

Titlul proiectului:

**MATERIALE SILICONICE
NANOSTRUCTURATE
MULTIFUNCTIONALE**

Acronim:

NANOSIMAT

Contract 52/2006

Director proiect: Dr. Maria Cazacu

Contractor principal:



Institutul de Chimie Macromoleculara "Petru Poni" Iasi

Director proiect: Dr. Maria Cazacu



Partener P1

**Universitatea Tehnica
"Gh. Asachi" Iasi -
UTI**

**Prof. Dr. Silvia
Curteanu**



Partener P2

**Universitatea "Al.
I. Cuza" Iasi - UAIC**

**Conf. Dr. Felicia
Iacomi**



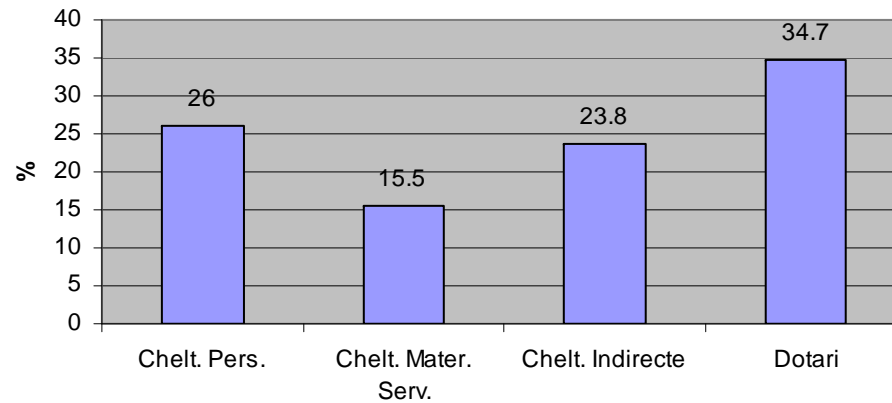
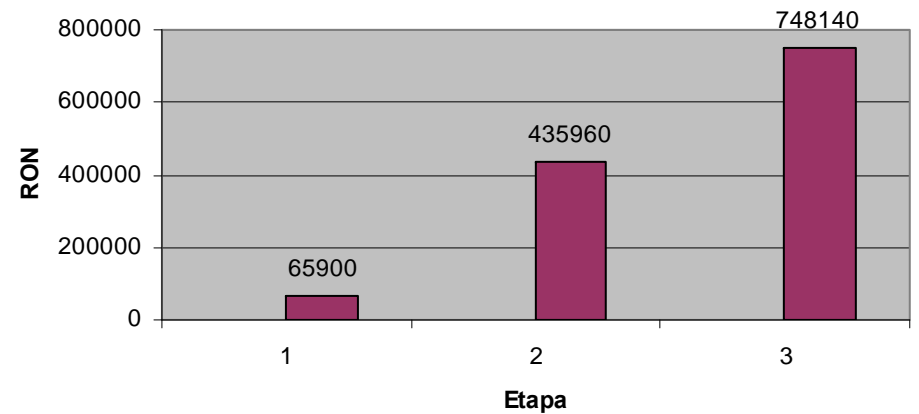
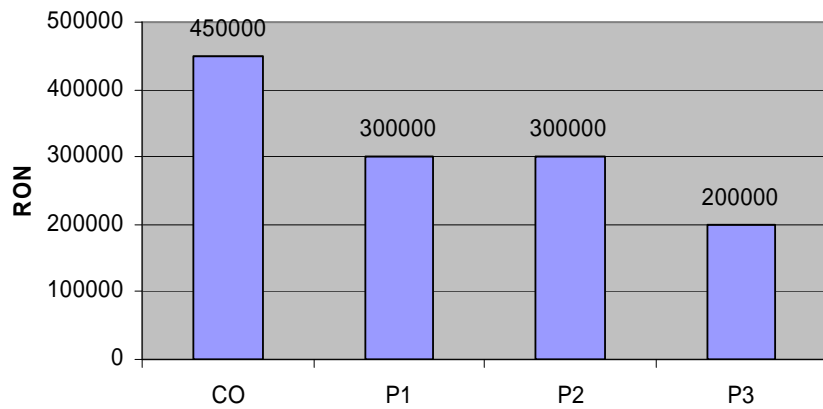
Partener P3

**Institutul National
pentru Cercetare-
Dezvoltare pentru
Inginerie Electrica
Bucuresti- INC DIE
ICPE-CA**

Dr. Petru Budruga

Valoare proiect de la buget: 1 250 000 lei

Cofinantare: -



Obiective generale

1. Dezvoltarea **activitatii de cercetare** intr-un domeniu specializat, cel al polimerilor si materialelor polimerice pe baza de siliciu, prin concentrarea si valorificarea optima a potentialului stiintific, pentru a atinge nivelul de excelenta recunoscut de normele internationale.
2. Dezvoltarea de **noi polimeri siliconici** si materiale pe baza lor cu proprietati noi printr-o abordare moderna folosind instrumente ale intellingei artificiale.
3. Punerea in valoare a noilor produse sintetizati prin **evaluarea proprietatilor**.
4. **Contributie la formarea resursei umane** prin abordarea simultana a elementelor stiintifice cu cele de formare si specializare a resurselor umane. Crearea unei scoli care sa pregateasca **resurse umane** in domeniul siliconilor.
5. Dezvoltarea **infrastructurii de cercetare** necesare.
6. Formarea si dezvoltarea unei **retele de cercetare** pe baza experientei si complementaritatii competentelor care sa pregateasca participarea la PC7.

Obiective specifice

- 1. Dezvoltari in domeniul copolimerilor siloxan-organici capabili de structurare prin separare de faza**
- 2. Noi polimeri lichid cristalini continand segmente siloxanice**
- 3. Polisiloxani modificati cu grupe polare sau complexante**
- 4. Structuri polimerice continand segmente siloxanice si unitati de metal complexat**
- 5. Nanocompozite siloxan-complecsi metalici prin tehnica sol-gel**
- 6. Tehnici ale inteligentei artificiale cu aplicatii la materialele polimerice pe baza de siliciu**

Tinte finale ale proiectului

Compusi si materiale noi

Tehnici de preparare imbunatatite, abordari noi pentru caracterizare si evaluare proprietati

Modele si tehnici de optimizare si clasificare

Pregatirea resursei umane

Imbunatatirea infrastructurii

Lucrari stiintifice in reviste de impact

Consolidarea unui grup in jurul unei tematici competitive pentru dezvoltarea de alte proiecte nationale si internationale

FAZA I (1.08-20.11.2006): *Dezvoltari in domeniul copolimerilor siloxan-organici capabili de structurare prin separare de faza*

Obiective realizate:

- 1. Actualizarea bazei de date prin evaluarea permanenta a stadiului si tendintelor cercetarii in domeniile proiectului.**
- 2. Obtinerea de structuri siloxan-organice cu diferite functiuni interne**
- 3. Investigarea proprietatilor compusilor sintetizati**
- 4. Sistematizarea referintelor bibliografice referitoare la instrumente ale inteligentei artificiale utilizate in ingineria proceselor de polimerizare**

Faza II (21.11.2006 – 30.05.2007) : *Noi polimeri lichid cristalini continand segmente siloxanice.*

Obiective realizate:

- 1. Dezvoltari in sinteza si aplicatiile cristalelor lichide polimere**
- 2. Obtinerea de noi copolimeri siloxan-organici cu proprietati de cristal lichid**
- 3. Tehnici ale inteligentei artificiale cu aplicatii la materialele polimerice pe baza de siliciu**
- 4. Algoritmi de clasificare utilizati pentru predictia de proprietati.**

Faza III (1.06.2007-15.10.2007) : *Polisiloxani modificati cu grupe polare sau complexante.*

Obiective realizate:

- 1. Obținerea de siloxani modificati cu grupe polare sau complexante**
- 2. Studiul proprietatilor siloxanilor modificati cu grupe polare**
- 3. Evaluarea potentialului aplicativ al polisiloxanilor modificati cu grupe polare**
- 4. Modelarea procesului de obtinere a nanoparticulelor polimerice stabilizate cu surfactanti siliconici, folosind rețele neuronale**
- 5. Studiul proprietatilor siloxanilor modificati cu grupe complexante**

Faza IV (6.10.2007-30.05.2008) : *Structuri polimerice continand segmente siloxanice si unitati de metal complexat*

Obiective realizate:

- 1. Obtinerea de noi polimeri continand segmente siloxanice si unitati de metal complexat**
- 2. Studiul proprietatilor polimerilor siloxanici cu unitati de metal complexat in catena principala**
- 3. Modelarea procesului de complexare cu metale a liganzilor pe baza de siliciu**

Faza V (1.06.2008-31.11.2008) : *Nanocompozite siloxan-complecsi metalici prin tehnica sol-gel*

Obiective realizate:

- 1. Obținerea de xerogeluri de silice dopate cu complecsi metalici**
- 2. Evaluarea proprietatilor multiple prin diverse tehnici**
- 3. Algoritmi genetici – instrumente ale Inteligentei Artificiale utilizate in optimizarea proceselor**

Tipuri de compusi sintetizati si studiatii in cadrul proiectului

- 1. Copolimeri siloxan-organici capabili de structurare prin separare de faza**
- 2. Polimeri lichid cristalini continand segmente siloxanice**
- 3. Polisiloxani modificati cu grupe polare sau complexante**
- 4. Nanocompozite siloxan/complecsi metalici prin tehnica sol-gel**

Echipamente achizitionate in cadrul proiectului

1.Tensiometru automat KSV Sigma 700 (CO)

2.Analizer pentru sorbtia dinamica de vapori (CO)

3.Spectrometru de rezonanta electronica de spin, RES (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 μ N

Contact Angle range 0-180°

Contact Angle resolution 0.01°

Calibration and locking Automatic

Stage speed 0.01-500 mm/min

Stage positioning resolution 0.015 μ m

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

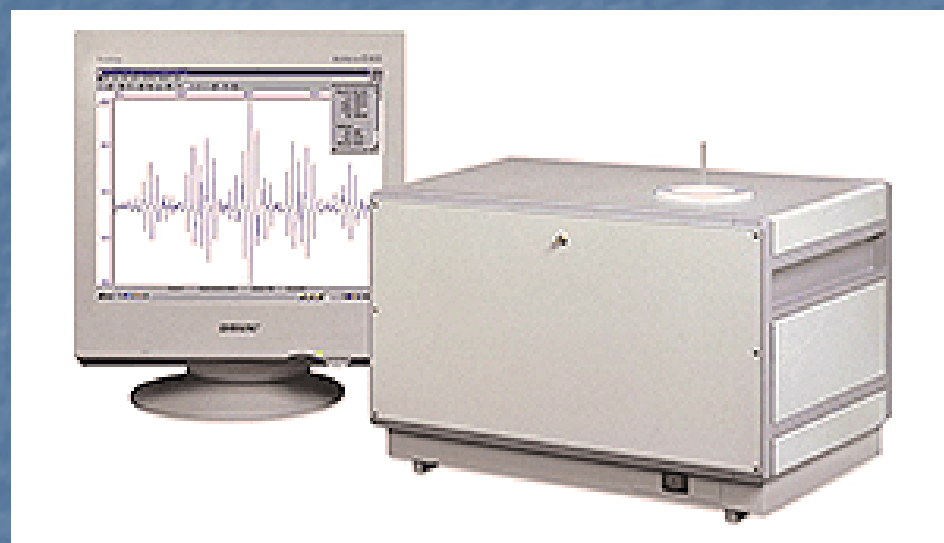
Density Software

Powder Wettability and Sedimentation Software

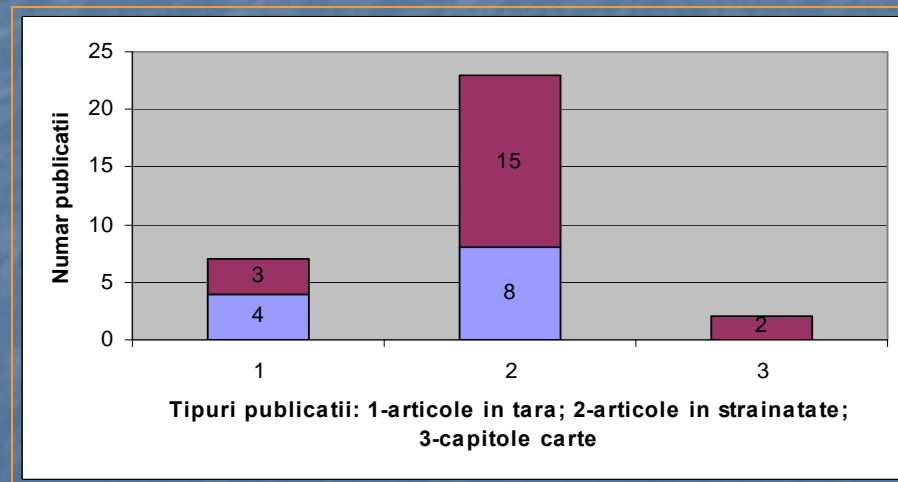
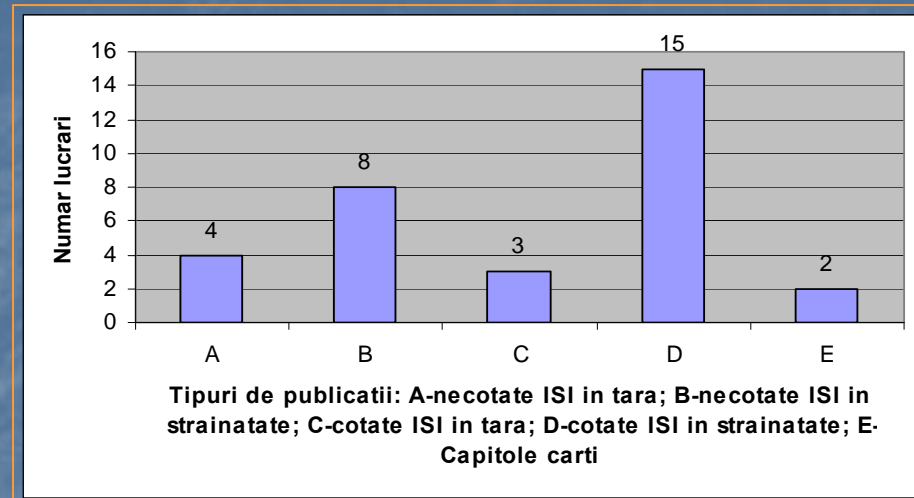
Dynamic Vapor Sorption Analyser



Compact Microwave Electron Spin Resonance Spectrometer



Diseminarea rezultatelor proiectului



Articole publicate in reviste cotate ISI:

In strainatate

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. Budrugaec, E. Segal, Applicability of the Kissinger equation in thermal analysis: revisited, *J. Therm. Anal. Calorim.*- 88 (3), 703-707, 2007.
5. P. Budrugaec, 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. Budrugaec, 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. Budrugaec, 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*

In tara:

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.

Articole publicate in alte reviste

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 Braşov, 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 Society, 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.*

Capitole carte:

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 Polymeric Materials Designed for Hi-Tech Applications “ (editor M. Nechifor), Research Signpost

Prezentari la manifestari stiintifice

In strainatate

Comunicari

1. M. Cazacu, A. Vlad, C. Racles, M. Alexandru, New functional silicone-based materials, *Comunicare : 8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
2. M. Alexandru, M. Cristea, M. Cazacu, A. Ioanid, F. Iacomì, Le renforcement des polysiloxanes avec de la silice obtenue in situ ou ex situ. Études comparatives, *Comunicare : 8ème COLLOQUE Franco-Roumain sur les POLYMERES, Grenoble 26-30 Août 2007*
3. V. Cozan, L. Marin, E. Avram, Comportement thermotrope de polysulfones aromatiques, polyazométhines et poly(azométhine-sulfone)s, *Comunicare: 8ème Colloque Franco-Roumain, Les polymères : des Matériaux Fonctionnels au cœur 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, *Comunicare: 8ème Colloque Franco-Roumain, Les polymères : des Matériaux Fonctionnels au cœur des Nouvelles Technologies, Grenoble, France, 26-30 Aout 2007, C8 pag. 5.*

Postere

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. Iacomì, 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 Balkan Physical Union, 22-26 august 2006, 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*

In tara **Conferinte**

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*

Postere

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 - ROMPHYSICHEM-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 Iași*, 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 Iași*, 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

Contributii la formarea resursei umane: Implicare tineret

Nr doctoranzi: 14

Participare la Scolii europene de iarna/primavara: 5 doctoranzi

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

University of Montpellier 2, Vilnius University, University of Erlangen-Nurnberg and Aristotle University of Thessaloniki (coordinator)-Marie Curie Actions co-funded by the European Commission within the Sixth Framework Programme (2002-2006).

George Stiubianu (CO)

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

Proiecte depuse:

- 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 proiecte castigate in parteneriat in competitia PN II 2007;**
- 4. 1 proiect Idei in competitia PN II 2007- acceptat la finantare;**
- 5. Implicare in 2 proiecte Idei competitia PN II 2008 – acceptate la finantare;**
- 5. Implicare in 2 proiecte parteneriat depuse in competitia PN 2008. Acceptate la finantare;**