *Annual Meeting of the Polymer Processing Society*, PPS-24, Salerno (Italy), 15 - 19 June 2008.

Book chapters:

1. M. Cazacu, Siloxane based Polymeric Structures containing Complexed Metals in “Advances in Organometallic Chemistry Research, (Kenji Yamamoto, Ed.), 2007, 227-256, Nova Science Publishers, ISBN: 1-60021-779-6
2. E. S. Dragan, M. Cazacu, “Ionic hybrid hydrogels” in "New Trends in Ionic (Co)Polymers and Hybrids” (Ecaterina Stela Dragan, Ed.), 145-164, Nova Science Publishers, 2007, ISBN: 1-60021-611-0
3. L. Marin, V. Cozan, E. Perju, Thermotropic Liquid Crystalline Poly(azomethine-ether-sulfone)s. Synthesis and Properties in “Functional Poymeric Materials Designed for Hi-Tech Applications “ (editor M. Nechifor), Research Signpost

International Conferences

Oral presentations

1. M. Cazacu, A. Vlad, C. Racles, M. Alexandru, New functional silicone-based materials, *8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
2. M. Alexandru, M. Cristea, M. Cazacu, A. Ioanid, F. Iacomi, Le renforcement des polysiloxanes avec de la silice obtenue in situ ou ex situ. Études comparatives, *8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
3. V. Cozan, L. Marin, E. Avram, Comportement thermotrope de polysulfones aromatiques, polyazomethines et poly(azomethine-sulfone)s, *8eme Colloque Franco-Roumain, Les polymeres : des Materiaux Fonctionnels au coeur des Nouvelles Technologies, Grenoble, France, 26-30 Aout 2007, C8 pag. 5.*
4. S. Curteanu, F. Leon, M. Cazacu, Méthodologie générale d’optimisation fondée sur des réseaux neuronaux et algorithmes génétiques, *8eme Colloque Franco-Roumain, Les polymeres : des Materiaux Fonctionnels au coeur des Nouvelles Technologies, Grenoble, France, 26-30 Aout 2007, C8 pag. 5.*

Posters

1.S. Curteanu, M. Cazacu Neural networks based prediction and optimization applied to siloxane-siloxane copolymers synthesis, *International Conference of Computational Methods in Science and Engineering” 2006, 27.10 – 1.11. 2006, Grecia.*
2. C. Racles, V. Cozan, Influence of chemical structure on processing and thermotropic properties of poly(siloxane-azomethine)s, *International Conference „Polycondensation 2006”, Istanbul, Turcia*
3. F. Iacomi, C. Baban, N. Iftimie, P.Prepelita, D. Luca, Influence of substrate nature and annealing on the electro-optical properties of ZnO thin films, *6th International Conference of the BalkanPhysical Union, 22-26 august2006, Istanbul, Turcia*
4. M. Cazacu, A. Vlad, C. Racles, Condensation polymers of the metallocenes and siloxane derivatives, *European Polymer Congress, Portoroz, 2007*

5. C. Racles, S. Curteanu, V. Cozan, M. Cazacu, Thermotropic poly(siloxane-Schiff bases): synthesis of new polymers and predictions of lc properties based on neural network, *European Polymer Congress, Portoroz, 2007*
6.C. Racles, Polysiloxanes portant des groupes mesogenes azo-aromatiques, *Poster: 8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
7. C. Racles, M. Alexandru, M. Cazacu, A. Ioanid, T. Hamaide, Obtention des elastomeres silicones en nanoreacteurs siloxanes-organiques, *Poster : 8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
8. M. Alexandru, M. Cristea, C. Racles, M. Cazacu, Reseaux interpenetres organo-inorganiques par la technique sol-gel, *Poster : 8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
9. C. Baban, G.G. Rusu, D. Macovei, C.M. Teodorescu, F. Iacomi, Structural, electrical and optical properties of ITO:Mn thin films grown by thermal evaporation, *EMRS-2007, Strasbourg, 28.mai - 1iunie 2007*
10. P. Budrugeac, Carmen Racles, Vasile Cozan, Maria Cazacu, Thermal and thermo-oxidative stabilities of some poly(siloxane-azomethine)s, *MEDICTA 2007, The 8-th Mediterranean Conference on Calorimetry and Thermal Analysis*

National Conferences

Oral Presentations

1. Maria Cazacu, C. Racles, A. Vlad, M. Alexandru, G. Stiubianu, Noi materiale polimere continand retele de silice, *Conferinta: Simpozionul "Micro/nano-interactii si sisteme pe baza de polimeri naturali sau sintetici", 28.09.2007*
2. F. Iacomi, Studies on some oxide diluted magnetic semiconductors, *IBWAP Constanta 2007-10-14-* Conferinta invitata

Posters

1. M. Alexandru, M. Cazacu, M. Cristea, Structuri reticulate pe baza de polisiloxani. I. Polisiloxani ranforsati cu silice precipitata in situ prin tehnica sol-gel, *A XXIX-a Conferinta de Nationala de Chimie, Calimanesti-Caciulata, Valcea, 4-6 oct. 2006*
2. E. Budeanu, M. Purica, F. Iacomi, C. Baban, Optically transparent electrodes for photoresponse enhancement of MSM photodetector, *International Semiconductor Conference 2006, Sinaia, Romania, 29th Edition, sept 27-29.*
3. P. Budrugeac, E. Segal, Applicability of the Kissinger equation in thermal analysis: revisited, *International Conference of Physical Chemistry - ROMPHYSCHEM-12, Bucuresti, 2006.*
4. M. Alexandru, Materiale siliconice nanostructurate multifunctionale, *Comunicare: AL X-LEA SIMPOZION NATIONAL MATNANTECH, CAP AURORA, 04-08 Iulie 2007*

5. L. Solcanu, M. Valentin Solcanu, S. Curteanu, Optimizare bazată pe algoritmi genetici cu aplicații în polimerizarea siloxanilor, *Zilele Facultății de Chimie Industrială Iaşi, 18 ianuarie 2007.*
6. M. Valentin Solcanu, L. Solcanu, S. Curteanu, Instrumente ale inteligenței artificiale cu aplicații în ingineria chimică, *Zilele Facultății de Chimie Industrială Iaşi, 18 ianuarie 2007*
7. A. Nistor, C. George Piuleac, M. Cazacu, S. Curteanu, Kinetics modeling of the equilibrium anionic polymerization of cyclic siloxanes by using neural networks, *10th Edition of Academic Days Timisoara, Chemistry, May 24-25, 2007.*
8. C. Lisa, S. Curteanu, Neural network based predictions for the liquid crystal properties of organic compounds, *17th European Symposium on Computer Aided process Engineering, ESCAPE 17, 27-30 mai, Bucuresti, 2007*
9. M. Alexandru, Materiale hibride organic-anorganice, *Comunicare Al XI-lea Simpozion MATNANTECH-CEEX, 19-22.11.2007, Sinaia*
10. C. Lisa, S. Curteanu, V. Bulacovschi, D. Apreutesei, Prediction of the liquid crystalline behavior for some symmetrically derivatives with two ferrocene units using the artificial intelligence methods, *Romanian International Conference on Chemistry and Chemical Engineering, RICCCE XV, Sinaia, september 19-22, 2007.*
11. M. Cazacu, A. Vlad, C. Racles, M. Alexandru, A. Airinei, P. Budrugeac, Linear and crosslinked polymeric structures containing complexed metals, *A 5–a Conferinta Nationala "DIRECTII NOI DE CERCETARE IN STIINTA MATERIALELOR", ARM – 5, 5-7 Septembrie, 2007, Sibiu, Romania.*
12. A. Vlad, M. Cazacu, A. Airinei, A new Lanthanum complex encapsulated in silica network by sol-gel technique, *A 5–a Conferinta Nationala "DIRECTII NOI DE CERCETARE IN STIINTA MATERIALELOR", ARM – 5, 5-7 Septembrie, 2007, Sibiu, Romania.*
13. A. Vlad, M. Marcu, M. Cazacu, A. Airinei, G. Munteanu, New functional materials based on siloxane-organic copolymers having quinone-imine units within the chain, *International Conference on Materials Science & Engineering, 22-24 February, Brasov, Romania*
14. F. Iacomi, I. Caraman, I. Caraman, Chemical and magnetical disorder in CdMnS nanocrystalline thin films, *ANC3 -International Workshop, Brasov 2007*
15. Maria Cazacu, Nanostructured polymeric materials, *Info- and brokerage event in new technologies and materials (FP7/2007: NMP/ICT), 22-23 martie, Bucuresti*

Contribution to the human resource formation

Ph.D students: 14

The participation of the youngs to the European schools:

Gabriela Calin (P2)

Marius Cazacu (P2)

Physics of Advanced Materials Winter School, "Growth and characterization of advanced materials focused on structural characterization", January 14-18, 2008, Thessaloniki, Greece

George Stiubianu (CO):

CEI Spring Workshop for Young Researchers from SE and Central European Countries: "Developing entrepreneurial skills for future carreer", 6-12.04.2008, Poznan, Poland

Applied Projects:

1. Siloxane-containing systems: from biphasic morphology towards nano-materials (NANOMATSiSYS), ERC Starting grants, Ref. Number FP7-204577-1.

2. Multifunctional materials developed on the silicone/silica backbones designed by experiment and simulation (MULTIFUNCSiES), ERC-2008-AdG_20080228, Ref. Number FP7-227654

3. 2 projects in partnership in PN II 2007 call;

4. 1 project Idea in PN II 2007 call and 2 in PN II 2008 call;

5. 2 PC projects financed in PN 2008 call.