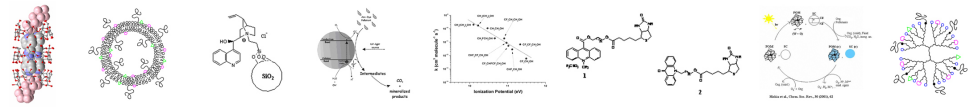
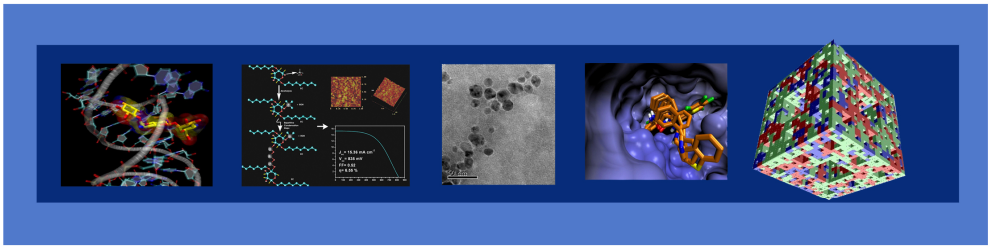
N.C.S.R. "Demokritos"

Institute of Physical Chemistry





http://ipc.chem.demokritos.gr/

ANNUAL REPORT

2007

NATIONAL CENTER FOR SCIENTIFIC RESEARCH "DEMOKRITOS"

INSTITUTE OF PHYSICAL CHEMISTRY

DIRECTOR

Falaras Polycarpos

DEPUTY DIRECTOR

Provata Astero

Address: Neapoleos & Patriarchou Grigoriou, Ag.Paraskevi, 15310, Athens GREECE

Contact:
Secreteriat: Tel + 3 210 650- 3652 - 3653, FAX: +3 210 6511 766, e-mail vdouvara@chem.demokritos,gr
Director: Tel. +3 210 650-3644 - 3652, e-mail papi@chem.demokritos.gr

Preface

The primary objective of the Institute is the fundamental research in physical chemistry which is pursued by both experimental and theoretical methods. Current research activities focus on nanomaterials, functional molecular and supramolecular materials, biomolecules and natural products, theoretical modelling, transport, catalytic and photoinduced processes, environmental technology and renewable energy. The Institute also provides specialized services to the private sector and public organizations, particularly in relation to environmental pollutants analysis, materials characterization, water quality, and glassblowing work.

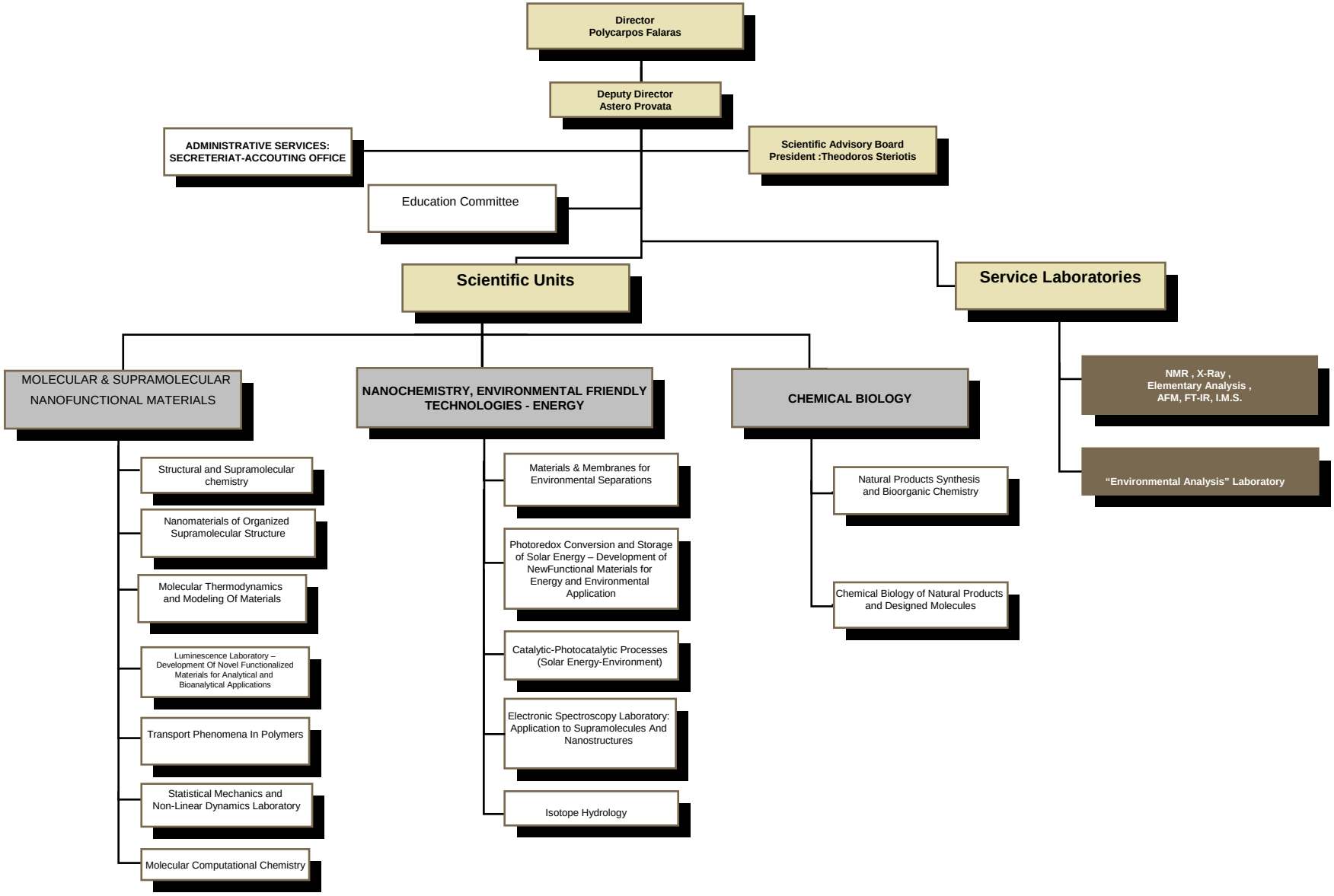
The main axes of research policy aim at establishing the Institute as a National as well as EU, Center of Excellence in the field of physical chemistry and comprise:

- Converging research activities focusing on topical subjects of fundamental research and technological applications in the field of Physical Chemistry
- Attraction of new capable research staff, including post-doctoral and PhD candidates
- Implementation of high level competitive research
- Establishment of long term scientific collaboration with research centers and universities (in Greece and abroad)
- Increase the Institute income from competitive projects
- Improvement of research infrastructure (including research facilities and buildings)

The year 2007 was dominated by the launching of the FP7 research programme and the Institute has made important effort to actively participate in European research projects. The first evaluation results are very positive and greater success is expected in the near future.

March 2008 Dr. Polycarpos FALARAS, Director

Institute of Physical Chemistry



Index page Number

Institute of Physical Chemistry 2007
Performance Indicators

Publications (International Journals) / in press	82 / 31
Conference Proceedings/ Abstracts	102
Lectures	44
Patents	5
PhD Theses	5
Master Degrees	5

Scientific Personnel

Name		Tel. / e-mail
1. Dr. Vourloumis Dionysios	Chemist	+30 210 650 3624,3795 vourloumis@chem.demokritos.gr
2. Dr. Giannakopoulou Konst.	Chemist	+30 210 650 3796, 3617 dyanna@chem.demokritos.gr
3. Dr. Zouridakis Nikolaos	Physicist	+30 210 650 3969, 3959 nizouri@chem.demokritos.gr
4. Dr. Kanellopoulos Nikolaos	Chem. Engin.	+30 210 650 3973, 3977 kanel@chem.demokritos.gr
5. Dr. Katsaros Fotis	Chemist	+30 210 650 3671 fkats@chem.demokritos.gr
6. Dr. Kontos Athanasios	Physicist	+30 210 650 3632 akontos@chem.demokritos.gr
7. Dr. Lazarou Ioannis	Chemist	+30 210 650 3623 lazarou@chem.demokritos.gr
8. Dr. Mavridis Irene M.	Chemist	+30 210 650 3793, 3617 mavridi@chem.demokritos.gr
9. Dr. Economou John	Chem. Engin.	+30 210 650 3963 economou@chem.demokritos.gr
10. Dr. Papadokostaki Kyriaki	Chemist	+30 210 650 3639, 3661 kpapadok@chem.demokritos.gr
11. Dr. Papadopoulos Kyriakos	Chemist	+30 210 650 3647, 3646 kyriakos@chem.demokritos.gr
12. Dr. Pitsinos Emmanouel	Chemist	+30 210 650 3689, 3654 pistolis@chem.demokritos.gr
13. Dr. Pistolis George	Chemist	+30 210 650 3637, 3422 pitsinos@chem.demokritos.gr
14. Dr. Provata Astero	Physicist	+30 210 650 3964 aprovata@limnos.chem.demokritos.gr
15. Dr. Romanos George	Chem. Engin.	+30 210 650 3981 groman@chem.demokrit
16. Dr. Sanopoulou Meropi	Chemist	+30 210 650 3785, 3620 sanopoul@chem.demokritos.gr os.gr
17. Dr. Saridakis Emmanouel	Physicist	+30 210 650 3981 esaridak@chem.demokritos.gr
18. Dr. Sideratou Oreozili	Chemist	+30 210 650 3616, 3638 zili@chem.demokritos.gr
19. Dr. Steriotis Theodoros	Physicist	+30 210 650 3614, 3636 tster@chem.demokritos.gr
20. Dr. Stefanopoulos Konst.	Physicist	+30 210 650 3606 stefan@chem.demokritos.gr
21. Dr. Tsiourvas Dimirtios	Chem. Engin	+30 210 650 3616 tsiourvas@chem.demokritos.gr
22. Dr. Falaras Polycarpos	Physicist	+30 210 650 3644, 3652 papi@chem.demokritos.gr
23. Dr. Hiskia Anastasia	Chemist	+30 210 650 3643, 3642 hiskia@chem.demokritos.gr

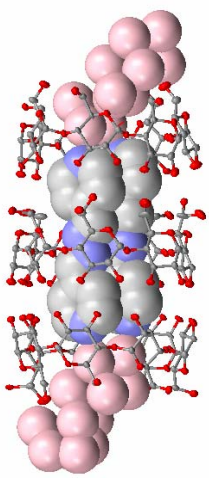
1st Scientific Programme

Molecular & Supramolecular Nanofunctional Materials

STRUCTURAL AND SUPRAMOLECULAR CHEMISTRY

Research Objectives / Activities

The activities of the laboratory involve the structure determination and the intermolecular interactions of supramolecular systems comprising cyclodextrins (CDs), proteins and nucleic acids. Specifically, the areas of research are:



1. *Host-guest systems.* We study the inclusion of biologically active molecules and model compounds in the CD cavity and determine the structure and detailed interactions using NMR in aqueous solutions and/or X-ray crystallography in the crystalline state. Thus we gain insight in host-guest recognition, non-bonding interactions, self-assembly, chiral discrimination and dynamics (when possible). Besides the fundamental understanding, applications such as controlled release, specific binding and drug formulations are of interest.

2. *Synthesis of novel, functional cyclodextrin derivatives for biomedical applications.* The derivatives: (a) Complex with small bio-active molecules. (b) Interact with biological macromolecules, such as DNA, RNA, proteins. (c) Penetrate cell membranes. (d) Complex with metal ions i.e. Gd(III) (new contrast agents for imaging). (e) Bind to each other non-covalently and form biomimetic structures.

3. *Synthesis of novel, functional cyclodextrin derivatives for nanotechnology applications*. The derivatives: (a) Attach onto surfaces (i.e. on Au). (b) When deposited on Si/SiO_2 surfaces form nanostructures in 2D or (c) become the substrate for 2D nanostructures for the electron or energy transfer at specific directions.

4. *Macromolecular Crystallography*. (a) Structure determination of natural and mutated members of the new family of 2[4Fe4S] ferredoxins from selected pathogenic bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*) with low and widely different reduction potentials (–460 and –650 mV) of the two metal clusters (b) Structure determination of complexes of DNA and RNA with modified cyclodextrins. (c) Structure determination of muscle proteins.

Publications

1. Mourtzis, N.; Eliadou, K.; Aggelidou, C.; Sophianopoulou, V.; Mavridis, I. M.; Yannakopoulou, K. "Synthesis and characterization of *per*(6-guanidino-6-deoxy)cyclodextrins and studies of their effect on DNA", *Org. Biomol. Chem*. **2007**, *5*, 125 - 131. Hot article.
2. Paulidou, A.; Giastas, P.; Mourtzis, N.; Yannakopoulou, K.; Mavridis, I. M. **"**Crystal and Molecular Structure of *Octakis*(6-bromo-6-deoxy)-γ-cyclodextrin. A novel stacking of a distorted macrocycle" *Carbohydr. Res.* **2007***, 342(11),* 1519-1524.
3. Chatziefthimiou, S. D.; Yannakopoulou, K.; Mavridis, I. M. "A novel packing of *β*-Cyclodextrin enclosing an unusual organization of guest: The inclusion complexes *β*-Cyclodextrin/4-pyridinealdazine" *Cryst. Eng. Commun*. **2007**, *9,* 976-979. Hot article.
4. Karathanos, V. T.; Mourtzinos, I.; Yannakopoulou, K.; Andrikopoulos, K. N. K. "Study of the solubility, antioxidant activity and structure of inclusion complex of vanillin with β-cyclodextrin", *Food Chem.* **2007**, *101*, 652-658.
5. Mourtzinos, I.; Salta, F.; Yannakopoulou, K.; Chiou, A.; Karathanos, V. T. "Encapsulation of olive leaf extract in β-Cyclodextrin"*J. Agr. Food Chem*. **2007**, *55*, 8088-8094.
6. *Hadjoudis, E.; Chatziefthimiou, S. D.; Mavridis, I. M. "Anils: Photochromism by H-transfer", Curr. Org. Chem, invited review. In print.*
7. *Mourtzis, N.; Paravatou, M.; Mavridis, I. M.; Roberts, M. L.; Yannakopoulou, K. "Synthesis, characterisation, and remarkable biological properties of cyclodextrins bearing guanidino-alkylamino and aminoalkylamino groups on their primary side", Chem. Eur. J., in print.*
8. *"Protein crystallization: from purified protein to diffraction-quality crystal", Chayen, N. E.; Saridakis, E. Nature Methods, in print.*

International Conferences

1. Maffeo, D.; Mavridis, I. M.; Yannakopoulou, K. "New ligands for lanthanide ions based on cyclodextrins", in COST D31, WG 0001-04, "*Organising Non-Covalent Chemical Systems with Selected Functions*" 3rd Workshop, 28-31 March **2007**, NCSR "Demokritos", Athens, Greece.
2. Paulidou, A.; Mavridis, I. M. "X-ray structure of the inclusion complex between β-cyclodextrin and tolbutamide", in COST D31, WG 0001-04, "*Organising Non-Covalent Chemical Systems with Selected Functions*" 3rd Workshop, 28-31 March **2007**, NCSR "Demokritos", Athens, Greece.
3. Aggelidou, C.; Yannakopoulou, K. "Study of the interaction of per(6-guanidino-6-deoxy)cyclodextrins with nucleotides and nucleosides" COST D31, WG 0001-04, "*Organising Non-Covalent Chemical Systems with Selected Functions*" 3rd Workshop, 28-31 March **2007**, NCSR "Demokritos", Athens, Greece.
4. Chatziefthimiou S. D.; Mavridis, I. M. "Unusual organization of host and guest molecules in the inclusion complex *β*-Cyclodextrin/4-pyridinealdazine",The 39th crystallographic meeting at Erice, "*Engineering of Crystalline Materials Properties: State-of-the-Art, Design and Applications*", June 7-17, **2007**, Erice, Italy.
5. Faiz, J. A.; Kyllönen, L. E. P.; Pikramenou, Z.; Williams, R. M.; de Cola, L.; Thanassoulas, A. ; Nounesis, G.; Mavridis, I. M.; Yannakopoulou, K. "Light switched energy transfer and detailed binding studies between an anthracene guest and trimeric Ru(II) cyclodextrin" *RSC UK Macrocyclic and Supramolecular Chemistry Group Meeting***,** Dec. 18-19, **2007**, Manchester, UK.

Funded projects

1. "Development of new pharmaceutical formulations. Molecular inclusion of antibiotics in cyclodextrins for resistant pathogen strains", PENED, 57.5 k€, 2006-2008.
2. "Uni-directional nanoscale supramolecular wires assembled by photo- and electro-active metallo-cyclodextrin cups" MC Research Training Network *UNI-NANOCUPS,* Collaboration with IMEL. Budget of IPC & IMEL: 202 k€, 1/1/2004 – 31/12/2007.
3. "Tools and Technologies for the Analysis and Synthesis of Nanostructures, STREP: TASNANO, Collaboration with IMEL. Budget of IPC 50 k€, 1/1/2005 – 31/6/2008.
4. "A Network for Bringing NANOtechnologies TO LIFE, *NANO2LIFE*" "Network of Excellence" Priority 3-NMP 3.4.1.2-1 Nanotechnology, The funding of the collaborating institutes IPC, IMEL and IRRP, varies evey year. For 2007: 71.9 k€, 1/2/2004 – 31/1/2008.
5. "Autoorganised supramolecular materials with electrical and optical properties" Empirikion Foundation, 12 k€, 2004-.
6. "Optical and electro-active molecular wires organised by aqueous cyclodextrin-assembly of metallounits", COST, Action 31, 2005-2009.
7. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008.
8. "Large Facilities Programme" for Access to the European Synchrotron Radiation Source DESY, Hamburg, Germany, EMBL Outstation under the EU Community. Financial Support for the projects "Natural and Derivatised Cyclodextrins and their Inclusion Complexes" and "Structure of Bacterial 2[4Fe-4S] Ferredoxins", 2000 – today, 1.3 k€.

International Collaborations

Dr. Zoe Pikramenou, Prof. M. J. Hannon, University of Birmingham; Dr. J.-M Moulis, CEA, Grenoble, France; Dr. V. Karginov, Innovative Biologics, Inc., USA, Dr. M. Wilmans, EMBL-Hamburg, Germany.

Infrastructure

250 and 500 MHz BRUKER NMR instruments (departmental); 4-Cyrcle diffractometer; Macromolecular data collection system (Rigaku, R-Axis IV); Low temperature for data collection (Oxford cryosystems); Autoclave (Parr); Circular dichroism spectrophotometer (JASCO), Microscope (Olympus).

Personnel

I. M. Mavridis: research director/group leader (permanent researcher); K. Yannakopoulou (permanent researcher); D. Maffeo, E. Saridakis (post doctoral associates, external funding); A. Paulidou (post doctoral associate, funding by NCSR "D"); Ch. Aggelidou (PhD student, funding by NCSR "D"); M.

Lambropoulou, L. Kyllonen, S. Hadjiefthimiou (PhD students, external funding); K. Fotiadou (MSc student, external funding); Dr. E. Hadjoudis (external senior researcher).

Contact

Dr. I. M.. Mavridis (mavridi@chem.demokritos.gr), Tel. +30 210 65033793, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

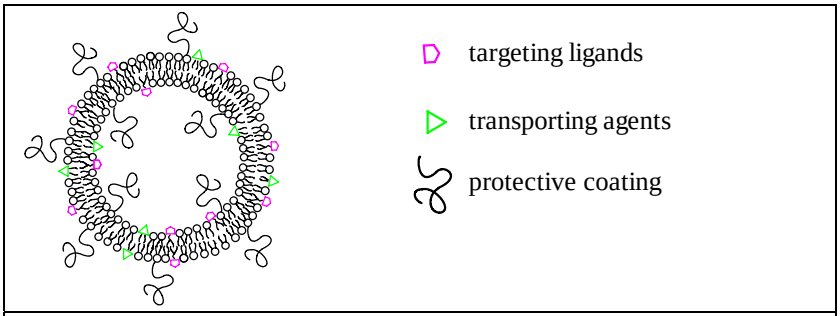
NANOMATERIALS OF ORGANIZED SUPRAMOLECULAR STRUCTURE

Research Objectives / Activities

The research activities are mainly focused on the synthesis and physicochemical characterization of functional nanomaterials, namely liposomes and dendritic polymers, giving emphasis on their applications as drug and gene delivery systems as well as, on the use of dendritic polymers for the removal of organic contaminants from water. Specifically, the scientific work is centered on:

1. Multifunctional Liposomes as Drug Delivery Systems.

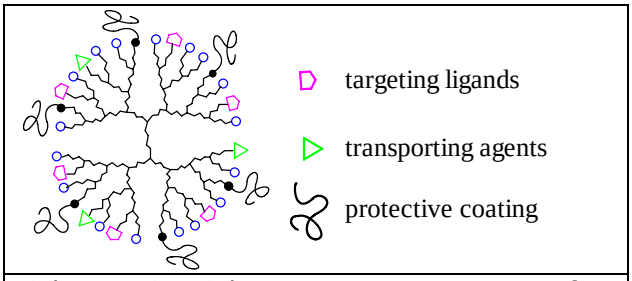
Liposomes bearing recognizable groups are employed in molecular recognition experiments with complementary liposomes or simple molecules in an attempt to simulate the behaviour of cells. The external surface of liposomes is modified with appropriate moieties for conducting the molecular recognition experiments with the final however objective to develop efficient drug or gene delivery systems combining stability, targeting and transporting properties, Scheme 1.



Scheme 1. Schematic representation of Multifunctional Liposomes

2. Multifunctional Dendrimeric and Hyperbranched Polymers as Drug and Gene Delivery Systems.

Multifunctionalization of dendrimeric and hyperbranched polymers (dendritic polymers) is conducted aiming at developing drug and gene delivery systems exhibiting targeting, stability and transport properties through cell membranes, Scheme 2. Active drug ingredients are incorporated in the nanocavities of dendritic polymers. On the other hand suitably designed positively charged dendritic polymers are also employed for the formation of complexes with DNA and studied either physicochemically or in *in vitro* experiments employing a variety of cell lines.



Scheme 2. Schematic representation of a Multifunctional Denritic Polymer

3. Dendritic Polymers with Application in the Production of Ultrapure Water.

Alkylated dendritic polymers have the property of behaving as "nanosponges", in the cavities of which hydrophobic water impurities are encapsulated. Ultrapure water is produced, in which the remaining impurities are at the ppb level. Furthermore, cross-linked hydrophobic dendrimeric and hyperbranched polymers have been developed for water purification. Work has also been performed for the preparation of organosilicon dendrimers which were applied at the surface of ceramic filters for the production of ultrapure water.

Publications 2007

1. Paleos, C.M., Tsiourvas, D., Sideratou, Z. "Molecular engineering of dendritic polymers and their application as drug and gene delivery systems" *Mol. Pharm.* **2007**, *4*, 169-188.
2. Paleos, C.M., Tsiourvas, D., Sideratou, Z. "Developing and applying a drug delivery model for liposomal and dendritic multifunctional nanoparticles" *Gene Therapy and Molecular Biology* **2007**, *11*, 117-131.
3. Tziveleka, L.A., Psarra, A-M.G., Tsiourvas, D., Paleos, C.M. **"**Synthesis and characterization of guanidinylated poly(propylene imine) dendrimers as gene transfection agents" *J. Controlled Release* **2007**, *117*, 137-146.
4. Tsogas, I., Sideratou, Z., Tsiourvas, D., Theodossiou, T.A., Paleos, C.M. "Interactive transport of guanidinylated poly(propylene imine) based dendrimers through liposomal and cellular membranes" *ChemBioChem* **2007**, *15*, 1865-1876.
5. Tsogas, I., Theodossiou, T., Sideratou, Z., Paleos, C.M., Collet, H., Rossi, J.C., Romestand, B., Commeyras, A. "Interaction and transport of poly(l-lysine) dendrigrafts through liposomal and cellular membranes: The role of generation and surface functionalization" *Biomacromolecules* **2007**, *8*, 3263-3270.
6. Allabashi, R., Arkas, M., Hörmann, G., Tsiourvas, D. "Removal of some organic pollutants in water employing ceramic membranes impregnated with cross-linked silylated dendritic and cyclodextrin polymers" *Water Research* **2007**, *41*, 476-486.
7. *Pantos, A., Tsogas, I., Paleos, C.M. "Guanidinium group: A versatile moiety inducing transport and multicompartmentalization in complementary membranes", Biochim. Biophys. Acta,-Biomembranes (in press).*
8. *Tziveleka, L.A., Psarra, A.-M.G., Tsiourvas, D., Paleos, C.M. "Synthesis and evaluation of functional hyperbranched polyether polyols as prospected gene carriers", Int. J. Pharm. (in press).*
9. *Tsetsekou, A., Arkas, M., Kritikaki, A., Simonetis, S., Tsiourvas, D. "Optimization of hybrid hyperbranched polymer/ceramic filters for the efficient absorption of polyaromatic hydrocarbons from water", J. Membr. Sci. (in press).*
10. *Kontoyianni, C., Sideratou, Z., Theodossiou, T., Tziveleka, L.-A., Tsiourvas, D., Paleos, C. M. "A novel micellar pegylated hyperbranched polyester as prospective drug delivery system for paclitaxel", Macromolecular Bioscience (in press).*
11. *Paleos, C. M., Tsiourvas, D., Non-Covalent Interactions of Liposomes, in "Bottom-up nanofabrication: Supramolecules, self-assemblies and organized films", American Scientific Publishers (in press).*

Conferences

1. Tziveleka, L.-A., Psarra, A.-M.G., Tsiourvas, D., Paleos, C.M. "Guanidinium functionalized poly(propylene imine) dendrimers as gene delivery systems", COST D31, Workshop on "Organising Non-Covalent Chemical Systems with Selected Functions", Athens, Greece, March 28-31, 2007.
2. Pantos, A., Tsiourvas, D., Nounesis, G., Paleos, C.M. "Molecular recognition of guanidinylated dendrimers with complementary multilamellar liposomes", COST D31, Workshop on "Organising Non-Covalent Chemical Systems with Selected Functions", Athens, Greece, March 28-31, 2007.
3. Tsogas, I., Theodosiou, T., Sideratou, Z., Paleos, C.M. "Transport of dendrimers bearing guanidinium surface groups through liposomal membranes", COST D31, Workshop on "Organising Non-Covalent Chemical Systems with Selected Functions", Athens, Greece, March 28-31, 2007.
4. Tsogas, I., Theodossiou, T.A., Sideratou, Z., Tsiourvas, D., Paleos, C.M., Collet, H., Rossi, J.C., Romestand, B., Commeyras, A. "Interaction and transport of poly(l-lysine) dendrigrafts through liposomal and cellular membranes: the role of generation and surface functionalization", 5th International Dendrimer Symposium, Toulouse, France, August 28- September 1, 2007, p. P-99.
5. Koumbi, D., Clement, J.C., Psarra, A.M., Sideratou, Z., Yaouanc, J.J., Chatzouli, M., Samara, M., Loukopoulos, D., Kollia, P. "Detailed studies on the mechanism and factors mediating lipofection potency of cationic phosphonolipid-based gene transfer into human cells", 4th International Conference on Stem Cell Gene Therapy, Thessaloniki, Halkidiki, Greece, September 13-17, 2007, .

6. Koumbi, D., Clement, J.C., Psarra, A.M., Yaouanc, J.J., Sideratou, Z., Chatzouli, M., Chiotoglou, I., Vamvakopoulos, N., Kollia, P. "Impact of lipoplex physicochemical properties upon transgene incorporation, stability and mode of nuclear targeting in cationic phosphonolipid- and lipophosphoramide-mediated transfection into human cells", 4th International Conference on Stem Cell Gene Therapy, Thessaloniki, Halkidiki, Greece, September 13-17, 2007.
7. Paleos, C.M., Tsiourvas, D., Sideratou, Z., Tziveleka, L.-A. "Functional dendritic_polymers as drug and gene delivery systems", International conference on Nanomedicine, Chalkidiki, Greece, September 9-11, 2007.
8. Paleos, C.M., Tsiourvas, D., Sideratou, Z., Theodossiou, T. "Modelling cellular membrane transport: Interaction and transport of guanidinylated dendritic polymers through liposomal membranes, International Liposome Society 2007, Liposome Advances: Progress in Drug and Vaccine Delivery, Annual Meeting, London, UK December 8-11, 2007.

Patents

1. Paleos, C.M., Tsiourvas, D., Sideratou, Z., Tsogas, I., Theodossiou, T. "Molecular dendritic transporters". International Application Filing No.: PCT/GR07/000038, Filing date: 23/07/2007.

Funded projects

1. "Targeted drug delivery systems based on liposomes and dendritic polymers", PAVET-NE 2004 04BEN4 project, 70 K€, 2005-2007.
2. "Development of a novel anticancer technique: Bioluminescence activated destruction of cancer cells employing targeted gene carriers based on liposomes and dendritic polymers", ENTEP 04EP 61 project, 78 K€, 2006-2008.
3. "Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics", 'NMP' INTEGRATED PROJECT, Contract No NMP4-CT-2006-026723, 537 K€, 2006-2010.
4. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008.
5. "Preparation and Properties of Functionalized Vesicles as Protocell Models", COST D27 "Prebiotic Chemistry and Early Evolution", 2002-2007.

Infrastructure

Optical and fluorescence microscopy with imaging facilities, Thermal analysis (DSC, TGA), Spectroscopic methods (NMR, FT-IR, UV-Vis, Fluorescence), Size exclusion chromatography, Dynamic Light Scattering, Multi-angle static light scattering, Zeta-potential, AFM microscopy, X-ray diffraction.

Collaborations

Psarra, A-M.G. (Foundation for Biomedical Research of the Academy of Athens, gene transfection), Allabashi, R. (Institute for Sanitary Engineering and Water Pollution Control, Austria, studies of water pollutants), Tsetsekou, A. (NTUA, ceramic membranes), Nounesis, G. (Institute of Radioisotopes & Radiodiagnostic Products, NCSR "Demokritos", microcalorimetry), Koumbi, D. (Fox Chase Cancer Center; Philadelphia, USA).

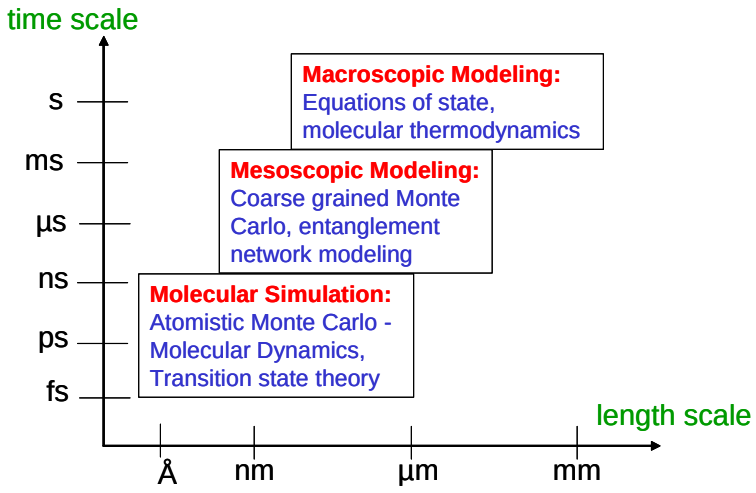
.

Contact

Dr D. Tsiourvas (tsiourvas@chem.demokritos.gr, Tel. +30 210 6503616, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

MOLECULAR THERMODYNAMICS AND MODELING OF MATERIALS

Research work



Research work in the Molecular Thermodynamics and Modeling of Materials Laboratory (MTMML) focuses on the development and implementation of novel hierarchical methods and algorithms for the computer modelling and calculation of advanced material properties at the molecular, mesoscopic and macroscopic levels. Through this work, quantitative links are established between chemical constitution, processing conditions, and physical (thermal, mechanical, rheological, transport, interfacial, optical, dielectric) properties, which are critical for the optimal design of industrial processes and also govern the end-use performance of commercial products. In parallel, the molecular mechanisms underlying structure - property - processing - performance relations are elucidated with the objective of designing new, tailor-made materials.

The hierarchical approaches developed and implemented at MTMML start with atomistic simulations addressing length scales on the order of tens of nanometers and time scales on the order of tens of nanoseconds (e.g., Monte Carlo, molecular dynamics, transition-state theory analysis of infrequent events) and proceed with mesoscopic methods (e.g., entanglement network modelling, kinetic Monte Carlo simulation, self-consistent field theory of inhomogeneous systems) to address longer time- and length scale phenomena. Finally, for the efficient design of novel processes mainly for the chemical and polymer industry, accurate macroscopic models, mostly in the form of equations of state (eos), are developed for phase equilibria and other thermodynamic properties of multicomponent mixtures. These eos are rooted to statistical mechanics and can be safely extrapolated to conditions where limited or no experimental data exist.

Research work in 2007 focused on:
(a) Molecular simulation of elastomeric and glassy polymers,
(b) Polymer solutions and blends,
(c) Sorption and diffusion of small molecules in silicon-containing polymers,
(d) Molecular simulation of polar homo- and co-polymers,
(e) Mesoscopic simulation of polydisperse colloids,
(f) Thermodynamic properties of polar fluids in pure and in mixture,
(g) Ionic liquids in pure and in mixture with supercritical carbon dioxide or water.

Personnel

Researchers: Dr. Ioannis G. Economou, Researcher A', Laboratory Director
Research Scientist: Dr. Niki Vergadou
Collaborating Researcher D': Dr. Nikolas Zacharopoulos (until May 2007, then part time collaborator)
Post-doctoral scientists in projects:
- ✓ Dr. Theodora Spyriouni (EU-STREP)
- ✓ Dr. Anastassia Rissanou (GSRT)
- ✓ Dr. Evangelia-Georgia Logotheti (INTAS)
- ✓ Dr. Hari Leontiadou (GSRT)
- ✓ Dr. Stelios Karanikas (GSRT – ENTER)

PhD students:
- ✓ Zoi Makrodimitri (GSRT – PENED)
- ✓ Marianna Yiannourakou

Senior undergraduate students:
- ✓ Eleni Androulaki (School of Applied Mathematics and Natural Sciences, NTUA)
- ✓ Vassilios Niotis (School of Chemical Engineering, NTUA)

Collaborating faculty:
- ✓ Professor Doros N. Theodorou, School of Chemical Engineering, NTUA

Publications in peer-reviewed journals

1. Z.A. Makrodimitri, R. Dohrn and I.G. Economou, "Atomistic Simulation of Poly(dimethylsiloxane): Force Field Development, Structure and Thermodynamic Properties of Polymer Melt and Solubility of *n*-Alkanes, *n*-Perfluoroalkanes, Noble and Light Gases", *Macromolecules,* **40**(5), 1720 – 1729 (2007).
2. I. Tsivintzelis, T. Spyriouni and I.G. Economou, "Modeling of Fluid Phase Equilibria with Two Thermodynamic Theories: Non-Random Hydrogen Bonding (NRHB) and Statistical Associating Fluid Theory (SAFT)", *Fluid Phase Equil.,* **253**, 19 – 28 (2007).
3. C. Panayiotou, I. Tsivintzelis and I.G. Economou, "Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 2. Multicomponent Mixtures", *Ind. Eng. Chem. Res.,* **46**(8), 2628 – 2636 (2007).
4. L.D. Peristeras, A.N. Rissanou, I.G. Economou and D.N. Theodorou, "Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends", *Macromolecules,* **40**(8), 2904 – 2914 (2007).
5. A.N. Rissanou, M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Amorphous and Crystalline States of Ultrasoft Colloids: A Molecular Dynamics Study", *Rheol. Acta,* **46**(5), 755 – 764 (2007).
6. A.N. Rissanou, L.D. Peristeras and I.G. Economou, "Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear – Tri-arm Polyethylene Blends from Monte Carlo Simulation", *Polymer,* **48**(13), 3883 – 3892 (2007).
7. I.G. Economou, Z.A. Makrodimitri, G.M. Kontogeorgis and A. Tihic, "Solubility of Gases and Solvents in Silicon Polymers: Molecular Simulation and Equation of State Modeling", *Molec. Simul.*, **33**(9-10), 851 – 860 (2007).
8. E.K. Karakatsani, I.G. Economou, M.C. Kroon, C.J. Peters and G.-J. Witkamp, "tPC-PSAFT Modeling of Gas Solubility in Imidazolium-Based Ionic Liquids", *J. Phys. Chem. C,* **111**(43), 15487 – 15492 (2007).
9. E.K. Karakatsani and I.G. Economou, "Phase Equilibrium Calculations for Multi-Component Polar Fluid Mixtures with tPC-PSAFT", *Fluid Phase Equil.,* **261**, 265 – 271 (2007).
10. T. Spyriouni, C. Tzoumanekas, D.N. Theodorou, F. Müller-Plathe and G. Milano, "Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts: Structure, Thermodynamic Properties, Chain Conformation, and Entanglements", *Macromolecules,* **40**(10), 3876 – 3885 (2007).

11. Z. Kechagia, C. Kiparissides and I.G. Economou, "Determination of Liquid – Gas Partition Coefficients of BuA and MMA by Headspace-Gas Chromatography Utilizing the Phase Ratio Variation Method", *Fluid Phase Equil.,* in press.
12. I.G. Economou, E.K. Karakatsani, G.E. Logotheti, J. Ramos and A. Vanin, "Multi-scale Modeling of Structure, Dynamic and Thermodynamic Properties of Imidazolium-Based Ionic Liquids: *Ab initio* DFT Calculations, Molecular Simulation and Equation of State Predictions", *Oil & Gas Sci. Tech.,* in press.
13. A. Grenner, I. Tsivintzelis, G.M. Kontogeorgis, I.G. Economou and C. Panayiotou, "Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the simplified Perturbed Chain-Statistical Associating Fluid Theory (sPC-SAFT). I. Vapor – Liquid Equilibria", *Ind. Eng. Chem. Res.*, in press.
14. I. Tsivintzelis, A. Grenner, I.G. Economou and G.M. Kontogeorgis, "Evaluation of the Non-Random Hydrogen Bonding (NRHB) Theory and the simplified Perturbed Chain-Statistical Associating Fluid Theory (sPC-SAFT). II. Liquid – Liquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems", *Ind. Eng. Chem. Res.*, in press.

Presentations in international conferences

1. Z.A. Makrodimitri and I.G. Economou, "Atomistic Simulation of Silicon-Containing Elastomers: Force Field Development, Structure and Thermodynamic Properties of Polymer Melt and Solubility of *n*-Alkanes, *n*-Perfluoroalkanes, Noble and Light Gases", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
2. A.N. Rissanou, L.D. Peristeras and I.G. Economou, "Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear - Tri-arm Polyethylene Blends from Monte Carlo Simulation", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
3. E.K. Karakatsani and I.G. Economou, "Prediction of Thermodynamic Properties and Phase Equilibria of Polar Multicomponent Mixtures from Perturbation Theory", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
4. T. Spyriouni, C. Tzoumanekas, and D.N. Theodorou, "Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts: Structure, Thermodynamic Properties, Chain Conformation, and Entanglements", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
5. N. Vergadou and D.N. Theodorou, "Computational Study of Permeability of Glassy Polymers to Gases", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
6. M.C. Kroon, E.K. Karakatsani, M. Montero, I.G. Economou, G.-J. Witkamp and C.J. Peters, "Experimental Measurements and Modeling using tPC-PSAFT of the Phase Behavior of the Ternary Ionic Liquid System CO_2 + water + [bmim]NO_3", *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* Hersonissos, Crete, Greece (2007).
7. E. Tritopoulou and I.G. Economou, "Molecular Simulation of Thermodynamic Properties of Glycols in Pure State and in Aqueous Solutions", *6th Greek Chemical Engineering Conference*, Athens, Greece (2007).
8. M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Phase Equilibria of Polydisperse Colloidal Systems", *6th Greek Chemical Engineering Conference*, Athens, Greece (2007).
9. N. Vergadou and D.N. Theodorou, "Molecular simulation towards the Prediction of Permeability of Glassy Polymers to gases", *6th Greek Chemical Engineering Conference*, Athens, Greece (2007).
10. I.G. Economou, A. Grenner, I. Tsivintzelis, C. Panayiotou and G.M. Kontogeorgis, "Evaluation of Statistical Mechanics-Based Equations of State for Complex Fluid Mixtures", *6th European Congress of Chemical Engineering,* Copenhagen, Denmark (2007).
11. I.G. Economou, E.K. Karakatsani, M.C. Kroon, C.J. Peters and G.-J. Witkamp, "Modeling of Ionic Liquid Binary and Ternary Mixture Phase Equilibria at Low and High Pressure With the tPC-PSAFT", *6th European Congress of Chemical Engineering,* Copenhagen, Denmark (2007).
12. I.G. Economou, Z.A. Makrodimitri, A. Tihic and G.M. Kontogeorgis, "Molecular Simulation and Macroscopic Modeling of Thermodynamic and Transport Properties of Silicon-Containing Rubbery Polymer – Solvent Mixtures", *6th European Congress of Chemical Engineering,* Copenhagen, Denmark (2007).

13. H. Leontiadou and I.G. Economou, "Structure and Thermodynamic Properties of Poly(ethylene oxide) from Molecular Dynamics Simulations", *Thermodynamics 2007,* Paris, France (2007).
14. G.-E. Logotheti, F.J. Ramos-Díaz and I.G. Economou, "Molecular Modelling of 1-n-hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide Ionic Liquid", *Thermodynamics 2007,* Paris, France (2007).
15. Z.A. Makrodimitri and I.G. Economou, "Molecular Modeling of Polydimethylsiloxane Mixtures", *International Conference on Computational Methods in Science and Engineering 2007,* Corfu, Greece (2007).
16. M. Yiannourakou, I.A. Bitsanis and I.G. Economou, "Phase Equilibrium of Colloid Systems with Particle Size Dispersity: A Molecular Dynamics Study", *International Conference on Computational Methods in Science and Engineering 2007,* Corfu, Greece (2007).
17. M. Yiannourakou, L. Marsella, F. de Meyer, B. Smit, "Clustering of Proteins Embedded in Lipid Bilayers: a Monte Carlo Study", *International Conference on Computational Methods in Science and Engineering 2007,* Corfu, Greece (2007).
18. F. de Meyer, M. Venturoli, M. Yiannourakou, L. Marsella, B. Smit, "Mesoscopic Simulation Study of Lipid-Mediated Interactions Between Intrinsic Membrane Proteins", *AIChE Annual Meeting*, Salt Lake City, Utah, USA (2007).
19. I.A. Bitsanis, M. Yiannourakou and I.G. Economou, "Amorphous and Crystalline States of Ultrasoft Colloids: A Molecular Dynamics Study", *APS Spring Meeting*, Denver, Colorado, USA (2007).
20. A.N. Rissanou, M. Yiannourakou, I.A. Bitsanis, I.G. Economou, "Thermal Vitrification and Crystallization in Concentrated Suspensions of Ultrasoft Colloids", *Soft, Complex, and Biological Matter Conference*, Città del Mare, Terrasini, Sicily (2007).

Invited lectures

1. I.G. Economou, "Prediction of Structure and Physical Properties of Complex Fluids Using Molecular Simulation", Department of Chemical Engineering, Technical University of Denmark, Lyngby, January 2007.

2. I.G. Economou, "Structural and Physical Properties of Complex Fluids via Molecular Simulation Methods", Department of Materials Science and Technology, University of Crete, Heraklion, Crete, Greece, April 2007.

3. I.G. Economou, "Solubility of Gases and Solvents in Silicon Polymers: Molecular Simulation and Equation of State Modeling", IVC-SEP Discussion Meeting, Department of Chemical Engineering, Technical University of Denmark, Helsingør, Denmark, June 2007.

4. I.G. Economou, "Materials Property Predictions Using Equation of State Theories", 2nd Innovative Modeling Technology Consortium Meeting and Seminar, National Technical University of Athens, Greece, June 2007.

5. I.G. Economou, "Molecular Simulation of Ionic Liquids: Structure, Thermodynamic and Dynamic Properties", Department of Chemical Engineering, IVC-SEP, Technical University of Denmark, Lyngby, November 2007.

Educational work

Teaching

A. Undergraduate courses

1. Ioannis G. Economou, "Physical Chemistry", 2nd year course in *Studies in Natural Sciences,* Open University of Greece, 2007 – 08.
2. Ioannis G. Economou, "Corrosion and Selection of Materials", Department of Chemical Engineering, Technical University of Denmark, Lyngby, Denmark, Fall 2007
3. Nikolas Zacharopoulos, "Simulation", 7th Semester, Department of Product and Systems Design, University of the Aegean, 2006 – 2007.

4. Nikolas Zacharopoulos, "Introduction to Probability and Statistics", 4th Semester, Department of Product and Systems Design, University of the Aegean, 2006 – 2007.
5. Nikolas Zacharopoulos, "Material Science Laboratory", 4th Semester, Department of Product and Systems Design, University of the Aegean, 2006 – 2007.
6. Nikolas Zacharopoulos, "Material Selection for Design", 9th Semester, Department of Product and Systems Design, University of the Aegean, 2006 – 2007.

B. Post-graduate courses
1. Ioannis G. Economou, "Molecular Simulation of Complex Chemical Systems with Emphasis to Practical Applications", PhD Program in *Chemical Engineering,* Technical University of Denmark, Lyngby, Denmark, January - February 2007.
2. Ioannis G. Economou, «Polymer Physics I». Post-graduate program in *Polymer Science and Its Applications,* Department of Chemistry, University of Athens, October – November 2007.

Post-graduate degree awarded

PhD degrees
Eirini Karakatsani, «Development and Evaluation of a New Equation of State for Polar Fluids: Pure Components and Mixtures», School of Chemical Engineering, NTUA, May 2007.

External funding

1. "Computer Aided Molecular Design of Multifunctional Materials with Controlled Permeability Properties" [MULTIMAT], *European Union, STREP FP6, Priority 3, NMP*. Scientific director: Doros N. Theodorou. Total funding for Institute of Physical Chemistry: 173.117 €, funding for MTMML: 86.308 €. Co-funding is provided by GSRT. Duration: 1 / 3 / 2005 – 28 / 2 / 2008.
2. "Reorganization of the Liaison Office of NCSR "Demokritos"", *Greek Secretariat of Research and Technology, Program for Support of Liaison Offices in Universities and Research Centers.* Scientific director: Ioannis G. Economou. Total funding: 300,000 €. Duration: January 1, 2005 – July 30, 2008.
3. "Development of New Molecular Simulation Methods and Macroscopic Models for the Calculation of Microscopic Structure and of Thermodynamic Properties of Complex Polymer Systems", *Greek Secretariat of Research and Technology, Program for Research Support (PENED).* Scientific director: Ioannis G. Economou. Total funding: 60,000 €. Duration: December 1, 2005 – November 30, 2008.
4. "Development of Sustainable Industrial Processes: Experimental, Theoretical and Computational Investigation of Thermodynamic Properties and Phase Equilibria of Ionic Liquid Mixtures", *INTAS.* Scientific director: Ioannis G. Economou. Total funding: 150,000 €. Funding for I.G. Economou: 12,500 €. Duration: September 1, 2006 – May 30, 2009.
5. "Investigation of Structure, Thermodynamic and Transport Properties of Poly(styrene-*co*-acrylonitrile) in High Temperatures", *Greek Secretariat of Research and Technology, ENTER 2003 Program.* Scientific director: Ioannis G. Economou. Total funding: 78,000 €. Duration: October 1, 2006 – September 30, 2008.
6. "Polymer Surfaces Responsive to Thermal and Chemical Stimuli: Towards the Micro-design of 'Intelligent' Materials", *Greek Secretariat of Research and Technology, Greece – USA Research and Technology Cooperation in Materials Research.* Scientific director: Ioannis G. Economou. Total funding: 50,000 €. Funding for I.G. Economou: 25,000 €. Duration: June 1, 2006 – May 31, 2008.

Collaborations

1. Professor Georgios Kontogeorgis, Department of Chemical Engineering, Technical University of Denmark. Development of thermodynamic models for non-ideal polymer systems.
2. Dr. Ioannis Bitsanis, Institute of Electronic Structure and Laser, Foundation of Research and Technology, Hellas, Heraklion, Crete. Mesoscopic simulation of colloids and polymers.
3. Professor Athanassios Z. Panagiotopoulos, Department of Chemical Engineering, Princeton University, USA. Molecular simulation of dendrimers.

4. Professor Costas Panayiotou. Department of Chemical Engineering, Aristotle University of Thessaloniki. Development of a lattice equation of state for non-ideal fluids.
5. Professor Cor Peters, Department of Chemical Engineering, Delft University of Technology, The Netherlands. Modeling thermodynamic properties of ionic liquids.
6. Δρ. J. Ramos-Díaz, Department of Macromolecular Physics, Instituto de Estructura de la Materia - CSIC, Madrid, Spain. Quantum-mechanics calculations for ionic liquids.
7. Professor Sophia Lambropoulou, NTUA. Statistical mechanics.

Other activities

Ioannis G. Economou

1. Scientific Director of Technology Transfer Office, NCSR "Demokritos".
2. Visiting Professor, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby.
3. Chairman, Working Group on Thermodynamics and Transport Properties, *European Federation of Chemical Engineering*.
4. Vice-chairman, International Organizing Committee, *11th International Conference on Properties & Phase Equilibria for Product and Process Design,* 20 – 25 May 2007, Hersonissos, Heraklion, Crete.
5. Referee for the following international scientific journals: *AIChE Journal, Chemical Engineering Research and Design, European Polymer Journal, Fluid Phase Equilibria, Industrial and Engineering Chemistry Research, Journal of the American Chemical Society, Journal of Chemical and Engineering Data, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Physical Chemistry B, Macromolecular Rapid Communications, Macromolecules.*
6. Evaluation of research proposals for funding from the agencies: *Secretariat of Research and Technology, Greece; INTAS, Belgium.*
7. External examiner for PhD thesis at Department of Physical Chemistry, Université Paris-Sud 11, Orsay, France.
8. Guest Editor, *Fluid Phase Equilibria,* **261**, 2007.
9. Consultant, Scienomics SARL, Paris.

Nikolas Zacharopoulos
Non-tenure teacher 407/80, Department of Product and Systems Design, University of the Aegean.

Marianna Yiannourakou
Visiting PhD fellow of Marie Curie EuroSim Programme, CECAM, Lyon, December 2006 – December 2007.

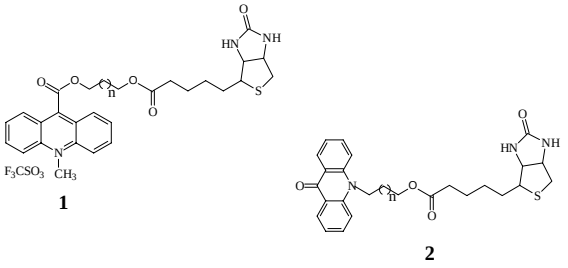
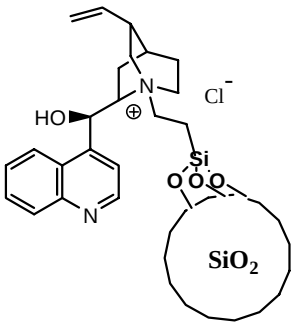
Contact

Dr Ioannis G. Economou (economou@chem.demokritos.gr, Tel. +30 210 6503963, Fax. +30 210 6511766)
Web site: http://www.mtmml.gr/

LUMINESCENCE LABORATORY – DEVELOPMENT OF NOVEL FUNCTIONALIZED MATERIALS FOR ANALYTICAL AND BIOANALYTICAL APPLICATIONS

Research Objectives/Activities

The main objective of the Laboratory is the development of novel functionalized materials and their application in Analytical and Clinical Chemistry. The most important functionalized materials prepared in our laboratory were (a) biotinylated luminescent materials, (b) paramagnetic europium complexes derivatives of diethylenetriaminopentacacetic acid, (c) functional ferric oxide nanoparticles and (d) hybridized organo-inorganic chiral materials. The first one were applied for the quantification of the proteins avidin and streptavidin and in combination with them to the quantification of mouse IgG protein. The protein could be determined down to a few femtomoles per assay (9,2±1.8 fmoles). From paramagnetic europium complexes were measured the relaxation times and found to be similar to those obtained for commercially available MRI agent Magnevist (4.34±0.27 mM^{-1} s^{-1} και 4.15±0.23 mM^{-1} s^{-1} for novel derivatives and 3.93±0.12 mM^{-1} s^{-1} for Magnevist). The novel functional ferric oxide nanoparticles were tested as catalyst in chemiluminescent determinations of reactive oxygen species. It was found that hydrogen peroxide could be determined down to a few micromoles per assay (2.08 ± 0.16 μmoles). Finally, the novel hybridized organo-inorganic materials tested in the asymmetric synthesis of some important optical active molecules, such as α-amino acids. The stereochemical yields of these reactions reached values up to 62%. At this point, it should be noted that beside the use of functionalized novel materials, a novel chemiluminescent technique was also developed in our laboratory and used for the estimation of the antioxidant activities of biological important materials as well as of natural products, such edible oils. The results were impressive and comparable to those obtained by the internationally accepted spectrophotometric DPPH-method.

	
Novel functionalized biotinylated materials	*Chiral functionalized inorganic material*

Publications 2007

1. T.M. Triantis, E. Yannakopoulou, A. Nikokavoura, D. Dimotikali and K. Papadopoulos, Chemiluminescent studies on the antioxidant activity of amino acids, *Anal. Chim. Acta*, **2007**, 591 106-111.
2. O. Lanitou, D. Dimotikali, E. Yannakopoulou and K. Papadopoulos, Studies on the catalytic activity of novel hybridized chiral organo-inorganic catalysts for epoxidation and alkylation reactions, *Chem. Eng. Journal*, **2007**, 134, 72-77.
3. J. Hrbac, V. Halouzka, R. Zboril, K. Papadopoulos and T. Triantis, Carbon electrodes modified by nanoscopic Iron (III) Oxides to assemble chemical sensors for the hydrogen peroxide amperometric detection, Electroanalysis, **2007**, 19, 1850-1854.
4. K. Kasviky, I.E. Stamatelatos, E. Yannakopoulou, P. Papadopoulou, J. Kalef-Esra, The accuracy of protein determination in large biological samples by prompt gamma neutron activation analysis, Nucl. Instr. & Methods in Phys. Res. Section B Beam Interactions with materials and atoms 2007, 263, 132-135.

Conferences

1. O. Lanitou, D. Dimotikali, K. Papadopoulos, Catalytic asymmetric synthesis of a-aminoacids under phase-transfer conditions, 2nd Hellenic Symposium on Organic Synthesis, from Chemistry to Biology, Medicine and Materials Science, Athens, Greece, April 19-21, 2007.
2. K. Agiamarnioti, T. Triantis, E. Yannakopoulou, K. Papadopoulos, Novel biotinylated fluorescent labels. Studies on the effect of spacer moieties upon binding to (strept)avidin, 2nd Hellenic Symposium on Organic Synthesis, from Chemistry to Biology, Medicine and Materials Science, Athens, Greece, April 19-21, 2007.
3. O. Lanitou, D. Dimotikali, K. Papadopoulos, Catalytic asymmetric synthesis of a-aminoacids by phase-transfer catalysis conditions, 9th Creek-Cyprus, Larnaka, Cyprus, 27-30 April 2007.
4. D. Christodouleas, K. Papadopoulos, A. Calokerinos, Development and validation of a chemiluminogenic assay for the estimation of antioxidant activities of edible oils, 2nd Panhellenic conference for lipids and oils, Athens, 7-8 June 2007.
5. K. Papadopoulos, E. Yannakopoulou, K. Agiamarnioti, D. Dimotikali, J. Hrbáč, R. Zbořil, Enhanced Chemiluminescence of Luminol-Hydrogen Peroxide using Nanometer-Sized Ferric Oxides, 4th International Workshop on Nanosciences and Nanotechnologies (NN07), Thessaloniki-Greece, 16-18 July 2007.
6. D. Christodouleas, K. Papadopoulos, A. Calokerinos, Antioxidant activity of edible oils using chemiluminescence, 5th international conference on instrumental methods of analysis, modern trends and applications, Rio Patras, Greece, 30 September-4 October 2007.

Funded projects

1. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008".
2. Sensitized chemiluminescence using ferric oxide nanoparticles. Bilateral collaboration between Greece and Czech Republic, 12 K€, 2006-2008.
3. Enhanced chemiluminescence using nanosized catalysts - prospects for analytical applications, internal funding from NCSR Demokriots, "DEMOEREVNA", 14 K€, 2006-2008.

Infrastructure

UV-Vis spectrophotometer (Jasco V-560), 2 fluorimeters (Jasco FP-777 and Fluostar Optima BMG), 3 luminometers (Bio-Orbit 1250), complete photolysis system 1000 watt (ORIEL), elemental analyzer CHN, Cobalt-60 source (Gamma Chamber 4000A), complete laboratory for the synthesis of organic compounds equipped with rotary evaporators, high vacuum oil pumps, magnetic stirrers, ovens and lines for working in inert atmosphere.

Personnel

K. Papadopoulos (Research director/Group leader, permanent researcher), E. Giannakopoulou (technical staff), D. Kalogiannidis (PhD student, NCSR "D" fellow), D. Christodouleas and O. Lanitou (unpaid PhD students).

Collaborations

D. Dimotikali (Chemical Engineering Department, NTUA Athens, Greece), A. Scorilas (Department for Biochemistry and Molecular Biology, University of Athens), M. Maia (Institute of Pharmaceutical Chemistry, University of Tbilisi, Georgia), R. Saicic (Faculty of Chemistry, University of Belgrade, Serbia), J. Hrbac (Faculty of Inorganic Chemistry, University of Olomouc, Czech Republic), A. Meghea (Polytechnique School of Bucharest, Romania).

Contact

Dr. K. Papadopoulos, kyriakos@chem.demokritos.gr
Tel. +30 210 6503647, Fax. +30 210 6511766)

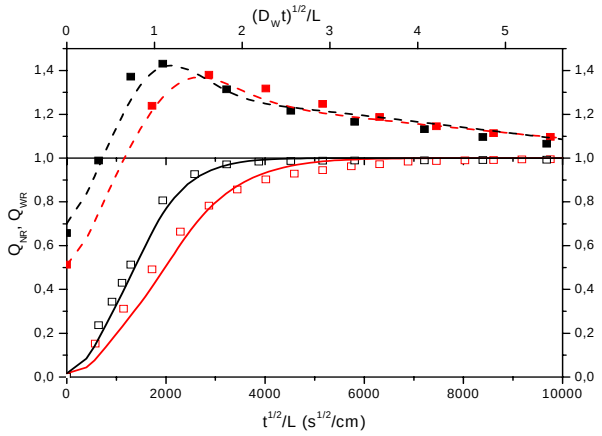
TRANSPORT PHENOMENA IN POLYMERS

Research Objectives / Activities

Research focuses on micromolecular sorption and transport in polymeric materials by a combination of theoretical and experimental approaches. The aim of this work is to help create the basic scientific background for the optimization of the design of polymeric materials for important applications (controlled release systems, permselective membranes, packaging, chemical sensors etc).The *theoretical* part involves computer-assisted modelling at both the molecular/nano and macroscopic levels, aiming primarily at (i) the predictive evaluation of sorption and diffusivity parameters and (ii) the realistic simulation of complex transport phenomena (including diffusion in relaxing polymers, in nonhomogeneous or in composite, media, as well as diffusion coupled with chemical reaction or other concurrent diffusion processes). The *experimental* part is primarily concerned with systematic investigation of (i) vapor or liquid sorption in polymer films, (ii) matrix controlled release devices (iii) transport in thin supported polymer films.
Current research activities include

1. Polymer -based controlled release systems

Development of controlled release devices aims at the regulated, prolonged delivery of drugs, agrochemicals or other bioactive agents. Matrix-type controlled release devices consist of a swellable polymer matrix incorporating the requisite bioactive solute and are activated by the ingress of water when placed in an aqueous environment. Research of our group in this area aims at the optimization of the design of these devices, in order to alleviate their main drawback of continuous decline of dose rate. Theoretical work focuses on the development of advanced, realistic models, simulating the release performance of single-layer as well as multilayered devices. Experimental work includes (i) Validation of models against experiment, based on model experimental systems (ii) Effect of chemical or physical treatment on drug release from hydrogels (iii) Effect of osmotic excipients on drug release from hydrophobic matrices (iv) development of multilaminate devices which constitute a promising design strategy for approaching the desired constant dose rate.



Validation against experiment of model simulating the functioning of matrix-type controlled release systems : Comparison of computed NaI release (continuous lines) and water uptake (dashed lines) curves with experimental data (points) from cellulose acetate matrices loaded with initial concentration of NaI, C_{N0} (g/g of dry polymer) 0.33(black points and lines), 0.20 (red points and lines),

2. Mechanisms of Micromolecular Non-Fickian Transport Kinetics in Glassy Polymers

Sorption and diffusion of micromolecular substances in glassy polymer films is of great importance in many technological applications (e.g. polymer film drying, controlled release systems, food packaging materials). Sorption kinetics in these systems exhibits a variety of deviations from normal Fickian behaviour, attributable to either (i) slow viscous relaxations of the swelling polymer, or (ii) differential swelling stresses generated by the constraints imposed on local swelling during sorption. Our group developes models based on both mechanisms, capable of simulating all basic features of observed non_Fickian kinetic behaviour, including Case II kinetics. Experimental work includes (i) sorption from the *vapour* phase. Carefully designed experimental sorption protocols, supplemented by measurement of longitudinal swelling kinetics of the polymer film, enable us to study various types of non-Fickian behaviour. On the basis of the models mentioned above, we develop general diagnostic criteria for distinguishing between the underlying mechanisms responsible for the observed experimental

behaviour. (ii) sorption from the *liquid* phase. Various optical techniques are used in order to obtain information not only on the rate and kinetics of penetration but also on penetrant concentration profiles and parallel deformation and structural relaxation of the swelling polymer. Combination of these techniques enables us to study in detail various types of non-Fickian penetration such as stress-dependent diffusion and Case II kinetics.

3. Transport in ultrathin supported films
In collaboration with the Institute of Microelectronics in Demokritos, we study the swelling behaviour of thin supported polymer films exposed to different vapour environments for the development of polymer-based chemocapacitive chemical sensor array.

Publications 2007

1. Jaczewska, J.; Budkowski, A.; Bernasik, A.; Raptis, I.; Raczkowska, J.; Goustouridis, D.; Rysz, J.; Sanopoulou, M. "Humidity and Solvent Effects in spin-coated Polythiophene- Polystyrene Blends", *J. Appl. Polym. Sci.* **2007**, *105*, 67-79.
2. Jaczewska, J.; Raptis, I.; Budkowski, A.; Goustouridis, D.; Raczkowska, J.; Sanopoulou, M. Pamuła, E.; Bernasik,; Rysz, J. "Swelling of Poly(3-alkylthiophene) Films Exposed to Solvent Vapors and Humidity: Evaluation of Solubility Parameters", *Synthetic Metals* 2007, *157*, 726-732
3. Iijima, T.; Petropoulos, J.H. "A proposed novel approach to the study of the dual-mode mechanism of dyeing nylon with acid dyes" J. Appl. Polym. Sci. 2007, *103*, 1055-1057
4. Papadopoulos, G.K., Petropoulos, J.H. Model study of the effect of pore structure and condensation on multilayer adsorbate transport in porous media *Langmuir* 2007 *23,* 12932-12936
5. *Sarantopoulou, E.; Kollia, Z.; Cefalas, A.C.; Manoli, K.; Sanopoulou, M.; Goustouridis, D.; Chatzandroulis, S. "Surface nano/micro functionalization of PMMA thin films by 157 nm irradiation for sensing application" Appl. Surface Sci. (in press).*
6. *Dallas, P.; Bourlinos, A.B.; Petridis, D.; Boukos, N.; Papadokostaki, K.; Niarchos, D.; Guskos, N. "Synthesis and characterization of 2-D and 3-D covalent networks derived from triazine central cores and bridging aromatic diamines" Polymer (in press).*
7. *Papadokostaki, K.G.; Stavropoulou, A.; Sanopoulou, M.; Petropoulos, J.H. "An advanced model for composite planar three-layer matrix-controlled release devices. Part I. Devices of uniform material properties and non-uniform solute load" J. Membrane Sci. (in press)..*

Conferences

1. Manoli, K.; Karonisa, E.; Chatzichristidi, M.; Goustouridis, D.; Chatzandroulis, S.; Raptis, I.; Sanopoulou, M. "A chemocapacitive sensor array for the detection of volatile organic compounds and humidity" 5th International Conference on Instrumental Methods of Analysis Modern Trends and Applications, IMA'07, 30 September-4 October 2007, Rio-Patras-Greece.

Funded Projects

1. "Computer aided molecular design of multifunctional materials with controlled permeability properties-Multimatdesign", FP6-NMP-STREP, 86 K€, 2005-2008.
2. "Facing pathogenic conditions by combined use of bio-medical methods and nanotechnology" Ypodomes, Metro 4.5, 4.4.1 Action «Consortia of research and technological development in sectors of National priorities», 2050-4/2, 50 k€,, 2005-2008.
3. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008.
4. "Morphological control of polymer blend nanofilms for organic (opto-) electronics" Joint research and technology programmes, Greece -Poland, 11.7 k€ , 2006 – 2008.

Infrastructure

Vacuum apparatuses for sorption and longitudinal dilation kinetic measurements on polymer samples including electronic microbalances (Cahn 2000 and MK2-M5 CI Electronics) or quartz spring balances, Polarizing and interferometric microscopes, Tensile tester in conjunction with optical setup, Thermal analysis instruments (Temperature Modulated DSC), Home-made apparatuses for kinetic release measurements, Abbe refractometer.

Personnel

M. Sanopoulou: research director/group leader, K. Papadokostaki: principal researcher, (permanent stuff); J.H. Petropoulos (emeritus researcher); D. Soulas, M. Herouvim, A. Hasimi, K. Manoli (4 PhD students, external funding).

Collaborations

Prof. A. Budkowski , M. Smoluchowski (Institute of Physics, Jagellonian University, Krakow, Poland, bilateral program); Prof. D. Hofmann (GKSS, Germany, STREP); Dr. I. Raptis, (NCSR "D", Inst. Of Microelectronics, chemical sensors); Dr. P. Argitis (NCSR "D" Inst. Of Microelectronics, DSC); Dr. P. Dallas (NCSR "D", Inst. of Material Science, DSC); Dr. I. Economou and Prof. D. Theodorou (NCSR "D", Inst. Of Physical Chemistry, STREP)

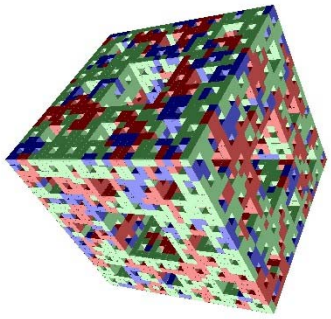
Contact

Dr. M. Sanopoulou (sanopoul@chem.demokritos.gr, Tel. +30 210 6503785, 30 210 6503661; fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

STATISTICAL MECHANICS AND NON-LINEAR DYNAMICS LABORATORY

Research Objectives/Activities

The Laboratory of "Statistical Mechanics and Non-linear Dynamics" was formed in 02/2004 as part of the Institute of Physical Chemistry. Its research focuses on the development of Statistical Mechanical and Non-linear Dynamical methods for the study of development of mesoscopic and macroscopic patterns and correlations due to the local interactions between particles at the microscopic level. Such structures include spatiotemporal patterns, aggregates, spiral and stripe formations, helices, fractals etc which can be experimentally observed in material science, physics, chemistry and biology. Our studies in particular include research on fractal pattern formation and correlations near the critical point in phase transitions (eg the gas-liquid phase transition) but also in open systems in constant exchange with the environment, such as in the noncoding DNA. Away from the critical point and in closed, isolated systems (such as in coding DNA), short range correlations and spatiotemporal patterns with well-defined length and time scales are studied (eg. spiral and stripe formations, helices etc.). The study of these structures at the micro-, meso- and macro scale and the interaction between these three levels of description has major technological impact in materials science and physical, chemical and biological processes.



Reactive Dynamics on Fractal Substrates
(The different colours correspond to different chemical species)

For the study of such complex systems in the lab we develop a) statistical methods/tools describing complex morphologies and b) modelling of the dynamics of pattern formation. Statistical methods include thermodynamic approaches, entropic (extensive and non-extensive) approaches, theory of long and short range distributions, and Levi distributions and the theory of random walks. For the study of the mechanisms creating complex patterns, non-linear dynamical systems of hierarchical complexity are used, together with mean-field theories, exact enumeration methods, real space renormalisation theory, theory of stochastic processes and numerical Monte Carlo Methods.

Applications in the lab include, among others, studies of surface phenomena and aggregates with fractal morphology, bioinformatics, statistical analysis and modelling of biological macromolecules, non-linear studies of open and closed catalytic surface reactions as well as the influence of diffusion on low dimensional catalysis..

Publications 2007

1. Oikonomou, Th., "Tsallis, Renyi and nonextensive Gaussian entropy derived from the respective multinomial coefficients", *Physica A*, 2007, 386, 119-134.
2. Provata, A.;, Oikonomou, T.;, "Power law exponents characterizing human DNA", *Phys. Rev. E* , 2007, 75, Art. No. 056102.

3. Sellis, D.; Provata, A.; Almirantis, Y.; "Alu and LINE1 distributions in the human chromosomes: Evidence of global genomic organization expressed in the form of power laws", *Mol. Biol. & Evol.* 2007 24 (11): 2385-2399.
4. Noussiou, V.K.; Provata, A.; "Surface reconstruction in reactive dynamics: A kinetic Monte Carlo approach", *Surface Science* 2007 601 (14): 2941-2951.
5. Provata, A.; "Non-extensive block entropy statistics of Cantor fractal sets", *Physica A*, 2007, 381, 148-154.
6. Provata, A.; Noussiou, V.K.; "Fractal pattern formation in the Ziff-Gulari-Barshad model", *J. Phys. C- Cond. Mat.* 2007, 19 (6): Art. No. 065128.
7. Oikonomou, Th., "Properties of the "non-extensive Gaussian" entropy", *Physica A*, 2007, 381, 381 155–163.
8. Oikonomou, Th.; Provata, A.;, Tirnakli, U.; "Nonextensive statistical approach to non-coding human DNA", *Physica A*, 2008, 387 2653–2659
9. Noussiou, V.K.; Provata, A.; Kinetic Monte Carlo simulations of the oscillatory CO oxidation at high pressures: the surface oxide model", *Chem. Phys.* 2008, accepted.
10. Kouvaris, N.; and Provata, A.; "Trimolecular reactive system with spatial disorder*", Nonlinear Phenomena in Complex Systems* 2008, accepted.

Conferences

1. Noussiou, V. K. ; Provata A.; "Kinetic Monte Carlo simulations of the oscillatory CO oxidation at high pressures: the surface oxide model", Summer School: Morphogenesis through the interplay of nonlinear chemical instabilities and elastic active media, 2 - 14 July 2007, Cargèse, France
2. Noussiou, V. K. ; Provata A.; "Kinetic Monte Carlo simulations of the oscillatory CO oxidation at high pressures: the surface oxide model", 20th International Conference / Summer School: NONLINEAR SCIENCE AND COMPLEXITY , 19 – 29 July 2007, Patras, Greece.
3. Oikonomou, Th; "Tsallis, Renyi and nonextensive Gaussian entropy derived from the respective multinomial coefficients", 20th International Conference / Summer School: NONLINEAR SCIENCE AND COMPLEXITY , 19 – 29 July 2007, Patras, Greece.
4. Kouvaris, N.; Provata,; "Complex Population Dynamics and Oscillations on Low Dimensional Lattices", Summer School on "Morphogenesis through the interplay of nonlinear chemical instabilities and elastic active media", Cargese, France (2007).
5. Kouvaris, N.; Provata,; "Complex population dynamics, coexistence of oscillatory steady state and frozen pattern", poster at 20th International Conference and Summer School on "Non Linear Science and Complexity", 19 – 29 July 2007, Patras, Greece.

Funded Projects

1. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008
2. "MOLSIMU: Forging the Missing Link: From Molecular Simulations to Nanoscale Experiments", COST Scientific Network, 10 K€ (from 400 000 € total budjet), 2004-2008 .

Infrastructure

1 computer Pentium IV, dual core + dual processor (Linux).
4 computers Pentium IV (Linux).
1 personal computer (Windows).

Personnel

A. Provata: research director/group leader (permanent researcher); P. Katsaloulis: (post doctoral associate, external funding); V. Nousiou, N. Kouvaris: (2 PhD students, NCSR "D" fellows), Th. Oikonomou: (PhD student, external funding).

Collaborations

Dr. Y. Almirantis (NCSR "Demokritos", Genome Organisation), Prof. G. Nicolis (Free University of Brussels, Service de Chimie-Physique, Brussels, Belgium, "Entropic Representations of DNA"), Prof. T. Bountis (Univ. of Patras, 'Statistical Properties and Correlations of Genomic Data and Biological Time Series'), Prof. Th. Theoharis (Univ. of Athens, 'Non-linear Dynamics in the Genome of Higher Eucaryotes'), Dr. A. Shabunin (University of Saratov, Russia, 'Non-linear reactive dynamics on low dimensional and fractal lattices'), Profs. A Tsekoutas and A. Koutselos (Univ. of Athens "Chemical Dynamics of Catalytic Reactions"), Prof. D.. Kougioumtzis (Univ. of Thessaloniki, "Pattern formation on low dimensional lattices"), Prof. B. Spagnolo (Univ. of Palermo, Dept of Physics, "Ecological Complex Systems). Prof. I. Sokolov and Prof. L. Schimansky-Geier (humbolt Universitaet Berlin, Dept. of Physics, "Reactive Dynamics with Diffusion on Low Dimensional Supports")

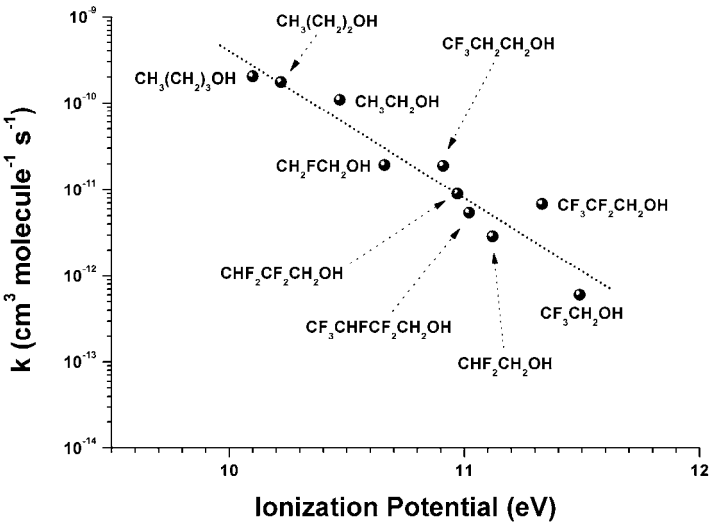
Contact

Dr. A. Provata (aprovata@chem.demokritos.gr, Tel. +30 210 6503964, Fax. +30 210 6511766)
Web site: http://limnos.chem.demokritos.gr/

MOLECULAR COMPUTATIONAL CHEMISTRY

Research Objectives/Activities

The research activity of Molecular Computational Chemistry Laboratory encompasses the study of chemical reactivity and tropospheric degradation of molecules as well as the reliable prediction of properties of molecular materials by theoretical methods.
More specifically, the environmental behavior of a series of fluorinated alcohols towards chlorine atoms has been studied, and their reactivity has been successfully correlated with reliably calculated molecular properties, such as C-H bond strengths and ionization potentials, in order to allow the assessment of the environmental impact for these candidate substitutes of Freons. In addition, the reactivity of chlorinated and fluorinated ethanols towards hydroxyl radicals in aqueous solutions was studied as a function of theoretically calculated molecular properties. The reactivity of naturally emitted diiodomethane CH_2I_2 towards chlorine atoms as well as the oxidation mechanism of the CH_2I και CHI_2 free radicals was clarified by quantum-mechanical calculations.
The tropospheric degradation rate of small organic molecules (CH_4, CH_3F, CH_2F_2, CHF_3 και CH_3OH) by chlorine atoms and hydroxyl radicals and the dependence of the rate on the number and position of water molecules attached is being studied by using *ab-initio* and DFT methods in the framework of Transition State Theory.
The electronic structure and the molecular properties of ML_2 complexes of first-row transition metals (M = Mn, Fe, Co, Ni, Cu, Zn) with ligands L as models of several metalloenzymes active sites are studied by DFT methods, in order to assess the role of the metal in the structural, optical and magnetic properties of complexes.
The coordination ability of lanthanide cations with substituted cyclodextrins is studied by semiempirical methods (AM1, PM3) in order to determine the structure of the complexes which may be employed in magnetic resonance imaging techniques (MRI).



Correlation diagram of fluorinated alcohols rate coefficients with chlorine atoms as a function of their ionization potentials.

Publications 2007

1. V. C. Papadimitriou, D. K. Papanastasiou, V. G. Stefanopoulos, A. M. Zaras, Y. G. Lazarou and P. Papagiannakopoulos, "Kinetic Study for the Reactions of Cl Atoms with $CF_3CH_2CH_2OH$, $CF_3CF_2CH_2OH$, $CHF_2CF_2CH_2OH$, and $CF_3CHFCF_2CH_2OH$", J. Phys. Chem. A **2007**, 111, 11608 - 11617.
2. *V.G. Stefanopoulos, V. C. Papadimitriou, Y.G. Lazarou and P. Papagiannakopoulos, "Absolute Rate Coefficient Determination and Reaction Mechanism Investigation for the Reaction of Cl Atoms with CH_2I_2 and the Oxidation Mechanism of CH_2I Radicals", J. Phys. Chem. A **2008**, 112, 1526 - 1535.*
3. *I. Morozov, S. Gligorovski, P. Barzaghi, D. Hoffman, Y.G. Lazarou, E. Vasiliev and H. Herrmann, "Hydroxyl Radical Reactions with Halogenated Ethanols in Aqueous Solution: Kinetics and Thermochemistry", Int. J. Chem. Kinet. **2008**, 40, 174 - 188.*

Conferences

1. Zaras, A.M., Lazarou Y.G. "Interaction of HNO_3 and HO_2 with water clusters: A theoretical investigation", Computational Chemistry Workshop, LAL, Orsay, France, December 3-4, 2007.
2. Zaras, A.M., Stefanopoulos V.G., Papanastasiou D.K., Papadimitriou V.C., Romanias M.N., Lazarou Y.G., Papagiannakopoulos, P. "Interaction of HNO_3 and HO_2 with water clusters: A theoretical investigation", 2nd Accent Symposium, ATMOSPHERIC COMPOSITION CHANGE, 'Causes and Consequences-Local to Global', Urbino, Italy, July 23-27, 2007.
3. Zaras, A.M., Lazarou Y.G., "HCl uptake on ice", Third SCOUT-O3 Annual Meeting, Heraklion, Crete, Greece, May 7-11, 2007.

Funded Projects

1. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 5.0 k€, 2006-2008.

Infrastructure

A cluster of personal computers running Linux Redhat and Fedora Core.

Personnel

Yannis G. Lazarou: group leader (permanent researcher); Aristotelis M. Zaras (PhD student)

Collaborations

Prof. P. Papagiannakopoulos (Chemistry Dept., University of Crete, chemical reactions of halogenated molecules, experimental studies, VLP reactor), Dr. I. Mavridis (Inst. Of Physical Chemistry, NCSR "D", complexes of substituted cyclodextrins), Dr. K. Yannakopoulou (Inst. Of Physical Chemistry, NCSR "D", complexes of substituted cyclodextrins), Prof. I. I. Morozov (Russian Academy of Sciences, Moscow, Russia, halogenated ethanols), Lect. P. Kyritsis (Inorganic Chemistry Lab, Chemistry Dept., University of Athens, calculations in metalloenzyme models), Dr. R. Prosmiti (Department of Atomic, Molecular and Cluster Physics, Institute of Fundamental Physics `Blas Cabrera', Spanish National Research Council (CSIC), Madrid, Spain, iodinated compounds).

Contact

Dr. Y. G.. Lazarou (lazarou@chem.demokritos.gr, Tel. +30 210 6503623, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

2nd Scientific Programme

Nanochemistry, Environmental Friendly Technologies - Energy

MATERIALS & MEMBRANES FOR ENVINONMENTAL SEPARATIONS LABORATORY

Research Objectives/Activities

- Characterization of Pore Structure (pore size distribution, surface area, pore volume, pore connectivity) : Nitrogen and Mercury porosimetry, absolute and relative permeability of gases (single – multi phase), Microscopy / Spectroscopy.
- Development – Modification of membranes with the following processes: Chemical Vapor Deposition [CVD], Deposition Langmuir-Blodgett, Plasma treatment, Phase Eversion, Carbonization – Activation
- Evaluation / Control of the behavior of porous materials (membranes, activated carbon filters etc) in various environmental and industrial applications (gas pollutants separations, gas permeability, reversed osmosis, control release systems, transcutaneous drug dosing)
- Simulation of mass and heat transfer processes in porous media with continuing (macroscopic) and discernible numerical models (networks)
- Visual representation of flow through porous media with the use of various techniques pore sizes.
- Numerical and experimental simulation and also visual representation of oil recovery techniques with the use of mathematical and experimental well defined geometry structures under environment and high pressure contitions
- Reconstruction of porous media with the use of scanning tomography which uses graphic methods floated by a computer

Publications 2007

1. E. Kouvelos, K. Kesore, T. Steriotis, H. Grigoropoulou, D. Bouloubasi, N. Theophilou, S. Tzintzos and N. Kanelopoulos, "High pressure N2/CH4 adsorption measurements in clinoptilolites", *Microporous and Mesoporous Materials*, **99**, 106-111 (2007).
2. F.K. Katsaros, Th.A. Steriotis, G.E. Romanos, M. Konstantakou, A.K. Stubos and N.K. Kanellopoulos, "Preparation and characterisation of gas selective microporous carbon membranes", *Microporous and Mesoporous Materials*, **99**, 181-189 (2007)
3. A. Lambropoulos, G. Romanos, Th. Steriotis, J. Nolan, F. Katsaros, E. Kouvelos, G. Charalambopoulou and N. Kanellopoulos, "Application of an innovative mercury intrusion technique and relative permeability to examine the thin layer pores of sol–gel and CVD post-treated membranes**"** *Microporous and Mesoporous Materials*, **99**, 206-215 (2007).
4. A.B. Bourlinos, Th. A. Steriotis, M. Karakassides, Y. Sanakis, V. Tzitzios, C. Trapalis, E. Kouvelos and A. Stubos, "Synthesis, characterization and gas sorption properties of a molecularly-derived graphite oxide-like foam", *Carbon*, **45 (4)**, 852-857 (2007).
5. A. Bakandritsos, A.B. Bourlinos, , V. Tzitzios, N. Boukos, E. Devlin, T.Steriotis, V. Kouvelos, D. Petridis, , Biopolymer networks for the solid-state production of porous magnetic beads and wires, *Advanced Functional Materials* 17 (8), 1409-1416 (2007).
6. A. Lambropoulos, G. E. Romanos, T. A. Steriotis, J. Nolan, F. K. Katsaros, E. Kouvelos, N. K. Kanellopoulos, Development of an innovative mercury intrusion technique to examine defects plugging after CVD treatment of NF composite membranes, *J Porous Mater*, DOI 10.1007/s10934-006-9055-5 (Available on line)
7. Konstantakou M.; Steriotis Th.A.; Papadopoulos G.K.; Kainourgiakis M.; Kikkinides E.S.; Stubos A.K. "Characterization of nanoporous carbons by combining CO_2 and H_2 sorption data with the Monte Carlo simulations", *Appl. Surf. Sci.* **2007**, *253*, 5715–5720.
8. G.N. Karanikolos, J.W. Wydra, J.A. Stoeger, H. García, A. Corma, and M. Tsapatsis "Continuous c-Oriented AlPO4-5 Films by Tertiary Growth", Chem. Μater., 19, 792 (2007)
9. Papageorgiou, S.K.; Kouvelos, E.P.; Katsaros, F.K. "Calcium alginate beads from Laminaria digitata for the removal of Cu+2 and Cd+2 from dilute aqueous metal solutions" Desalination in press

10. *A. De Stefanis, A.A.G. Tomlinson, Th.A. Steriotis, G.Ch. Charalambopoulou and U. Keiderling, "Study of structural irregularities of smectite clay systems by Small-Angle Neutron Scattering and adsorption", Applied Surface Science, in press, Available online 8 January 2007*
11. *A.A. Sapalidis, F.K. Katsaros, G.E. Romanos, N.K. Kakizis and N.K. Kanellopoulos, "Preparation and characterization of novel poly-(vinyl alcohol)–Zostera flakes composites for packaging applications", Composites Part B: Engineering, in press, Available online 30 October 2006*
12. *N.I. Papadimitriou, G.E. Romanos, G.Ch. Charalambopoulou, M.E. Kainourgiakis, F.K. Katsaros and A.K. Stubos, "Experimental investigation of asphaltene deposition mechanism during oil flow in core samples", Journal of Petroleum Science and Engineering, in press,*

Conferences

1. Steriotis Th. "Study of pore confined CO_2 by sorption with in situ neutron diffraction" (Invited), 2nd BENSC Adsorption Workshop, February 2, 2007, Berlin, Germany.
2. Lelong G.; Price D.L.; Bhattacharyya S.; Brady J.W.; Steriotis T.; Charalambopoulou G.; Brandt A.; Saboungi M.-L.; "Neutron Scattering: A tool to probe structure and dynamics in porous silica", 2nd International School & Workshop of INSIDE-POReS NoE, 24-28 February 2007, Thessaloniki, Greece.
3. De Stefanis A.; Tomlinson A.A.G.; Steriotis Th.A.; Charalambopoulou G.Ch.; Keiderling U.; "Characterisation of the nanostructure of smectite clay systems based on SANS and adsorption data", BENSC User's Meeting, Hahn-Meitner Institute, Berlin-Germany, 23-24 May 2007.
4. De Stefanis A.; Tomilnson A.A.G.; Στεριώτης Θ.Α.; Χαραλαμποπούλου Γ.Χ.; Keiderling U.; «Συνδυασμός δεδομένων ρόφησης και μικρογωνιακής σκέδασης νετρονίων για το χαρακτηρισμό της νανοδομής σμεκτιτών», 3ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών Θεσσαλονίκη, 1-2 Νοεμβρίου 2007.
5. Fotis Katsaros, Th. Steriotis, A. Stubos and N. KanellopouloPreparation and Characterisation of carbon powders by pyrolysis of Phenolic resins, s, 2nd International School and Workshop on IN-Situ Study and DEvelopment of Processes Involving PORous Solids (INSIDE-POReS) CERTH, THESSALONIKI GREECE 24 -28th February 2007
6. S. Papageorgiou, F. Katsaros, E. Kouvelos, N. Kanellopoulos, Alginate Beads From Laminaria Digitata For Single And Binary Metal Sorption, Fundamentals of Adsorption (FOA) 09, May 20-25, 2007, Giardini Naxos, Sicily, Italy
7. 3. F.K. Katsaros, S. Papageorgiou, T.A. Steriotis and N.K. Kanellopoulos Preparation and characterization of carbon powders by pyrolisis of Alginate salts, 3rd International Workshop on IN-Situ Study and DEvelopment of Processes Involving PORous Solids (INSIDE-POReS) ALICANTE (SPAIN) 24 -26th September 2007

Funded Projects

coordinator:

1. EE 1195 – INSIDE_PORES NMP3-CT-2004-500895, "In-Situ Study and Development of Processes Involving Nano-Porous Solids", Network of Excellence in nanotechnology FP6, Priority 3 – NMP, Thematic priority 3.4.1.1. Partners to NCSR "D": Centre Nationale de la Researche Scientifique (France), Imperial College (United Kingdom), University of Leipzig (Germany), University of Antwerp (Belgium), University of Stuttgart (Germany), Institute of Energy and Technology (Norway), TuDelft (The Netherlands), University of Alicante (Spain), Instituto di Chimica dei Mateiali (Italy), Centre for Research and Technology Hellas (Greece), University of Hannover (Germany), SINTEF(Norway),TNO (The Netherlands). Total Budget: 6.800.000 €, NCSR "D" Budget: 1.844834 €. (October 2004- October 2008).
2. EE 1399 - HYCONES NMP3-CT-2006-032970, "Hydrogen Storage in Carbon Cones", Partners to NCSR "D": Institute for Energy Technology (NO), The University of Nottingham (UK), Institute of Nuclear Physics, Polish Academy of Sciences (PL), Scatec AS (NO) Total Budget 2.564.000 €, NCSR"D" Budget: 577.000 € (November 2006-September 2009).
3. EE 1112 - EPAN-HYDROCELL E-22 F.P. 39 14010/19-10-2003, "Development of Production Technologies for Hydrogen used in Fuel Cells", GREEK NATIONAL OPERATIONAL PROGRAMME "COMPETITIVENESS", AXIS 4 – MEASURE 4.5, CONCERTED PROGRAMME "RENEWABLE ENERGY SOURCES & ENERGY SAVING". Partners to NCSR "D": Silver & Baryte Co S.A.,

Phosphorous Fertilizers Industry, Motor Oil Hellas S.A., DEYAMV, ENOIA S.A. Total Budget 1.084,533 €, NCSR"D" Budget: 299.400 € (September 2003-August 2006).

4. EE 1242 - EPAN-NANOFOOD TP-21, "Development of ceramic membranes for applications in food industries", GREEK NATIONAL OPERATIONAL PROGRAMME "COMPETITIVENESS", AXIS 4 – MEASURE 4.5, CONCERTED PROGRAMME "Food Agriculture", Partners to NCSR "D": Tsantalis S.A., Greek Sugar Industry, Zenon S.A., Technological Educational Institute (T.E..I.) of Athens, EVGA S.A. Total Budget 600.200 €, NCSR"D" Budget: 112.800 € (November 2004-October 2007).
5. EE 1232 - HUNGARY–GREECE JOINT RESEARCH AND TECHNOLOGY PROGRAMMES 2003 – 2006, "Preparation of Highlyt Selective Carbon for CO_2/CO Separation", Partners to NCSR "D": Department of Physical Chemistry Budapest University of Technology and Economics (Hungary), SUC Hellas (Greece). NCSR"D" Budget: 23.460 € (January 2005-December 2006)
6. EE 1290- EPAN – Ο3ΕΔ181, "Design and development of carbon and silicon nanostructures. Theoretical and experimental investigation of their application in hydrogen, or other gas, mixtures separation and storage processes." GREEK NATIONAL OPERATIONAL PROGRAMME "COMPETITIVENESS", MEASURE 8.3, CONCERTED PROGRAMME "Nanotechnology". Partners to NCSR "D": University of Athens, University of Illinois Chicago, SUC HELLAS Ltd (IPEL). Total Budget: 111.660 €, NCSR "D" Budget: 67.642 € (December 2005 – December 2008)
7. POLAND-GREECE 157-ε, Development and Testing of Ordered Porous Materials for Olefin-Paraffin Gas Separations, JOINT RESEARCH AND TECHNOLOGY PROGRAMMES 2005 – 2007, Partner to NCSR "D": Institute of Chemical Engineering-Polish Academy of Sciences (PO). Budget NCSR "D": 11.740 € (October 2006-March 2008).
8. Ανάπτυξη Πρωτότυπων Συστημάτων Αφαλάτωσης και Επεξεργασίας Υγρών Αποβλήτων με Χρήση Κοίλων Μεμβρανών Διπλής Στοιβάδας (ΑΦΕΠ) Development of Desalination Systems and Waste Water Treatment with the use of Hollow fibers

NCSRD budget: 141.500 euros

Partners

1. FUSION "Fundamental Studies of Transport in Inorganic Nanostructures", FP6, Thematic priority 3.4.2.1-2. Partners to NCSR "D": University College Dublin (Ireland), University of Edinburgh (UK), Delft University of Technology (The Netherlands), Warsaw University of Technology (Poland), VTT Technical Research Centre of Finland, EcoCeramics B.V. (The Netherlands). Total budget: 2.137.000 €, NCSR"D" Budget: 180.000 €. (December 2004-November 2007).
2. ERA Pilot MiNa TSI "European Research Area Pilot Action onMicroNano Technology Systems Integration", FP6 Priority. Partners to NCSR "D": VDI/VDE Innovation + Technik GmbH (Germany), Österreichische Forschungsförderungsgesellschaft (Austria), University Of Tartu (Estonia), Ministerio De Educacion Y Ciencia (Spain), Association Eurimus Office (France), Association For Pidea (France), Commissariat A L'Energie Atomique (France), Ente Per Le Nuove Tecnologie, L'Energia E L'Ambiente (Italy), Israeli Industry Centre For Research and Development (Israel), Fondazzjoni Temi Zammit (Malta), Slovenska Technicka Univerzita v Bratislave (Slovakia). Total Budget: 850.000 €. NCSR"D" Budget: 42.366 €. (July 2005-July 2007).

Infrastructure

1. Nitrogen porosimeter with Krypton upgrade - Quantachrome
2. Mercury Porosimeter - Quantachrome
3. Low pressure single component permeability rig
4. High pressure 70 bar single component permeability rigς (2)
5. Two high pressure mass flow controlled permeability/selectivity rigs (one up to 50 bar and the second up to 100 bar-up to 3 gas components each-flow rates 0-50 ml/min or 0-1000 ml/min)
6. One low-medium pressure mass flow controlled permeability/selectivity rig (one up to 5 bar-3 gas components each-flow rates 0-1000 ml/min)
7. Gas chromatographers (3) with auto sampling capabilities
8. Mass spectrometer – Residual gas analyzer - Pfeiffer
9. Several Flow systems
10. Hybrid Membrane Sorption Unit for the removal of Organic Chemicals
11. Gravimetric analyzer - HIDEN IGA

12. Gravimetric systems with magnetic suspension (2) - Rubotherm
13. Low pressure gravimetric systems (3) – CI balances
14. Langmuir-Blodgett (LB) trough of thin films
15. Chemical Vapor Deposition reactor
16. Grazing incidence infrared GIIR reflection unit
17. Advanced Imaging Equipment, including a Computerized Video Unit for the Investigation of Flow Phenomena through Porous Systems
18. Extensive IT and Network infrastructure available including UNIX servers, access to supercomputer clusters for advanced modeling applications, T3 Network Lines etc.
19. Quartz crystal microbalances (2) – Q-sense, ThinkSRS
20. High vacuum systems
21. High pressure volumetric apparatus for isotherms - VTI
22. Gas and vapour permeability apparatus for polymers and nano-composites (oxygen permeability – Danseror PBI
23. AFM - Veeco Innova
24. FTIR Nicolet 6700
25. High pressure cell for FT-IR
26. Ultra pure water
27. Ion chromatography system – Dionex
28. HPLC - Dionex
29. Calorimeter Calvet - Setaram
30. Thermal analysis (TGA) - Setaram
31. Zero length Chromatography

Personnel

N.Kanellopoulos (Research director-permanent researcher), Th. Steriotis, K. Stefanopoulos, F. Katsaros, G. Romanos,N. Kakizis, V. Kouvelos, A. Sapalidis, V. Favvas, S. Papageorgiou, C. Athanasekou, G. Pilatos A. Gotzias(permanent researchers, S. Christou, E. Zinger (2 research Associates,external funding), E. Vermisoglou, A. Labropoulos, H. Veziri, V. Akillas, (phd students, external funding)

Collaborations

A. Roussis(UOA),N. Theofilou (S&B), A. Dimitriadis (Tsantali),G. Theodoridis (VFL S.A.) S. Ravani(EVZ S.A.) H. Foteinopoulos (Motor Oil)

Contact

Nick Kanellopoulos
MESL - Materials & Membranes for Environmental Applications Laboratory HYPERLINK "http://mesl.chem.demokritos.gr"http://mesl.chem.demokritos.gr
NCSRD - National Center for Scientific Research "Demokritos"
15310 Agia Paraskevi, Athens, Greece

Network of Excellence: INSIDE_POReS - IN-SItu study and DEvelopment of processes involving nano-PORous Solids.
HYPERLINK "http://www.inside-pores.gr"http://www.inside-pores.gr

tel: 0030-210-6503977, 6535294
fax: 0030-210-6511766
mobile: 0030-6944-787050
e-mail: HYPERLINK "mailto:kanel@chem.demokritos.gr"kanel@chem.demokritos.gr
HYPERLINK "mailto:mesl@chem.demokritos.gr"mesl@chem.demokritos.gr

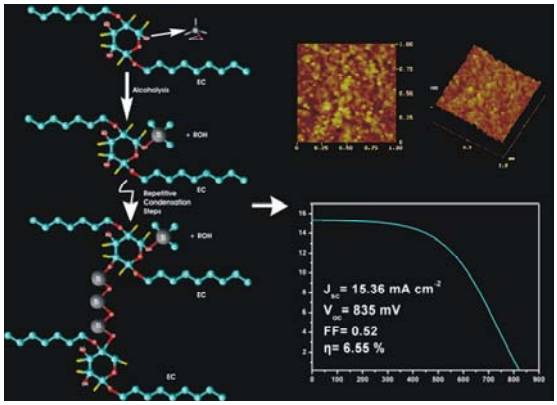
PHOTOREDOX CONVERSION AND STORAGE OF SOLAR ENERGY – DEVELOPMENT OF NEW FUNCTIONAL MATERIALS FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

Research Objectives / Activities

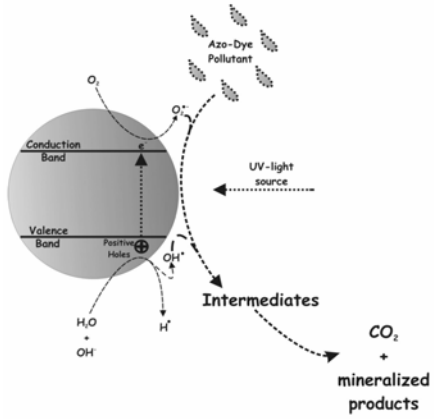
The research activities are mainly centered on the investigation of photoinduced processes and their application to direct conversion of solar energy to electricity as well as to environmental cleaning and health protection. The scientific work is centered on:

1. Dye-sensitization of large band-gap semiconductors

The direct conversion of solar energy to electricity is investigated by developing heterojunctions consisting of large band-gap semiconductors sensitized by light harvesting molecular antennas-transition metal complexes. The main objectives concern the investigation, tuning and optimization of photoinduced processes taking place at the semiconductor/dye/electrolyte interface. Essential emphasis is given to the design, synthesis/preparation, characterization, theoretical analysis/modeling and evaluation of performance of multifunctional inorganic photonic compounds [metal oxide thin films (nanopartıculate and nantube), transition metal complexes) and redox nanocomposite polymer electrolytes as well as their efficient incorporation in photoelectrochemical devices. Based on its intensive research activity, the team has established fruitful collaborations with research institutions and foreign companies for development of dye-sensitized solar cells (DSSCs) and their optimization in terms of efficiency, life-time and stability. Besides technology transfer, the perspectives of this collaboration include the creation of a DSSC manufacturing facility in Greece and demonstration activities in the field of building integrated photovoltaics.



Sol-gel synthesis of fractal nanotitania and I-V characteristic of the corresponding DSSC



Degradation of pollutants using TiO_2 photocatalysis

2. Innovative nanostructured photocatalysts for environmental cleaning and health protection

Heterogeneous photocatalytic processes and related applications are investigated, involving functional photonic materials in the nanometer scale. The scientific effort aims at improving the efficiency of photocatalytic processes via: a) increase of the photocatalyst effective surface area; b) efficient separation of the photogenerated charge carriers (e^- and h^+); c) photocatalytic sensitization into the Vis light region-shift of the absorption onset; d) judicious balance of photocatalytic and superhydrophylic properties on multi-dynamic surfaces able to photochemically decompose harmful organics, kill bacteria and viruses and being easily self-cleaned; e) increased anticancer and anticoagulant action of titanium dioxide on neoplasm and inflammatory cells.

Publications 2007

1. Faiz, J.; Philippopoulos, A.I.; Kontos, A.G.; Falaras, P.; Pikramenou, Z. "Functional supramolecular ruthenium cyclodextrin dyes for nanocrystalline solar cells" *Adv. Funct. Mater.* 2007 *, 17* , 54-58.
2. Tsoukleris, D.S. ; Kontos, A. I. ; Aloupogiannis, P.; Falaras, P. "Photocatalytic properties of screen printed titania", *Catal. Today* 2007, *124*, 110-117.
3. Kontos, A. I.; Kontos, A. G.; Tsoukleris, D. S.; Vlachos, G. D.; Falaras, P. "Superhydrophilicity and photocatalytic property of nanocrystalline Titania sol-gel films" *Thin Solid Films* 2007, *515*, 7370-7375.
4. Krstajic, N.V.; Vracar,L.M.; Radmilovic,V.R.; Neophytides, S.G.; Labou,M.; Jaksic, J.M.; Tunold, R.; Falaras, P; Jaksic, M.M. "Advances in Interactive Supported Electrocatalysts for Hydrogen and Oxygen Electrode Reactions" *Surface Science* 2007, *601*, 1449-1966.
5. Ibhadon, A.O.; Arabatzis, I.M.; Falaras, P. "The Design and Photoreaction Kinetic Modeling of a Gas-Phase Titania Foam Packed Bed Reactor", *Chem. Eng. J.* 2007 , *133*, 317-323.
6. Mitsopoulou, C.A.;Veroni, V.; Philippopoulos, A.I.; Falaras, P. "Synthesis, characterization and sensitization properties of two novel mono and bis carboxyl-dipyrido-phenazine ruthenium (II) charge transfer complexes", *J. Photochem. Photob. A: Chem.* 2007, *191*, 6-12.
7. Tsoukleris, D.S.; Maggos, T.; Vassilakos, C.; Falaras, P. "Photocatalytic degradation of volatile organics on TiO_2 embedded glass spherules", *Catal. Today* 2007, *129*, 96-101.
8. Hahn, R.; Stergiopoulos, T.; Macak, J.M.; Tsoukleris, D.; Kontos, A.G.; Albu, S.; Kim, D.; Ghicov, A.; Kunze, J.; Falaras, P.; Schmuki, P. "Efficient solar energy conversion using TiO_2 nanotubes produced by rapid breakdown anodization - acomparison", *Phys. Status Solidi (RRL)* 2007, *1*, 135-137.
9. Chatzivasiloglou, E.; Stergiopoulos, T.; Kontos, A.G.; Alexis, N.; Prodromidis, M.; Falaras, P. "The influence of the metal cation and the filler on the performance of dye-sensitized solar cells using polymer-gel redox electrolytes", *J. Photochem. Photob. A: Chem.* 2007, *192*, 49-55.
10. Al-mutlaq, F.A.; Potvin, P.G.; Philippopoulos, A.I.; Falaras, P. "Catechol-Bearing Dipyrazinylpyridine Complexes of Ruthenium(II)", *Eur J. Inorg. Chem.* 2007, 2121–2128.
11. Jaksic, J.M.; Krstajic, N.V.; Vracar, L.M.; Neophytides, S.G.; Labou, D.; Falaras, P.; Jaksic, M.M. "Spillover of primary oxides as a dynamic catalytic effect of interactive hypo-d-oxide supports", *Electrochim. Acta* 2007, *53*, 349-361.
12. Maletin, M.; Kontos, A.G.; Devlin, E.; Cvejić, Ž.; Srdić, V.V.; Moshopoulou, E.G. "Synthesis and structural characterization of In-doped $ZnFe_2O_4$ nanoparticles", *J. Eur. Ceram. Soc.* 2007, *27*, 4391-94.
13. Philippopoulos, A.I.; Terzis, A.; Raptopoulou, C.P.; Catalano, V.J.; Falaras, P. "Synthesis, characterization and sensitizing properties of heteroleptic Ru(II) complexes based on 2,6-bis(N-pyrazolyl)pyridine and 4,4'-dicarboxy-2,2'-bipyridine ligands", *Eur. J. Inorg. Chem.* 2007, 5633-5644.
14. *Kontos, A.I.; Kontos, A.G.; Tsoukleris, D.S.; Bernard, M.; Spyrellis, N.; Falaras, P. "Nanostructured TiO_2 films for DSSCS prepared by combining doctor blade and sol gel techniques", J. Mater.. Process. Tech (in press).*
15. *Kontos, A.G.; Stergiopoulos, T.; Tsiminis, G.; Raptis, Y.S.; Falaras, P. "In-situ micro- and macro- Raman investigation of the redox couple behavior in dsscs", Inorg. Chim. Acta, invited paper (in press).*
16. *Katsanaki, A.; Tsoukleris, D.S.; Falaras P; Karayianni, H.S. "Preparation and characterization of nanocrystalline Pt/TCG counter electrodes for dye-sensitized solar cells", J. Sol. Energy Eng. (in press).*

Conferences

1. Ghicov, A.; Hahn, R.; Albu, S.P.; Kim, D.; Macak, J.M.; Stergiopoulos, T.; Tsoukleris, D.; Kontos, A.G.; Kunze, J.; Falaras, P.; Schmuki, P. "Efficient solar energy conversion using TiO_2 nanotubes", EuroNanoForum 2007, Düsseldorf, Germany, June 19-21. p. 279.
2. Hahn, R.; Stergiopoulos, T.; Ghicov, A.; Albu, S.P.; Kim, D.; Macak, J.M.; Tsoukleris, D.; Kontos, A.G.; Kunze, J.; Falaras, P.; Schmuki, P. "Use of Anodic TiO_2 Nanotubes in Dye-Sensitized Solar Cells", Nano Europe 2007, St. Gallen, Switzerland, 11-13 September 2007.

3. Falaras, P.; Tulloch, G.; Harikisun, R.; Desilvestro, H.; Stergiopoulos, T.; Likodimos, V.; Kontos, A.G. "Micro-Raman analysis-Aged IV characteristics of DSC", Abstract in Proceedings of Nano Europe 2007, St. Gallen, Switzerland, 11-13 September 2007, invited.
4. Vasilopoulou, M.; Stathopoulos, N.; Falaras, P.; Pistolis, G.; D. Davazoglou, D.; Argitis, P. "An all-organic optocoupler based on polymer light-emitting diodes (PLEDs)", P II.38, 3rd International Conference MICRO&NANO 2007 on Micro-Nanoelectronics, Nanotechnology & MEMs, Athens, 18-21 November 2007.
5. Macak, J.; Hahn,R.; Stergiopoulos, T.; Ghicov, A.; Tsoukleris, D.; Albu, S.; Kunze, L.; Kim, D.; Falaras, P.; Schmuki, P. "Use of Anodic TiO_2 Nanotubes in Solar Cell", Symposium H: Nanostructured Solar Cells, 2007 MRS Fall Meeting, Hynes Convention Center and Sheraton Boston Hotel, Boston, MA, , **November 26 - 30, 2007.**
6. Lagopati, N.; Kontos, A.I.; Venieratos, P.; Kitsiou, P.; Tsilibari, E.F.; Falaras P. "Photoinduced Cancer Treatment Using Nanostructured Titanium Dioxide Solution and Corresponding Molecular Mechanisms", International conference on nanomedicine, Porto Carras Grand Resort, Chalkidiki, Greece, September 9 –11, 2007.
7. Kyrkou, A.; Kontos, A.I.; Papavasileiou, G.; Charitidis, C.; Falaras, P. "Investigation of the Structural Properties and Photocatalytic Activity Control of Monodispersed TiO_2 Nanospheres", THE INTERNATIONAL CONFERENCE ON STRUCTURAL ANALYSIS OF ADVANCED MATERIALS - ICSAM, Session 8A-NANOMATERIALS, Lect. 8A-4, Patras, Greece, September 2-6, 2007.

Funded Projects

1. "Molecular Engineering of Interfaces of Photonic Devices based on Mesoscopic Oxide layers", COST Action D35- "From Molecules to Molecular Devices", 2005-2009.
2. "Ti-nanotubes", FP6-NMP-STREP, 300 K€, 2006-2009.
3. "Facing pathogenic conditions by combined use of bio-medical methods and nanotechnology" Ypodomes, Metro 4.5, 4.4.1 Action «Consortia of research and technological development in sectors of National priorities», 2050-4/2, 300 k€,, 2005-2008.
4. "Organic Solar Cells" PENED 03ΕΔ 118 project, Coordinator P. Falaras: 144 k€, 2005-2008.
5. "Development of composite nanostructured titania. Incorporation into photocatalytic construction materials and application in the decomposition of model liquid and gas pollutants", PENED 03ΕΔ 963 project, 51 k€, 2005-2008.
6. "Development of integrated control analytical methods and advanced oxidation processes for the detoxification of natural water and treated wastes", PENED 03ΕΔ 926 project, 2005-2008.
7. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008.
8. "Developing of a managing system for monitoring the concentration of suspended particles and the estimated population exposure in Attica", PEP Attikis, 30 k€, 2006-2008.
9. "OrgaPVNet – Coordination Action towards stable and low cost organic solar cell technologies and their application", FP6-Energy-CA, 2006-2009.

Patents

1. Falaras, P., "Modified nanostructured titania materials and methods of manufacture", Pub. No.: WO/2007/085911, Publication Date: 02.08.2007, International Application No: PCT/IB2006/004163, International Filing Date: 19.12.2006

Infrastructure

Micro-Raman spectrometer with visible and IR excitation, photoelectrochemistry unit, cyclic and linear sweep voltametry, screen printing and spin coating deposition facilities, photocatalytic reactors, contact angle meter and viscosity meter.

Personnel

P. Falaras: research director/group leader (permanent researcher); T. Stergiopoulos, A.G. Kontos, V. Likodimos: (3 post doctoral associates, external funding); E. Chatzivassiloglou, G. Konti: (2 PhD students, NCSR "D" fellows); A.I.Kontos, G. Kantonis, E.Rozi, N. Alexaki, A. Katsanaki: (5 PhD students, external funding); D.Tsoukleris: (technical staff, external funding).

Collaborations

M. Grätzel (EPFL Lausanne, Switzerland, DSSCs), G. Tulloch (Dyesol, Australia, Light ant Thermal Stress on DSSCs.), J. Kunze (Erlangen, Germany, Ti-Nanotubes), V. Catalano (Nevada, USA, Ligands for Ru-dyes), P. Potvin (Toronto, Canada, Dyes for DSSCs), Z. Picramenou (Birmingham, UK, Supramolecular Dyes), A. Ibhandon (Hull University, UK, Photoreactors).

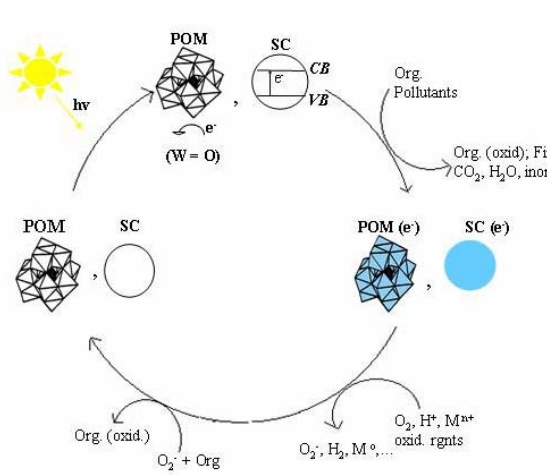
Contact

Dr. P. Falaras (papi@chem.demokritos.gr, Tel. +30 210 6503644, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

CATALYTIC-PHOTOCATALYTIC PROCESSES (SOLAR ENERGY-ENVIRONMENT)

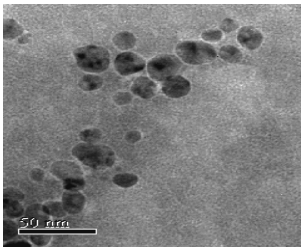
Research Objectives / Activities

Catalytic photocatalytic reactions for solar energy utilization, environmental detoxification and environmentally friendly processes. In particular aggregates of metal oxides, mainly TiO_2, and polyoxometallates (POM) mainly of W, are used in thermal photochemical reactions for: (a) Water splitting (hydrogen production), (b) photoelectro-chemical produdtion of electricity, (c) modification of electrodes (photoelectron-chemical reactions), (d) selective oxidation-synthesis of organic chemicals, (e) non-selective oxidation (photodegradation) of organic pollutants to CO_2, H_2O and inorganic anions, (f) reduction-removal of metallic ions and (g) synthesis of metal nanoparticles and



Hiskia et al., Chem. Soc. Rev., 30 (2001), 62

Current research interests: (a) immobilization of photocatalysts in optically active and/or inert substrates, (b) synthesis of nanocomposite films of polymer/POM with layer by layer (LbL) technique, characterization and investigation of their photocatalytic properties (c) photocatalytic synthesis of metallic nanoparticles deposited in nanostructured multilayer films (d) sensitisation of photocatalysts towards the visible light and (e) development of new methods of analysis for trace organic pollutants.



Hiskia et. al., Angew. Chem. Int. Ed. 41 (2002) 1911-1914

Ag **Au** **Pd** **Pt**

Publications 2007

1. Kormali, P.; Triantis, T.; Dimoticali, D.; Hiskia, A.; Papaconstantinou, E. "On the Photooxidative behavior of TiO_2 and Polyoxometalate $PW_{12}O_{40}^{3-}$. OH radicals vs holes.", *Applied Catalysis B: Environmental* **2006**, 68, 139-146.
2. Troupis, A.; Gika, E.; Hiskia, A.; Papaconstantinou, E. "Photocatalytic Reduction of Metals using Polyoxometallates: Recovery of Metals or Synthesis of Metal Nanoparticles." *Comptes Rendus Chimie* **2006**, 9, 851-857.
3. Hiskia, A.; Troupis, A.; Antonaraki, S.; Gkika, E.; Kormali, P.; Papaconstantinou, E. "Polyoxometallate photocatalysis for decontaminating the aquatic environment from organic and inorganic pollutants.", *Inter. J. Environ. Anal. Chem.* **2006**, 86, 233-242.
4. Gkika, E.; Troupis, A.; Hiskia, A.; Papaconstantinou, E. "Photocatalytic Reduction of Chromium and Oxidation of Organics by Polyoxometalates" *Applied Catalysis B: Environmental* **2006**, 62, 28-34.
5. Agiamarnioti K., Triantis T., Papadopoulos K., Scorilas A., "10-(2-Biotinyloxyethyl)-9-acridone: A novel fluorescent label for (strept)avidin–biotin based assays", *J. Photochem. Photobiology A: Chemistry*, **2006**, 181, 126-131.
6. Eliades, Th.; Hiskia, A.; Eliades G.; Athanasiou, A. "Assessment of bisphenol-A release from orthodontic adhesives" *American Journal of Orthodontics and Dentofacial Orthopedics*, in press.

7. Troupis, A.; Gkika, E.; Hiskia, A.; Papaconstantinou, E. "Photocatalytic Reductive Destruction of Azo Dyes by Polyoxometalates", *JAOT*, in press.
8. Troupis, A.; Gkika, E.; Triantis, T.; Hiskia, A.; Papaconstantinou, E. "Photocatalytic Reductive Destruction of Azo Dyes by Polyoxometellates: Naphthol Blue Black.", *J. Photochem. Photobiology A: Chemistry*, in press.

Conferences

1. Kaloudis, T.; Thanasoulias, N.; Kousouris, L.; Tzoumerkas, P.; Triantis, T.; Gkika, E; Tsimeli K.; Hiskia, A. "Development of an integrated laboratory system for the monitoring of cyanotoxins in surface and drinking waters." 5th International Conference on Instrumental Methods of Analysis, IMA, Πάτρα, 30 Σεπτεμβρίου-4 Οκτωβρίου 2007.
2. Tsimeli, K.; Triantis, T.M.; Dimotikali, D.; Hiskia, A. "Development of a rapid and sensitive method for the simultaneous determination of 1,2-Dibromoethane, 1,4-Dichlorobenzene and Naphthalene residues in honey using HS-SPME coupled with GC-MS." 3th International Symposium on Recent Advances in Food Analysis, Prague, Czech Republic, 7-9 November 2007.

Funded Projects

1. "Photocatalysis for the mild and selective Functionalization of non-activated C-H bonds", COST Action D29, 2004-2008.
2. "Development of an integrated system for the monitoring of cyanobacteria toxins in surface and processed water by advanced analytical methods", PABET 2005, 32.7 K€, 2006-2008.
3. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 9.5 k€, 2006-2008.
4. "Integrated National Center for Environmental Technology" EPAN, 36 K€, 2006-2008.

Infrastructure

Photolysis apparatus, Catalytic/ Photocatalytic reactors, Spectrophotometers UV-VIS-near IR, GC equipped with FID, ECD and TCD, HPLC equipped with UV-VIS and FLD, GC/MS, HPLC/MS/MS triple tetrapole, IC, Polarographic unit, TOC, SPE and SPME apparatus, oven, ultrasound bath, analytical balances, pHmeter, Rotary evaporator, ultrapure water apparatus.

Personnel

A. Hiskia: research director/group leader (permanent researcher); T. Triantis: (post doctoral associates); A. Tsimeli, G. Alexakos: (2 PhD students, NCSR "D" fellows); S. Antonaraki, P. Kormali, E. Chasioti, I. Dimitracopoulos, S. Anagnostou: (5 PhD students, without pay); E. Papaconstantinou, T. Caloudis: (adjunct scientists).

Collaborations

Prof. D. Dionysiou (University of Cincinnati, USA, AOP for cyonobacteria toxins destruction), Dr. S. Lacorte (Dep. of Environ. Chem., CID-CSIC, Barcelona, Analytical method development), Dr. T. Caloudis, (EYDAP, trace organic analysis in water)

Contact

Dr. A. Hiskia (hiskia@chem.demokritos.gr, Tel. +30 210 6503643, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

ELECTRONIC SPECTROSCOPY LABORATORY: APPLICATION TO SUPRAMOLECULES AND NANOSTRUCTURES

Research Objectives / Activities

- Guest stability and Dynamics in Nanocavities.
- Dynamics, kinetics and thermodynamics of conformers in the ground and excited state.
- Organized Supramolecular Assemblies: Non- covalently bonded Nanotubes.
- Photophysics and Dynamics of Linear and Dendronized Photonic Polymers

Publications 2007

1. Vasilopoulou, M.; Pistolis, G.; Georgiadou, D.; Argitis, P. "Tuning the emitting colour of Organic Light Emitting Diodes through photochemically induced transformations: towards single layer, patterned, full colour displays and white lighting applications", *Adv. Funct. Mater.* **2007** , *17* , 3477-3485.
2. Balomenou, I.; Pistolis, G. "Experimental evidence for a highly reversible excited state equilibrium between s-cis and s-trans rotational isomers of 2-methoxynaphthalene in solution", *J. Am. Chem. Soc.* 2007, *129*, 13247.
3. Boukos, N.; Chandrinou, C.; Giannakopoulos, K.; Pistolis, G.; Travlos, A. "Growth of ZnO nanorods by a simple chemical method", *Appl. Phys. A* 2007, *88*, 35.

Conferences

2. Vasilopoulou, M.; Pistolis, G.; Botsialas, A.; Stathopoulos, N.; Rangoussi, M.; Argitis, P.; Patterning scheme based on photoacid induced spectral changes for single layer, patterned full color light emitting diodes, in *Organic Electronics — Materials, Devices and Applications*, edited by F. So, G.B. Blanchet, Y. Ohmori (Mater. Res. Soc. Symp. Proc. 965E, Warrendale, PA, 2007), paper no 0965-S03-24
3. Vasilopoulou, M.; Palilis, L.C.; Botsialas, A.; Georgiadou, D.; Bayiati, P.; Vourdas, N.; Petrou, P.S.; Pistolis, G.; Stathopoulos, N.; Argitis, P. "Flexible Organic Light Emitting Diodes (OLEDs) based on blue emitting polymers", Micro&Nano 2007, Athens, Greece, 18-22 November 2007.Georgiadou, D.; Vasilopoulou, M.; Pistolis, G.; Dimotikali D.; Argitis, P. "Energy transfer processes among emitters dispersed in a single polymer layer for colour tuning in OLEDs", Micro&Nano 2007, Athens, Greece, 18-22 November 2007.
4. Vasilopoulou, M.; Stathopoulos, N.; Falaras, P.; Pistolis, G.; D. Davazoglou, D.; Argitis, P. "An all-organic optocoupler based on polymer light-emitting diodes (PLEDs)", P II.38, 3rd International Conference **MICRO&NANO 2007 on Micro-Nanoelectronics, Nanotechnology & MEMs, Athens, 18-21 November 2007**.
5. Vasilopoulou, M.; Georgiadou, D.; Palilis, L.C.; Pistolis, G.; Argitis, P. "Single layer white organic light-emitting diodes for lighting applications", 5th European Conference on Organic Electronics (ECOER07), Varenna, Italy, 01-04 October 2007.

Funded Projects

1. PEP Attikis

Infrastructure

LS-50B Perkin-Elmer Fluorometer and a ns pulsed flash-lamp fluorometer (Edinburgh Instruments).

Personnel

G. Pistolis: research director/group leader (permanent researcher); I. Balomenou, : (PhD student, NCSR "D" fellow), A. Kaloudi-Chantzea: (PhD student).

Collaborations

Prof. I. Kallitsis, Department of Chemistry University of Patras.
Dr. P. Argitis, Institute of Microelectronics NCSR Demokritos.

Contact

Dr. G. Pistolis (pistolis@chem.demokritos.gr, Tel. +30 210 6503637, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

ISOTOPE HYDROLOGY

Research Objectives / Activities

The program deals with the analysis of the isotopic characteristics of the underground and surface waters and the use of the corresponding results, for the resolution of problems related with the exploitation of aquatic resources and geothermal energy. Such problems are the supply mechanism of aquatic horizons, their potential, the speed of flow of the underground water, the interconnection of the aquatic horizons or their communication with surface reservoirs, as well as the origin of geothermal fluids.

Another research activity is the development of a methodology for the determination of the concentration of natural ^{14}C in the atmosphere and the study of the change of the isotopic ratios $^{13}C/^{12}C$ and $^{18}O/^{16}O$ in the atmospheric CO_2.

Furthermore, a method for the determination of the concentration of ^{222}Rn in water and atmospheric samples using the Liquid Scintillation technique was developed and applied in the Laboratory.

The Laboratory of Isotope Hydrology is responsible for radioactive tracing in assessed stages of a hydrologic system.

Personnel

N. Zouridakis: research director/group leader (permanent researcher)
E.Arnidi: (technical staff, under contract).

Contact

Dr. N. Zouridakis (nizouri@chem.demokritos.gr, Tel. +30 210 6503969, Fax. +30 210 6503956)
Web site: http://ipc.chem.demokritos.gr/

TRACE ELEMENT STUDIES LABORATORY

Research Objectives / Activities

In 2007 the project "Particulate matter and heavy metals in the atmospheric aerosol of an industrial and an urban area in Athens, Greece", a cooperation of the Laboratory of Inorganic and Analytical Chemistry of the NTUA and the Laboratory of Trace Element Studies and the Environmental Radioactivity Laboratory of the NCSR "Demokritos", which was co-funded by the European Social Fund (75%) and National Resources (25%) – (EPEAEK II) – PYTHAGORAS, could be successfully finished.

The areas of interest were Aspropyrgos (industrial area), center of Athens (Patission Str. , urban area) and NCSR Demokritos (suburban area)

In the industrial area there was an enrichment in coarse particulates ($PM_{10-2.5}$), whereas the urban area was enriched in fine particulates ($PM_{2.5}$). The high concentrations of the investigated metals that were found in the industrial area, suggests the influence of local sources. Although the concentrations of Pb, Cd, Ni and Mn do not exceed the WHO limits of 500, 5, 20 and 150 ng/m^3, respectively, it is an issue of concern for the population living in this area as far as the long term health effects is concerned. Additionally, the relationship between the metal concentrations measured and the wind direction was investigated by demonstrating time-weighted concentration roses to provide information of the major emission sources. From the statistical evaluation of the results, some of the local air pollution sources could be identified.

The last activity of the Laboratory was the investigation of screen printed electrodes for the application in trace element analysis.
With the end of 2007 the Laboratory for Trace Element Studies is without person responsible. The Laboratory, initially called "Laboratory of Analytical Chemistry" (with activation by neutrons) , belongs to one of the oldest Laboratories not only at the Institute of Physical Chemistry, but at the NCSR Demokritos. It was founded by Dr.A.Grimanis, who used the neutron activation analysis for his research. In that time the neutron activation analysis was one of the most powerful analytical methods in the field of inorganic chemistry. The neutron activation analysis allowed to analyze a large number of elements at concentrations 1000 times lower as it was possible by the convenient methods in those days. In cooperation with his wife Maria, Dr.Grimanis worked successful in different scientific fields, such as environment, archaeometry and health related topics, which are up to now topics of the Laboratory. When Dr.Grimanis retired the Laboratory was handed over to Dr.G.Kanias and than to Dr.K.M.Ochsenkuehn. The reseach of Dr.G.Kanias covered the investigation of trace elements recommended daily allowances required for the growth and the maintenance of human life. With Dr.K.M.Ochsenkuehn the research fields were extended to geochemistry and to speciation analysis, an important but difficulty topic in environmental investigations. In 2004, the year of the Olympic games in Greece, the activities concerning the neutron activation analysis had to stop as the only reactor in Greece, the one of the NCSR Demokritos, had to stop working (for safety reasons, as it was said). As the reactor does not run up to now the the analytical work was continued by using other analytical techniques such as electroanalytical methods, especially anodic stripping voltammetry, but also ion chromatography and AAS. The shut down of the reactor was also the reason to rename the Laboratory to "Laboratory for Trace Element Studies".

Publications 2007

1. R.Argyropoulou, M.Ochsenkühn-Petropoulou, C.Dounis, P.Karaboulis, A.Alzoumailis, K.M.Ochsenkühn. "Comparison of the behavior of the three superconductors YBCO, Bi-2212 and MgB2 in different environmental conditions" *J.Mat.Process.Tech*. **181,** 2-5 **(2007)**
2. Klaus-Michael Ochsenkühn, Theopisti Lyberopoulou, G. Koumarianou, M.Ochsenkühn-Petropoulou,"Ion chromatographic and spectrometric determination of water-soluble compounds in airborne particulates and their correlations in an industrial area in Attica, Greece", *Microchim.Acta* DOI 10.1007/s00604-007-0830-z (**2007)**

3. Klaus-Michael Ochsenkühn, Maria Ochsenkühn-Petropoulou, "Anodic Stripping Voltammetry a Tool for the Analysis of some Acid Leachable Heavy Metals in Airborne Particulate Matter", accepted for publication in *Fresenius Environ. Bull.* (2007)

Conferences

1. Ochsenkühn,K.M., Lyberopoulou,Th., Razos,P., Karagiannis,K., Ochsenkühn-Petropoulou, M. "Ionic composition of $PM_{10}/PM_{2.5}$ in an industrial area in Greece", *4. Conference über Ionenanalyse*, 12.-14. March 2007, Berlin, Germany , p.75 (2007)
2. K.M. Ochsenkühn, M. Ochsenkühn-Petropoulou," Spectroscopic investigation of airborne particulate matter on filters from low and high volume samplers of an industrial area in Greece",*Colloquium Spectroscopicum Internationale XXXV*, September 23-27, Xiamen, China p.428 (2007)

Contact

Dr.Ochsenkühn Klaus (oxenkuen@chem.demokritos.gr) Retired, 31/12/2007)

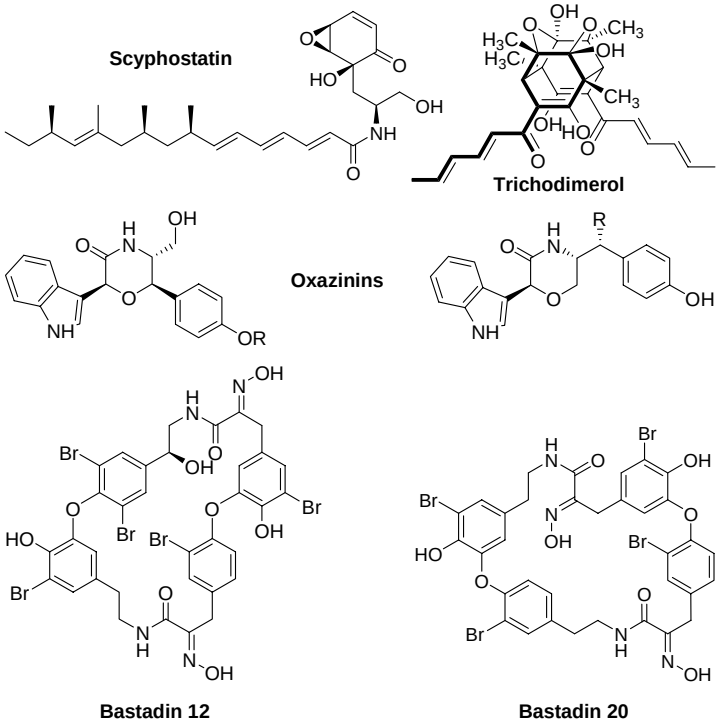
3rd Scientific Programme

Chemical Biology

NATURAL PRODUCTS SYNTHESIS AND BIOORGANIC CHEMISTRY

Research Objectives / Activities

Our group is involved in the design and synthesis of organic compounds. The targeted molecules are mainly natural products or designed analogues with the aim to prepare and study novel compounds with interesting and/or improved biological activity and possible pharmaceutical applications. The evaluation of their biological activity is performed through collaboration with specialized laboratories. In parallel, the expertise of the team in the design and synthesis of complex organic molecules is exploited for the preparation of organic molecules with possible technological applications (e.g. photoresist etch enhancement additives, linkers for the preparation of polymers) or molecules with interesting supramolecular behavior.



The team has also initiated research in the area of combinatorial chemistry introducing the use of polymorphic scaffolds for the generation of libraries of pharmacophoric structures. Other current research activities include the total synthesis of the natural products Bastadins, Radicicol and Adociasulfate-2 as well as the design and synthesis of Scyphostatin and Alkanin analogues.

Publications 2007

1. Pitsinos, E.N.; Cruz, A.; Giannis, A.; Waschолowski, V. "Synthesis of novel scyphostatin analogues and evaluation as neutral sphingomyelinase inhibitors", *Naunyn-Schmiedeberg's Arch. Pharmacol.* 2007, *374*, 322-323.
2. Pitsinos, E.N.; Moutsos, V.I.; Vageli, O. "Synthesis of enantiopure (*S*)-7-hydroxy-3-amino-3,4-dihydro-2*H*-1-benzopyran en route to (+)-schophostatin", *Tetrahedron Lett.* 2007, *48*, 1523-1526.
3. Ziemińska, E.; Stafiej, A.; Pitsinos, E.N.; Couladouros, E.A.; Moutsos, V.; Kozłowska, H.; Toczyłowska, B.; Łazarewicz, J.W. "Synthetic bastadins modify the activity of ryanodine receptors in cultured cerebellar granule cells", *NeuroSignals* 2006-07, *15*, 283-292.
4. Ziemińska, E.; Stafiej, A.; Pitsinos, E.N.; Couladouros, E.A.; Moutsos, V.; Kozłowska, H.; Toczyłowska, B.; Łazarewicz, J.W. "Synthetic bastadins modify the activity of ryanodine receptors in cultured cerebellar granule cells", *Pharmacological Reports* 2007, *59*, 33-33.

5. Ciminiello, P.; Dell'Aversano, C.; Fattorusso, E.; Forino, M.; Grauso, L.; Santelia, F.U.; Tartaglione, L.; Moutsos, V.I.; Pitsinos, E.N.; Couladouros, E.A. "Stereo-structural determination of three novel oxazinins isolated from Adriatic mussels via a synthetic and NMR-based approach", *Eur. J. Org. Chem.* 2007, 5434-5439.
6. Stathopoulos, G.T.; Kollintza, A.; Moschos, A.; Psallidas, I.; Sherrill, T.P.; Pitsinos, E.N.; Vassiliou, S.; Karatza, M.; Papiris, S.A.; Graf, D.; Orphanidou, D.; Light, R.W.; Roussos, C.; Blackwell, T.S.; Kalomenidis, I. "Tumor necrosis factor-α promotes malignant pleural effusion", *Cancer Res.* 2007, *67*, 9825-9834.
7. Couladouros, E.A.; Strongilos, A.T.; Neokosmidis, E. "Formal synthesis of the piperidine alkaloid (+/-)-prosophylline using polymer-supported dihydro-2H-pyridin-3-one", *Tetrahedron Lett.* 2007, *48*, 8227-8229.
8. Michaelakis, A.; Mihou, A.P.; Koliopoulos, G.; Couladouros, E.A. "Attract-and-kill strategy. Laboratory studies on hatched larvae of Culex pipiens", *Pest Management Science* 2007, *63*, 954-959.
9. Couladouros, E.A.; Moutsos, V.I.; Lampropoulou, M.; Little, J.L.; Hyatt, J.A. "A short and convenient chemical route to optically pure 2-methyl chromanmethanols. Total asymmetric synthesis of beta-, gamma-, and delta-tocotrienols", *J. Org. Chem.* 2007, *72*, 6735-6741.
10. Drygiannakis, D.; Patsis, G.P.; Raptis, I.; Niakoula, D.; Vidali, V.; Couladouros, E.; Argitis, P.; Gogolides, E. "Stochastic simulation studies of molecular resists", *Microelectronic Engineering* 2007, *84*, 1062-1065.
11. Mihou, A.P.; Michaelakis, A.; Krokos, F.D.; Mazomenos, B.E.; Couladouros, E.A. "Prolonged slow release of (Z)-11-hexadecenyl acetate employing polyurea microcapsules", *J. Appl. Entomol.* 2007, *131*, 128-133.

Patents

1. "Molecular resists based on polycarbocycle derivatives", P. Argitis, E. Gogolides, D. Niakoula, V. Vidali, E. Couladouros, R. Gautam, Greek Patent (OBI) appl. 20050100472/ 16-9-2005, GR no 1005438/14-2-2007, PCT International Patent Application PCT/GR06/000050 19/9/2006.

Conferences

1. Pitsinos, E.N.; Cruz, A.; Moutsos, V.; Vageli, O.; Giannis, A.; Waschołowski, V.; Stathopoulos, G.; Kalomenidis, J. "From scyphostatin to kotylostatin: chemistry and biology of new inhibitors of neutral sphingomyelinases", 8th Conference Medicinal Chemistry: Drug Discovery and Design, Patras, Greece, 15-17 March 2007, p. 24.
2. Couladouros, E.A. "Chemical synthesis of bioactive natural products; Early steps in the discovery of new drugs", 8th Conference Medicinal Chemistry: Drug Discovery and Design, Πάτρα, 15-17 Μαρτίου 2007, Πρακτικά σελ. 23.
3. Dakanali, M.I.; Vidali, V.P.; Couladouros, E.A. "Development of a general method for the synthesis of polyprenylated acylphloroglucinols", 8th Conference Medicinal Chemistry: Drug Discovery and Design, Patras, Greece, 15-17 March 2007, p. 73.
4. Maranti, A.G.; Bouzas, E.A.; Couladouros, E.A. "Studies of enone-ene ring closing metathesis. Total synthesis of monocillin II", 8th Conference Medicinal Chemistry: Drug Discovery and Design, Patras, Greece, 15-17 March 2007, p. 94.
5. Pratsinis, H.; Kletsas, D.; Bouzas, E.A.; Mechaelakis, A.; Strongilos, A.T.; Couladouros, E.A. "Synthesis and in vitro activity of shikalkin derivatives", 8th Conference Medicinal Chemistry: Drug Discovery and Design, Patras, Greece, 15-17 March 2007, p. 107.
6. Pitsinos, E.N.; Cruz, A.; Moutsos, V.; Vageli, O.; Giannis, A.; Waschołowski, V.; Stathopoulos, G.; Kalomenidis, J. "From scyphostatin to kotylostatin: chemistry and biology of new inhibitors of neutral sphingomyelinases", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 54.
7. Couladouros, E.A. "New routes towards the synthesis of natural products and designed derivatives", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 34.
8. Maranti, A.G.; Bouzas, E.A.; Couladouros, E.A. "Synthetic studies towards monocillins I, II and III", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 67.

9. Dakanali, M.I.; Vidali, V.P.; Couladouros, E.A. "Synthesis of the bicyclic common core of hyperforin and related polycyclic polyprenylated acylphloroglucinols", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 68.
10. Bouzas, E.A.; Magos, A.D.; Chiotellis, A.E.; Salama, T.A.; Couladouros, E.A. "Studies towards an improved synthesis of the new anti-MRSA & VRSA polyketide, abyssomicin C", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 69.

Funded Projects

1. "Structure-related pharmacological effects of synthetic bastadins in neurons", Κοινά Ερευνητικά και Τεχνολογικά Προγράμματα Ελλάδας-Πολωνίας 2005-2007, 11,74 k€.
2. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 10 k€, 2006-2008
3. "Inhibitors of angiogenesis: design, synthesis and biological exploitation (AngioKem)", COST Action CM0602, 2007-2011.

Infrastructure

Polarimeter, parallel synthesizer, HPLC.

Personnel

E.N. Pitsinos: researcher B level (permanent researcher); V. Vidali: (research fello NCSR "D"); A. Kazantzis, A. Chiotellis, A. Strongilos: (3 post doctoral associates, external funding); O. Vageli : (PhD student, NCSR "D" fellow); M. Dakanali, C. Mitsopoulou, K. Tsiliouka, N. Athinaios : (4 PhD students, external funding).

Collaborations

Prof. A. Giannis (Universität Leipzig, Fakultät für Chemie und Mineralogie, Insitut für Organische Chemie), Prof. E. Fattorusso (Dipartimento di Chimica delle Sostanze Naturali, Università degli Studi di Napoli "Federico II"), Prof. J.W. Lazarewicz (Medical Research Centre, Polish Academy of Sciences), Prof. E.-I. Negishi (Purdue University, Purdue University, West Lafayette, Indiana, USA).

Contact

Dr. E.N. Pitsinos (pitsinos@chem.demokritos.gr, Tel. +30 210 6503789, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/

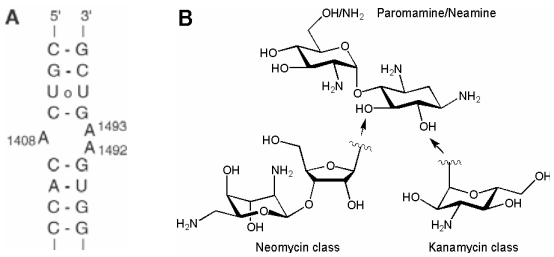
CHEMICAL BIOLOGY OF NATURAL PRODUCTS AND DESIGNED MOLECULES

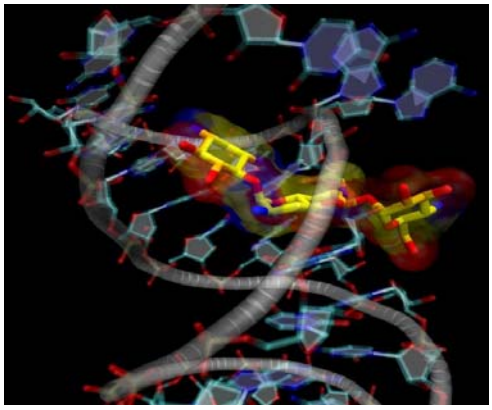
Research Objectives / Activities

Our laboratory represents a new function within the Institute of Physical Chemistry, namely the "Chemical Biology of Natural Products and Designed Molecules", which was initiated in July 2005. Our studies incorporate molecular design and analysis, total synthesis, structure/activity relationship observations, combinatorial synthesis and biological investigations. Our research focuses on the study of biological systems, DNA, RNA and proteins, through their interaction with small molecules of natural or synthetic origin, targeting the development of new and improved pharmaceutical entities. Our goal is the total synthesis of natural products and designed analogs with improved potencies and pharmacological profiles, the development of new synthetic methodologies in solution and solid phase and the development of new *in vitro* biological assays for the evaluation of the new synthetic entities. Our design will be based on crystallographic information and molecular modeling studies. Currently, we are involved in the areas of Cancer (topoisomerase II inhibitors, apoptosis), bacterial infections (aminoglycosides and A-site ribosomal-RNA) and anti-virals (Hepatitis C virus, HIV). Some of our ongoing projects are described bellow in more detail.

1. Study of RNA components by the synthesis of small molecules

The proposed research is intended to exploit RNA as a pharmaceutical target by the synthesis of rationally designed small molecules as lead structures and could potentially result in the development of novel antibiotics. The work will initially focus on substrates that bind specifically to the ribonucleic acid (RNA) components of the bacterial ribosome, which is a validated target for many known antibiotics. Additionally, technologies currently used for the global analysis of protein function, exemplified by the biotin-small molecule conjugates, will be explored for the identification of novel RNA components as potential targets for small molecule interactions with therapeutic significance. Finally, exploration of RNA tertiary structure will be performed by the synthesis of "dynamic libraries", where the individual final products will be generated in the presence of the biological target, resembling the outcome of a natural selection. Our approach will be expandable to other RNA-domains, like the GTPase associated domain in 23S rRNA, target of the antibiotic thiostrepton, or the internal ribosome entry sites (IRES), which are important targets for the treatment of viral pathogens such as polio and hepatitis C.





This project represents an interdisciplinary approach, comprising of synthetic, spectroscopic, biological, and computational studies and is expected to elucidate the pharmacological profile of various RNA components and increase our understanding for their individual function. In addition to the obvious training opportunities for young researchers in the different scientific fields involved, its successful completion will place EU in the lead of the world stage in the field of RNA, will create new opportunities for the development of biotechnology and pharmaceutics and will improve overall our quality of life.

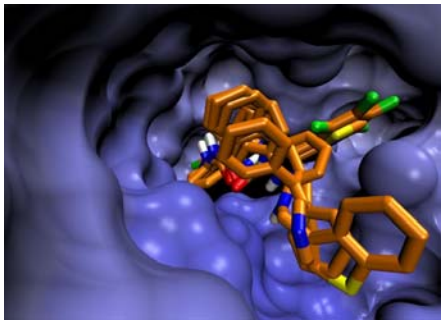
2. Nanoscale functionalities for targeted delivery of biopharmaceutics

The present research aims at the development of innovative multidisciplinary approaches for the design, synthesis and evaluation of molecular, nano- and micro-scale functionalities for targeted delivery of therapeutic peptides and proteins (biopharmaceutics). New protein- and peptide-based drugs are being discovered every day and their increased availability offers new ways to treat diseases. However, the structure, physicochemical properties, stability, pharmacodynamics, and pharmacokinetics of these new biopharmaceutics place stringent demands on the way they are delivered into the body. Carrier-based drug delivery systems can improve the bioavailability and diminish the toxicity of Peptidic/Proteinic (P/P) drugs. Furthermore, the carrier specificity can be

enhanced, through proper functionalization, and the release of the therapeutic peptide/protein can be controlled on demand. Artificial nanostructures being of the same size as biological entities can readily interact with biomolecules both on the cell's surface and within the cell. Thus, the development of functionalized nanocarriers and nanoparticle-based microcarriers for P/P delivery is both an important scientific challenge and potentially a business breakthrough for the biopharmaceutical industry.

3. Design and synthesis of selective VEGF-R2 inhibitors

Angiogenesis is the process by which new blood capillaries sprout from pre-existing blood vessels, and it is well recognized that angiogenesis is an important mechanism governing tumor growth and metastasis. The recent clinical success of Avastatin® has provided a proof of principle for the potential of anti-angiogenic cancer therapy with anti-vascular enthothelial growth factor (VEGF) agents. This dimeric glycoprotein interacts with two high-affinity transmembrane tyrosine kinase receptors, VEGF-R1 (originally Flt-1) and VEGF-R2 (or human KDR), and results in the proliferation of the endothelial cells and their development into new blood vessels.



One of the potential therapeutic approaches utilizes VEGF-R tyrosine kinase inhibitors that target the intracellular signal transduction. Within the last 5 years there has been considerable effort to produce selective VEGF-R inhibitors, therefore structures of several nanomolar binders of VEGF-R2 have been obtained. Computational chemistry analysis of these results will lead to the design, synthesis and biological evaluation of novel VEGF-R2 inhibitors.

Publications 2007

1. Psomas G., Tarushi A., Efthimiadou E.K., Sanakis Y., Raptopoulou C.P., Katsaros N., "Synthesis, Structure and Biological Activity of Copper(II) Complexes with Oxolinic Acid.", *J. Inorg. Biochem.* **2006**, *100*, 1764-1773. (not included in the **2006** report)
2. Efthimiadou E.K, Thomadaki H., Sanakis Y., Raptopoulou C.P., Katsaros N., Scorilas A., Karaliota A., Psomas G., "Structure and biological properties of the copper(II) complex with the quinolone antibacterial drug N-propyl-norfloxacin and 2,2'-bipyridine." *J. Inorg. Biochem.* **2007**, *101*, 64-73.
3. Efthimiadou E.K, Sanakis Y., Katsaros N., Karaliota A., Psomas G., "Transition metal complexes with the quinolone antibacterial agent pipemidic acid: Synthesis, characterization and biological activity." *Polyhedron* **2007**, *26*, 1148-1158.
4. Efthimiadou E.K, Psomas G., Sanakis Y., Katsaros N., Karaliota A., "Metal complexes with the quinolone antibacterial agent N-propylnorfloxacin: Synthesis, structure and bioactivity.", *J. Inorg. Biochem.* **2007**, *101*, 525-535.
5. Katsarou M.E., Efthimiadou E.K., Psomas G., Karaliota A., Vourloumis D., "Novel Copper(II) Complex of *N*-Propyl-norfloxacin and 1,10-Phenanthroline with Enhanced Antileukemic and DNA Nuclease Activities", *J. Med. Chem.* **2008**, *51*, 470-478. (published on the web in **2007**)

Conferences

1. Dionisios Vourloumis, "Targeting RNA with small molecules." EMBO Conference on "Viral RNA: Structure, Function and Targeting", Invited speaker, EMBL Heidelberg, Germany, March 5–7, **2007**.

International Patents

1. K.C. Nicolaou, Y. He, S. Ninkovic, J. Pastor, F. Roschangar, F. Sarabia, H. Vallberg, D. Vourloumis, N. Winssinger, Z. Yang, N.P. King, M.R.V. Finlay, "Epothilone Analogs." *US* **7,173,137 B2**, publication date: Feb. 6, 2007.
2. D. Vourloumis, D.E. Murphy, T.J. Prins, F. Ruebsam, C.V. Tran, S.J. Berthel, R.F. Kester, R. "Oxime Glucokinase Activators." U.S. Provisional Patent Application No. **23198 US** (pending).

Funded Projects

1. Marie Curie Excellence Grants, "Study of RNA components by the Synthesis of Small Molecules", Contract No. MEXT-CT-2006-039149, Dr. Dionisios Vourloumis, € 1.620 k€, 2/2007–1/2011).
2. 'NMP' INTEGRATED PROJECT, "Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics", Contract No. NMP4-CT-2006-026723, € 537 k€, 10/2006-9/2010).
3. ENTER2004, GSRT, "Design of Selective Inhibitors of Vascular Endothelial Growth Factor Receptor-2 (VEGF-R2) Using Structural Methods for the Treatment of Cancer." Contract No. 04EP63, Dr. Dionisios Vourloumis, € 58.5 k€, 2/07-10/08)
4. "Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography", PEP Attikis, 10 k€, 2006-2008.

Personnel

D. Vourloumis: research director (permanent researcher); A. Zografos, I. Katsoulis, G. Kythreoti, A. Papakyriakou, M. Katsarou: (5 post doctoral associates, external funding); E. Efthimiadou, G. Mavridis: (2 PhD students, NCSR "D" fellows); P. Anastasopoulou, A. Papadopoulou: (2 PhD students, external funding); C. Georgaki: (administrative assistant, external funding).

Collaborations

T. Hermann (UCSD, San Diego USA, RNA biochemistry), E. Theodorakis (UCSD, San Diego USA, Organic Synthesis), D. Georgiadis (UOA, Athens Greece, Organic Synthesis/Spectroscopy).

Contact

Dr. D. Vourloumis (vourloumis@chem.demokritos.gr, Tel. +30 210 6503624, Fax. +30 210 6511766)
Web site: http://vourloumis_group.chem.demokritos.gr/index.html

Service Laboratories

SERVICE LABORATORY "ENVIRONMENTAL ANALYSIS"

Objectives/Activities

Contamination of water supplies with organic pollutants such as PAHs, PCBs and cyanotoxins is one of the most important global problems. Recent EU Directives propose the determination of these target pollutants in drinking and surface water and set their maximum concentration. Resulting from the above, it is mandatory to monitor these analytes using appropriate methods. The availability of rapid, reliable screening method is prerequisite when a large number of samples must be analyzed, but on the other hand there is an urgent need of a confirmatory method for the analysis of these contaminants which belong to the priority pollutants list. Disadvantages of conventional methods of analysis can be overcome by using liquid chromatography-mass spectrometry (LC/MS/MS). In the frame of the accreditation of our laboratory in PAHs determination in potable and surface water by using LC/MS/MS it has been funded (2005-2008) by Antagonistikotita (Ministry of Development) with 311.3 KEuro. This will upgrade the instrumentation of our laboratory (HPLC/UV-Vis or FL or CD, IC, GC/ECD or FID and GC/MS), mainly by the purchase of the LC/MS/MS analytical device and will give new opportunity to our research and service activities.

Current interests of our Laboratory are focused into the following:

- Method Development for the determination of toxic pollutants in trace level in water, foodstuff and environmental samples (pesticides, PCBs, PBRBs, chlorophenols, PAHs, BTX, VOCs, drug residues, cyanotoxins, organic halides)
- Method Development for the determination of Polychlorinated Biphenyls (PCBs) in water and Organic Halides in foodstuff (honey) by Solid Phase Microextraction (SPME) in combination with GC/ECD and GC/MS.
- Method Development for the determination of Polycyclic Aromatic Hydrocarbons (PAHs) in potable and surface water by using LC/MS/MS.
- Method Development for the determination and identification of cyanotoxins in surface and drinking water by using SPE and LC/MS-MS.
- Elaboration of MSc and PhD Thesis.
- Accreditation of the laboratory in PAHs determination in potable and surface water by using LC/MS/MS (being the only Laboratory in Greece for that purpose).
- Services for the determination of toxic organic residues in trace level.

Personnel

A. Hiskia: director (permanent researcher); T. Triantis: (quality manager); A. Tsimeli, T. Caloudis: (adjunct scientist).

Funded Projects

1. "Development of analytical infrastructure of the Environmental Analysis Laboratory, EKEFE Demokritos", Antagonistikotita (Ministry of Development), Coordinator Dr. A. Hiskia, 311,3 K€, 2006-2008.
2. "Chemical Analysis of sediments for heavy metals and chlorinated organic compounds", in the frame of services to EDRASOMICHANIKI, 3,3 K€.
3. "Chemical Analysis of sediments for heavy metals and chlorinated organic compounds", in the frame of services to ALTEC, 3,3 K€.

Infrastructure

Spectrophotometers UV-VIS-near IR, GC equipped with FID, ECD and TCD, HPLC equipped with UV-VIS and FLD, GC/MS, HPLC/MS/MS triple tetrapole, IC, Polarographic unit, TOC, SPE and SPME apparatus, oven, ultrasound bath, analytical balances, pHmeter, Rotary evaporator, ultrapure water apparatus.

Collaborations

Dr. Jussi Meriluoto (Abo Akademi University, Finland, Method development for the determination and identification of cyanotoxins in surface and drinking water by using SPE and LC/MS-MS), Prof. D. Dionysiou (University of Cincinnati, USA, AOP for cyonobacteria toxins destruction), Dr. S. Lacorte (Dep. of Environ. Chem., CID-CSIC, Barcelona, Analytical method development), Dr. T. Caloudis, (EYDAP, trace organic analysis in water)