NATIONAL CENTER FOR SCIENTIFIC RESEARCH “DEMOKRITOS”

INSTITUTE OF PHYSICAL CHEMISTRY

DIRECTOR

Falaras Polycarpos

DEPUTY DIRECTOR

Provata Astero

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

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

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

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

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

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

March 2008

Dr. Polycarpos FALARAS, Director
Institute of Physical Chemistry

Director
Polycarpos Falaras

Deputy Director
Astero Provata

Scientific Advisory Board
President: Theodoros Steriotis

Education Committee

Scientific Units

Service Laboratories

MOLECULAR & SUPRAMOLECULAR
NANOFUNCTIONAL MATERIALS

Structural and Supramolecular chemistry
Nanomaterials of Organized Supramolecular Structure
Molecular Thermodynamics and Modeling of Materials
Luminescence Laboratory - Development Of Novel Functionalized Materials for Analytical and Biomedical Applications
Transport Phenomena in Polymers
Statistical Mechanics and Non-Linear Dynamics Laboratory
Molecular Computational Chemistry

NANOQUICKER, ENVIRONMENTAL FRIENDLY
TECHNOLOGIES - ENERGY

Materials & Membranes for Environmental Separations
Catalytic-Photocatalytic Processes (Solar Energy-Environment)
Electronic Spectroscopy Laboratory Application to Supramolecules and Nanostructures
Isotope Hydrology

CHEMICAL BIOLOGY

Natural Products Synthesis and Bioorganic Chemistry
Chemical Biology of Natural Products and Designed Molecules

“Environmental Analysis” Laboratory

NMR, X-Ray, Elementary Analysis, AFM, FT-IR, I.M.S.
Scientific Activities

Personel

Scientific Programms

1st Scientific Programme: Molecular & Supramolecular Nanofunctional Materials

1. Structural and Supramolecular Chemistry
2. Nanomaterials of Organized Supramolecular Structure
3. Molecular Thermodynamics and Modeling Of Materials
4. Luminescence Laboratory – Development Of Novel Functionalized Materials for Analytical and Bioanalytical Applications
5. Transport Phenomena In Polymers
6. Statistical Mechanics and Non-Linear Dynamics Laboratory
7. Molecular Computational Chemistry

2nd Scientific Programme: Nanochemistry, Environmental Friendly Technologies – Energy

1. Materials & Membranes for Environmental Separations Laboratory
3. Catalytic-Photocatalytic Processes (Solar Energy-Environment)
4. Electronic Spectroscopy Laboratory: Application to Supramolecules And Nanostructures
5. Isotope Hydrology
6. Trace Element Studies Laboratory

3rd Scientific Programme: Chemical Biology

1. Natural Products Synthesis and Bioorganic Chemistry
2. Chemical Biology of Natural Products and Designed Molecules

Service laboratories

1. Environmental Analysis Laboratory
### Institute of Physical Chemistry 2007
#### Performance Indicators

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<td>Publications (International Journals) / in press</td>
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<td>1. Dr. Vourloumis Dionysios</td>
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<td>2. Dr. Giannakopoulou Konst.</td>
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<td>5. Dr. Katsaros Fotis</td>
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<td>6. Dr. Kontos Athanasios</td>
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<td>9. Dr. Economou John</td>
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<td>13. Dr. Pistolis George</td>
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<td>22. Dr. Falaras Polycarpos</td>
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<td>23. Dr. Hiskia Anastasia</td>
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1st Scientific Programme

Molecular & Supramolecular Nanofunctional Materials
Research Objectives/Activities

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

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

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

3. **Synthesis of novel, functional cyclodextrin derivatives for nanotechnology applications.** The derivatives: (a) Attach onto surfaces (i.e. on Au). (b) When deposited on Si/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 natural and mutated members of the new family of 2[4Fe4S] ferredoxins from selected pathogenic bacteria (Escherichia coli, Pseudomonas aeruginosa) with low and widely different reduction potentials (–460 and –650 mV) of the two metal clusters (b) Structure determination of complexes of DNA and RNA with modified cyclodextrins. (c) Structure determination of muscle proteins.

Publications


International Conferences


Funded projects


5. "Autoorganised supramolecular materials with electrical and optical properties” Empirikon Foundation, 12 k€, 2004-.


8. "Large Facilities Programme” for Access to the European Synchrotron Radiation Source DESY, Hamburg, Germany, EMBL Outstation under the EU Community. Financial Support for the projects “Natural and Derivatised Cyclodextrins and their Inclusion Complexes” and “Structure of Bacterial 2[4Fe-4S] Ferredoxins”, 2000 – today, 1.3 k€.

International Collaborations

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

Infrastructure

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

Personnel

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

Research Objectives / Activities

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

1. Multifunctional Liposomes as Drug Delivery Systems.

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


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

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

Alkylated dendritic polymers have the property of behaving as "nanosponges", in the cavities of which hydrophobic water impurities are encapsulated. Ultrapure water is produced, in which the remaining impurities are at the ppb level. Furthermore, cross-linked hydrophobic dendrimeric and hyperbranched polymers have been developed for water purification. Work has also been performed for the preparation of organosilicon dendrimers which were applied at the surface of ceramic filters for the production of ultrapure water.
Publications 2007


Conferences


**Patents**


**Funded projects**


**Infrastructure**

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

**Collaborations**

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

**Contact**

Dr D. Tsiourvas (tsiourvas@chem.demokritos.gr, Tel. +30 210 6503616, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/
Research work in the Molecular Thermodynamics and Modeling of Materials Laboratory (MTMML) focuses on the development and implementation of novel hierarchical methods and algorithms for the computer modelling and calculation of advanced material properties at the molecular, mesoscopic and macroscopic levels. Through this work, quantitative links are established between chemical constitution, processing conditions, and physical (thermal, mechanical, rheological, transport, interfacial, optical, dielectric) properties, which are critical for the optimal design of industrial processes and also govern the end-use performance of commercial products. In parallel, the molecular mechanisms underlying structure - property - processing - performance relations are elucidated with the objective of designing new, tailor-made materials.

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

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

Researchers: Dr. Ioannis G. Economou, Researcher A', Laboratory Director
Research Scientist: Dr. Niki Vergadou
Collaborating Researcher D': Dr. Nikolas Zacharopoulos (until May 2007, then part time collaborator)

Post-doctoral scientists in projects:
- Dr. Theodora Spyriouni (EU-STREP)
- Dr. Anastassia Rissanou (GSRT)
- Dr. Evangelia-Georgia Logotheti (INTAS)
- Dr. hari Leontiadou (GSRT)
- Dr. Stelios Karanikas (GSRT – ENTER)

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

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

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

Publications in peer-reviewed journals


Presentations in international conferences

Invited lectures


Educational work

Teaching

A. Undergraduate courses

2. Ioannis G. Economou, "Corrosion and Selection of Materials”, Department of Chemical Engineering, Technical University of Denmark, Lyngby, Denmark, Fall 2007

B. Post-graduate courses

Post-graduate degree awarded
PhD degrees

External funding


Collaborations
1. Professor Georgios Kontogeorgis, Department of Chemical Engineering, Technical University of Denmark. Development of thermodynamic models for non-ideal polymer systems.
3. Professor Athanassios Z. Panagiotopoulos, Department of Chemical Engineering, Princeton University, USA. Molecular simulation of dendrimers.
5. Professor Cor Peters, Department of Chemical Engineering, Delft University of Technology, The Netherlands. Modeling thermodynamic properties of ionic liquids.
7. Professor Sophia Lambropoulou, NTUA. Statistical mechanics.

Other activities

Ioannis G. Economou
1. Scientific Director of Technology Transfer Office, NCSR “Demokritos”.
2. Visiting Professor, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby.
6. Evaluation of research proposals for funding from the agencies: Secretariat of Research and Technology, Greece; INTAS, Belgium.
7. External examiner for PhD thesis at Department of Physical Chemistry, Université Paris-Sud 11, Orsay, France.

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

Marianna Yiannourakou

Contact
Dr Ioannis G. Economou (economou@chem.demokritos.gr, Tel. +30 210 6503963, Fax. +30 210 6511766)
Web site: http://www.mtmml.gr/
LUMINESCENCE LABORATORY – DEVELOPMENT OF NOVEL FUNCTIONALIZED MATERIALS FOR ANALYTICAL AND BIOANALYTICAL APPLICATIONS

Research Objectives/ Activities
The main objective of the Laboratory is the development of novel functionalized materials and their application in Analytical and Clinical Chemistry. The most important functionalized materials prepared in our laboratory were (a) biotinylated luminescent materials, (b) paramagnetic europium complexes derivatives of diethyleneetriaminopentacetic acid, (c) functional ferric oxide nanoparticles and (d) hybridized organo-inorganic chiral materials. The first one were applied for the quantification of the proteins avidin and streptavidin and in combination with them to the quantification of mouse IgG protein. The protein could be determined down to a few femtomoles per assay (9.2±1.8 fmoles). From paramagnetic europium complexes were measured the relaxation times and found to be similar to those obtained for commercially available MRI agent Magnevist (4.34±0.27 mM$^{-1}$s$^{-1}$ και 4.15±0.23 mM$^{-1}$s$^{-1}$ for novel derivatives and 3.93±0.12 mM$^{-1}$s$^{-1}$ for Magnevist). The novel functional ferric oxide nanoparticles were tested as catalyst in chemiluminescent determinations of reactive oxygen species. It was found that hydrogen peroxide could be determined down to a few micromoles per assay (2.08 ± 0.16 µmoles). Finally, the novel hybridized organo-inorganic materials tested in the asymmetric synthesis of some important optical active molecules, such as α-amino acids. The stereochemical yields of these reactions reached values up to 62%. At this point, it should be noted that beside the use of functionalized novel materials, a novel chemiluminescent technique was also developed in our laboratory and used for the estimation of the antioxidant activities of biological important materials as well as of natural products, such edible oils. The results were impressive and comparable to those obtained by the internationally accepted spectrophotometric DPPH-method.

Novel functionalized biotinylated materials | Chiral functionalized inorganic material
Publications 2007

Conferences

Funded projects

Infrastructure
UV-Vis spectrophotometer (Jasco V-560), 2 fluorimeters (Jasco FP-777 and Fluostar Optima BMG), 3 luminometers (Bio-Orbit 1250), complete photolysis system 1000 watt (ORIEL), elemental analyzer CHN, Cobalt-60 source (Gamma Chamber 4000A), complete laboratory for the synthesis of organic compounds equipped with rotary evaporators, high vacuum oil pumps, magnetic stirrers, ovens and lines for working in inert atmosphere.
**Personnel**
K. Papadopoulos (Research director/Group leader, permanent researcher), E. Giannakopoulou (technical staff), D. Kalogiannidis (PhD student, NCSR “D” fellow), D. Christodouleas and O. Lanitou (unpaid PhD students).

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

**Contact**
Dr. K. Papadopoulos, kyriakos@chem.demokritos.gr
Tel. +30 210 6503647, Fax. +30 210 6511766)
TRANSPORT PHENOMENA IN POLYMERS

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

Current research activities include

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

Validation against experiment of model simulating the functioning of matrix-type controlled release systems : Comparison of computed NaI release (continuous lines) and water uptake (dashed lines) curves with experimental data (points) from cellulose acetate matrices loaded with initial concentration of NaI, C_{0} (g/g of dry polymer ) 0.33 (black points and lines), 0.20 (red points and lines),

2. Mechanisms of Micromolecular Non-Fickian Transport Kinetics in Glassy Polymers
Sorption and diffusion of micromolecular substances in glassy polymer films is of great importance in many technological applications (e.g. polymer film drying, controlled release systems, food packaging materials). Sorption kinetics in these systems exhibits a variety of deviations from normal Fickian behaviour, attributable to either (i) slow viscous relaxations of the swelling polymer, or (ii) differential swelling stresses generated by the constraints imposed on local swelling during sorption. Our group 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. Various optical techniques are used in order to obtain information not only on the rate and kinetics of penetration but also on penetrant concentration profiles and parallel deformation and structural relaxation of the swelling polymer. Combination of these techniques enables us to study in detail various types of non-Fickian penetration such as stress-dependent diffusion and Case II kinetics.

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

Publications 2007

Conferences

Funded Projects

Infrastructure
Vacuum apparatuses for sorption and longitudinal dilation kinetic measurements on polymer samples including electronic microbalances (Cahn 2000 and MK2-M5 CI Electronics) or quartz spring balances, Polarizing and interferometric microscopes, Tensile tester in conjunction with optical setup, Thermal analysis instruments (Temperature Modulated DSC), Home-made apparatuses for kinetic release measurements, Abbe refractometer.
**Personnel**
M. Sanopoulou: research director/group leader, K. Papadokostaki: principal researcher, (permanent staff); J.H. Petropoulos (emeritus researcher); D. Soulas, M. Herouvim, A. Hasimi, K. Manoli (4 PhD students, external funding).

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

**Contact**
Dr. M. Sanopoulou (sanopoul@chem.demokritos.gr, Tel. +30 210 6503785, 30 210 6503661; fax. +30 210 6511766)
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 (e.g., 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 (e.g., 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 Levy distributions and the theory of random walks. For the study of the mechanisms creating complex patterns, non-linear dynamical systems of hierarchical complexity are used, together with mean-field theories, exact enumeration methods, real space renormalisation theory, theory of stochastic processes and numerical Monte Carlo Methods.

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

Publications 2007


**Conferences**

1. Noussiou, V. K. ; Provata A.; "Kinetic Monte Carlo simulations of the oscillatory CO oxidation at high pressures: the surface oxide model", Summer School: Morphogenesis through the interplay of nonlinear chemical instabilities and elastic active media, 2 - 14 July 2007, Cargèse, France

**Funded Projects**

1. “Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography”, PEP Attikis, 9.5 k€, 2006-2008

**Infrastructure**

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

**Personnel**

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

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

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

Research Objectives/Activities

The research activity of Molecular Computational Chemistry Laboratory encompasses the study of chemical reactivity and tropospheric degradation of molecules as well as the reliable prediction of properties of molecular materials by theoretical methods.

More specifically, the environmental behavior of a series of fluorinated alcohols towards chlorine atoms has been studied, and their reactivity has been successfully correlated with reliably calculated molecular properties, such as C-H bond strengths and ionization potentials, in order to allow the assessment of the environmental impact for these candidate substitutes of Freons. In addition, the reactivity of chlorinated and fluorinated ethanol towards hydroxyl radicals in aqueous solutions was studied as a function of theoretically calculated molecular properties. The reactivity of naturally emitted diiodomethane CH$_2$I$_2$ towards chlorine atoms as well as the oxidation mechanism of the CH$_2$I και CHI$_2$ free radicals was clarified by quantum-mechanical calculations.

The tropospheric degradation rate of small organic molecules (CH$_4$, CH$_3$F, CH$_2$F$_2$, CHF$_3$ και CH$_3$OH) by chlorine atoms and hydroxyl radicals and the dependence of the rate on the number and position of water molecules attached is being studied by using ab-initio and DFT methods in the framework of Transition State Theory.

The electronic structure and the molecular properties of ML$_2$ complexes of first-row transition metals (M = Mn, Fe, Co, Ni, Cu, Zn) with ligands L as models of several metalloenzymes active sites are studied by DFT methods, in order to assess the role of the metal in the structural, optical and magnetic properties of complexes.

The coordination ability of lanthanide cations with substituted cyclodextrins is studied by semiempirical methods (AM1, PM3) in order to determine the structure of the complexes which may be employed in magnetic resonance imaging techniques (MRI).

Correlation diagram of fluorinated alcohols rate coefficients with chlorine atoms as a function of their ionization potentials.
Publications 2007


Conferences


Funded Projects

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

Infrastructure

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

Personnel

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

Collaborations

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

Contact

Dr. Y. G. Lazarou (lazarou@chem.demokritos.gr), Tel. +30 210 6503623, Fax. +30 210 6511766
Web site: http://ipc.chem.demokritos.gr/
2nd Scientific Programme

Nanochemistry,
Environmental Friendly Technologies - Energy
MATERIALS & MEMBRANES FOR ENVIRONMENTAL SEPARATIONS LABORATORY

Research Objectives/Activities

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

Publications 2007


Conferences


Funded Projects

1. EE 1195 – INSIDE_PORES NMP3-CT-2004-500895, “In-Situ Study and Development of Processes Involving Nano-Porous Solids”, Network of Excellence in nanotechnology FP6, Priority 3 – NMP, Thematic priority 3.4.1.1. Partners to NCSR "D": Centre Nationale de la Recherche Scientifique (France), Imperial College (United Kingdom), University of Leipzig (Germany), University of Antwerp (Belgium), University of Stuttgart (Germany), Institute of Energy and Technology (Norway), TuDelft (The Netherlands), University of Alicante (Spain), Instituto di Chimica dei Materiali (Italy), Centre for Research and Technology Hellas (Greece), University of Hannover (Germany), SINTEF(Norway), TNO (The Netherlands). Total Budget: 6.800.000 €, NCSR "D" Budget: 1.844834 €. (October 2004- October 2008).

2. EE 1399 - HYCONES NMP3-CT-2006-032970, “Hydrogen Storage in Carbon Cones”, Partners to NCSR "D": Institute for Energy Technology (NO), The University of Nottingham (UK), Institute of Nuclear Physics, Polish Academy of Sciences (PL), Scatec AS (NO) Total Budget 2.564.000 €, NCSR"D" Budget: 577.000 € (November 2006-September 2009).


8. Ανάπτυξη Πρωτότυπων Συστηµάτων Αφαλάτωσης και Επεξεργασίας Υγρών Αποβλήτων µε Χρήση Κόλλων Μεµβρανών Διπλής Στοιβάδας (ΑΦΕΠ) Development of Desalination Systems and Waste Water Treatment with the use of Hollow fibers NCSRD budget: 141.500 euros

**Partners**

1. FUSION "Fundamental Studies of Transport in Inorganic Nanostructures", FP6, Thematic priority 3.4.2.1-2. Partners to NCSR "D": University College Dublin (Ireland), University of Edinburgh (UK), Delft University of Technology (The Netherlands), Warsaw University of Technology (Poland), VTT Technical Research Centre of Finland, EcoCeramics B.V. (The Netherlands). Total budget: 2.137.000 €, NCSR "D" Budget: 180.000 € (December 2004-November 2007).

2. ERA Pilot MiNa TSI "European Research Area Pilot Action on MicroNano Technology Systems Integration”, FP6 Priority. Partners to NCSR "D": VDI/VDE Innovation + Technik GmbH (Germany), Österreichische Forschungsförderungsgesellschaft (Austria), University Of Tartu (Estonia), Ministerio De Educacion Y Ciencia (Spain), Association Eurimus Office (France), Association For Pidea (France), Commissariat A L'Energie Atomique (France), Ente Per Le Nuove Tecnologie, L'Energia E L'Ambiente (Italy), Israeli Industry Centre For Research and Development (Israel), Fondazzioni Temi Zammit (Malta), Slovenska Technicka Univerzita v Bratislave (Slovakia). Total Budget: 850.000 €. NCSR "D" Budget: 42.366 €. (July 2005-July 2007).

**Infrastructure**

1. Nitrogen porosimeter with Krypton upgrade - Quantachrome
2. Mercury Porosimeter - Quantachrome
3. Low pressure single component permeability rig
4. High pressure 70 bar single component permeability rig(2)
5. Two high pressure mass flow controlled permeability/selectivity rigs (one up to 50 bar and the second up to 100 bar-up to 3 gas components each-flow rates 0-50 ml/min or 0-1000 ml/min)
6. One low-medium pressure mass flow controlled permeability/selectivity rig (one up to 5 bar-3 gas components each-flow rates 0-1000 ml/min)
7. Gas chromatographers (3) with auto sampling capabilities
8. Mass spectrometer – Residual gas analyzer - Pfeiffer
9. Several Flow systems
10. Hybrid Membrane Sorption Unit for the removal of Organic Chemicals
11. Gravimetric analyzer - HIDEN IGA
12. Gravimetric systems with magnetic suspension (2) - Rubotherm
13. Low pressure gravimetric systems (3) – CI balances
14. Langmuir-Blodgett (LB) trough of thin films
15. Chemical Vapor Deposition reactor
16. Grazing incidence infrared GIIR reflection unit
17. Advanced Imaging Equipment, including a Computerized Video Unit for the Investigation of Flow Phenomena through Porous Systems
18. Extensive IT and Network infrastructure available including UNIX servers, access to supercomputer clusters for advanced modeling applications, T3 Network Lines etc.
19. Quartz crystal microbalances (2) – Q-sense, ThinkSRS
20. High vacuum systems
21. High pressure volumetric apparatus for isotherms - VTI
22. Gas and vapour permeability apparatus for polymers and nano-composites (oxygen permeability – Danseror PBI
23. AFM - Veeco Innova
24. FTIR Nicolet 6700
25. High pressure cell for FT-IR
26. Ultra pure water
27. Ion chromatography system – Dionex
28. HPLC - Dionex
29. Calorimeter Calvet - Setaram
30. Thermal analysis (TGA) - Setaram
31. Zero length Chromatography

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

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

Contact
Nick Kanellopoulos
NCSRД - National Center for Scientific Research "Demokritos"
15310 Agia Paraskevi, Athens, Greece


tel: 0030-210-6503977, 6535294
fax: 0030-210-6511766
mobile: 0030-6944-787050
e-mail: HYPERLINK "mailto:kanel@chem.demokritos.gr" kanel@chem.demokritos.gr
HYPERLINK "mailto:mesl@chem.demokritos.gr" mesl@chem.demokritos.gr
PHOTOREDOX CONVERSION AND STORAGE OF SOLAR ENERGY – DEVELOPMENT OF NEW FUNCTIONAL MATERIALS FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

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

1. Dye-sensitization of large band-gap semiconductors
   The direct conversion of solar energy to electricity is investigated by developing heterojunctions consisting of large band-gap semiconductors sensitized by light harvesting molecular antennae-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 (nanoparticulate and nantube), transition metal complexes] and redox nanocomposite polymer electrolytes as well as their efficient incorporation in photovoltaic devices. Based on its intensive research activity, the team has established fruitful collaborations with research institutions and foreign companies for development of dye-sensitized solar cells (DSSCs) and their optimization in terms of efficiency, life-time and stability. Besides technology transfer, the perspectives of this collaboration include the creation of a DSSC manufacturing facility in Greece and demonstration activities in the field of building integrated photovoltaics.

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 superhydrophobic properties on multi-dynamic surfaces able to photochemically decompose harmful organics, kill bacteria and viruses and being easily self-cleaned; e) increased anticancer and anticoagulant action of titanium dioxide on neoplasm and inflammatory cells.
Publications 2007


Conferences


Funded Projects


Patents


Infrastructure

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

Personnel

P. Falaras: research director/group leader (permanent researcher); T. Stergiopoulos, A.G. Kontos, V. Likodimos: (3 post doctoral associates, external funding); E. Chatzivassiloglou, G. Konti: (2 PhD students, NCSR "D" fellows); A.I.Kontos, G. Kantonis, E.Rozi, N. Alexaki, A. Katsanaki: (5 PhD students, external funding); D.Tsoukleris: (technical staff, external funding).
Collaborations
M. Grätzel (EPFL Lausanne, Switzerland, DSSCs), G. Tulloch (Dyesol, Australia, Light ant Thermal Stress on DSSCs.), J. Kunze (Erlangen, Germany, Ti-Nanotubes), V. Catalano (Nevada, USA, Ligands for Ru-dyes), P. Potvin (Toronto, Canada, Dyes for DSSCs), Z. Picramenou (Birmingham, UK, Supramolecular Dyes), A. Ibhandon (Hull University, UK, Photoreactors).

Contact
Dr. P. Falaras (papi@chem.demokritos.gr, Tel. +30 210 6503644, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/
CATALYTIC-PHOTOCATALYTIC PROCESSES  
(SOLAR ENERGY-ENVIRONMENT)

Research Objectives/Activities
Catalytic photocatalytic reactions for solar energy utilization, environmental detoxification and environmentally friendly processes. In particular aggregates of metal oxides, mainly TiO$_2$, and polyoxometallates (POM) mainly of W, are used in thermal photochemical reactions for: (a) Water splitting (hydrogen production), (b) photoelectro-chemical 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$_2$O and inorganic anions, (f) reduction-removal of metallic ions and (g) synthesis of metal nanoparticles

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 2007

Conferences

Funded Projects

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

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

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

Contact
Dr. A. Hiskia (hiskia@chem.demokritos.gr, Tel. +30 210 6503643, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/
ELECTRONIC SPECTROSCOPY LABORATORY: APPLICATION TO
SUPRAMOLECULES AND NANOSTRUCTURES

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

Publications 2007

Conferences

Funded Projects
1. PEP Attikis

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

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

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

Contact
Dr. G. Pistolis (pistolis@chem.demokritos.gr, Tel. +30 210 6503637, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/
Research Objectives/Activities
The program deals with the analysis of the isotopic characteristics of the underground and surface waters and the use of the corresponding results, for the resolution of problems related with the exploitation of aquatic resources and geothermal energy. Such problems are the supply mechanism of aquatic horizons, their potential, the speed of flow of the underground water, the interconnection of the aquatic horizons or their communication with surface reservoirs, as well as the origin of geothermal fluids.

Another research activity is the development of a methodology for the determination of the concentration of natural $^{14}$C in the atmosphere and the study of the change of the isotopic ratios $^{13}$C/$^{12}$C and $^{18}$O/$^{16}$O in the atmospheric CO$_2$.

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

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

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

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

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

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

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

The last activity of the Laboratory was the investigation of screen printed electrodes for the application in trace element analysis.

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

Publications 2007


**Conferences**


**Contact**

Dr. Ochsenkühn Klaus (oxenkuen@chem.demokritos.gr) Retired, 31/12/2007
3rd Scientific Programme

Chemical Biology
Research Objectives/Activities

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

![Chemical structures of Scyphostatin, Trichodimerol, Oxazinins, Bastadin 12, and Bastadin 20](image)

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

Publications 2007


Patents

Conferences


7. Couladouros, E.A. "New routes towards the synthesis of natural products and designed derivatives", 2nd Hellenic Symposium on Organic Synthesis; From Chemistry to Biology, Medicine and Materials Science, Athens, 19-21 April 2007, p. 34.


**Funded Projects**


2. “Development of innovative bio-active magnetic nanomaterials for diagnosis and monitoring of pathogenic conditions by magnetic tomography”, PEP Attikis, 10 k€, 2006-2008


**Infrastructure**

Polarimeter, parallel synthesizer, HPLC.

**Personnel**

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

**Collaborations**

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

**Contact**

Dr. E.N. Pitsinos (pitsinos@chem.demokritos.gr, Tel. +30 210 6503789, Fax. +30 210 6511766)
Web site: http://ipc.chem.demokritos.gr/
Research Objectives/Activities
Our laboratory represents a new function within the Institute of Physical Chemistry, namely the “Chemical Biology of Natural Products and Designed Molecules”, which was initiated in July 2005. Our studies incorporate molecular design and analysis, total synthesis, structure/activity relationship observations, combinatorial synthesis and biological investigations. Our research focuses on the study of biological systems, DNA, RNA and proteins, through their interaction with small molecules of natural or synthetic origin, targeting the development of new and improved pharmaceutical entities. Our goal is the total synthesis of natural products and designed analogs with improved potencies and pharmacological profiles, the development of new synthetic methodologies in solution and solid phase and the development of new in vitro biological assays for the evaluation of the new synthetic entities. Our design will be based on crystallographic information and molecular modeling studies. Currently, we are involved in the areas of Cancer (topoisomerase II inhibitors, apoptosis), bacterial infections (aminoglycosides and A-site ribosomal-RNA) and anti-virals (Hepatitis C virus, HIV). Some of our ongoing projects are described 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 pharmaceutics and will improve overall our quality of life.

2. Nanoscale functionalities for targeted delivery of biopharmaceutics
The present research aims at the development of innovative multidisciplinary approaches for the design, synthesis and evaluation of molecular, nano- and micro-scale functionalities for targeted delivery of therapeutic peptides and proteins (biopharmaceutics). New protein- and peptide-based drugs are being discovered every day and their increased availability offers new ways to treat diseases. However, the structure, physicochemical properties, stability, pharmacodynamics, and pharmacokinetics of these new biopharmaceutics place stringent demands on the way they are delivered into the body. Carrier-based drug delivery systems can improve the bioavailability and diminish the toxicity of Peptidic/Proteinic (P/P) drugs. Furthermore, the carrier specificity can be
enhanced, through proper functionalization, and the release of the therapeutic peptide/protein can be controlled on demand. Artificial nanostructures being of the same size as biological entities can readily interact with biomolecules both on the cell’s surface and within the cell. Thus, the development of functionalized nanocarriers and nanoparticle-based microcarriers for P/P delivery is both an important scientific challenge and potentially a business breakthrough for the biopharmaceutical industry.

3. Design and synthesis of selective VEGF-R2 inhibitors

Angiogenesis is the process by which new blood capillaries sprout from pre-existing blood vessels, and it is well recognized that angiogenesis is an important mechanism governing tumor growth and metastasis. The recent clinical success of Avastatin® has provided a proof of principle for the potential of anti-angiogenic cancer therapy with anti-vascular 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 2007**


**Conferences**


**International Patents**


**Funded Projects**


**Personnel**

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

**Collaborations**


**Contact**

Dr. D. Vourloumis (vourloumis@chem.demokritos.gr, Tel. +30 210 6503624, Fax. +30 210 6511766)
Web site: http://vourloumis_group.chem.demokritos.gr/index.html
Service Laboratories
**SERVCE LABORATORY “ENVIRONMENTAL ANALYSIS”**

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

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

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

**Funded Projects**
2. "Chemical Analysis of sediments for heavy metals and chlorinated organic compounds", in the frame of services to EDRASOMICHANIKI, 3,3 K€.
3. "Chemical Analysis of sediments for heavy metals and chlorinated organic compounds", in the frame of services to ALTEC, 3,3 K€.
**Infrastructure**
Spectrophotometers UV-VIS-near IR, GC equipped with FID, ECD and TCD, HPLC equipped with UV-VIS and FLD, GC/MS, HPLC/MS/MS triple tetrapole, IC, Polarographic unit, TOC, SPE and SPME apparatus, oven, ultrasound bath, analytical balances, pHmeter, Rotary evaporator, ultrapure water apparatus.

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