

**NATIONAL CENTER FOR SCIENTIFIC
RESEARCH “DEMOKRITOS”**

INSTITUTE OF PHYSICAL CHEMISTRY
<http://ipc.chem.demokritos.gr/>

Scientific Report 2009

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Introduction

The primary objective of the Institute of Physical Chemistry (IPC) of the National Center for Scientific Research "Demokritos" (NCSR "D") 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, but also on equilibrium, transport, catalytic and photoinduced processes as well as environmental technologies and renewable energy issues. The Institute also provides specialized services to the private sector and public organizations, particularly in relation to environmental pollutants analyses, materials characterization, water quality assessment, and glassblowing work.

The year 2008 was characterized by the intensification of the Institute's effort to achieve a series of research and technological objectives, via the implementation of a research and growth policy based on concrete strategy and clearly determined goals.

The main axes of the Institutes research policy aim at establishing it as a National, but also a European, Center of Excellence in the field of physical chemistry and consist of:

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

The performance of IPC research groups for 2008 (papers in international journals and conference proceedings, citations, patents, PhD theses and external funding) is remarkable. More specifically, about 120 articles were published in international refereed journals of high impact factor, the research work of the Institute received more from 1900 citations (excluding self-citations), 6 patents were submitted and 3 international conferences were organized. Additionally, IPC presented intense educational activity as indicated by the organization of 3 summer schools, the co-ordination of postgraduate courses (COSA network) as well as the completion of 6 PhD, 4 Master and 5 diploma theses.

IPC has attracted significant external funding. Currently, 8 European projects are under implementation in the frame of FP6, 2 of them being Networks of Excellence ([NoE]) (one coordinated by IPC). The Institute has also put substantial effort to actively participate in new research projects. The initial participation in FP7 was particularly successful, as already 6 new proposals have been approved and the corresponding projects are either running or under negotiation. The first results are very positive and

greater success is expected in the near future, from both European and Greek financing sources.

Particular emphasis was given in the preparation of the Institute for the imminent evaluation of Research Centres (organized by the General Secretariat of Research and Technology, GSRT). In this respect, restructuring of the Institute's Research Programs is currently underway. This is coupled with the establishment of a modern and functional organogramme that is anticipated to highlight the Institute's uniqueness, but also to strengthen the collaboration between the different IPC research groups and thus allow for optimal exploitation of its research potential.

Considerable effort and capital was also invested in the development of the Institute's infrastructure. A completely new research facility for the assessment of nanomaterials' hydrogen storage capacity (unique in Greece) was established. New and modern systems (including SEM, new AFM, Electrochemical Impedance, Intensity Modulated Photocurrent and Photovoltage Spectroscopies) were acquired. The laboratory of Characterization of Molecular and Supramolecular Systems infrastructure was upgraded with the integration of a Raman Spectrometer and the improved of the old AFM microscope (Nanoscope III of Digital Instruments). The accreditation of the Laboratory of Environmental Analyses for "Determination of polyaromatic hydrocarbons in potable and surface waters" (the only accredited analytic unit in Greece) was completed.

The detailed activity report that follows underlines the ascendant course of IPC . The data presented confirm the production of important research results, awarding the hard effort of the personnel, despite the fact that this work is many times carried out under objectively difficult conditions.

February 2009,

Dr. Polycarpos FALARAS, Director

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3. Molecular Computational Chemistry
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5. Chemical Biology of Natural Products and Designed Molecules

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Service laboratories.....
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1. Environmental Analysis
2. Isotopic Analysis, Radiocarbon Dating, and Radon Measurements
3. Other Service Laboratories NMR, Macromolecular Crystallography Lab (X-RAY), Elemental Analyzer, AFM, FT-IR, Thermal analysis lab, Micro raman

Education Activities.....
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Institute of Physical Chemistry 2008 Performance Indicators

Publications (International Journals)	72/ 28*
Conference Proceedings/ Abstracts	88/35
Citations	
Technical Reports	
Invited Lectures	58
Patents	5
PhD Dissertations	11
Master's Theses	4

*** in press**

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1st Scientific Programme

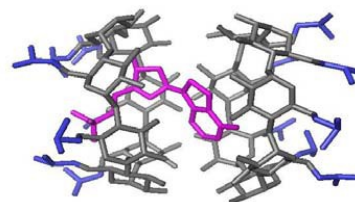
Molecular & Supramolecular Nanofunctional Materials - Chemical Biology

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, nucleic acids and bioactive compounds. Specifically, the areas of research are:

1. *Host-guest systems*: The inclusion of biologically active molecules and model compounds in the CD cavity is studied. The structure and detailed host-guest interactions are determined by NMR in aqueous solutions and/or X-ray crystallography in the crystalline state. Thus insight in host-guest recognition, non-bonding interactions, self-assembly, chiral discrimination and dynamics (when possible) is gained. In addition, pharmaceutical applications are of interest, such as controlled release and specific binding of drugs, as well as formulations.

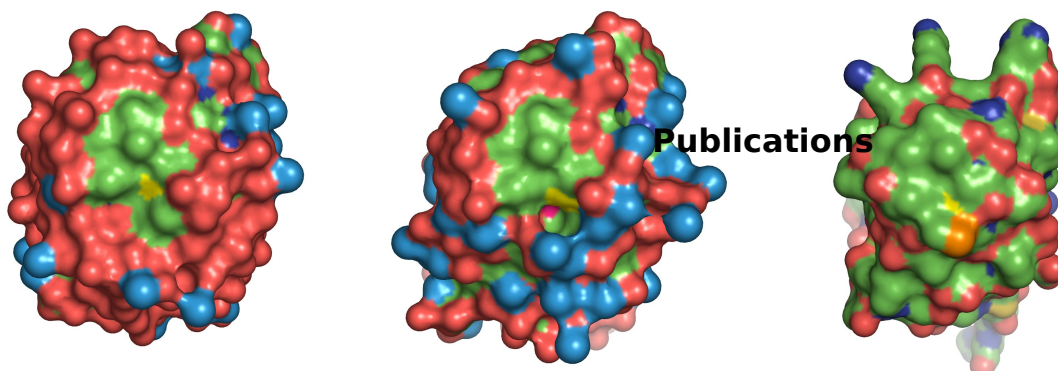


Complex of 6-perguanidilated- β -Cyclodextrin with the nucleotide 5'-dAMP, *Eur. J. Org. Chem.* **2009**, 2299-2305

2. *Synthesis of novel, functional cyclodextrin derivatives for biomedical applications*. The derivatives: (a) Complex with small bio-active molecules, e.g. nucleotides. (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 magnetic 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/SiO₂ 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 muscle proteins, specifically myomesin in collaboration with EMBL-Hamburg Outstation, Germany (Dr M. Wilmanns). (b) Structure determination of RNA with small synthetic molecules of pharmaceutical interest for the development of new antibiotic in collaboration with the Laboratory of *Chemical Biology of Natural Products and Designed Molecules* of IPC (Dr D. Vourloumis). (c) Proteins that synthesize or degrade silica, silica, silicatein & silicase, in collaboration with the Institut für Physiologische Chemie und Pathobiochemie, Universitätsmedizin der Johannes Gutenberg-Universität, Mainz, Germany (Professors W.E.G. Müller & H.C. Schröder). (d) Structure determination of natural and mutated members of the new family of 2[4Fe4S] ferredoxins from selected pathogenic bacteria.



Solvent accessibility surfaces of members of the new family of 2[4Fe4S] ferredoxins: two mutated from the bacterium *A. vinosum* and the natural one from *E. coli* (atom color code: red: oxygen, blue: nitrogen, green: carbon, yellow: sulfur), *J. Biol. Inorg. Chem.* **2009**, 14, 783-799.

reduction potentials of $[4\text{Fe-4S}]^{2+/+}$ clusters: Crystal structures of the *Allochrochromatium vinosum* ferredoxin variants C57A and V13G and the homologous *Escherichia coli* ferredoxin" *J. Biolog. Inorg. Chem.* **2009**, *14*, 783-799.

2. C. Aggelidou, I. M. Mavridis, K. Yannakopoulou "Binding of nucleotides and nucleosides to per(6-guanidino-6-deoxy)-cyclodextrins in solution", *Eur. J. Org. Chem.* **2009**, 2299-2305.
3. E. Hadjoudis, S. D. Chatziefthimiou, I. M. Mavridis, "Anils: Photochromism by H-transfer", *Current Org. Chem.* **2009**, *13*, 269-286. [Invited review](#)
4. E. Saridakis, N.E. Chayen "Towards a 'universal' nucleant for protein crystallization" *Trends Biotechnol.* **2009**, *27*, 99-106. [Invited review](#)
5. P. Asanithi, E. Saridakis, L. Govada, I. Jurewicz, E.W. Brunner, R. Ponnusamy, J.A.S. Cleaver, A.B. Dalton, N.E. Chayen, R.P. Sear, "Carbon-nanotube based materials for protein crystallisation." *ACS Appl. Mat. Interf.* **2009**, *1*, 1203-1210.
6. A. Paulidou, D. Maffeo, K. Yannakopoulou, I.M. Mavridis "Similar modes of inclusion in complexes of β -cyclodextrin with sulfonylurea hypoglycemic drugs" *Cryst. Eng. Comm.* **2010**, *12*, 517-525.
7. D. Maffeo, M. Lampropoulou, M. Fardis, Y. G. Lazarou, I. M. Mavridis, D. A.I. Mavridou, E. Urso, H. Pratsinis, D. Klestas, K. Yannakopoulou, "Novel Polycarboxylated EDTA-Type Cyclodextrins as Ligands for Lanthanide Binding: Study of Their Luminescence, Relaxivity Properties of Gd(III) Complexes, and PM3 Theoretical Calculations" *Org. Biomol. Chem.*, in print
8. N. Kalogeropoulos, K. Yannakopoulou, A. Gioxari, A. Chiou, D. P. Makris, "Polyphenol characterization and encapsulation in β -cyclodextrin of a flavonoid-rich *Hypericum perforatum* (St John's wort) extract ", *LWT- Food Science and Technology*, in print.

Conferences

1. I. M. Mavridis, S. D. Chatziefthymiou, A. Paulidou " β -Cyclodextrin inclusion complexes of L- and D-tryptophan. Chiral discrimination", 25th European Crystallographic Meeting, 16-21 Sept. 2009, Istanbul, Turkey, book of abstracts.
2. E. Saridakis, P. Giastas, J.-M. Moulis, P. Kyritsis, I. M. Mavridis "Insight into the reduction potentials of *Allochrochromatium vinosum*-like ferredoxins", 25th European Crystallographic Meeting, 16-21 Sept. 2009, Istanbul, Turkey, book of abstracts.
3. M. Lampropoulou, K. Misiakos, K. Yannakopoulou, "Synthesis of cyclodextrin based novel glycoclusters and studies on their interactions with lectins by White Light Interferometry", 3^o Ελληνικό Συμπόσιο Οργανικής Σύνθεσης, "Από τη Χημεία στη Βιολογία, στην Ιατρική και στην Επιστήμη Υλικών", 15 - 17 Οκτωβρίου 2009, Πανεπιστήμιο Αθηνών, book of abstracts.
4. M. Manouilidou, K. Yannakopoulou, "Synthetic approaches toward cyclodextrin dimers and trimers", 3^o Ελληνικό Συμπόσιο Οργανικής Σύνθεσης, "Από τη Χημεία στη Βιολογία, στην Ιατρική και στην Επιστήμη Υλικών", 15 - 17 Οκτωβρίου 2009, Πανεπιστήμιο Αθηνών, book of abstracts.
5. C. Aggelidou, T.A. Theodossiou, C. Staggel, G. Velegraki, A. G. Coutsolelos, I. M. Mavridis, K. Yannakopoulou, "Novel conjugates of carboxylated porphyrins with cyclodextrins for biological applications", 3^o Ελληνικό Συμπόσιο Οργανικής Σύνθεσης, "Από τη Χημεία στη Βιολογία, στην Ιατρική και στην Επιστήμη Υλικών", 15 - 17 Οκτωβρίου 2009, Πανεπιστήμιο Αθηνών, book of abstracts.

6. I. M. Mavridis, Petros Giastas, Emmanuel Saridakis, Panayotis Kyritsis, Jean-Marc Moulis, "High resolution structures of several 2[4Fe-4S] ferredoxins explain the reduction potential of [4Fe-4S] clusters", Structural Biology and Chemistry Symposium, The National Hellenic Research Foundation, Athens, 30-31 Oct. 2009, book of abstracts.

Funded projects

1. "Development of new pharmaceutical formulations. Molecular inclusion of antibiotics in cyclodextrins for resistant pathogen strains", PENED , 57.5 k€, 1/1/2006 - 30/6/2009.
2. "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 every year. For 2009: € 26.26 k€, 1/2/2004 - 30/9/2008.
3. "Novel tools for crystallisation of macromolecules" *TOPCRYST*, EU People-IAPP (Industry-Academia Partnerships and Pathways) 241.3 k€, 1/3/2008 - 29/2/2012.
4. "Biom mineralization: Understanding of basic mechanisms for the design of novel strategies in nanobiotechnology" BIOMINTEC, EU People- ITN (Networks for Initial Training), 184.4 k€ 1/9/2008 - 31/08/2012.
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. Network Coordinator of the *Initial Training Network «CYCLON*", *ITN237962* "Novel multifunctional cyclodextrin-based nanocarriers for drug encapsulation and delivery as a strategy to overcome current therapeutic drawbacks" 411.4 k€ 1/10/2009-30/09/2013).

Patent Applications

«EDTA-type cyclodextrin derivatives for metal ion binding and their complexes with gadolinium(III) for use in magnetic resonance imaging.», K. Yannakopoulou, I. M. Mavridis, M. Fardis, D. Maffeo, M. Lampropoulou, Greek Patent application # 200990100531, September 22nd, 2009.

International Collaborations

Dr. Zoe Pikramenou & Prof. M. J. Hannon, University of Birmingham, UK (on cyclodextrin derivatives); Dr. J.-M Moulis, CEA, Grenoble, France (on Ferredoxins); Dr. V. Karginov, Innovative Biologics, Inc., USA (biological studies of cyclodextrin derivatives); Dr. M. Wilmans, EMBL-Hamburg, Germany (structure of muscle proteins); Prof. N. E. Chayen, Imperial College, London, UK (on protein crystallisation); Drs. E. Urso and G. Torri, Institute for Chemical and Biochemical Research "G. Ronzoni", Milan, Italy (MS of large modified cyclodextrins); Professors W.E.G. Müller & H.C. Schröder, Johannes Gutenberg-Universität, Mainz, Germany.

Infrastructure

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

Personnel

I. M. Mavridis: research director/group leader (Researcher A); K. Yannakopoulou (Researcher A); E. Saridakis (researcher D); A. Paulidou (post doctoral associate, funding by NCSR "D", up to 30/6/2009); M-D. Manouilidou (PhD student, funding by NCSR "D"); M. Lambropoulou (PhD student, external funding); Ch. Aggelidou (PhD student); Eduard Baquero Salazar (PhD student, external funding, since 1/5/2009); K. Fotiadou (MSc student, partial external funding); Dr. E. Hadjoudis (external senior researcher).

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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 focusing on:

1. Multifunctional Liposomes as Drug Delivery Systems.

The laboratory is involved in the development of efficient, multifunctional liposomal drug delivery systems that combine stability in the biological environment, cell specificity and membrane transporting properties that are realized by appropriate modification of their external surfaces. Drug encapsulation and release, membrane transport, subcellular localization and phototoxicity were assessed for liposomal formulations that were employed as a novel route for photodynamic therapy. Liposomal formulations are characterized by atomic force and optical microscopy dynamic light scattering, ζ -potential, and various spectroscopic methods while the thermodynamics of liposomal interactions are investigated by microcalorimetric methods.

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

Functionalized dendrimers developed in our laboratory through the modification of commercially available dendrimers are studied as potential drug delivery systems. Active drug ingredients are incorporated in the dendrimers' interior and their release properties are studied. Multiple functionalization of dendrimers or hyperbranched polymers promotes enhanced targeting properties (through the introduction of recognizable groups), stability (by attaching poly(ethylene glycol) chains) and transport properties through cell membranes (through the introduction of guanidinium groups). The materials are characterized by a variety of physicochemical methods including spectroscopy (NMR, FTIR, UV-Vis), dynamic light scattering, multi-angle static light scattering and ζ -potential. Cell toxicity and subcellular localization are studied on various cell lines.

Suitably designed positively charged dendrimers or hyperbranched polymers are also employed for complexation with DNA. The resulting polyplexes are physicochemically characterized, while transfection efficiency is assessed *in vitro* on several cell lines. The effect of macromolecular architecture and end group modifications on gene transfection efficiency is investigated.

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

Alkylated dendrimeric and hyperbranched polymers are used as novel "nanosponges", able to encapsulate hydrophobic water impurities. Ultrapure water is thus produced, with remaining impurities at the ppb level. Furthermore, cross-linked hydrophobic dendrimeric and hyperbranched polymers are also suitable for water purification. Nanosponges' impregnation into ceramic membranes affords filter modules with advanced retention characteristics that can be easily integrated in existing water purification units. Further work has been performed on the preparation of organosilicon dendrimers which were covalently attached to the pore surface of ceramic filters for the production of hybrid organic-inorganic water purification modules.

4. Environmentally friendly biomimetic synthesis of nanoparticles

Organic-inorganic hybrid silica nanospheres were prepared through a biomimetic silicification process in water at ambient conditions, by the interaction of low cost poly(ethylene imine) hyperbranched polymer with silicic acid. The so-produced hybrid nanoparticles were successfully employed for the removal of two completely different categories of pollutants, i.e. metal ions and polycyclic aromatic hydrocarbons.

Amino terminated dendritic polymers and synthetic polypeptides have also been utilized for the formation of hydroxyapatite nanoparticles. The impact of hydroxyapatite nanoparticles on cellular function was studied by cell culture experiments on the viability and morphology of osteogenic cells.

Publications 2009

1. Z. Sideratou, N. Sterioti, D. Tsiourvas, C. M. Paleos, "Structural features of interacting complementary liposomes promoting the formation of multicompartments structures", *ChemPhysChem*, **2009**, *10*, 3083-3089.
2. M. Arkas, D. Tsiourvas, "Organic/inorganic hybrid nanospheres based on hyperbranched poly(ethylene imine) encapsulated into silica for the sorption of toxic metal ions and polycyclic aromatic hydrocarbons from water", *J. Hazardous Mater.*, **2009**, *170*, 35-42.
3. C. M. Paleos, L.-A. Tziveleka, Z. Sideratou, D. Tsiourvas, "Gene Delivery Using Functional Dendritic Polymers", *Expert Opin. Drug Delivery*, **2009**, *6*, 27-38.
4. S. Giatrellis, G. Nikolopoulos, Z. Sideratou, G. Nounesis, Calorimetric Study of the Interaction of Binary DMTAP/DOTAP Cationic Liposomes with Plasmid DNA, *Journal of Liposome Research*, **2009**, *19*, 220-230.
5. T. A. Theodossiou, D. Tsiourvas, J. S. Hothersall, "Hypericin Hydroquinone: Potential as a Red-Far Red Photosensitizer?", *Photochem. Photobiol.*, in press.

Chapters in Books

1. C. M. Paleos, D. Tsiourvas, "Non-Covalent Interactions of Liposomes", in "Bottom-up Nanofabrication: Supramolecules, Self-Assemblies and Organized Films", Edited by Katsuhiko Ariga, and Hari Singh Nalwa, Vol 2, Chapter 9, pp 245-262, American Scientific Publishers, 2009.

Conferences

1. S. Cohen, Z. Sideratou, C. M. Paleos and R. Korenstein, "Uptake and Adsorption of Nano-carrier Based on PEGylated Hyperbranched Polyesters by Different Cell Lines", Fifth Workshop, The Center of Nanoscience and Nanotechnology, February 22-24, 2009, Tel Aviv University, Israel, Book of Abstracts, p. 89.
2. T. A. Theodossiou, L.A. Tziveleka, Z. Sideratou, J. Tsogas, D. Tsiourvas and C. M. Paleos, "The Adaptive Solubility Behaviour of Guanidinylated Dendritic Polymers Facilitates their Transport through Cells Membrane", Second European Conference for Clinical Nanomedicine, Basel Switzerland, April 27-29, 2009, Conference Proceedings Part III, p. 77.
3. C. M. Paleos, D. Tsiourvas, Z. Sideratou, A. Pantos, "Guanidinium Group: A Group Inducing Membrane Transport and Multicompartments System Formation", Chembiogenesis 2009, COST ACTION CM0703, Lake Balaton, Hungary, October 23-27, 2009.

4. N. Sterioti, Z. Sideratou, D. Tsiourvas, C. M. Paleos, Synthesis and Characterization of Guanidinylated Poly(L-lysine) DendriGrafts as Prospective Insulin Delivery systems, Young Researchers' Technical Workshop in the frame of EuroNanoMedicine 2009, Bled, Slovenia, September 28, 2009.

Patents

- D. Tsiourvas, M. Arkas, "The use of metal and/or metalloid oxide nanoparticles produced through an environmentally safe process for the removal of pollutants from water, solvents or fluids", Application Number: 20080100395; Filing Date: 09/06/2008. Patent Number 1006559, 24-9-2009.

Funded projects

1. "Nanoscale Functionalities for Targeted Delivery of Biopharmaceutics", 'NMP' INTEGRATED PROJECT, Contract No NMP4-CT-2006-026723, 537 K€, 2006-2010.

Infrastructure

Well-equipped organic synthesis laboratory and Cell-culture facilities, Optical and fluorescence microscopy with imaging facilities, Thermal analysis (DSC, TGA), Spectrophotometers (UV-Vis, Fluorescence), Dynamic Light Scattering, Multi-angle static light scattering, ζ -potential.

Personnel

Dr Dimitris Tsiourvas Research Director, Dr Zili Sideratou Researcher, Dr. Michael Arkas, Assisting Scientific personnel. Collaborating Scientists: Dr Constantinos M. Paleos, Dr Leto-Aikaterini Tziveleka, Dr Theodossis Theodossiou, M Sc. Nikoletta Sterioti. Graduate Students: Maria Agathokleous.

Collaborations

Cohen, S. (Marian Gertner Institute for Medical Nanosystems, Tel-Aviv University, development of novel drug delivery systems based on dendritic polymers); Tsetsekou, A. (NTUA, hybrid organic/ceramic membranes), Nounesis, G. (Institute of Radioisotopes & Radiodiagnostic Products, NCSR "Demokritos", microcalorimetry studies).

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LUMINESCENCE LABORATORY - DEVELOPMENT OF NOVEL PHOTOMETRIC METHODS FOR ANALYTICAL APPLICATIONS

Research Objectives/Activities

The main object of our Laboratory research is the development of novel chemiluminescent methods for the determination of quality factors of natural products. Recently, we have developed and published a chemiluminescent method for the adulteration of olive oils with cheaper seed oils and another one regarding the estimation of antioxidant activity of hydrophilic and hydrophobic compounds as well as the antioxidant activity of natural products (publication 1, presentations 4 and 5). A novel chemiluminescent method is also developed for the determination of hydroperoxides in edible oils and will be published, soon. Sensitized chemiluminescent method has been developed for the determination of active compounds in pharmaceutical formulations by using for the first time nanostructured organo-inorganic catalysts. The chemiluminescent signals increased up to 10-fold (presentation 3).

In frame of a collaboration with the Institute of Farmacochemistry (Tbilisi, Georgia), 3-(3,4-dihydroxyphenyl)-3-glyceric acid has been synthesized and its antioxidant activity and its prostate anti-cancer properties determined (publications 2, presentation 1). The novel glyceric derivative is the basic moiety of a polymeric polyether which presents important prostate anti-cancer properties.

Parallel to the above mentioned activities our laboratory is also active in the synthesis of organo-inorganic hybridized catalysts and their applications in catalytic chemiluminescent reactions as well as in catalytic asymmetric synthetic reactions of bioorganic molecules (presentation 2).

Publications

1. D. Christodouleas, C. Fotakis, K. Papadopoulos, E. Yannakopoulou, A.C. Calokerinos, Development and validation of a chemiluminogenic method for the evaluation of antioxidant activity of hydrophilic and hydrophobic antioxidants, *Anal. Chim. Acta*, 652 (2009) 295-302.
2. M. Merlani, V. Barbakadze, L. Gogilashvili, L. Amiranashvili, K. Mulkijanyan, E. Yannakopoulou, K. Papadopoulos, Enantioselective synthesis and antioxidant activity of 3-(3,4-dihydroxyphenyl)glyceric acid. Monomer of a biologically active polyether isolated from *Symphytum asperum* and *S. caucasicum*, *Chirality*, in press.
3. M.N. Alberti, G.C. Vougioukalakis, M. Orfanopoulos, Photosensitized oxidations of substituted pyrroles: Unanticipated radical-derived oxygenated products, *J. Org. Chem.* 2009, 74, 7274-7282.
4. G.C. Vougioukalakis, I. Stamatopoulos, N. Petzetakis, C.P. Raptopoulou, V. Psycharis, A. Terzis, **P. Kyritsis**, M. Pitsikalis, Hadjichristidis, Controlled vinyl-type polymerization of norbornene with a Nickel(II) diphosphinoamine methylaluminumoxane catalytic system, *J. Polym. Sci. Part A: Polym. Chem.* 2009, 47, 5241-5250.

5. G.C. Vougioukalakis, M.M. Roubelakis, M. Orfanopoulos, Open-Cage Fullerenes: Towards the construction of nanosized molecular containers, *Chem. Soc. Rev.* in press.
6. G.C. Vougioukalakis, R.H. Grubbs, Ruthenium-based heterocyclic carbene-coordinated olefin metathesis catalysts, *Chem. Rev.* in press.

Conferences

1. S. Shrotiya, G. Deep, N. Walie, V. Barbakadze, K. Mulkijanyan, M. Merlani, K. Papadopoulos, L. Gogilashvili, L. Amiranashvili, E. Shaburishvili, R. Agarwal, *Anti-cancer efficacy of novel polymer from Caucasian species of comfrey and its synthetic monomer against androgen-dependent and independent human prostate cancer cells*, American Association for Cancer Research, 100th Annual Meeting 2009, Denver, Colorado, April 18-22, 2009.
2. Ο. Λανίτου, Δ. Δημοτίκαλη, Κ. Παπαδόπουλος, Μελέτη της καταλυτικής δράσης χειρόμορφων υβριδικών οργανο-ανόργανων καταλυτών σε αντιδράσεις εποξειδωσης και αλκυλίωσης, *10 Συνέδριο Χημείας Ελλάδας-Κύπρου*, 2-5 Ιουλίου 2009, Ηράκλειο Κρήτης. (Oral Presentation)
3. K. Papadopoulos, T. Triantis, E. Yannakopoulou, N. Menegas, D. Dimotikali, *Direct chemiluminescence determination of hydroquinidine in pharmaceutical formulation using the oxidation reaction of sodium dithionite with cerium oxide nanoparticles*, 6th International Conference on Nanosciences & Nanotechnologies (NN09), Thessaloniki, Greece, July 13-15, 2009.
4. A. Nikokavoura, D. Christodouleas, K. Papadopoulos, E. Yannakopoulou, D. Dimotikali, A. Calokerinos, *Estimation of total antioxidant activity of edible oils using fluorescence and chemiluminescence techniques*, 6th International Conference on Instrumental Methods of Analysis – Modern Trends and Applications, October 4-8, 2009, Athens, Greece.
5. D. Christodouleas, C. Fotakis, E. Yannakopoulou, K. Papadopoulos, A. Calokerinos, *Evaluation of total antioxidant activity of edible oils by the DPPH-Method*, 6th International Conference on Instrumental Methods of Analysis – Modern Trends and Applications, October 4-8, 2009, Athens, Greece.
6. C. Fotakis, K. Kokkotou, D. Christodouleas, A. Calokerinos, M. Liouni, P. Zoumpoulakis, M. Zervou, *Metabolic monitoring of Greek beverages using HR NMR spectroscopy* 6th International Conference on Instrumental Methods of Analysis – Modern Trends and Applications, October 4-8, 2009, Athens, Greece.
7. T. Tsiaka, D. Christodouleas, A. Calokerinos, P. Kefalas, *Development and validation of a chemiluminometric method for the measurement of peroxide value of olive oil* 6th International Conference on Instrumental Methods of Analysis – Modern Trends and Applications, October 4-8, 2009, Athens, Greece.
8. Vougioukalakis, G. C., Grubbs, R. H. “Ruthenium-Based Metathesis Catalysts Coordinated with Heterocyclic Carbene Ligands: Synthesis, Structure, and Catalytic Activity, 3rd Hellenic Symposium on Organic Synthesis, Athens, Greece, October 2009. (Oral Presentation)

Patent

G.C. Vougioukalakis, R.H. Grubbs, US Patent Application 12/515,702 and European Patent Application EP2104566: "Olefin Metathesis Initiators Bearing Thiazol-2-ylidene Ligands"

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), Dr G. C. Vougioukalakis (Researcher D), E. Yannakopoulou (technical staff), D. Christodouleas and O. Lanitou (unpaid PhD students), A. Pinaka (PhD student).

Collaborations Contact

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)

MOLECULAR COMPUTATIONAL CHEMISTRY

Research Objectives/Activities

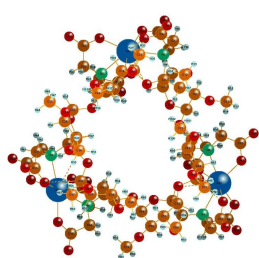
The research activity of Molecular Computational Chemistry Laboratory is focused on the study of the chemical reactivity and the degradation mechanism of molecules in the atmosphere as well as on the reliable prediction of the properties of molecular materials by using theoretical methods (semiempirical, density functional and *ab-initio*).

The theoretical study using density functional theory (DFT) of the heterogeneous chemical reactions of ozone with aromatic compounds in the presence of photosensitizers was completed as well as the elucidation of the origin of tropospheric degradation products which lead to the formation of atmospheric aerosols. At the same time, by using DFT and the semiempirical PM3 method, the study of the structure of complexes of α -, β - and γ - cyclodextrins containing $-\text{N}(\text{CH}_2\text{COOH})_2$ and $-\text{SCH}_2\text{CH}_2\text{COOH}$ groups with lanthanide cations (Eu^{+3} , Gd^{+3} and Tb^{+3}) was completed. The theoretical predictions are in accordance with experimental results which suggest the application of these complexes as paramagnetic contrast enhancing agents in magnetic resonance imaging (MRI) techniques.

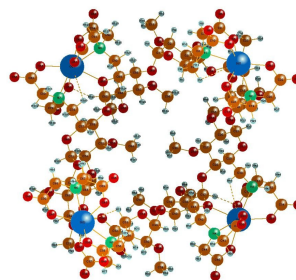
The study of the degradation mechanism of fluorinated unsaturated organic compounds (as promising substitutes for certain categories of freons) by using DFT is still in progress. This study aims at exploring the thermochemical efficiency of the overall reaction scheme and the prediction of the final oxidation pathways of the free radicals generated after the initial hydrogen atom abstraction by the "detergents of the atmosphere" OH, Cl and NO_3 .

The chemical reactions of $\text{CH}_{(3-n)}\text{X}_n\text{COOH}$ ($\text{X}=\text{F}, \text{Cl}$, $n=1-3$) with Cl atoms are being studied by DFT, in order to compare the theoretical predictions with kinetic data available by using structure-activity relationships.

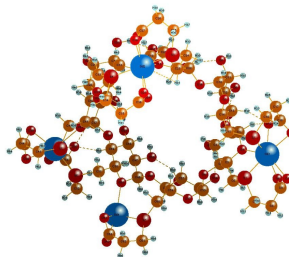
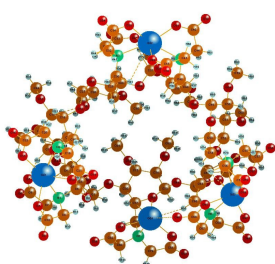
The detailed description of the first step in reactions of alkyl halides with halogen atoms and in particular the stability of the intermediate adducts is studied by using reliable and costly *ab-initio* methods (MP2, CCSD(T)) in order to accurately explain the kinetic parameters for these reactions.



Gd₃-AEDTA



Gd₄-GEDTA



Gd₄-BEDTA

Gd₄-BPSP

Structures of substituted cyclodextrin complexes with the maximum attainable number of Gd⁺³ cations, calculated by the PM3 method

Publications

1. S. Net, L. Nieto-Gligorovski, S. Gligorovski, B. Temime-Rousell, S. Barbati, Y. G. Lazarou, H. Wortham, "Heterogeneous light-induced ozone processing on the organic coatings in the atmosphere", *Atmos. Environ.* **2009**, 43, 1683 - 1692.

Infrastructure

A cluster of personal computers running Microsoft Windows XP, Linux Redhat and Fedora Core.

Personnel

Yannis G. Lazarou: group leader (permanent researcher); Christina Tsonaki (PhD student)

Collaborations

Prof. P. Papagiannakopoulos and Dr. V. C. Papadimitriou (Chemistry Dept., University of Crete, chemical reactions of halogenated molecules, chemical kinetics experiments), 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), Dr. J. B. Burkholder (Earth System Research Laboratory, National Oceanic and Atmospheric Administration, Boulder, Colorado, USA, fluorinated unsaturated organic compounds), Dr. R. Prosmiiti (Department of Atomic, Molecular and Cluster Physics, Institute of Fundamental Physics 'Blas Cabrera', Spanish National Research Council (CSIC), Madrid, Spain, iodinated compounds), Prof. I. I. Morozov (Russian Academy of Sciences, Moscow, Russia, halogenated ethanols), Dr. Sasho Gligorovski (Universités d'Aix-Marseille, France, reactions of ozone with organic compounds).

Contact

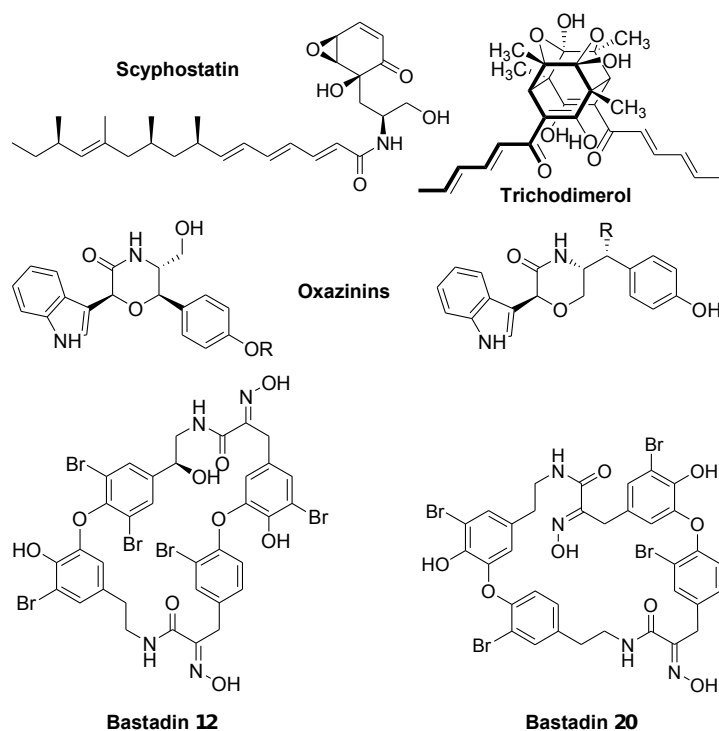
Dr. Y. G. Lazarou (lazarou@chem.demokritos.gr, Tel. +30 210 6503623, Fax. +30 210 6511766)

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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 develop novel synthetic strategies, explore the potential of new synthetic methods, and prepare and study novel compounds with interesting and/or improved biological activity and possible pharmaceutical applications. Modern synthetic methods and techniques, including combinatorial chemistry, are exploited for their preparation (either in solution or on solid support) and 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.



Indicative accomplishments of the group are the total synthesis of **Trichodimerol** (TNF- α inhibitor), **Bastadins** (a family of marine natural products that modulate Ca^{2+} homeostasis and have antiangiogenic activity), **Oxazinins** (marine toxins related to "red tide" incidents), and the efficient and short synthesis of the pharmacophoric core of **Scyphostatin** (selective inhibitor of Neutral Sphingomyelinase, N-Smase).

Publications 2009

1. Athinaios, N.; Kazantzis, A.; Putzker, K.; Lewis, J.; Pitsinos, E.N. "Synthesis of novel laurenditerpenol analogues and their evaluation as HIF-1 activation inhibitors", *Lett. Org. Chem.*, 2009, 6, 269-271.
2. Michaelakis, A.; Strongilos, A.T.; Bouzas, E.A.; Koliopoulos, G.; Couladouros, E.A. "Larvicidal activity of naturally occurring naphthoquinones and

- derivatives against the West Nile virus vector *Culex pipiens*”, *Parasitol. Res.*, 2009, *104*, 657-662.
3. Argitis, P.; Niakoula, D.; Douvas, A.M.; Gogolides, E.; Raptis, I.; Vidali, V.P.; Couladouros, E.A. “Materials for lithography in the nanoscale”, *Int. J. Nanotechnol.*, 2009, *6*, 71-87.
 4. Michaelakis, A.; Mihou, A.P.; Koliopoulos, G.; Couladouros, E.A. “Influence of the microencapsulated pheromone from aged infusion as an oviposition medium of the west Nile virus vector *Culex pipiens*”, *Parasitol. Res.*, 2009, *104*, 1005-1009.
 5. Couladouros, E.A.; Dakanali, M.; Demadis, K.D.; Vidali, V.P. “A short biomimetic approach to the fully functionalized bicyclic framework of type A acylphloroglucinols” *Org. Lett.*, 2009, *11*, 4430-4433.
 6. Pitsinos, E.; Athinaios, N.; Xu, Z.; Wang, G.; Negishi, E.-i. “Total synthesis of (+)-Scyphostatin featuring a fully enantioselective and highly efficient route to the side-chain via Zr-catalyzed asymmetric carboalumination of alkenes (ZACA)”, *Chem. Commun.*, 2010, *46*, DOI:10.1039/B920261G.

Conferences

1. Pitsinos, E.N.; Athinaios, N.; Kazantzis, A. “Synthesis of novel Laurenditerpenol analogues and their evaluation as HIF-1 activation inhibitors”, Medicinal Chemistry: Drug Discovery and Design, 10th Conference with international participation, Conference and Cultural Center, University of Patras, Patras, Greece, March 18-20, **2009**, P32, Abstract Book p. 88.
2. Pitsinos, E.N.; Athinaios, N. “Total synthesis of Laurenditerpenol, a novel HIF-1 activation inhibitor”, 3rd Hellenic Symposium on Organic Synthesis: From chemistry to biology, medicine and materials science, University of Athens, October 15-17, **2009**, P01, Abstracts p. 61.
3. Mitsopoulou, K.P.; Vidali, V.P.; Couladouros, E.A. “Design and synthesis of novel Hyperforin analogues”, 3rd Hellenic Symposium on Organic Synthesis: From chemistry to biology, medicine and materials science, University of Athens, October 15-17, **2009**, P02, Abstracts p. 62.
4. Vidali, V.P.; Dakanali, M.; Demadis, K.D.; Mitsopoulou, K.P.; Couladouros, E.A. “Recent advances in the synthesis of Hyperforin”, COST CM0804: Chemical Biology with Natural Products, Workshop 2009, Certosa di Pontignano, Italy, December 3-6, **2009**, O21, Abstracts p. 31.
5. Anastasopoulou, P.; Efthimiadou, E.K.; Katsarou, M.E.; Katsoulis, I.A.; Kythreoti, G.; Mavridis, I.; Nahmias, V.R.; Papakyriakou, A.; Pitsinos, E.N.; Pyrkotis, C.; Zografos, A.I.; Vourloumis, D. “Antibiotics, anti-angiogenics and diagnostics”, COST CM0804: Chemical Biology with Natural Products, Workshop 2009, Certosa di Pontignano, Italy, December 3-6, **2009**, O23, Abstracts p. 33.
6. Athinaios, N.; Kazantzis, A.; Vidali, V.P.; Pitsinos, E.N. “An olefin cross-metathesis approach for the stereoselective total synthesis of Laurenditerpenol, a novel HIF-1 inhibitor”, COST CM0804: Chemical Biology with Natural Products, Workshop 2009, Certosa di Pontignano, Italy, December 3-6, **2009**, O26, Abstracts p. 38.

Invited lectures

1. Pitsinos, E.N. “Natural Products in Chemistry & Biology: Scyphostatin a Potent and Selective N-Smase Inhibitor”, University of California, San Diego, Department of Chemistry and Biochemistry, 16 June **2009**, invited lecture.
2. Pitsinos, E.N. “Scyphostatin, a potent and selective N-SMase inhibitor”, invited talk at ESF-COST High-Level Research Conference: Natural Products Chemistry, Biology and Medicine II, Hotel Villa del Mare, Acquafredda di Maratea, Italy, 29 August - 3 September **2009**.

Funded Projects

1. "Inhibitors of angiogenesis: design, synthesis and biological exploitation (AngioKem)", COST Action CM0602, 2007-2011.
2. "Chemical biology with natural products", COST Action CM0804, 2009-2012.

Infrastructure

Polarimeter, parallel synthesizer, HPLC.

Personnel

E.N. Pitsinos: researcher A level (permanent researcher); E.A. Couladouros: collaborating faculty (Professor, Agricultural University of Athens); V. Vidali: research fellow (NCSR "D"); N. Athinaios: PhD student (NCSR "D" fellow, National Kapodistrian University of Athens); C. Mitsopoulou: PhD student external funding, Agricultural University of Athens), H. Chrisochou: undergraduate student (National Kapodistrian University of Athens).

Collaborations

Prof. A. Giannis (Universität Leipzig, Fakultät für Chemie und Mineralogie, Institut für Organische Chemie, Leipzig, Germany), Dr. Joe Lewis (Chemical Biology Core Facility, EMBL Heidelberg, Heidelberg, Germany), Prof. J.W. Lazarewicz (Medical Research Centre, Polish Academy of Sciences, Warsaw, Poland), Prof. E.-I. Negishi (Purdue University, Purdue University, West Lafayette, Indiana, USA).

Contact

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Web site: <http://ipc.chem.demokritos.gr/>

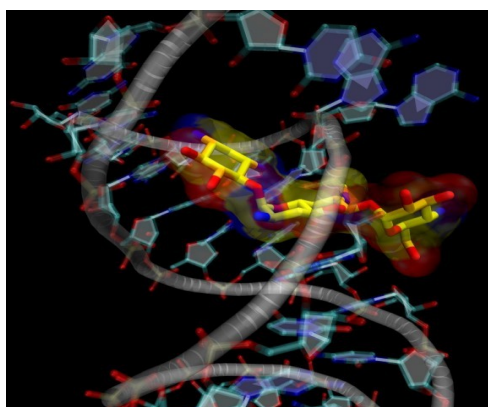
CHEMICAL BIOLOGY OF NATURAL PRODUCTS AND DESIGNED MOLECULES

Research Objectives/Activities

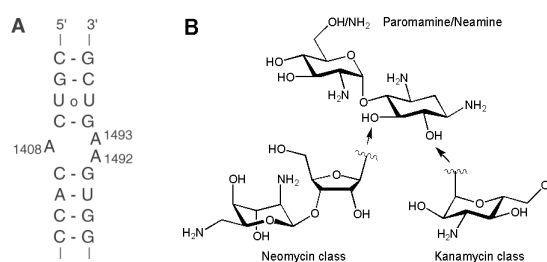
Our laboratory represents a new function within the Institute of Physical Chemistry, namely the "Chemical Biology of Natural Products and Designed Molecules", which was initiated in July 2005. Our studies incorporate molecular design and analysis, total synthesis, structure/activity relationship observations, 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 analogues 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 modelling studies. Currently, we are involved in the areas of Cancer (topoisomerase II inhibitors, apoptosis, angiogenesis), bacterial infections (aminoglycosides and A-site ribosomal-RNA) and anti-virals (Hepatitis C virus, HIV). Some of our ongoing projects are described below 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 pharmaceuticals and will improve overall our quality of life.



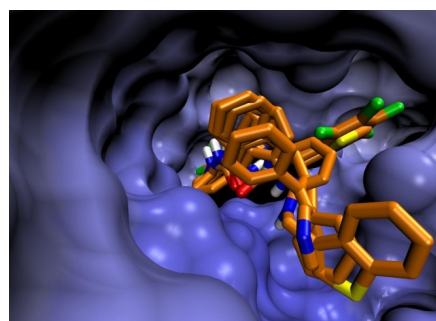
2. Nanoscale functionalities for targeted delivery of biopharmaceutics

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 endothelial 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 2009

1. A. Papakyriakou, D. Vourloumis, F. Tzortzatou-Stathopoulou, M. Karpusas, "Conformational dynamics of the EGFR kinase domain reveals structural features involved in activation." *Proteins: Structure and Bioinformatics* **2009**, 76 (2), 375-386.
2. Evnouchidou I., Papakyriakou A., Stratikos E. "A new role for Zn(II) aminopeptidases: Antigenic peptide generation and destruction" *Curr. Pharm. Design* **2009**, 15 (31), 3656-3670.
3. Dalkas, G.A., Papakyriakou, A., Vlamis-Gardikas, A., Spyroulias, G.A. "Insights into the anthrax lethal factor-substrate interaction and selectivity using docking and molecular dynamics simulations", *Protein Science* **2009**, 18 (8), 1774-1785.
4. Katsoulis, I.A.; Pyrkotis, C.; Papakyriakou, A.; Kythreoti, G.; Zografos, A.L.;

Mavridis, I.; Nahmias, V.R.; Anastasopoulou, P.; Vourloumis, D., "Unnatural rigid scaffolds targeting the bacterial ribosome", *ChemBioChem* **2009**, *10*, 1969-1972.

5. Papakyriakou, M.E. Katsarou, M. Belimezi, M. Karpusas, D. Vourloumis, "Discovery of Potent Vascular Endothelial Growth Factor Receptor-2 Inhibitors Assisted by Computational Methods", *ChemMedChem* **2010**, in press.

Conferences 2009

- a. Dionisios Vourloumis "Unnatural Rigid Scaffolds Targeting the Bacterial Ribosome" 10th International Conference in Medicinal Chemistry: Drug discovery and design, University of Patra, Greece, March 18-20, **2009**.
- b. Dionisios Vourloumis et al. "Chemical Biology of Novel Rigid Scaffolds with Antibiotic Potential" 10th International Conference in Medicinal Chemistry: Drug discovery and design, University of Patra, Greece, March 18-20, **2009**, book of abstracts, P26.
- c. Pyrkotis, C.; Katsoulis, I.A.; Papakyriakou, A.; Kythreoti, G.; Zografos, A.L.; Mavridis, I.; Nahmias, V.R.; Anastasopoulou, P.; Vourloumis, D., "Unnatural rigid scaffolds targeting the bacterial ribosome", 10th Tetrahedron Symposium, "Challenges in Organic and Bioorganic Chemistry", Paris, France, June 23-26, **2009** book of abstracts, C026.
- d. Mavridis, I.; Anastasopoulou, P.; Katsoulis, I.A.; Pyrkotis, C.; Papakyriakou, A.; Kythreoti, G.; Zografos, A.L.; Nahmias, V.R.; Vourloumis, D., "Chemical Biology of Novel Rigid Scaffolds with Antibiotic Potential", International Symposium on Advances in Synthetic and Medicinal Chemistry, Kiev, Ukraine, August 23-27, **2009** book of abstracts, page 168, P040.
- e. Katsoulis, I.A.; Pyrkotis, C.; Papakyriakou, A.; Kythreoti, G.; Cottin, T.; Zografos, A.L.; Mavridis, I.; Nahmias, V.R.; Anastasopoulou, P.; Vourloumis, D., "Novel Spirocyclic Aminocyclitols: Simplified Rigid Structures with Antibiotic Activity", 3rd Hellenic Symposium on Organic Synthesis, "From Chemistry to Biology, Medicine and Materials Science", Athens, Greece, October 15-17, **2009** book of abstracts, L08.
- f. Anastasopoulou, P.; Nahmias, V.R.; Zografos, A.L.; Pyrkotis, C.; Katsoulis, I.A.; Papakyriakou, A.; Kythreoti, G.; Mavridis, I.; Vourloumis, D., "Novel Orthogonally Functionalized 2-DOS Analogues", 3rd Hellenic Symposium on Organic Synthesis, "From Chemistry to Biology, Medicine and Materials Science", Athens, Greece, October 15-17, **2009** book of abstracts, P03.
- g. Anastasopoulou, P.; Efthimiadou, E.; Katsarou, M.; Katsoulis, I.A.; Kythreoti, G.; Mavridis, I.; Nahmias, V.R.; Papakyriakou, A.; Pitsinos, E.N.; Pyrkotis, C.; Zografos, A.L.; Vourloumis, D., "Antibiotics, anti-Angiogenics and Diagnostics", COST CM0804, "Chemical Biology with Natural Products", Workshop 2009, Certosa di Pontignano, Siena, Italy, December 03-06 **2009**, book of abstracts, O23.
- h. Athanasios Papakyriakou, Michael Karpusas, Dionisios Vourloumis, "Targeted Molecular Dynamics of the EGFR Kinase Domain Reveals Structural Features Involved in Activation", 4th Conference of the Hellenic Society for Computational Biology, December 18-20 **2009**, NHRF, Athens, Greece.

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. COST action CM0804, Chemical Biology with Natural Products, 2008-2012.

Personnel

D. Vourloumis: research director (permanent researcher); C. Stathakis, I. Katsoulis, G. Kythreoti, A. Papakyriakou, M. Katsarou, T. Cottin, C. Pyrkotis: (7 post doctoral associates, external funding); E. Efthimiadou, G. Mavridis: (2 PhD students, NCSR "D" fellows); P. Anastasopoulou, A. Papadopoulou, C. Koltsida: (2 PhD students, external funding); N. Lymperea, K. Xanthopoulos (2 undergraduate students); C. Georgaki: (administrative assistant, external funding).

Collaborations

T. Hermann (UCSD, San Diego USA, RNA biochemistry), E. Theodorakis (UCSD, San Diego USA, Organic Synthesis), Prof. A. Giannis (University of Leipzig, Germany, angiogenesis), T. Mpoulikas (REGULON A.E., angiogenesis), D. Georgiadis (UOA, Athens Greece, Organic Synthesis/Spectroscopy), A. Karaliota (UOA, Athens Greece, Inorganic Chemistry), S. Stratikos (NCSR "Demokritos", IRRP, immunomodulation).

Contact

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Web site: http://vourloumis_group.chem.demokritos.gr/index.html

2nd Scientific Programme

**Nanochemistry,
Environmental Friendly
Technologies - Energy**

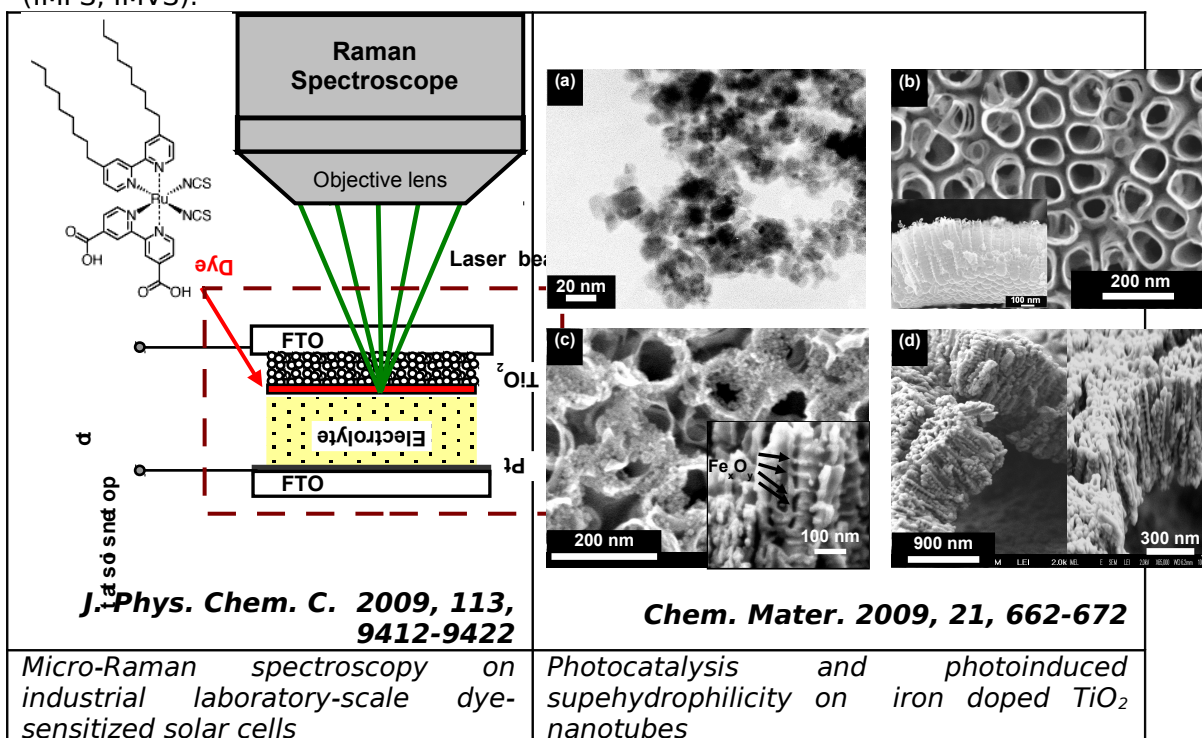
PHOTOREDOX CONVERSION AND STORAGE OF SOLAR ENERGY DEVELOPMENT OF INNOVATIVE FUNCTIONAL MATERIALS FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

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 (of nanoparticles, nanospheres and nanotubes), transition metal complexes, quantum dots and redox nanocomposite polymer electrolytes as well as their efficient incorporation in the photoelectrochemical device. Intensive research activity aims at controlling the photoelectrode nanostructure using sol-gel templating synthesis and electrochemical self-assembly supported by versatile deposition techniques: screen-printing, doctor-blade, spin-coating, dip-coating, anodic oxidation in corrosive media (aqueous and organic). In addition, the team has intensive research activity, for the development of dye-sensitized solar cells (DSSCs) and their optimization in terms of efficiency, life-time and stability, combining state of the art microscopic (AFM), spectroscopic (Raman) and electrochemical techniques (IMPS, IMVS).



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 superhydrophilic 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. Special emphasis is paid to the combination of advanced oxidation processes, titania modified nanomaterials and nanotechnology for water treatment.

Publications

1. Pandiyaraj, K.N.; Selvarajan, V.; Pavese, M.; Falaras, P.; Tsoukleris, D. "Investigation on surface properties of TiO_2 modified by DC glow discharge plasma", *Current Applied Physics*, 2009, 9, 1032-1037.
2. Kontos, A.G.; Kontos, A.I.; Tsoukleris, D.; V.Likodimos, V.; Kunze, J.; Schmuki, P.; Falaras, P. "Photo-induced effects on self-organized TiO_2 nanotube arrays: Influence of surface morphology", *Nanotechnology*, 2009, 20, 045603.
3. Kontos A.I; Likodimos V.; Stergiopoulos T.; Tsoukleris D.; Rabias ; Papavassiliou G.; Kim D.; Kunze J.; Schmuki P.; Falaras P. "Self-Organized Anodic TiO_2 Nanotube Arrays Functionalized by Iron Oxide Nanoparticles", *Chem. Mater.* 2009, 21, 662-672.
4. Pelaez, M.; de la Cruz, A.A.; Stathatos, E.; Falaras P.; Dionysiou D.D.; "Visible Light-activated N-F-codoped TiO_2 Nanoparticles for the Photocatalytic Degradation of Microcystin-LR in Water", *Catalysis Today*, 2009, 144, 19-25.
5. Ghicov A.; Albu S. P.; Hahn R.; Kim D.; Stergiopoulos T.; Kunze J.; Schiller C.-A.; Falaras P.; Schmuki P. " TiO_2 Nanotubes in Dye-Sensitized Solar Cells: Critical Factors for the Conversion Efficiency", *Chemistry-An Asian Journal*, 2009, 4, 520-525.
6. Likodimos V.; Stergiopoulos T.; Falaras P.; Harikisun R.; Desilvestro J.; Tulloch G. "Prolonged light and thermal stress effects on dye sensitized solar cells: a micro-Raman investigation on the long-term stability of aged cells", *J. Phys. Chem. C*, 2009, 113, 9412-9422.
7. Alexaki N.; Stergiopoulos T.; Kontos A. G.; Tsoukleris D. S.; Katsoulidis A. P.; Pomonis P. J.; LeClere D. J.; Skeldon P.; Thompson G. E.; Falaras P. "Mesoporous titania nanocrystals prepared using hexadecylamine surfactant template: crystallization progress monitoring, morphological characterization and application in dye-sensitized solar cells", *Microporous and Mesoporous Materials*, 2009, 124, 52-58.
8. Stergiopoulos T.; Valota A.; Likodimos V.; Speliotis Th.; Niarchos D.; Skeldon P.; Thompson G. E.; Falaras P. "Dye-sensitization of self-assembled titania nanotubes prepared by galvanostatic anodization of Ti sputtered on conductive glass", *Nanotechnology*, 2009, 20, 365601.
9. Stergiou D. V.; Stergiopoulos T.; Falaras P.; Prodromidis M. I. "Solid Redox Polymer Electrolyte-Based Amperometric Sensors for the Direct Monitoring of Ozone in Gas Phase", *Electrochem. Commun.* 2009, 11, 2113-2116.
10. Konti, G.; Chatzivasiloglou, E.; Likodimos, V.; Kantonis, G.; Kontos, A. G.; Philippopoulos, A. I.; Falaras, P. "Influence of the pyridine ligands nature and corresponding Ruthenium (II) dye molecular structure on the performance of dye sensitized solar cells", *Photochem. Photobiol. Sciences*, 2009, 8, 726-732.

11. Philippopoulos, A. I.; Tsantila, N.; Demopoulos, C. A.; Raptopoulou, C. P.; Likodimos, V.; Falaras, P. "Synthesis, characterization and crystal structure of the *cis*-[RhL₂Cl₂]Cl complex with the bifunctional ligand (L) 2-(2'-pyridyl)quinoxaline. Biological activity towards PAF (Platelet Activating Factor) induced platelet aggregation", *Polyhedron*, 2009, 28, 3310-3316.
12. Karatasios, I.; Katsiotis, M.S.; Likodimos, V.; Kontos, A. I.; Papavassiliou, G.; Falaras, P.; Kilikoglou, V. "Photo-induced carbonation of lime-TiO₂ mortars", *Applied Catalysis B: Environmental, Appl. Catal. B: Environ.*, accepted.

Conferences (International)

1. Falaras, P.; Likodimos, V.; Aloupogiannis, P. "Nanotechnology for clean water: Water detoxification using innovative visible nanophotocatalysts", Euro Nano Forum ENF 2009, Nanotechnology for Sustainable Economy, European and International Forum on Nanotechnology, Parallel SESSION B3 - 3.2 Nanotechnology for health and environment - Nanotechnology applications for water treatment, Prague Congress Centre, Prague, Czech Republic, 2-5 June 2009, O-31, Proceedings, p.50.
2. Kim D.; Ghicov A.; Albu S.; Hahn R.; Stergiopoulos T.; Kunze J.; Falaras P.; Schmuki P. "TiO₂ Nanotubes for Dye-Sensitized Solar Cells", Euro Nano Forum (ENF), Prague, 2-5 June 2009, P-010, Proceedings, p.103.
3. Valota A.; Stergiopoulos T.; Likodimos V.; Speliotis Th.; Niarchos D.; Skeldon P., Thompson G. E.; Falaras P. "Dye-sensitization of self-assembled titanium oxide nanotubes", LATEST Researchers Symposium, Victoria Park, Manchester, 22 September 2009, Poster.
4. Stergiou D.; Stergiopoulos T.; Falaras P.; Prodromidis M. I. "On-site ozone monitoring based on solid-state redox electrolyte-modified gold electrodes, 6th International Conference on Instrumental Methods of Analysis, 4-8 October 2009, Athens PB60/p. 252.
5. Stefanou, E.; Falaras P. "Anticancer activity of titanium dioxide under UV irradiation", 2nd European Conference on Environmental Applications of Advanced Oxidation Processes-EAAOP2, Oral Presentation, Nicosia, Cyprus, September 9 -11, 2009, CD of Proceedings.
6. Katsanaki, A.; Kontos, A.I.; Maggos, T.; Vassilakos, C.; Kontos, A.G.; Falaras, P. "Photocatalytic decomposition of nitrogen oxide (NO) under U.V & Vis-Irradiation employing backed and non-backed N-doped TiO₂ nanostructures", 2nd European Conference on Environmental Applications of Advanced Oxidation Processes-EAAOP2, Poster Presentation, Nicosia, Cyprus, September 9 -11, 2009, CD of Proceedings.
7. Spanou, S.; Kontos, A.I.; Pavlatou, E.A.; Falaras P. "TiO₂ reinforced Ni matrix coatings for photoinduced applications", 2nd European Conference on Environmental Applications of Advanced Oxidation Processes-EAAOP2, Poster Presentation, Nicosia, Cyprus, September 9 -11, 2009, CD of Proceedings.
8. Stergiopoulos, T.; Rozi, E.; Ghicov, A.; Likodimos, V.; Kontos, A. G.; Kunze, J.; Schmuki, P.; Falaras, P. "Polymer redox electrolytes filled with anodic titania nanotubular powder: application in dye-sensitized solar cells", Oral Presentation, 5th Kurt Schwabe Symposium, Erlangen, Germany, 24-28 May 2009, CD of Abstracts.
9. Katsanaki, A.; Kontos, A. G.; Likodimos, V.; Maggos, T.; Falaras, P.; Ghicov, A.; Kunze, J.; Schmuki, P. "Photo-induced reactivity of self-organized TiO₂ nanotube arrays prepared by electrochemical anodization", Poster presentation, 5th Kurt Schwabe Symposium, 24-28 May 2009, Erlangen, Germany, CD of Abstracts.
10. Kim, D.; Roy, P.; Lee, K.; Berger, S.; Paramasivam, I.; Ghicov, A.; Albu, S. P.; Stergiopoulos, T.; Hahn, R.; Falaras, P.; Schmuki, P. "TiO₂ Nanotubes for Dye-Sensitized Solar Cells", Poster presentation, 5th Kurt Schwabe Symposium, 24-28 May 2009, Erlangen, Germany, CD of Abstracts.

11. Falaras, P.; Philippopoulos, A. I. "Synthesis and characterization of new ruthenium photosensitizers for solar cell applications", Cost D35 Workshop "Dithiolenes and non-innocent redox-active ligands", Vravra, Attica, June 17-19 2009, poster presentation, Abstracts, p.47.

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. "Organic Solar Cells" PENED 03EΔ 118 project, Coordinator P. Falaras: 144 k€, 2005-2009.
4. "Development of composite nanostructured titania. Incorporation into photocatalytic construction materials and application in the decomposition of model liquid and gas pollutants", PENED 03EΔ 963 project, 51 k€, 2005-2009.
5. "Development of integrated control analytical methods and advanced oxidation processes for the detoxification of natural water and treated wastes", PENED 03EΔ 926 project, 2005-2009.
6. "OrgaPVNet - Coordination Action towards stable and low cost organic solar cell technologies and their application", FP6-Energy-CA, 2006-2009.
7. "Clean Water-Water detoxification using innovative vi-nanocatalysts", FP7-ENV-NMP-2008-2 STREP, 580 K€, 2009-2012, Coordination of the project.
8. "SANS- Sensitizer Activated Nanostructured Solar Cells", FP7-NMP-2009 SMALL-3, 466 K€, 2009- .

Infrastructure

Micro-Raman spectrometer with visible and IR excitation, UV-Vis spectrometer with integrating sphere, cyclic and linear sweep voltametry, Autolab with possibility of electrochemical impedance spectroscopy (EIS), intensity modulated photocurrent spectroscopy (IMPS) and intensity modulated photovoltage spectroscopy, photoelectrochemistry unit, screen printing and spin coating deposition facilities, photocatalytic reactors, contact angle meter, viscosity meter, autoclave.

Personnel

P. Falaras, research director/group leader (permanent researcher); A.G. Kontos (permanent researcher); T. Stergiopoulos, V. Likodimos: (2 post doctoral associates, external funding); N. Vaenas: (PhD student, NCSR "D" fellows); A. I. Kontos, G. Konti, G. Kantonis, E.Rozi, N. Alexaki, A. Katsanaki, K. Skandali: (7 PhD students, external funding); D.Tsoukleris: (technical staff, external funding).

Collaborations

M. Grätzel (EPFL Lausanne, Switzerland, DSSCs), G. Tulloch (Dyesol, Australia, Light and Thermal Stress on DSSCs.), P. Schmuki/ J. Kunze (Erlangen, Germany, Ti-Nanotubes), G. Thompson (Manchester, UK, Ti-Nanotubes) V. Catalano (Nevada, USA, Ligands for Ru-dyes), P. Potvin (Toronto, Canada, Dyes for DSSCs), Z. Picramenou (Birmingham, UK, Supramolecular Dyes), A. Ibbandon (Hull University, UK, Photoreactors), D.D. Dionysiou (UC, USA, Photocatalytic water treatment), Prof. J. Bisquert (Universitat Jaume I, Castello, Spain, Quantum dot based solar cells), Dr. A. Katsoulidis (Northwestern University-Chicago, TiO₂ nanocrystals characterization),

Contact

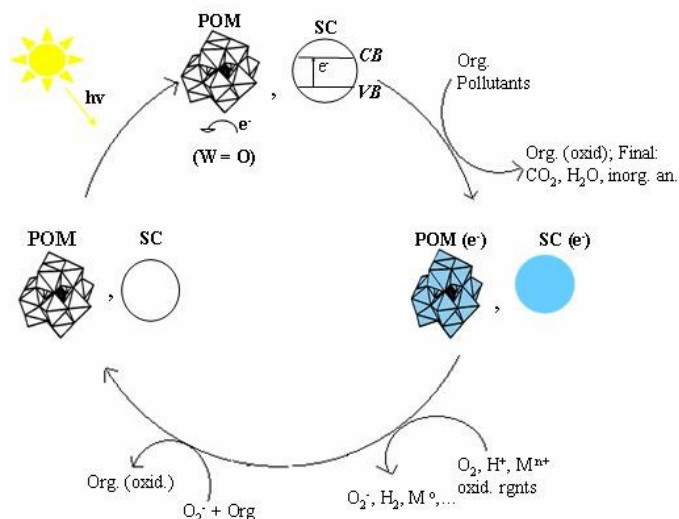
Dr. P. Falaras (papi@chem.demokritos.gr, Tel. +30 210 6503644, Fax. +30 210 6511766)

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CATALYTIC-PHOTOCATALYTIC PROCESSES (SOLAR ENERGY-ENVIRONMENT)

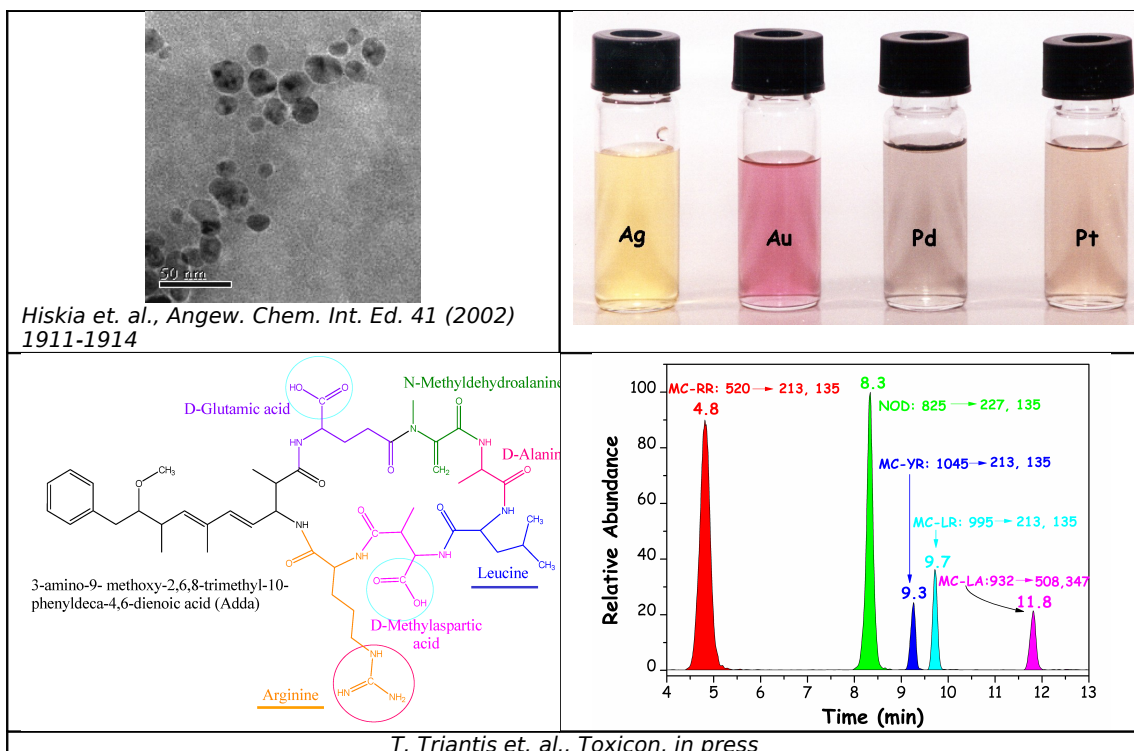
Research Objectives/Activities

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 and photochemical reactions for: (a) Water splitting (hydrogen production), (b) photoelectro-chemical production 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



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.



Publications 2009

1. T. Triantis, A. Troupis, E. Gkika, G. Alexakos, N. Boukos, E. Papaconstantinou, A. Hiskia, "Photocatalytic Synthesis of Se Nanoparticles using Polyoxometalates", *Catalysis Today*, **2009**, 144, 2-6.
2. A. Troupis, T.M. Triantis, E. Gkika, A. Hiskia and E. Papaconstantinou, "Photocatalytic Reductive-Oxidative Degradation of Acid Orange 7 by Polyoxometalates." *Applied Catalysis B: Environmental*, **2009**, 86, 98-107.
3. T. Triantis, K. Tsimeli, T. Kaloudis, N. Thanassoulas, E. Lytras, A. Hiskia, "Development of an integrated laboratory system for the monitoring of cyanotoxins in surface and drinking waters" *Toxicon*, **in press**.
4. "Photocatalytic Degradation of Lindane by Polyoxometalates. Intermediates and Mechanistic Aspects." S. Antonaraki, T.M. Triantis, E. Papaconstantinou, A. Hiskia, *Catalysis Today*, **in press**.
5. M. Pelaez, M.G. Antoniou, D.D. Dionysiou, A.A. de la Cruz, K. Tsimeli, T. Triantis, A. Hiskia, T. Kaloudis, C. Williams, M. Aubel, A. Chapman, A. Foss, U. Khan, K.E. O'Shea, J. Westrick, "Sources and Occurrence of Cyanotoxins Worldwide" in D.F. Kassinis, K. Bester, K. Kümmerer (Eds), "Xenobiotics in the Urban Water Cycle: Mass Flows, Environmental Processes, Mitigation and Treatment Strategies (Environmental Pollution Series, Vol. 16)", Springer-Verlag, New York, **2010**, Chapter 6, p. 101-127.

Conferences

1. K. Tsimeli, T. Triantis, T. Kaloudis, A. Hiskia, "Determination of cyanotoxins in drinking and surface water by LC-MS/MS", Food and Environment Conference, Athens, 13-14 February 2009.
2. T. Triantis, G. Alexakos, N. Boukos, E. Papaconstantinou, A. Hiskia, "Size controlled synthesis and photocatalytic properties of Se nanoparticles", International Polyoxometalate Symposium, Jacobs University, Bremen, Germany, 28 July - 1 August, 2009.
3. K. Papadopoulos, T. Triantis, E. Yannakopoulou, N. Menegas, D. Dimotikali, "Direct chemiluminescence determination of hydroquinidine in pharmaceutical formulation using oxidation reaction of sodium dithionite with cerium oxide nanoparticles", 6th International Conference on Nanosciences & Nanotechnologies, Thessaloniki, Greece, July 13-15, 2009, pg 218.
4. T. Triantis, A. Troupis, G. Alexakos, Elias Papaconstantinou, A. Hiskia, "Environmentally Friendly Synthesis of Nanoparticles using Polyoxometalates", 3rd Symposium on Green Chemistry, Thessaloniki, 25-27 September, 2009.
5. S. Antonaraki, T. Triantis, E. Papaconstantinou, A. Hiskia, "Photocatalytic Degradation of Lindane by Polyoxometalates", 2nd European Conference on "Environmental Applications of Advanced Oxidation Processes-EAAOP2", Nicosia, Cyprus, September 9-11, 2009.
6. K. Tsimeli, T. Triantis, T. Kaloudis, A. Hiskia, "Development of a New Analytical Method for the High Sensitivity Analysis Of Eu 8 Priority Pollutant PAHs in Surface and Drinking Water by LC-APPI-MS/MS", 6th International Conference "Instrumental Methods of Analysis - IMA 2009", Athens, Greece, 4th - 8th October, 2009.
7. I. Dimitrakopoulos, T. Kaloudis, A. Hiskia, N. Thomaidis, M. Koupparis, "Development of a Fast and Selective Method for the Sensitive Determination of Anatoxin-A in Lake Waters using Liquid Chromatography-Tandem Mass Spectrometry and D5-Phenylalanine as Internal Standard", 6th International Conference "Instrumental Methods of Analysis - IMA 2009", Athens, Greece, 4th - 8th October, 2009.

Funded Projects

9. «Water detoxification using innovative V-Nanocatalysts» FP7-ENV-NMP-2008-2, Co-ordinator: P. Falaras, 117 K€, Duration 36 months, Beginning of the program: 2/6/2009.
10. “Development of a multi-residue method for the determination of pesticides in water by LC-MS/MS. Determination of pesticides and cyanotoxins in drinking and surface water”, Research project funded by EYDAP SA, 25 K€, 2008-2009.

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, I. Dimitracopoulos, S. Anagnostou, S. Zervou: (5 PhD students, without pay); E. Papaconstantinou, T. Kaloudis: (adjunct scientists).

Collaborations

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

Contact

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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 $^{13}\text{C}/^{12}\text{C}$ and $^{18}\text{O}/^{16}\text{O}$ 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).

I. Matiatis: (PhD student)

K. Lakten: (technical staff)

Demo

1. N.Zouridakis, E.Arnidi, I.Matiatis, Isotopic analysis of O-18 and Tritium of the atmospheric precipitation in Greece, demo 2009/1G, Athens 2009.
2. N.Zouridakis, E.Arnidi, I.Matiatis, Oxygen-18 and Tritium isotopes in groundwater samples for the period 2004-2008, demo 200/2G, Athens 2009.

Collaborations

P.Sabatakakis, (IGME analysis of isotopic water samples in Peloponnese, Aegean islands), E.Nikolaou (IGME of Epirus, of isotopic water samples in Epirus), Dr. I.Dimitriou (HCMR, analysis of isotopic water samples in Crete, Program «Life-Nature 2004»), Dr.S.Pavlidou (IGME of Crete, analysis of isotopic water samples in Crete), Prof. I.Diamantis (Polytechnic School of Xanthi, Radon analysis in springs and drills of Xanthi), Prof. A.Aravantinos (TEI of Athens (application of infrared camera)

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3rd Scientific Programme

Membranes and Novel Nanostructured Materials for Energy and Environmental Processes

ELECTRONIC SPECTROSCOPY LABORATORY: APPLICATION TO SUPRAMOLECULES AND NANOSTRUCTURES

Research Objectives/Activities

- Guest stability and Dynamics in Nanocavities.
- Organized Supramolecular Assemblies: Non-covalently bonded Nanotubes.
- Spectroscopic research of conformers in ground and excited state.
- Photophysics and Dynamics of Linear and Dendronized Photonic Polymers: Applications to Organic Light Emission Diodes (OLEDs) and Optical Lithography

Publications 2009

1. I. Balomenou and **G. Pistolis*** *"Torsional Photoisomerization Proceeding Adiabatically Through a Volume-Conserving Pathway in Uninhibited Fluid Media"* Chem. Eur. J., 2009, 15, 4228.
2. I. Balomenou and **G. Pistolis*** *Pure Isolation and Stabilization of Energetically highly Disfavored Geometric Isomers by Controlling the Stereoselectivity of Supramolecular Interactions in Tailored Host-Guest Systems.* J. Phys. Chem. B (published in web 17 Dec 2009)

Conferences 2009

1. D. G. Georgiadou, L. Murphy, M. Vasilopoulou, L. C. Palilis, **G. Pistolis**, D. Dimotikalli, J.A.G. Williams and P. Argitis "Photochemical Tuning of the Photo- and Electroluminescence Spectrum of a Phosphorescent Pt Complex inside PVK matrix", 2nd International Symposium on Flexible Organic Electronics (IS-FOE), Halkidiki, Greece, July 2009.

Funded Projects

11. Financial Support from internal programme of Physical Chemistry Institute.

Infrastructure

A Perkin-Elmer Lambda-16 UV - Visible spectrophotometer, a LS-50B Perkin-Elmer Fluorometer, a time correlated single photon counter FL900 of Edinburgh Instruments, a pH meter.

Personnel

G. Pistolis: research director/group leader (permanent researcher);
N. Karakwstas: post doctoral associates (from August-)
I. Balomenou, : PhD student, (NCSR "D" fellow), A. Kaloudi-Chantzea: PhD student, (NCSR "D" fellow from November-).

Collaborations

- J. K. Kallitsis, Professor in Department of Chemistry, University of Patras.
- G. Bokias, Assistant Professor in Department of Chemistry, University of Patras.
- P. Argitis, Researcher in Institute of Microelectronics, NCSR “Demokritos”.
- A. Zarkadis Assistant Professor in Department of Chemistry, University of Ioannina.
- M. Siskos Assistant Professor in Department of Chemistry, University of Ioannina.
- A. Michailidis Associate Professor in Department of Chemistry, University of Ioannina.
- S. Skoulika Associate Professor in Department of Chemistry, University of Ioannina.
- C. Mitsopoulou Associate Professor in Department of Chemistry, University of Ioannina.
- Dr. Ralf Hermann in Faculty of Chemistry and Mineralogy, University of Leipzig, Germany.

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MATERIALS & MEMBRANES FOR ENVIRONMENTAL SEPARATIONS LABORATORY

Research Objectives/Activities

- Pore Structure Analysis & Characterisation (pore size distribution, specific surface analysis, pore volume, pore connectivity): nitrogen and mercury porosimetry, absolute and relative gas and gas vapours permeability (single and multi phase),
- Microscopy (Scanning Electron-Field Emission, Atomic Force),
- Spectroscopy (HPLC, GC, MS),
- Development, modification and optimization of membranes, filters and membrane systems: Chemical Vapour Deposition [CVD], Langmuir-Blodgett Deposition, Plasma Treatment, Phase Inversion, Carbonisation - Activation.
- Characterisation, evaluation and performance validation of porous materials (membranes, activated carbon, etc.) under the framework of various environmental and industrial applications (separation of gaseous pollutants, gas-liquid-vapour permeability-selectivity, reverse osmosis, control drug release and transcutaneous dosing systems, other biotechnological applications etc.).
- Mass and heat transfer process simulation in porous media by means of continuous (macroscopic) and discernible numerical modeling (networks) processes.
- Visual reconstruction and representation of flow phenomena through porous media and various pore sizes by means of different techniques.
- Numerical, experimental and visual, realistic representation of oil recovery processes and techniques by means of mathematical models and experimental process reconstruction structures of well-defined geometry and under realistic conditions (realistic high pressure and temperature deposit conditions).
- Reconstruction of porous media with the use of scanning tomography and computer graphic simulations.
- Preparation and characterization of hybrid nanocomposite materials (Polymer/clay nanocomposites).
- Modification and utilisation of natural algal products and processing by-products (i.e. polysaccharides, alginic acids etc.) in environmental applications and pollutant separations (i.e. heavy metal and pesticide removal from water streams, waste and brackish water treatment etc..).
- Development and characterization of single and multi-walled carbon nanotubes.
- Development and characterization of nanostructured materials for hydrogen storage.
- Preparation and characterization of material systems for biotechnological applications and packaging materials of improved barrier properties.
- Synthesis and characterisation of materials for single and multi-layer film and hollow-fibre structures.
- Synthesis and characterisation of zeolitic membranes.
- Synthesis and characterisation of metal nanoparticles.

Publications 2009

1. Eleni C. Vermisoglou, Georgios N. Karanikolos, Georgios Pilatos, Eamon Devlin, Georgios E. Romanos, Charitomeni U. Veziri, and Nick K. Kanellopoulos Aligned Carbon Nanotubes with Ferromagnetic Behavior, *Advanced Materials* (in press),
2. E.C. Vermisoglou, A. Labropoulos, G.E. Romanos, E. Kouvelos, S. Papageorgiou, G.N. Karanikolos, F. Katsaros, N.K. Kanellopoulos, *Hydrogen*

- Storage in Polymer-Functionalized Pd-Decorated Single Wall Carbon Nanotubes *Journal of Nanoscience and Nanotechnology* (in press)
- Sergios K. Papageorgiou, Evangelos P. Kouvelos, Evangelos P. Favvas, Andreas A. Sapalidis, George E. Romanos, Fotios K. Katsaros, Metal-carboxylate interactions in metal-alginate complexes studied with FTIR spectroscopy, *Carbohydrate Science* (in press).
 - N. Pasadakis, G. Romanos, V. Perdikatsis, A.E. Foscolos "Physical and chemical activation of Greek lignites. A comparative study" *Energy Sources, Part A: Recovery, Utilization, and Environmental Effects*, (in press)
 - A. Gotzias, H. Heiberg-Andersen, M. Kainourgiakis, Th. Steriotis, Grand Canonical Monte Carlo Simulations of Hydrogen Adsorption in Carbon Cones, *Appl. Surf. Sci.*, in press
 - M. Kainourgiakis, Th. Steriotis, G. Charalambopoulou, M. Strobl, and A. Stubos, Determination of the spatial distribution of multiple fluid phases in porous media by USANS, *Appl. Surf. Sci.*, in press.
 - M. Konstantakou, Th. Steriotis, E. Kikkinides and A. Stubos, "Monte Carlo simulations of CO₂ sorption in nanoporous carbons", *J. of Porous Media*, in press.
 - V. Georgakilas, A.B. Bourlinos, R. Zboril, Th. A. Steriotis, P. Dallas, A.K. Stubos and Ch. Trapalis, Organic functionalisation of graphenes, *Chem. Commun.* In press.
 - A. Bourlinos, Th. Steriotis, R. Zboril, V. Georgakilas and A. Stubos, "Direct synthesis of carbon nanosheets by the solid-state pyrolysis of betaine", *J. Mater. Sci.* 44, 1407-1411 (2009).
 - C. Zlotea, P. Moretto and Th. Steriotis, "A round robin characterisation of the hydrogen sorption properties of a carbon based material", *Int. Journal of Hydrogen Energy*, 34, 3044-3057 (2009).
 - A.B. Bourlinos, V. Georgakilas, R. Zboril, T.A. Steriotis, A.K. Stubos, C. Trapalis, Aqueous-phase exfoliation of graphite in the presence of polyvinylpyrrolidone for the production of water-soluble graphenes, *Solid State Communications*, 149, 2172-2176 (2009).
 - A.B. Bourlinos, V. Georgakilas, R. Zboril, Th.A. Steriotis and A.K. Stubos, Liquid-Phase Exfoliation of Graphite Towards Solubilized Graphenes, *Small*, 5(16), 1841-1845 (2009).
 - Veziri, Ch.M., Karanikolos, G.N., Pilatos, G., Vermisoglou, E.C., Giannakopoulos, K., Stogios, Ch., Kanellopoulos, N.K. "Growth and morphology manipulation of carbon nanostructures on porous supports ", *Carbon* 47 (9), **2009** pp. 2161-2173,
 - Labropoulos, A.I., Romanos, G.E., Karanikolos, G.N., Katsaros, F.K., Kakizis, N.K., Kanellopoulos, N.K. "Comparative study of the rate and locality of silica deposition during the CVD treatment of porous membranes with TEOS and TMOS" *Microporous and Mesoporous Materials* 120 (1-2), **2009** pp. 177-185
 - Favvas, E.P., Sapalidis, A.A., Stefanopoulos, K.L., Romanos, G.E., Kanellopoulos, N.K., Kargiotis, E.K., Mitropoulos, A.Ch. "Characterization of carbonate rocks by combination of scattering, porosimetry and permeability techniques", *Microporous and Mesoporous Materials* 120 (1-2), **2009** pp. 109-114
 - Athanasekou, C.P., Papageorgiou, S.K., Kaselouri, V., Katsaros, F.K., Kakizis, N.K., Sapalidis, A.A., Kanellopoulos, N.K. "Development of hybrid alginate/ceramic membranes for Cd²⁺ removal", *Microporous and Mesoporous Materials* 120 (1-2), **2009** pp. 154-164
 - Papageorgiou, S.K., Katsaros, F.K., Kouvelos, E.P., Kanellopoulos, N.K. "Prediction of binary adsorption isotherms of Cu²⁺, Cd²⁺ and Pb²⁺ on calcium alginate beads from single adsorption data", *Journal of Hazardous Materials* 162 (2-3), **2009** pp. 1347-1354
 - Bourlinos, A.B., Georgakilas, V., Zboril, R., Steriotis, T.A., Stubos, A.K., Trapalis, C." Aqueous-phase exfoliation of graphite in the presence of

- polyvinylpyrrolidone for the production of water-soluble graphenes”, *Solid State Communications* 149 (47-48), **2009** pp. 2172-2176
19. Zlotea, C., Moretto, P., Steriotis, T. “A Round Robin characterisation of the hydrogen sorption properties of a carbon based material”, *International Journal of Hydrogen Energy* 34 (7), **2009** pp. 3044-3057
 20. Bourlinos, A.B., Steriotis, T.A., Zboril, R., Georgakilas, V., Stubos, A. “Direct synthesis of carbon nanosheets by the solid-state pyrolysis of betaine”, *Journal of Materials Science* 44 (5), **2009** pp. 1407-1411.
 21. Karatasios, I., Theoulakis, P., Kalagri, A., Sapolidis, A., Kilikoglou, V. “Evaluation of consolidation treatments of marly limestones used in archaeological monuments”, *Construction and Building Materials* 23 (8), **2009** pp. 2803-2812.
 22. Orsolya Czakkel, Gyorgy Onyestyak, George Pilatos, Vangelis Kouvelos, Nick Kanellopoulos, Krisztina Lászlo, “Kinetic and equilibrium separation of CO and CO₂ by impregnated spherical carbons”, *Microporous and Mesoporous Materials* 120 (2), **2009** pp. 76-83.
 23. G. E. Romanos, O. C. Vangeli, K. L. Stefanopoulos, E. P. Kouvelos, S. K. Papageorgiou, E. P. Favvas and N. K Kanellopoulos, “Methods of evaluating pore morphology in hybrid organic-inorganic porous materials”, *Microp. Mesop. Mater.*, 120, 2009, 53 - 61.
 24. Vermisoglou, E.C. Romanos, G.E., Tzitzios, V. , Karanikolos, G.N. , Akylas, V. , Delimitis, A. , Pilatos, G. , Kanellopoulos, N.K. “Synthesis of nanocrystalline gold-carbon nanotube composites and evaluation of their sorption and catalytic properties”, *Microporous and Mesoporous Materials* 120, 1-2, 2009
 25. Belessi, V. , Romanos, G., Boukos, N, Lambropoulou, D., Trapalis, C. “Removal of Reactive Red 195 from aqueous solutions by adsorption on the surface of TiO₂ nanoparticles”, *Journal of Hazardous Materials* 170, 2-3, **2009** 836,

Conferences & Proceedings 2009

1. A.A. Sapolidis, F.K. Katsaros, Th. A. Steriotis, N.K. Kanellopoulos, «Highly ordered PVA/ Bentonite nanocomposites: Effect of matrix properties on the orientation of inorganic layers», 5th International Conference on Nanostructured Polymers And Nanocomposites, Paris - France, April 15-17, 2009
2. E.C. Vermisoglou, G.E. Romanos, G. Pilatos, N.K. Kanellopoulos “Aligned Carbon Nanotube Supported Alumina Membranes for Gas Separations” 5th International Conference on Diffusion in Solids and Liquids (DSL 2009) Rome (Italy), during 24-26 June, 2009.
3. Th. Steriotis, A.K. Stubos, “Metal doped carbon foams for hydrogen Storage”, 2009 Gordon Research Conference on Hydrogen-Metal systems, Barga, Italy, 12-17 July 2009 (invited).
4. Th. Steriotis, G. Charalambopoulou, A. Stubos, “Solid Storage for Hydrogen”, 3rd International Workshop on Hydrogen, Rabat - Morocco, 28-31 October 2009 (invited).
5. G. Charalambopoulou, Th. Steriotis, G. Derrien, J. Zajac, U. Keiderling, “Study of olefin selective porous aluminosilicates with in situ sorption and SANS”, 7th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis (ISSHAC 7), Kazimierz Dolny - Poland, 5 - 11 July 2009.
6. J. D. F. Ramsay, Th. A. Steriotis, G. Charalambopoulou, M. Kainourgiakis, “In situ SANS studies of benzene sorption on silica gels”, 7th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis (ISSHAC 7), Kazimierz Dolny - Poland, 5 - 11 July 2009.

7. M. Kainourgiakis, Th. Steriotis, G. Charalambopoulou, M. Strobl, A. Stubos, "Determination of the spatial distribution of multiple fluid phases in porous media by USANS", 7th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis (ISSHAC 7), Kazimierz Dolny - Poland, 5 - 11 July 2009.
8. A. Gotzias, H. Heiberg-Andersen, M. Kainourgiakis, Th. Steriotis, "Grand Canonical Monte Carlo Simulations of Hydrogen Adsorption in Carbon Cones", 7th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis (ISSHAC 7), Kazimierz Dolny - Poland, 5 - 11 July 2009.
9. E.C. Vermisoglou, G.E. Romanos, N.K. Kanellopoulos, Study of the Catalytic NOx Reduction by Polymer-Functionalized Rh-decorated SWNTs, The Seventh International Symposium Effects of Surface Heterogeneity in Adsorption and Catalysis on Solids - ISSHAC-7, 5-11 July 2009, Kazimierz Dolny, Poland.
10. N.K. Kakizis, "EU Research Priorities in FP7, Priority 6: Environment incl. Climate Change, Developing joint research initiatives with the EECA region countries", The EU-Eastern European & Central Asian Countries WorkShop, EU-EECA Committee Proceedings, 15/10/2009, Athens, Greece.
11. N.K. Kakizis, "EU Research Priorities in FP7, Priority 6: Environment incl. Climate Change, Developing joint research initiatives with the LARINET region countries", The EU-Latin American Countries Network WorkShop, EU-LARINET Committee Proceedings, 17-18/11/2009, Bogota, Colombia.
12. N. Kakizis, A. Baldoukas, A. Tassios "Introducing science and technology issues through the 'Technological Recycling' concept: a phenomographic study of primary and secondary school students in Greece and Italy concerning technology in daily life" e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
13. N. K. Kakizis, A. Baldoukas, A. Tasios, C. Kechagias, M. Tzani "Technological Recycling of Materials: A novel concept framework for reinforcing communication and strengthening synergetic integrated education in science and technology principles", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
14. N. K. Kakizis, A. Baldoukas, M. Tsigonias, S. Louzi, N. Kazachkova "Black Boxes or science for society: the 'TechnoRecycle' concept framework supports the process of an educational reversion to basic scientific concepts and provides a sustainable means for revealing technology and reaching the essence of science", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
15. N. K. Kakizis, A. Baldoukas, A. Tasios, C. Kechagias, M. Tzani "The exchange of S&T experiences and the cognitive integration of generations through the implementation of the 'Technological-Recycling' concept framework: developing a framework for the exchange of experiences, views and scientific knowledge between parents, pupils and teachers", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International

- Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
16. N. Kakizis, A. Baldoukas, A. Tasios, C. Kechagias, M. Tzani "The integration of scientific knowledge and technological experiences through hands-on science communication workshops", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 17. N. K. Kakizis, A. Baldoukas, M. Tsigonias, S. Louzi, N. Kazachkova "Researching or Experiencing Science & technology: Discussing best practice cases and approaches on the organization of successful science communication and technology familiarization events", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 18. N. Kazachkova, A. Baldoukas, N. K. Kakizis "The developing of cognitive skills in science and ecological knowledge by means of science presentations of new format called 'Paradox Show', e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 19. A. Baldoukas, N. K. Kakizis "Revealing energy conservation and motion-related principles through a clock-work car made of recycling materials", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 20. A. Baldoukas, N. K. Kakizis, G. Demosthenous, A. Tsatsaris, F. Soukatzidis "Hands-on experience with the construction and calibration of a weight balance constructed through up-cycling of recycled materials and according to the 'Technological-Recycling of Materials' educational method", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 21. A. Baldoukas, N. K. Kakizis "An interactive hands-on scenario explaining the ultrasonic tester working mechanism", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
 22. A. Baldoukas, N. K. Kakizis, A. Tsatsaris, G. Demosthenous, F. Soukatzidis "How does a telescope stimulate on a certain star during earth spinning? An educational device constructed of raw materials", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009

23. A. Baldoukas, N. K. Kakizis, F. Soukatzidis "An air propeller water pump made of raw materials, as an interactive teaching tool or an exhibition item in science museum", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
24. A. Baldoukas, N. K. Kakizis, G. Demosthenous, A. Tsatsaris, F. Soukatzidis "Correlating the tension force on the supporting cables of a scaled hanging bridge, with a car position moving along it", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
25. A. Baldoukas, N. K. Kakizis "Educating on jet-propulsion principles by means of plastic bottles, yogurt cups and balloons", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
26. A. Baldoukas, N. K. Kakizis, A. Tsatsaris, G. Demosthenous, F. Soukatzidis "How could the construction characteristics of a noise production device, made of recycling material, affect the it's digital analysis voice curve", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
27. A. Baldoukas, N. K. Kakizis, F. Soukatzidis "A rotating clock-work one-wheel bicycle made of recycling materials, as an educational toy connecting physics, math and environment", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
28. M. K. Tsigonias, A. Politis, N. K. Kakizis, A. Baldoukas "Environmental tele-education as a part of the highest level Education lesson 'holistic packaging construction', e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
29. N. K. Kakizis, M. K. Tsigonias, A. Baldoukas "Packaging up-cycling and reuse as a means for experiential environmental education of pupils", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
30. M. K. Tsigonias, N. K. Kakizis, A. Baldoukas "Green Packaging: Increasing environmental awareness by means of novel technologies and alternative education", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009

31. N. K. Kakizis, J. Nolan, E. G. Karagiannes, N. K. Kanellopoulos "The establishment of the European Academic Poles of Excellence and the dissemination of their disruptive and incremental technologies through the operation of pioneering fourth generation Virtual Technology Parks", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
32. N. K. Kakizis, E.G. Carayiannis, N. K. Kanellopoulos "Virtual Institutes and Virtual Research How To Enhance Educational output and experience development", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
33. N. K. Kakizis, G. Pilatos, M. K. Tsigonias, G.E. Romanos, P. Andrianopoulos, N. K. Kanellopoulos "Development of multilayer fabric assemblies with improved gas barrier properties containing activated carbon monolayer's", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
34. M. Tsigonias, N. K. Kakizis, G.E. Romanos, A. Baldoukas " Activated biological carbons: A new means for the analysis of cumulative pollution of aquatic environments or a case of "techno-mimesis", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
35. N. K. Kakizis, E.G. Carayiannis, N. K. Kanellopoulos "Science maturity, innovation development, organizational restructuring and virtual institutes", e RA - 4: The Conference for the contribution of Information Technology to Science, Economy, Society and Education & International Scientific Conference SynEnergy Forum (S.E.F.) - 2: The conference for International Synergy in Energy, Environment, Tourism and Information Technology Spetses Island, Greece, 24 - 26 September 2009
36. Romanos, G.; Falaras, P. "Clean Water, Nanotechnology for Clean Water", Euro Nano Forum ENF 2009, Nanotechnology for Sustainable Economy, European and International Forum on Nanotechnology, Workshop: Nanotechnology for environment and water treatment, Prague Congress Centre, Prague, Czech Republic, 2-5 June 2009.
37. Romanos, G.; Falaras, P.; Likodimos, V. "Solar light promoted nanotechnology for water cleaning" (Project CleanWater), Euro Nano Forum ENF 2009, Nanotechnology for Sustainable Economy, European and International Forum on Nanotechnology, Press Briefing 1: Nanotechnology for the environment, Prague Congress Centre, Prague, Czech Republic, 2-5 June 2009.
38. Romanos, G., Falaras, P.; Likodimos, V. "Nanotechnology for clean water: Water detoxification using innovative visible nanophotocatalysts", Euro Nano Forum ENF 2009, Nanotechnology for Sustainable Economy, European and International Forum on Nanotechnology, Parallel SESSION B3 - 3.2 Nanotechnology for health and environment - Nanotechnology applications for water treatment, Prague Congress Centre, Prague, Czech Republic, 2-5 June 2009, O-31, Proceedings, p.50.

39. Κ.Λ. Στεφανόπουλος “Μεταπτυχιακές Σπουδές στο ΕΚΕΦΕ «Δημόκριτος»: Δυνατότητες και Προοπτικές” Θερινό Σχολείο 2009, ΕΚΕΦΕ «Δημόκριτος», 6-17 Ιουλίου 2009.
40. Marios Tsigonias, Nickolas Kakizis and Antonis Baldoukas, BIOCARBONS AS INDICATORS OF CUMULATIVE POLLUTION OF HEAVY METALS AND RADIOACTIVE AGENTS IN AQUATIC ENVIRONMENTS – CASE STUDY: THE CYCLADES AND THE CENTRAL AEGEAN SEA, EuroScience Mediterranean Event ESME – 2009, Present Challenges – Future Opportunities, Athens 15-19 October 2009, Technopolis - Athens Gazi Industrial Archaeological Park
41. Antonis Baldoukas, Nickolas. Kakizis, Good practice in revealing energy conservation and motion-related principles through a clock-work car made of recycling materials EuroScience Mediterranean Event ESME – 2009, Present Challenges – Future Opportunities, Athens 15-19 October 2009, Technopolis - Athens Gazi Industrial Archaeological Park
42. Ε. Π. Φάββας, Κ.Λ. Στεφανόπουλος, Ν.Κ. Κανελλόπουλος και Α.Χ. Μητρόπουλος “Χαρακτηρισμός μεμβρανών άνθρακα με πειράματα διαπερατότητας και συνδυασμό προσρόφησης με ακτίνες-Χ σε μικρές γωνίες (SAXS)” 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Ιουλίου 2009.
43. Χ.Μ. Βεζύρη, Γ.Ν. Καρανικολός, Ν.Κ. Κανελλόπουλος, και Μ. Τσαπατσής “Δευτεροταγής ανάπτυξη ΑFI υμενίων και μεβρανών”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Ιουλίου 2009.
44. Χ. Αθανασέκου , Γ. Ρωμανός και Ν. Κανελλόπουλος “Τροποποίηση μεμβρανών αργιλίας με αλγινικό οξύ για απομάκρυνση Cd++ από απόβλητα”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Ιουλίου 2009.
45. Ο. Βαγγέλη, Γ. Ρωμανός, Κ. Μπέλτσιος, Δ. Φωκάς και Ν. Κανελλόπουλος “Τροποποίηση πυριτικών πορωδών υποστρωμάτων με ιοντικά υγρά για εφαρμογές διαχωρισμού αερίων”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Ιουλίου 2009.
46. Ν. Κανελλόπουλος “Νανοπορώδεις Μεμβράνες και συστοιχίες νανοσωλήνων άνθρακα”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Ιουλίου 2009.
47. Α. Γκότζιας, Θ. Στεριώτης, Μ. Καινουργιάκης, “Μελέτη ρόφησης υδρογόνου σε απομονωμένους νανο- σωλήνες και νανο-κώνους άνθρακα”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Οκτωβρίου 2009.
48. Α. Μπουρλίνος, Δ. Γιασαφάκη, Ε. Κούβελος, Α. Στούμπος, Γ. Χαραλαμποπούλου, Θ. Στεριώτης, “Μελέτη αποθήκευσης υδρογόνου σε νανοςύνθετα υλικά άνθρακα-μετάλλου”, 4ο Πανελλήνιο Συμπόσιο Πορωδών Υλικών, Πάτρα, 22-23 Οκτωβρίου 2009.

Funded Projects

Coordinator:

1. 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).

Partner:

1. NEXT-GTL, NMP-2008-4.0-2, Innovative catalytic technologies & materials for next gas to liquid processes (NEXT-GTL), Start Date: 2009-11-01, 48 months, Project Cost: 12.57 million euro, Contract Type: Large-scale integrating project, End Date: 2013-10-31, Project Funding: 8.39 million euro, NCSR(480000€)
2. "Environment NCPs cooperating to improve their effectiveness", (ENV-NCP-Together-21249), Coordination Support Action, N. Kakizis, Partners to NCSR"D" the Network of the 36 National Contact Point Organisations in Europe, Asia and N. Africa, Budget: 2997000€, NCSR"D" budget: 73.345€, 2008-2013.

Research Infrastructure & Facilities

1. Nitrogen Porosimeter with Krypton Upgrade - Quantachrome
2. Mercury Porosimeter - Quantachrome
3. Low Pressure Permeability rig
4. High Pressure permeability rigs (2, up to 70 bars)
5. High pressure selectivity rigs (2, gaseous phase)
6. Low pressure selectivity rig (gaseous phase)
7. Gas chromatographers (3) with automated sampling capabilities
8. Gas Chromatographer - Mass Spectrometer - Pfeiffer
9. Dynamic gas adsorption rig
10. Hybrid fluidised bed - membrane system for the removal of volatile organic compounds
11. High pressure automated gravimetric sorption analyser - HIDEN IGA
12. Magnetic suspension gravimetric analysers (2) - Rubotherm
13. Low pressure sorption gravimetric analysers (3) - CI balances
14. Langmuir-Blodgett (LB) trough for the preparation of thin films
15. Chemical Vapour Deposition reactors
16. Grazing incidence infrared GIRR 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, hydrogen volumetric sorption apparatus for isotherms - (VTI,HPVA 100)
22. Gas and vapour permeability apparatus for polymers and nano-composites (oxygen permeability - Danseror PBI)
23. AFM -VeeCo, diInnova
24. FTIR Nicolet 6700
25. High pressure cell for FT-IR
26. Ultra pure water production unit
27. Ion chromatography system - Dionex
28. HPLC - Dionex
29. Calorimeter Calvet - Setaram
30. Thermal analysis (TGA) - Setaram
31. Zero length Chromatography
32. Field emission scanning electron microscope, (FE-SEM) Jeol -JSM-7401F

Personnel

(Research Director); Dr. Nick Kanellopoulos, Researcher A', (4 Researchers); Dr. Theodore Steriotis, Researcher B', Dr. Kostas Stefanopoulos, Researcher C', Dr. Fotis Katsaros, Researcher C', Dr. George Romanos, Researcher C', (8 Research & Technical Personnel); Dr. Nickolas Kakizis, Dr. Sergios Papageorgiou, Evaggelos Kouvelos, Andreas Sapolides, Evaggelos Favvas, George Pilatos, Chrysa Athanasekou, Anastasios Gontzias, (2 post-doctoral associates, external funding); Dr. George Karanikolos, Dr. John Nolan; (6 PhD Students); Charitomeni Veziri, Eleni Vermisoglou, Anastasios Labropoulos, Victoras Akylas, Marios Tsigonias, Olga Vaggeli (4 MSc Students); Eleni Chatzidaki, Panagiotis Karatzis, Panagiota Tatsiou, Nikos Iliopoulos,

Collaborations - Invited Visits

Prof. Michael Tsapatsis (Department of Chemical Engineering and Materials Science, University of Minnesota, Development of Porous Films and Membranes), Prof. Avelino Corma (Instituto de Tecnologia Quimica, CSIC-UPV, Universidad Politecnica de Valencia, Development of oriented Nanotubes).

Contact

Nick Kanellopoulos

MESL - Materials & Membranes for Environmental Applications Laboratory

URL: <http://www.demokritos.gr>, <http://mesl.chem.demokritos.gr>

NCSR - 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.

URL: <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: kanel@chem.demokritos.gr"kanel@chem.demokritos.gr,
mesl@chem.demokritos.gr"mesl@chem.demokritos.gr

National Contact Point EU FP7, Thematic Priority 6: “Environment, including climate change”, Programme Cooperation

Since 2006 the National Centre for Scientific Research “Demokritos” and especially the Institute of Physical Chemistry, is the hosting organisation of the Hellenic National Contact Point of the 7th framework programme for research and technological development of the European Union in Hellas, Programme Cooperation, Thematic Priority 6: “Environment, including Climate Change”. Following a call for proposals by the Hellenic General Secretariat for Research and Technology (GSRT), the NCP has been staffed by members of the Membranes and Nanomaterials for Environmental Separations Laboratory (MESL) research team. During the two-year period of its operation the NCP has provided high level consulting and liaisoning services to over 60 Hellenic organisations (both private and public) with respect to their participation in the FP7-related initiatives, while over 270+ research project proposals have been submitted (that included at least one partner from Hellas) to the various call for the submission proposals under the framework of the specific thematic priority. At the same time, the NCP has provided high level consultation and liaisoning to the Hellenic scientific and research community with respect to the development of research consortia and the development, submission and implementation of research proposals, research projects and development and funding of scientific and technological innovation.

Aiming to the coverage of existing requirements at the greatest possible extent and the promotion of the participation of Hellenic organisations in the respective initiatives and calls for proposals, the NCP has organised and co-organised 9 National Infodays and has participated in the NCP Network meetings (4). Furthermore, it has been invited to participate at the proceedings of “Water Supply & Sanitation-WSSTP” and “Hydrogen and Fuel Cell Technology Platform-HFP” European Technology platforms and make invited presentation on a number of subjects pertaining to advances in the respective areas of interest. Under the same framework, the Hellenic NCP has undertaken the task of presenting research activities and research “ideas” on behalf from both research groups from NCSR “Demokritos” as well as from other Hellenic academic and research organisations in various EU organised Infodays and Brokerage events on environmental technologies.

For 2009 a multi-thematic National Infoday Event was organised entitled: Για το 2009 διοργανώθηκε πολυθεματική ημερίδα ενημέρωσης και πληροφόρησης με τίτλο: “Calls for Research Proposals in FP7 2009-2010, Best practice cases in research and RTD ethics”, 13-11-2009, NCSR “Demokritos”. At the International level a Technology Brokerage & Networking Event in the Field of Water Management & Sanitation Europe-Africa-EECA (Eastern European and Central Asian Countries), was organised in Vienna, Austria on 16-17 September 2009. The event attracted 5 scientific representations from Greek research organisations that presented 6 technological ideas or research proposals while 9 international scientific-research co-operations were established.

At the national level, the NCP has organised more than 112 consultation sessions with representatives from Hellenic Organisations with respect to the development, submission and support of research project proposals. Moreover, extensive efforts have been undertaken with respect to the organisation of visits and invited working sessions and infodays with organisations all around Hellas in order to fulfil specific regional requirements.

Apart from the full coverage of its contractual obligations towards the GSRT and the Hellenic Ministry of Development the Hellenic NCP “Environment, including climate change” aims at the proactive representation and support of the research groups of NCSR “Demokritos” and the promotion of NCSR “Demokritos” as one of the most prominent Hellenic research centres at the European and International level.

Personnel

(2 National Contact Points); Dr. Theodore Steriotis, Dr. Nickolas Kakizis

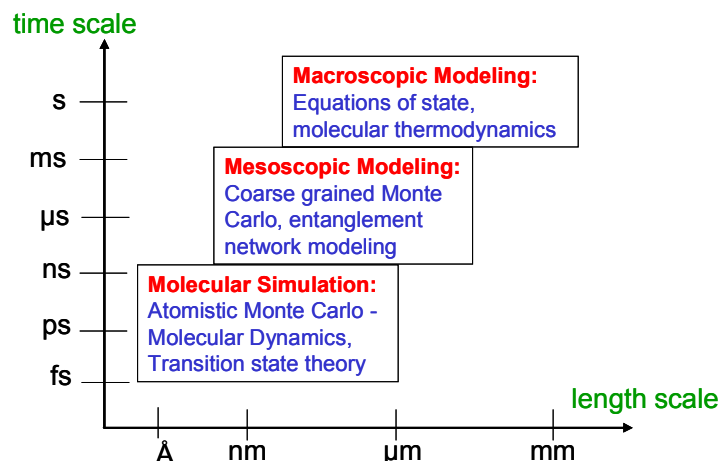
Contact

Dr. Nickolas Kakizis

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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, polymer and pharmaceutical 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 2009 focused on:

- (a) Molecular simulation of elastomeric and glassy polymers,
- (b) Sorption and diffusion of small molecules in silicon-containing polymers,
- (c) Molecular simulation of polar homo- and co-polymers,
- (d) Mesoscopic simulation of polydisperse colloids,
- (e) Thermodynamic properties of polar fluids in pure and in mixture,
- (f) Ionic liquids in pure and in mixture with supercritical carbon dioxide or water,
- (g) Development of a new EoS based on lattice theory for pharmaceutical solutions,
- (h) Development of a new molecular model for the prediction of solubility of pharmaceuticals in water and other solvents,
- (i) Prediction of solubility and diffusivity of CO, H₂ and H₂O in heavy hydrocarbons (new activity in 2009),
- (j) Modeling of properties of pure and mixtures of CO₂ (new activity in 2009).

The research services project on *Molecular Simulation and Thermodynamics of Fluids and Advanced Materials* co-ordinated by Dr. I. Economou was very successfully in fund raising from the European industry. In 2009, two new research contracts were signed for a total amount of € 687.352.

More information about MTMML can be found at: www.mtmml.gr.

Personnel

Researchers: Dr. Ioannis G. Economou, Researcher A', Laboratory Director

Research Scientist: Dr. Niki Vergadou

Collaborating Researcher: Dr. Nikolas Zacharopoulos (faculty under contract, University of the Aegean)

Post-doctoral scientists in projects:

Dr. Theodora Spyriouni (funded by industrial research contracts)

Dr. Georgios Lithoxoos (funded by industrial research contracts)

Dr. Zoi Makrodimitri (funded by industrial research contracts)

PhD students:

Eleni Androulaki (Demokritos PhD fellow)

Nikos Diamantonis (funded by EU project)

Visiting researchers:

Rasmus Lundsgaard (PhD student in Chemical Engineering, Technical University of Denmark)

Collaborating faculty:

Professor Doros N. Theodorou, School of Chemical Engineering, NTUA.

Publications in peer-reviewed journals

1. I. Tsivintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Solid - Liquid Equilibrium in Pharmaceutical - Solvent Mixtures: Systems with Complex Hydrogen Bonding Behavior", *AIChE J.*, **55**(3) 756 - 770 (2009).
2. I. Tsivintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents", *J. Phys. Chem. B*, **113**(18), 6446 - 6458 (2009).
3. G.E. Logotheti, J. Ramos, I.G. Economou, "Molecular Modeling of Imidazolium-Based [Tf₂N] Ionic Liquids: Microscopic Structure, Thermodynamic and Dynamic Properties and Segmental Dynamics", *J. Phys. Chem. B*, **113**(20), 7211 - 7224 (2009).
4. M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Phase Equilibrium of Colloidal Suspensions with Particle Size Dispersity: A Monte Carlo Study", *J. Chem. Phys.*, **130**(19), 194902-1 - 194902-10 (2009).
5. N.M. Garrido, A.J. Queimada, M. Jorge, E.A. Macedo and I.G. Economou, "1-Octanol / Water Partition Coefficients of n-Alkanes from Molecular Simulations of Absolute Solvation Free Energies", *J. Chem. Theory Comput.*, **5**(9), 2436 - 2446 (2009).
6. N.M. Garrido, M. Jorge, A.J. Queimada, I.G. Economou and E.A. Macedo, "Molecular Simulation of the Hydration Gibbs Energy of Barbiturates", *Fluid Phase Equilib.*, in press (2009).
7. P. Ahlström, K. Aim, R. Dohrn, J.R. Elliott, G. Jackson, J.-N. Jaubert, E.A. Macedo, J.-P. Pokki, K. Reczey, A. Victorov, L. Fele Žilnik, and I.G. Economou, "A Survey of the Role of Thermodynamics and Transport Properties in ChE University Education in Europe and the USA", *Chem. Eng. Ed.*, in press (2009).
8. M. Jorge, N.M. Garrido, A.J. Queimada, I.G. Economou and E.A. Macedo, "Effect of Integration Method on the Accuracy and Computational Efficiency of Free Energy Calculations Using Thermodynamic Integration", *J. Chem. Theory Comput.*, in press (2009).

9. I.G. Economou, N.M. Garrido and Z.A Makrodimitri, "Prediction of Microscopic Structure and Physical Properties of Complex Fluid Mixtures Based on Molecular Simulation", *Fluid Phase Equil.*, in press (2009).
10. N.M. Garrido, M. Jorge, A.J. Queimada, I.G. Economou and E.A. Macedo, "Molecular Simulation of Absolute Hydration Gibbs Energies of Polar Compounds", *Fluid Phase Equil.*, in press (2009).

Presentations in international conferences

1. I.A. Bitsanis, I.G. Economou and M. Yiannourakou, "Phase Equilibrium of Size-Dispersed Colloid Systems with Soft Pair Interactions: A Monte Carlo Study", *American Physical Society Meeting*, Session Z10, Pittsburgh, Pennsylvania, USA (2009).
2. X. Krokidis, T. Spyriouni and I.G. Economou, "Predictive Models for Thermodynamic Properties and Phase Equilibria of Complex Fluid Mixtures Based on Molecular Theory, Molecular Simulations and Equations of State", *ACHEMA 2009*, Frankfurt Am Main, Germany (2009).
3. Z.A. Makrodimitri and I.G. Economou, "Molecular Dynamics Simulation of Microscopic Structure and Physicochemical Properties of Elastomer Polymers", *7th Greek Chemical Engineering Conference*, Patras, Greece (2009).
4. I. Tsvintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents", *7th Greek Chemical Engineering Conference*, Patras, Greece (2009).
5. I.A. Bitsanis, A.N. Rissanou, M. Yiannourakou and I.G. Economou, "Simulations of Temperature Induced Ageing and Crystallization in Dense Suspensions of Ultrasoft Colloids", *7th Greek Chemical Engineering Conference*, Patras, Greece (2009).
6. M. Yiannourakou, I.G. Economou and I.A. Bitsanis, "Analysis of Structure and Dynamics of Polydisperse Colloidal Systems", *7th Greek Chemical Engineering Conference*, Patras, Greece (2009).
7. I.G. Economou, T. Spyriouni and X. Krokidis, "Thermodynamics of Pharmaceutical Mixtures: From Molecular Modeling to Equation of State Predictions with MAPS", *24th European Symposium on Applied Thermodynamics*, Santiago de Compostela, Spain (2009).
8. N.M. Garrido, M. Jorge, A.J. Queimada, I.G. Economou and E.A. Macedo, "Molecular Simulation of the Hydration Free Energies of Substituted Barbiturates", *24th European Symposium on Applied Thermodynamics*, Santiago de Compostela, Spain (2009).
9. N.M. Garrido, A.J. Queimada, M. Jorge, E.A. Macedo and I.G. Economou, "1-Octanol / Water Partition Coefficients Based on Molecular Simulation of Absolute Solvation Energies", *24th European Symposium on Applied Thermodynamics*, Santiago de Compostela, Spain (2009).
10. R. Lundsgaard, G.M. Kontogeorgis, I.G. Economou and N.M. Garrido, "Modeling of Partition Coefficients of Additives in Polymer / Polymer and Polymer / Solvent Systems by Free Energy Calculations", *24th European Symposium on Applied Thermodynamics*, Santiago de Compostela, Spain (2009).
11. I. Tsvintzelis, I.G. Economou and G.M. Kontogeorgis, "Modeling the Solubility of Pharmaceuticals in Liquid and Supercritical Pure and Mixed Solvents", *24th European Symposium on Applied Thermodynamics*, Santiago de Compostela, Spain (2009).
12. G.M. Kontogeorgis, I. Tsvintzelis and I.G. Economou, "Modeling Phase Equilibria of Pharmaceutical - Solvent Mixtures: Towards a Predictive Approach for Complex Hydrogen Bonding Systems", *Danish Colloid and Interface Symposium 2009*, Aarhus, Denmark (2009). Invited talk.
13. I.G. Economou, Z.A. Makrodimitri, G. Tsolou and V.G. Mavrantzas, "Molecular Simulation of Elastomer Polymers and Their Fluid Mixtures: Microscopic Structure and Physical Properties", *Thermodynamics 2009*, Imperial College London, United Kingdom (2009).
14. N.M. Garrido, A.J. Queimada, M. Jorge, E.A. Macedo and I.G. Economou, "Octanol - Water Partition Coefficients from Molecular Simulation of Solvation Free Energies", *Thermodynamics 2009*, Imperial College London, United Kingdom (2009).

15. G.M. Kontogeorgis, A. Tihic, G. Folas, I. Tsivintzelis, A. Grenner, N. von Solms, L. Constantinou, I.G. Economou and M.L. Michelsen, "Capabilities and Limitations of Association Theories", *Thermodynamics 2009*, Imperial College London, United Kingdom (2009).
16. I.G. Economou, "Prediction of Thermodynamic and Transport Properties of Complex Fluid Mixtures Based on Molecular Simulation", *VIII Ibero-American Conference on Phase Equilibria and Fluid Properties for Process Design EQUIFASE 2009*, Praia da Rocha, Algarve, Portugal (2009). Invited talk.
17. N.M. Garrido, A.J. Queimada, M. Jorge, I.G. Economou and E.A. Macedo, "Molecular Simulation of Absolute Free Energies of Polar Compounds", *VIII Ibero-American Conference on Phase Equilibria and Fluid Properties for Process Design EQUIFASE 2009*, Praia da Rocha, Algarve, Portugal (2009).
18. N.M. Garrido, A.J. Queimada, M. Jorge, E.A. Macedo and I.G. Economou, "Predicting the Hydration Free Energy of Psychotropic Drugs from Molecular Simulation", *VIII Ibero-American Conference on Phase Equilibria and Fluid Properties for Process Design EQUIFASE 2009*, Praia da Rocha, Algarve, Portugal (2009).

Invited lectures

1. Ioannis G. Economou, "From Computational Chemistry to the Design of Advanced Materials and Chemical Processes", Department of Chemistry, University of Athens, January 2009.
2. Ioannis G. Economou, "Calculation of Physical Properties for Chemical Product and Process Design from Molecular Simulation and Theory", Department of Chemical Engineering, United Arab Emirates University, Al Ain, United Arab Emirates, February 2009.
3. Ioannis G. Economou, "The Role of Molecular Simulation and Molecular Thermodynamics for Novel Process Design", The Petroleum Institute, Abu Dhabi, United Arab Emirates, June 2009.
4. Ioannis G. Economou, "Molecular Simulation of Macromolecular Systems: From Microscopic Structure to Macroscopic Physical Properties", Department of Macromolecular Physics, Instituto de Estructura de la Materia, Consejo Superior de Investigaciones Cientificas, Spain, July 2009.

Educational work

Teaching

A. Undergraduate courses

1. Ioannis G. Economou, "Physical Chemistry", 2nd year course in *Studies in Natural Sciences*, Open University of Greece,, 2008 - 09.
2. Nikolas Zacharopoulos, "Simulation", 7th Semester, Department of Product and Systems Design, University of the Aegean, 2008 - 2009.
3. Nikolas Zacharopoulos, "New Materials", 7th Semester, Department of Product and Systems Design, University of the Aegean, 2008 - 2009.
4. Nikolas Zacharopoulos, "Material Selection for Design", 9th Semester, Department of Product and Systems Design, University of the Aegean, 2008 - 2009.

B. Post-graduate courses

1. Ioannis G. Economou, "Environmental Management", MBA Program, Graduate School, American College of Greece, January - April 2009.
2. Ioannis G. Economou, "Technology and Innovation Management", MBA Program, Graduate School, American College of Greece, April - June 2009.

3. Nikolas Zacharopoulos, "Materials", 2nd Semester, Graduate program on *Design of functional and industrial products and systems*, Department of Product and Systems Design, University of the Aegean, 2008 - 2009.

PhD theses defended

1. Z. Makrodimitri, March 2009, "Molecular Dynamics Simulation of Microscopic Structure and Physical Chemical Properties of Elastomeric Polymers". Ph.D. granted from the Department of Chemistry, University of Athens, Greece.
2. M. Yiannourakou, April 2009, "Thermodynamic, Structural and Dynamic Properties of Soft Materials with Coarse Grained Simulations". Ph.D. granted from the School of Chemical Engineering, National Technical University of Athens, Greece.

Current External Funding

Basic Research Projects

1. "Development of Sustainable Industrial Processes: Experimental, Theoretical and Computational Investigation of Thermodynamic Properties and Phase Equilibria of Ionic Liquid Mixtures", *INTAS*. Project Director: Ioannis G. Economou. Total funding: 150,000 €. Funding for NCSR "Demokritos": 12,500 €. Duration: 1 / 9 / 2006 - 28 / 2 / 2009.
2. "Development of New Molecular Simulation Methods and Macroscopic Models for the Calculation of Microscopic Structure and Thermodynamic Properties of Complex Polymer Systems", *General Secretariat of Research and Technology, PENED 2003 Program*. Project Director: Ioannis G. Economou. Total funding: 57,660 €. Duration: 1 / 12 / 2005 - 30 / 6 / 2009.
3. "Quantitative Failure Consequence Hazard Assessment for Next Generation CO₂ Pipelines: The Missing Link", *European Commission 7th Framework Programme: Energy*. Project Director: Ioannis G. Economou. Funding for NCSR "Demokritos": 307,476 €. Duration: 1 / 12 / 2009 - 30 / 11 / 2012.

Applied Research Projects

1. "Implementation of Computer Codes for Physical Properties of Polymer and Non-Polymer Systems into MAPS - Phase II", *Contract Research Services, Scienomics SARL, Paris, France*. Project Director: Ioannis G. Economou. Total funding: 18,200 €. Duration: 1 / 9 / 2008 - 28 / 2 / 2009.
2. "Molecular Simulation of Diffusion of Hydrogen, Carbon Monoxide and Water in Heavy *n*-Alkanes at High Temperatures and Pressures", *Contract Research Services, Shell Global Solutions, Amsterdam, The Netherlands*. Project Director: Ioannis G. Economou. Total funding: 15,000 €. Duration: 15 / 12 / 2008 - 15 / 4 / 2009.
3. "Molecular Simulation of Diffusion and Solubility of Hydrogen, Carbon Monoxide and Water in Heavy *n*-Alkanes - Phase II", *Contract Research Services, Shell Global Solutions, Amsterdam, The Netherlands*. Project Director: Ioannis G. Economou. Total funding: 52,000 €. Duration: 15 / 6 / 2009 - 14 / 6 / 2010.
4. "Quantitative Materials Informatics Systems for Virtual High-Throughput Screening for Industrial R & D Applications", *Contract Research Services, Scienomics SARL and OSEO, Paris, France*. Project Director: Ioannis G. Economou. Funding for NCSR "Demokritos": 635,352 €. Duration: 1 / 3 / 2009 - 31 / 12 / 2011.

Current Collaborations

1. Professor Georgios Kontogeorgis, Department of Chemical Engineering, Technical University of Denmark. Development of thermodynamic models for pharmaceuticals.
2. Dr. Xenophon Krokidis, Scienomics SARL, France. Development of scientific software for prediction of material properties and design of chemical processes.
3. Professor Sofia Lampropoulou, School of Applied Mathematics and Physical Sciences, National Technical University of Athens, Statistical Mechanics Theory
4. Professor Maria Eugénia Rebello de A. Macedo, Department of Chemical Engineering, University of Porto, Portugal. Molecular simulation of the solubility of pharmaceuticals in water.
5. Professor Vlasis Mavrantzas, Department of Chemical Engineering, University of Patras. Molecular simulation of polymers.
6. Dr. Ioannis Bitsanis, Institute of Electronic Structure and Laser, Foundation of Research and Technology, Hellas, Heraklion, Crete, Greece. Mesoscopic simulation of colloids and polymers.
7. Professor Costas Panayiotou. Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece. Development of a lattice equation of state for non-ideal fluids.
8. Professor Cor Peters, Department of Chemical Engineering, Delft University of Technology, The Netherlands. Modeling thermodynamic properties of ionic liquids.
9. Dr. J. Ramos-Díaz, Department of Macromolecular Physics, Instituto de Estructura de la Materia - CSIC, Madrid, Spain. Quantum-mechanics calculations for ionic liquids.

Other activities

Ioannis Economou

1. Visiting Professor, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby, Denmark.
2. Visiting Professor, American College of Greece, Graduate School, Aghia Paraskevi Attikis.
3. Adjunct Professor, Open University of Greece.
4. Chairman, Working Group on Thermodynamics and Transport Properties, *European Federation of Chemical Engineering*.
5. Member of the Editorial Board, *Scientific Bulletin of University Politehnica of Bucharest, Series B: Chemistry and Materials Science*.
6. Referee for the following international scientific journals: *AIChE Journal*, *Canadian Journal of Chemical Engineering*, *Chemical Engineering Research and Design*, *Chemical Physics Letters*, *Colloid and Polymer Science*, *Computers in Chemical Engineering*, *Energy & Fuels*, *Environmental Science and Technology*, *European Polymer Journal*, *Fluid Phase Equilibria*, *Industrial and Engineering Chemistry Research*, *International Journal of Refrigeration*, *Journal of the American Chemical Society*, *Journal of Chemical and Engineering Data*, *Journal of Chemical Physics*, *Journal of Computational Chemistry*, *Journal of Physical Chemistry*, *Macromolecular Rapid Communications*, *Macromolecules*, *Polymer*, *Theoretical Chemistry Accounts*.
7. Consultant, Scienomics SARL, Paris, France.

Nikolas Zacharopoulos

Non-tenure teacher 407/80, Department of Product and Systems Design, University of the Aegean.
10.

Contact

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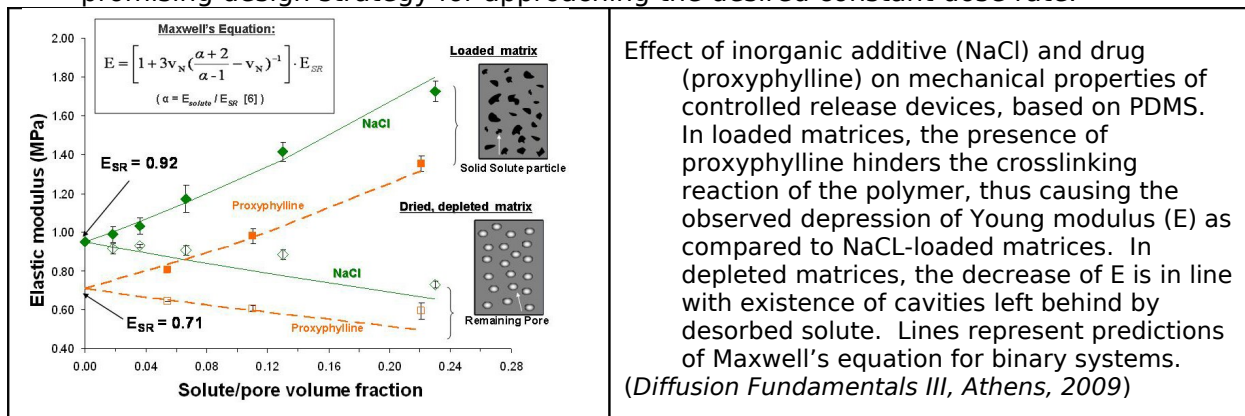
TRANSPORT PHENOMENA IN POLYMERS

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). 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 multilaminar devices which constitute a promising design strategy for approaching the desired constant dose rate.



Effect of inorganic additive (NaCl) and drug (proxyphylline) on mechanical properties of controlled release devices, based on PDMS. In loaded matrices, the presence of proxyphylline hinders the crosslinking reaction of the polymer, thus causing the observed depression of Young modulus (E) as compared to NaCl-loaded matrices. In depleted matrices, the decrease of E is in line with existence of cavities left behind by desorbed solute. Lines represent predictions of Maxwell's equation for binary systems. (Diffusion Fundamentals III, Athens, 2009)

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

Sorption kinetics in glassy polymers 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 develops 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. Combination of various optical 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 evaluate the swelling behaviour polymeric materials in the form of thin supported films upon exposure to different vapour environments, for subsequent use as the sensing layer of chemocapacitive chemical sensors. The activity aims at the development of sensor

arrays for specific applications concerning the detection of analytes in complex vapor environments.

Publications 2008

1. Papadokostaki, K.G.; Sanopoulou, M.; Petropoulos, J.H. "An advanced model for composite planar three-layer matrix-controlled release devices. Part II. Devices of non-uniform material properties and a practical example" *J. Membrane Sci.* **2009**, 343, 128-136
2. Soulas, D.; Sanopoulou, M.; Papadokostaki, K.G., "A comparative study on the release kinetics of osmotically active solutes from hydrophobic elastomeric matrices, combined with the characterization of the depleted matrices", *J. Appl. Polymer Sci.* **2009**, 113, 936-949
3. Papadokostaki, K.G. "Experimental realization of sustained simple kinetic regimes of release of particulate solutes subject to slow dissolution in the containing matrix" *J. Membrane Sci.* **2009**, 326, 503-506
4. Papadokostaki, K.G.; Savidou, A., "Study of leaching mechanisms of caesium ions incorporated in Ordinary Portland Cement", *J. Hazardous Materials* **2009**, 171, 1024-1031.
5. Vlachopoulou, M.E.; Tserepi, A.; Pavli, P.; Argitis, P.; Sanopoulou, M.; Misiakos, K. "A low temperature surface modification assisted method for bonding plastic" *J. Micromech. and Microeng.* **2009**, 19, 015007
6. Oikonomou, P.; Manoli, K.; Goustouridis, D.; Raptis, I.; Sanopoulou, M. "Polymer/BaTiO₃ nanocomposites based chemocapacitive sensors", *Microelectronic Eng.*, **2009**, 86, 1286-1288.
7. Manoli, K.; Goustouridis, D.; Oikonomou, P.; [Chatzandroulis, S.](#); Raptis, I.; Sanopoulou, M. "Capacitive sensor arrays with controllable deposition of the sensing polymer area for VOCs applications: Design and measurement considerations", *Procedia Chemistry* **2009**, 1, 176-179
8. K. Manoli, D. Goustouridis, I. Raptis, E. Valamontes, M. Sanopoulou "Vapor- induced swelling of supported methacrylic and siloxane polymer films: Determination of interaction parameters" *J. Appl. Polym. Sci.*, 2009, in press

Conferences

1. Petropoulos, J. H.; Sanopoulou, M.; Papadokostaki, K. G. "Beyond Fick: How best to deal with non-Fickian behavior in a Fickian spirit" Diffusion Fundamentals III, August 23-28, 2009, Athens, Greece, Proceedings pp.103-123 (invited lecture).
2. Stamatialis, D. F.; Soulas, D. N.; Sanopoulou, M. "Mechanisms of non-Fickian micromolecular diffusion in glassy polymer films: Analysis of experimental sorption and concurrent dilation kinetics in the light of a Differential Swelling Stress model", Diffusion Fundamentals III, August 23-28, 2009, Athens, Greece, Proceedings pp.132-133.
3. Soulas, D. N.; Papadokostaki, K.G. "Experimental investigation of the release mechanism of hydrophilic solutes from hydrophobic matrices" Diffusion Fundamentals III, August 23-28, 2009, Athens, Greece, Proceedings pp.130-131
4. Oikonomou P., Goustouridis D., Raptis I., Manoli K., Sanopoulou M. "Must fermentation progress monitoring by polymer coated capacitive vapour sensor arrays", IEEE Sensors 2009, October 25-28, 2009, Christchurch, Canterbury, New Zealand, Proceedings pp.1443-1446
5. Manoli, K.; D. Goustouridis, P. Oikonomou, S. Chatzandroulis, M. Sanopoulou, I. Raptis, "Capacitive sensor arrays with controllable deposition of the sensing polymer area for VOCs applications: Design and measurement considerations" Eurosensors 2009, September 6-9, Lausanne, Switzerland
6. Oikonomou, P.; K. Manoli, D. Goustouridis, I. Raptis, M. Sanopoulou, "In Situ monitoring of Must Fermentation by Polymer-coated Interdigitated Sensor Arrays",

6th International Conference on Instrumental Methods of Analysis : Modern Trends and Applications (IMA 2009) October 4-8, Athens

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, Dissolution tester equipped with fraction collector and UV-Vis spectrophotometer (Jasco).

Personnel

M. Sanopoulou: research director/group leader, K. Papadokostaki: principal researcher (permanent staff); J.H. Petropoulos (emeritus researcher); D. Soulas (post-doctoral collaborating researcher); A. Hasimi, K. Manoli , M. Konidari, Athanasia Panou (4 PhD students).

Collaborations

Dr. I. Raptis, (NCSR "D", Inst. Of Microelectronics, chemical sensors); Dr. P. Argitis (NCSR "D" Inst. of Microelectronics, DSC)

Contact

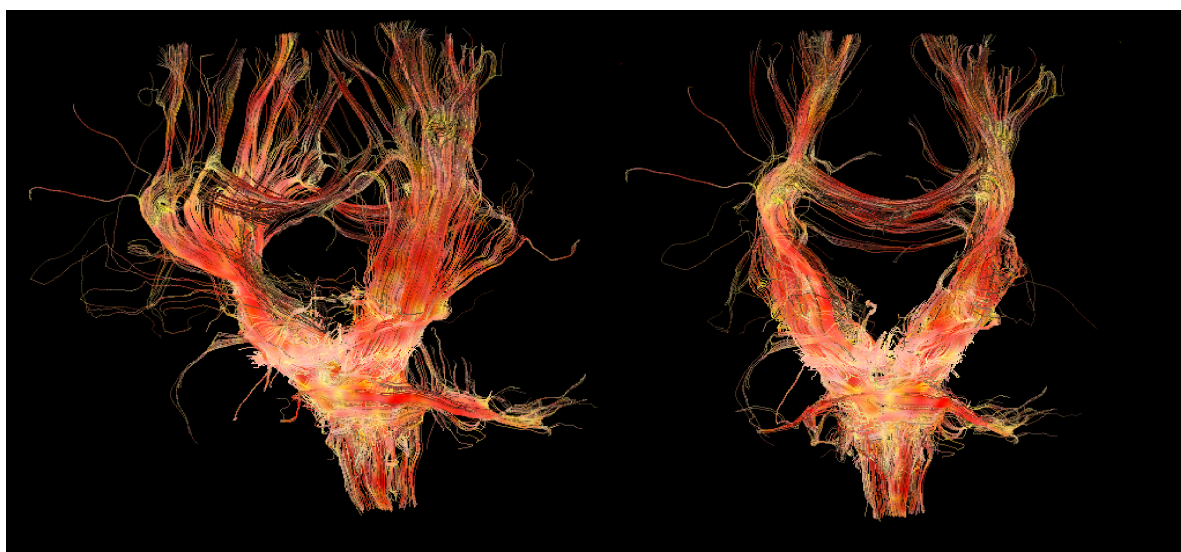
Dr. M. Sanopoulou (sanopoul@chem.demokritos.gr, Tel. +30 210 6503785, +30 210 6503661; fax. +30 210 6511766)

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.



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 2009

1. Kouvaris, N.; and Provata, A.; "Synchronization, stickiness effects and intermittent oscillations in coupled nonlinear stochastic networks", Eur. Phys. J. B, **2009**, 70, 535-541.
2. Kouvaris N.; Provata A.; Kugiumtzis D.; "Detecting synchronization in coupled stochastic ecosystem networks", Physics Letters A, **2009**, doi:10.1016/j.physleta.2009.11.047.
3. Katsaloulis, P.; Theoharis, Th.; Provata, A.; "Long range clustering of oligonucleotides containing the GC signal" J. Theor. Bio., **2009**, 258 (1): 18-26.
4. Katsaloulis, P.; Verganelakis, D.; Provata, A.; "Fractal Dimension and Lacunarity of Tractography Images of the Human Brain", Fractals, **2009**, 17 (2): 181-189 .
5. Oikonomou Th.; Tirnakli U.; "Generalized entropic structures and non-generality of Jaynes' Formalism", Chaos, Solitons and Fractals, **2009** 42 3027-3034
6. Oikonomou Th.; Bagci G.B.; "A note on the definition of deformed exponential and logarithm functions", JOURNAL OF MATHEMATICAL PHYSICS **2009** 50 103301(1-9)
- 7.** Provata A.; and Katsaloulis P.; "A note on the definition of deformed exponential and logarithm functions", Physical Review E, 2010 (accepted).

Conferences

1. Kouvaris N.; Provata A.; Kugiumtzis D.; "Synchronization in nonlinear coupled stochastic networks", poster at the 22th International Conference on "Non Linear Science and Complexity", Pescara, 2009.
2. Kouvaris N.; Provata A.; Kugiumtzis D.; "Detecting synchronization in coupled stochastic ecosystem networks", poster at International workshop on "Collective dynamics and pattern formation in active matter systems", Berlin, 2009.
3. Katsaloulis, P.; Verganelakis, D. A.; "2-D and 3-D Fractal Analysis of Diffusion Tensor Images of the Human Brain", 4th Conference of the Hellenic Society for Computational Biology, 18-20 December 2009, NHRF, Athens , Greece.

4. Provata A . ; Synchronization due to long distance coupling in stochastic, reactive networksh, Internatinal Conference on Nonlinear Science and Complexity, Pescara, Italy, 30 July 2009.
5. Oikonomou Th.; “On the definition of deformed In-exp-functions”, XXXII Encontro Nacional de Fisica da Materia Condensada, Águas de Lindoia, Brasil, 11/05-15/05 2009.
6. Provata; “Pattern Formation in Chemistry and Biology”, 22nd International Summer School - Conference on Nonlinear Science and Complexity, Patras, Greece, 21 July 2009.

Funded Projects

1. The research grant which funds the PhD degree of Nikos Kouvaris is provided by the grant “Sonderforschungsbereich 555” (sfb555), which is given by the German Science Foundation, **01/09/2009 - 30/06/2010**.
2. “Molecular Simulations in Biosystems and Material Science (SimBioMa)”, ESF Research Networking Programme, 05/2006-05/2011.

Infrastructure

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

Personnel

A. Provata: research director/group leader (permanent researcher); P. Katsaloulis: (post doctoral fellow, NCSR “Demokritos”); V. Nousiou (postdoctoral fellow until 08/2009), Dr, Thomas Oikonomou (postdoctoral fellow, from 6/2009), N. Kouvaris: (PhD student, NCSR “D” fellows), Prof. George Tsironis (visiting scholar).

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 V. Havredaki 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. U. Tirnakli, (Ege University, “Entropic Forms”), Prof. I. Sokolov and Prof. L. Schimansky-Geier (humbolt Universitaet Berlin, Dept. of Physics, “Reactive Dynamics with Diffusion on Low Dimensional Supports and “Sthochastic dynamics of excitable systems - Neuronal Networks”); Prof. Christian Beck (Queen Mary College, University of London, “Complex Pattern Formation - Superposition of Statistics).

Contact

Dr. A. Provata (aprovata@chem.demokritos.gr, Tel. +30 210 6503964, Fax. +30 210 6511766)

Web site: <http://limnos.chem.demokritos.gr/>

Service Laboratories

SERVICE LABORATORY “ENVIRONMENTAL ANALYSIS”

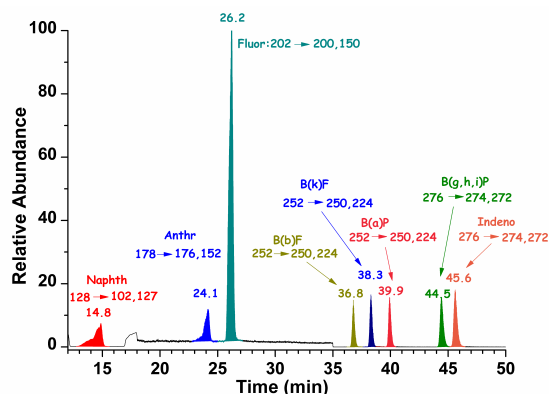
Objectives/Activities

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 (2005-2009) 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. The Environmental Analysis Laboratory has been accredited by ESYD (N. of Accreditation 580) on 17/7/2009.

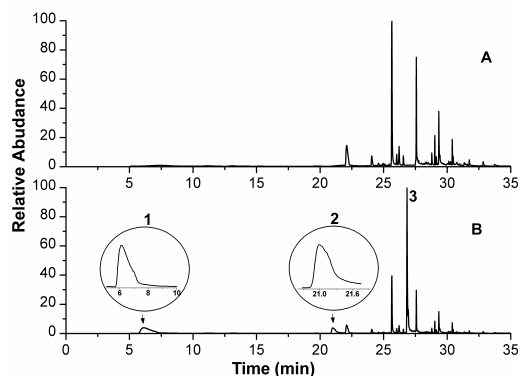


Current interests of our Laboratory are focused into the following:

- 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 cyanotoxins 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.



LC-MS/MS SRM chromatograms of a standard solution of the eight PAHs ($100 \mu\text{g L}^{-1}$ for the six target compounds and $1000 \mu\text{g L}^{-1}$ for Naphth, Fluor).



Selective GC/MS ion chromatograms (A) of a blank honey sample and (B) of a spiked honey sample at the concentration of $25 \mu\text{g kg}^{-1}$ for *p*-DCB (2), naphthalene (3) and at $250 \mu\text{g kg}^{-1}$ for 1,2-DBE (1) K. Tsimeli et al., *Analytica Chimica Acta*, 617 (2008) 64-71

Personnel

A. Hiskia: director (permanent researcher); T. Triantis: (quality manager); A. Tsimeli (analyst), S. Zervou, I. Dimitrakopoulos, T. Kaloudis: (adjunct scientist).

Funded Projects

1. "Development of analytical infrastructure of the Environmental Analysis Laboratory, EKEFE Demokritos", Antagonistiotita (Ministry of Development), Coordinator Dr. A. Hiskia, 311,3 K€, 2006-2008.
2. «Chemical analysis of air filters for the determination of Benzo(a)pyrene», in the frame of services to PLINIOS SA, 7,31 K€.
3. "Chemical analysis of soil and water samples for the determination of Polycyclic Aromatic Hydrocarbons (PAHs)", in the frame of services to PREFECTURE of DRAMA, 3,0 K€.
4. "Chemical analysis of air filters, wood and building materials for the determination of PCBs, PAHs, pentachlorophenol, hydroquinone and benzoquinone", in the frame of services to PLINIOS SA, 2,7 K€.
5. "Determination of odor-causing compounds in water" Research project funded by EYDAP SA, 20 K€, 2008-2009.

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

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

Εργαστήριο Παροχής Υπηρεσιών «Ραδιοχρονολογήσεις, Ισοτοπικές Αναλύσεις και Μετρήσεις Ραδονίου»

Προσωπικό

Υπεύθυνος Έργου: Δρ.Ν.Ζουριδάκης

Μέλη: Ε.Αρνίδη, Πτυχιούχος ΤΕΙ, σύμβαση έργου

Αντικείμενο

Ισοτοπική Υδρολογία είναι ο διεπιστημονικός κλάδος που ασχολείται με τη ανίχνευση των σταθερών και ραδιενεργών ισοτόπων (^{18}O , ^2H , ^{15}N , ^{13}C , ^3H , ^{14}C , ^{222}Rn κ.ά.) στον κύκλο του νερού στη φύση. Οι συγκεκριμένες αναλύσεις μπορούν να δώσουν απαντήσεις σε σημαντικά ζητήματα που αφορούν την εφαρμοσμένη έρευνα για την αξιοποίηση και την ορθολογική διαχείριση του υδάτινου δυναμικού όπως:

- Εκτίμηση του υψόμετρου τροφοδοσίας των υπόγειων υδροφόρων οριζόντων
- Ταχύτητα ροής και χρόνος παραμονής του νερού στο υπέδαφος.
- Ποσοστό ανάμειξης διαφορετικών υδροφόρων οριζόντων καθώς και της ανάμειξης επιφανειακών και υπόγειων νερών.
- Προσδιορισμός της προέλευσης της ρύπανσης των επιφανειακών και υπόγειων νερών από διάφορες ρυπογόνες εστίες (πχ. Νιτρορύπανση από αγροτικές και αστικές δραστηριότητες).
- Προσδιορισμός της ενθαλπίας των γεωθερμικών πεδίων.
- Εκτίμηση του δυναμικού των υπόγειων αποθεμάτων νερού.
- Επίδραση των κλιματικών αλλαγών στα υδατικά συστήματα.
- Μελέτη της υφαλμύρωσης των παράκτιων πηγών.
- Προσδιορισμός της βασικής ροής σε υδρογεωλογικές λεκάνες.
- κ.α.

Πέραν των εφαρμογών στην Υδρολογία και Υδρογεωλογία ο εξοπλισμός του Εργαστηρίου μπορεί να αξιοποιηθεί και σε άλλα πεδία έρευνας όπως:

- Προσδιορισμός της ηλικίας κάθε μορφής δειγμάτων για την αρχαιολογική έρευνα και την έρευνα του παλαιοπεριβάλλοντος.
- Μελέτες παλαιοδίαιτας.
- Έρευνα των μεταβολών της στάθμης της θάλασσας στο παρελθόν.
- Παλαιοκλιματολογικές έρευνες.
- Προσδιορισμό της συγκέντρωσης του ραδιενεργού ραδονίου σε εσωτερικούς χώρους και στα συστήματα ύδρευσης.
- Καθοριστική ανίχνευση της νοθείας των αλκοολούχων ποτών.
- Προσδιορισμό του ποσοστού προέλευσης του εκλυόμενου διοξειδίου του άνθρακα από την καύση των πετρελαιοειδών (αυτοκίνητα, κεντρική θέρμανση, βιομηχανία) στις αστικές περιοχές.
- Μελέτες της ραδιενέργειας της ατμόσφαιρας εξαιτίας των πυρηνικών δοκιμών την δεκαετία του '60.
- κ.α.

Έσοδα-Έξοδα 2009

Υπόλοιπο από προηγούμενα έτη	16.402,26 €
Ετήσια έσοδα Εργαστηρίου (από άλλα έργα)	14.400 €
Ετήσια έξοδα Εργαστηρίου	26.277,26 €

Το Εργαστήριο Ισοτοπικής Υδρολογίας υλοποιεί Συμβάσεις Έργου Παροχής Υπηρεσιών με το ΙΓΜΕ ύψους 110.000 ευρώ κατά τα έτη 2006, 2007, 2008.

Κοστολόγιο Ισοτοπικών Αναλύσεων

Οι τιμές για παροχή υπηρεσιών χωρίς Φ.Π.Α. των αναλύσεων δειγμάτων που πραγματοποιούνται στο εργαστήριο είναι οι παρακάτω:

Ραδιοχρονολογήσεις κάρβουνου, ξύλου, τύρφης	250 ευρώ
Ραδιοχρονολογήσεις κοχυλιών, χόρτων, CaCO ₃	280 ευρώ
Ραδιοχρονολογήσεις ασβεστοκονιαμάτων	350 ευρώ
Ραδιοχρονολογήσεις οστών	500 ευρώ
Ραδιοχρονολογήσεις νερού	600 ευρώ
Ισοτοπικές αναλύσεις ¹⁸ O σε δείγματα νερών	80 ευρώ
Ισοτοπικές αναλύσεις D σε δείγματα νερών	100 ευρώ
Προσδιορισμός συγκέντρωσης Ραδονίου στα νερά	60 ευρώ
Προσδιορισμός συγκέντρωσης Ραδονίου σε κλειστούς χώρους	80 ευρώ
Προσδιορισμός συγκέντρωσης Τριτίου σε δείγματα νερών	150 ευρώ
Ισοτοπικές αναλύσεις ¹⁸ O σε στερεά δείγματα	100 ευρώ

INTITUTE INSTRUMENTATION AND SERVICES

The following Research facilities provide support for the research projects in IPC and also offer services to other research Laboratories or industry.

- **NMR Laboratory**

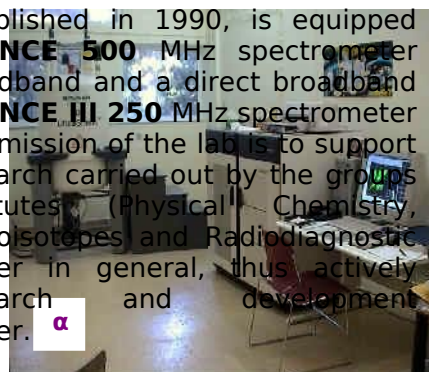
[nmrlab@chem.demokritos.gr](mailto:nmr@chem.demokritos.gr) ; <http://ipc.chem.demokritos.gr/Projects/nmr/nmr.html>

Responsible Scientists : *Dr. K. Yannakopoulou (IPC), Dr. M. Pelecanou (IB) , Dr. L. Leondiadis (RRP); Special Technical Scientist: Dr. A. Panagiotopoulou*

The laboratory, with a Bruker with an indirect probe and a Bruker with a dual probe. high quality of the participating Biology, Products) and the participating in the activities of the

A portion of providing service academic the industry.

established in 1990, is equipped **AVANCE 500** MHz spectrometer broadband and a direct broadband **AVANCE III 250** MHz spectrometer. The mission of the lab is to support research carried out by the groups institutes (Physical Chemistry, Radioisotopes) and Radiodiagnostic center in general, thus actively research and development center. α



spectrometer time is devoted to requested mainly from other institutions and occasionally from



a. AVANCE 500 MHz b. AVANCE III 250 MHz

- **Macromolecular Crystallography Lab (X-RAY)**

(<http://ipc.chem.demokritos.gr/raxis/index.html>)

Scientists in charge: Drs. Irene M. Mavridis, Metaxia Vlasi, George Nounesis

The laboratory was established in 1998, after the creation of the "Network of Macromolecular Crystallography" by 10 academic laboratories in the Athens area. It is equipped with a Rotating anode (Rigaku) generator, Image Plate Raxis IV (Molecular Structure corporation), Low Temperature apparatus (Oxford Cryosystems) an offer by the Hellenic Pasteur Institute, computing and molecular graphics facilities, Circular Dichroism spectrometer (Jasco J-715). The mission of the lab is to support research carried out by the participating laboratories of the network (three of which are institutes in NCSR Demokritos: Physical Chemistry, Biology, Radioisotopes and Radiodiagnostic Products) by providing macromolecular data collection facilities and studies by Circular Dichroism. Thus the laboratory actively helps structural biology research in Greece. The laboratory is also equipped with a 4-circle diffractometer, mainly for use of the Institute of Physical Chemistry.

- **Elemental Analyzer** (elyan@chem.demokritos.gr) Scientist in charge: E. Yannakopoulou

The laboratory was established in the 90s. It is equipped with a Perkin-Elmer 2400 (C,H,N) Elemental Analyzer, which performs a fast and accurate analysis of elements C,H,N. The method is based on the combustion of the sample in an oxygen atmosphere at 925°C. The Elemental Analyzer provides services to all institutes of NCSR "Demokritos", as well as to other research and academic institutions and private section.

- **AFM** (asap@chem.demokritos.gr) Scientist in charge:A. Sapalidis

The laboratory, established in the 90s, is equipped with the MultiMode scanning probe Nanoscope III microscope from Digital Instruments. NanoScope III controller is capable of scanning the maximum scan size (16x16 μm) as low as few nanometers with full 16-bit resolution on all scan waveforms and on each axis. This versatile, high-resolution metrology and imaging tool performs a complete range of AFM techniques for surface characterization of properties like topography, elasticity, friction, adhesion, and electrical/magnetic fields.

The mission of the lab is to support high quality research carried out by the groups of the Physical Chemistry Institute together as well as the other institutes in 'Demokritos'. A portion of microscope's time is devoted to providing service requested mainly from other academic institutions and occasionally from the private sector

- **FT-IR** (fkats@chem.demokritos.gr) Scientist in charge: Dr. F. Katsaros

The laboratory is equipped with a Thermo Scientific Nicolet 6700 FTIR spectrometer with N₂ purging system. In addition a single reflection ATR (Attenuated Total Reflection) SmartOrbit accessory, equipped with a single-bounce diamond crystal can be used. This accessory offers many advantages, including the ability to analyze hard, abrasive, or caustic materials, without any sample preparation. The spectrometer supports the research activities carried out by many groups of NCSR Demokritos. It also provides services to academic and industrial users.

- **Thermal analysis lab** (kpapadok@chem.demokritos.gr) Scientist in charge: Dr. K. Papadokostaki

The laboratory, established in 2003, is equipped with a **TA Instruments** 2920 Temperature Modulated Differential Scanning Calorimeter (**MDSC**). MDSC offers all the benefits of standard DSC and provides further information for greater understanding of material properties, because it can separate overlapping events that are difficult or impossible to do by standard DSC. The lab supports research carried out by the Institute of Physical Chemistry and Demokritos Centre in general, related to thermal characterization of polymers and other materials used in various scientific and technological areas. It also provides service to industry.

- **Micro Raman** (likodimo@chem.demokritos.gr) Scientist in charge: Dr. P. Falaras, Dr. A. Kontos, Dr. V. Likodimos

The laboratory, established in 2007, is equipped with a Renishaw inVia Reflex micro-Raman microscope utilizing an Ar⁺ ion laser (λ=514.5 nm) and a high power near infrared (NIR) diode laser (λ=785 nm) as excitation sources. The spectrometer is equipped with 1800 and 1200 lines/mm diffraction gratings together with holographic notch and

dielectric edge Rayleigh rejection filters and a high sensitivity deep depletion CCD detector. Raman spectra can be continuously acquired over an extended spectral range of 100-3500 cm^{-1} in a single scan (SynchroScan mode), while measurements down to 10 cm^{-1} from the laser line, can be performed by the use of the near excitation tunable filter (NEXT). Confocal Raman measurements are implemented by varying the spectrograph entrance slit and CCD area, while the laser line can be focused on the sample surface using the $\times 5$, $\times 20$, $\times 50$ and $\times 100$ objectives on a Leica DMLM microscope at variable laser power. Polarization measurements can also be performed.

The mission of the lab is to support high quality research on the vibrational properties of materials and the characterization of devices carried out in the Institute of Physical Chemistry and NCSR, in general. A portion of spectrometer time is devoted to providing service requested from other academic institutions as well as the private sector.

Education Activities

Graduate Studies at the Institute of Physical Chemistry

Responsible: Dr K.L. Stefanopoulos

Deputy: Dr G. Romanos

The training of young scientists (PhD or Master's candidates, post-doctoral fellows) is one of the most important activities of the Institute of Physical Chemistry.

High quality research activities constitute the core of the graduate studies offered. It is supplemented by advanced courses, offered either by NCSR "Demokritos" or by collaborating Universities, as well as lectures by invited speakers from Greece and abroad.

Since the Institute is not entitled by law to operate an independent graduate school, all graduate students are enrolled in university graduate programmes. Indeed, the Institute is actively participating in several such programmes that are financially supported by the Greek Ministry of Education (EPEAEK).

The majority of the graduate students working at the Institute receive financial support either by NCSR "Demokritos" (scholarship) or through their participation in research programmes (national, european or international). Thus, out of about fifty (50) graduate students that perform research at the Institute, seventeen (17) are financially supported by NCSR "Demokritos".

Finally, during 2009, eleven (11) PhD and four (4) Master's degrees were awarded to graduate students of the Institute.

Ph.D dissertations

1. E.K. Efthimiadou, "*Synthesis and Characterization of Coordination Compounds for Medical and Pharmaceutical Applications*", School of Chemical Engineering, National Technical University of Athens
2. G. Kantonis, "*Development and Improvement of Dye-Sensitized Solar Cells of Nanocrystallized Titania*", School of Chemical Engineering, National Technical University of Athens
3. A.I. Kontos, "*Development of Photocatalytic and Super-Hydrophilic materials based on Titanium Dioxide*", School of Chemical Engineering, National Technical University of Athens
4. P. Kormali, "*Photocatalytic Degradation of Organic Pollutants in the presence of $H_3PW_{12}O_{40}$ and TiO_2 . Comparison of the Photooxidation Mechanisms*", School of Chemical Engineering, National Technical University of Athens
5. L.E.P. Kyllönen, "*Supramolecular Wires Based on Cyclodextrins: Synthesis of Surface Active Hosts and Metallo Guests, Host-Guest Binding and Surface Identification of the Assemblies*", School of Chemistry, The University of Birmingham
6. A.I. Labropoulos, "*Development of Nanostructured Carbon and Silicon Composite Membranes for Separation of Gas Mixtures and Study of Carbon Nanostructures for Hydrogen Storage*", Department of Chemistry, University of Athens
7. M. Lambropoulou, "*Synthesis, structural characterization and properties of specific modified cyclodextrins. Studies of molecular inclusion of antimicrobial and other drugs*", Department of Science, Agricultural University of Athens
8. Z.A. Makrodimitri, "*Molecular Dynamic Simulation of Microscopic Structure and Physicochemical Properties of Elastomeric Polymers*", Department of Chemistry, University of Athens
9. E. Rozi, "*Development of Electrolytes for Organic Solar Cells*", School of Chemical Engineering, National Technical University of Athens

10. E.C. Vermisoglou, *"Synthesis and Chemical Modification of Carbon Nanostructures Aiming at the Optimization of their Gas and Vapour Storage Properties"*, Department of Chemistry, University of Athens
11. M. Yiannourakou, *"Thermodynamic, Structural and Dynamic Properties of Soft Materials Using Coarse-Grained Simulations"*, School of Chemical Engineering, National Technical University of Athens

Master's dissertations

1. G. Alexakos, *"Photocatalytic Synthesis and Characterization of Selenium Nanoparticles in Aqueous Solution"*, Department of Chemistry, University of Athens
2. E. Chatzidaki, *"Study of polyaniline/polymide blend membranes"*, Department of Chemistry, University of Athens
3. K. Fotiadou, *"Study of interactions between positively and negatively charged cyclodextrins in polar solutions by NMR spectroscopy and Isothermal Titration Calorimetry"*, Department of Chemistry, University of Athens
4. M. Konidari, *"Effect of functionalized and pristine single-wall carbon nanotubes on the properties of poly(vinyl alcohol)"*, Department of Chemistry, University of Athens