# YEARBOOK 2010

Institute of Materials and Environmental Chemistry
CHEMICAL RESEARCH CENTER ♦ HAS

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# PREFACE

The current research activities of the institute are based on the experience we have gained during several decades. Our research objectives pertain basically to the fields of materials science and environmental science, but the actual projects generally share features related to both disciplines. Most of our materials science projects involve environmental protection aspects either directly or indirectly. For instance, we develop and use environment-friendly production technologies, our research is aimed at the extension of the lifetime of various raw materials and we put an emphasis on using biodegradable components. Very often, the primarily environmental chemistry projects dealing with the reduction of the environmental impact of certain harmful materials are not restricted to eliminating the compounds themselves; instead, their transformation into value-added materials is also the goal of the research.

The knowledge accumulated in the fields of materials and environmental science is a solid fertile ground to grow new ideas and findings at the present time and in the future. It also allows us to carry out research in a wide national and international network. Together with our commercial partners we are interested in utilizing the results of scientific research. In addition to our R&D activities we participate in university education and contribute to talent development focusing on gifted secondary school students.

Our strong background also provides the necessary flexibility to survive economically difficult periods and to go by contemporary concerns of the society. As an example of the latter, the institute played a major role in surveying the environmental impacts caused by the red mud flood in Ajka region, October 2010.

In the present yearbook, you will find some details of our work briefly mentioned above. We shall be pleased if our activities would meet your interest.

Budapest, May 2011

János Szépvölgyi
director

## PLASMA CHEMISTRY

### *Surface and Nanolayer Chemistry*

*Contact persons: András Tóth, Miklós Mohai*

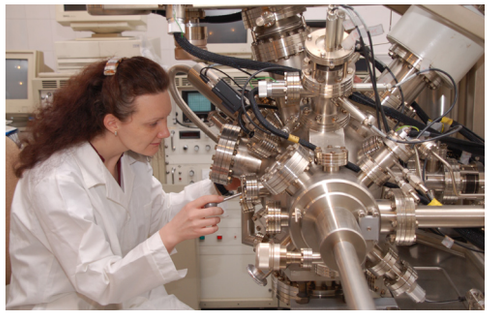
The principal profile of the laboratory is surface analysis, surface modification and layer deposition. The main areas of collaboration or service offered are as follows:

#### X-ray photoelectron spectroscopy (XPS or ESCA)

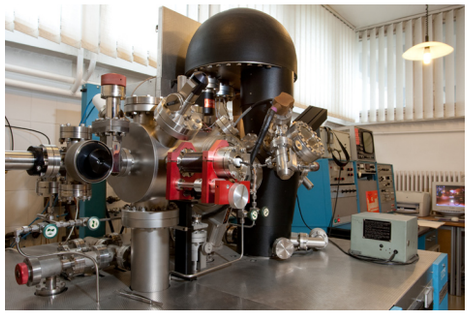
This versatile surface analytical method gives information on:

- Elements present in the surface layer (qualitative analysis)
- Surface composition (quantitative analysis)
- Chemical bonding mode, including oxidation state of the elements (chemical state)
- Depth profile (by sample tilting or ion etching)
- Layer thickness

Surface analysis by XPS provides information necessary to solve problems regarding: surface contamination, adhesion, printability, metallization, wettability, corrosion, functional groups, surface reactivity, wear resistance, flame-proofing, biocompatibility, antistatic, and antibacterial properties.



*Surface analysis by XPS*



*Kratos XSAM800 XPS spectrophotometer*

#### Nanomechanical and nanotribological studies

Two types of measurements are performed in this area:

- Dynamic, depth-sensitive nanoindentation, for determining hardness and elastic modulus of the surface layer of materials
- Dynamic scratch-, wear and topographic tests, for determining resistance to scratch and abrasive wear, and establishing surface roughness, and layer thickness

The layer thickness studied ranges between a few nm and several m. During the dynamic test the load applied to the diamond head, and the penetration depth, are followed simultaneously.

### Wettability studies

Static contact angle is studied by the sessile drop method and the surface free energy is calculated by various methods.

### Surface modification and lab-scale deposition of thin layers

- The surfaces of polymers, ceramics, glasses, metals, composites and biomaterials are modified by plasmas and particle beams like glow discharge, plasma beam, fast atom beam, plasma immersion ion implantation (PIII). In particular, PIII can be used to modify uniformly, in a single step the surface of irregularly-shaped devices (nitriding, carburizing, etc.), with the aim of improving hardness, wear resistance and other properties (e.g., wettability).
- Lab-scale deposition of hard and corrosion resistant (nitride, carbide or carbon-based) coatings is performed by RF and DC magnetron sputtering or PECVD under various conditions, to achieve targeted compositions and properties.

## *Thermal Plasma*

Research projects of the laboratory aim at the study of the chemical reactions occurring at high temperatures. For this purpose we operate several tube and muffle furnaces up to 1600°C in ambient air or inert/reactive atmospheres. For thermal plasma reactions we apply a 27 MHz/4 kW and a 3-5 MHz/30 kW radiofrequency (RF) plasma reactor, and direct current (DC) transferred and non-transferred arc plasma systems of 40 kW power. Synthesized powders are further processed by a sintering facility operating by spark plasma energy. For the characterization of the starting materials and the products, the following methods are used: bulk and surface chemical composition (ICP-AES, XRF, N/O analysis, XPS), phase composition (XRD), microscopic techniques (SEM, TEM), particle size analysis (LDA), physi- and chemisorptions.

### Formation of micro and nanopowders with special morphology

*Contact persons: János Szépvölgyi, Ilona Mohai, Zoltán Károly*

- Functional, micron and nanosized ceramic and composite powders having special chemical, electric, magnetic or mechanical properties,
- Catalyst supports,
- Spherical dense or hollow ceramic powders,
- Fullerenes and other carbon nanostructures,
- Nanofibers, nanotubes,
- Core/shell particles





*Preparation for atmospheric plasma spraying*

*High temperature tube furnace of spark plasma sintering equipment*

### Deposition of metallic and ceramic layers by atmospheric plasma spraying

*Contact persons: János Szépvölgyi, Ilona Mohai, Zoltán Károly*

### Sintering of ceramic, metallic and composite materials by spark plasma (SPS) method

*Contact persons: János Szépvölgyi, Zoltán Károly*

- Fast and efficient sintering of simple and composite nanopowders to achieve special, nanostructured morphology with increased mechanical and other special properties

### Processing of hazardous organic and inorganic wastes and their conversion into valuable secondary row materials

*Contact persons: János Szépvölgyi, Ilona Mohai, Zoltán Károly*

- Conversion of metallurgical and other wastes having high metal content
- Decompositon of organic and halogenated organic compounds and processing of inorganic materials contaminated by organics

## *Functional Nanoparticles*

The main activities of the Laboratory involve crystallization, granulation, coating, drying, mixing, grinding as well as modeling of these processes. Besides keeping in activities the conventional methods of particle technology our research work is expanded to the investigations on the preparation of new, tailored nano- and micro structured pure or composite materials. The research activities are the followings:

### Studies on colloid chemistry and nanostructure of solid products

*Contact persons: Tivadar Feczkó, Andrea Kardos-Fodor*

Preparation of pure and composite materials of micron and nanometer sizes using precipitation (salting-out and chemical), co-precipitation, spherical agglomeration and emulsion methods (controlled drug release formulations, support for biocatalysts).

### Chemical and process engineering research

*Contact person: Judit Tóth*

Elaboration of chemical, physical, mechanical and other (e.g., combined) processes to prepare and to treat micron size composite particles with suitable nanostructure, in order to establish new production methods, techniques and equipment for these kinds of products. Among them, product recovery by fluid dryer and granulator, drying of heat sensitive materials in spouted bed reactors, etc. are studied.

*Granulation of a food hydrocolloid*

*Mechanically spouted bed dryer with inert packing*

### Studies on physical, chemical and structural characteristics of materials

*Contact person: Tivadar Feczkó, Judit Tóth*

Material structure study of prepared individual or composite particles: crystal and/or amorphous phase composition, particle size and size distribution, morphology and inner microstructure of the surface, investigations on functional properties (e.g., chemical quality, stability, release, decomposition).

### Available devices

Reactors for batch crystallization, fluid granulator and dryer, mechanically spouted bed dryer, different grinders, freeze-dryer, ultrasonic homogenizator, ultracentrifuge, Malvern Mastersizer 2000 particle size analyzer, Malvern Zetasizer Nano ZS zeta-potential, particle size and molecular mass analyzer.





## *Metalkomplexes*

### Re-utilization of industrial and dangerous wastes

### Chemical methods for the treatment of dangerous wastes

### Synthesis of porous composite materials

*Contact person: László Kótai*

Composition of ash granulates as eco-fertilizers, various liquid absorbing and storage systems, bleaching earths.

### Preparation and investigation of essential metal complexes

*Contact person: Klára Szentmihályi*

- Preparation and investigation of essential metal complexes
- Significance and role of metal complexes in the function of human body
- Supplementation possibilities of metals by natural mode or by polygalacturonate and other metal complexes with natural origin

### Analytical techniques

IR, TG, XPS, ICP-OES, polarographic-voltammetric methods, potentiometry, UV-VIS spectrometry.

### Analytical investigations in multicomponent biological samples

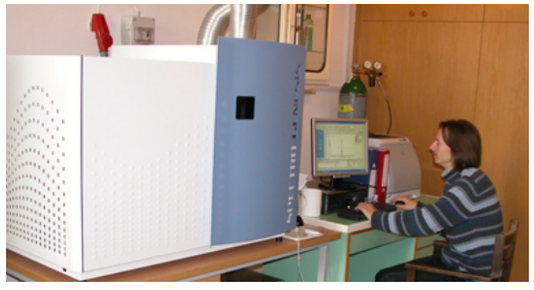
*Contact person: Klára Szentmihályi*

The determination of inorganic components and active organic ingredients in e.g., medicinal plants and extracts.

### Analytical techniques

ICP-OES, polarographic-voltammetric methods, potentiometry, UV-VIS spectrometry.

*O and N content analysis*



*Measurement on ICP system*

## POLYMER CHEMISTRY AND MATERIAL SCIENCE

Based on our expertise and inventions, our Department has a long history of successful research and development contracts (R&D) and cooperations with both domestic and foreign companies ranging from small enterprises to multinational firms on the areas listed below.

### Synthesis of Polymers with New Structures

*Contact person: Béla Iván*

R&D on the synthesis of a large variety of polymers as well as their block copolymers, e. g. polyisobutylenes, polystyrenes, other vinyl polymers (acrylates, methacrylates, etc.), polymers containing heteroatoms, branched and cross-linked macromocules with unique topologies and properties etc., with well-defined structure and molecular weights, with small polydispersities (suitable for GPC/SEC standards as well), and with functional groups by various polymerization techniques is carried out by us up to 100 g amounts. The potential applications of such R&D materials include drug carriers, biomaterials, new type of coatings with small amount of solvents (low VOC coatings), additives for motor oils, nonionic surface active materials, cosmetics, polymer additives, nanocarriers, nanotemplates, nanohybrids, polymers of nanomedicine etc.

### Biomaterials, Nanocomposites, Nanohybrids Based on Nanostructured Amphiphilic Polymer Conetworks

*Contact person: Béla Iván*

These new and very promising materials are made only by few research groups in the world. Our Department is carrying out pioneering R&D with these novel macromolecular structures. By orders, as well in the framework of R&D contracts we can offer

- synthesis of amphiphilic conetworks
- wide range of investigations on their physical, chemical and biological properties
- search for new unconventional applications and development of them

### Degradative Transformations and Recycling of Polymers

*Contact person: Béla Iván*

In the field of the degradative decomposition and search for possibilities of new type reuse of industrial polymers, such as PVC, we have elaborated several new procedures. Our accumulated know-how can be utilized in further R&D projects to investigate further potential possibilities.





## APPLIED POLYMER CHEMISTRY AND PHYSICS

Our Department forms a Joint Laboratory with the Laboratory of Plastics and Rubber Technology, Department of Physical Chemistry and Material Science, Budapest University of Technology and Economics.

### Degradation and stabilization of polymers

*Contact persons: Béla Pukánszky, Enikő Földes*

The effects determining the degradation and stability of polymers are studied on theoretical and applied research levels. The effects of processing and application conditions, as well as those of different additives and additive systems on the stability of polymers are investigated. Relationships are established between the chemical processes taking place during degradation and the changes in chemical, physical, rheological and mechanical characteristics of polymer. The chemical and physical parameters affecting the efficiency of additives are analyzed. Optimal additive compositions are developed to solve practical problems on the bases of conclusions drawn from theoretical studies. Partner: TVK

*The gel permeation chromatography equipment with multidetector system for the determination of molecular weight distributions and average molecular weights of polymers*

*Injection molding machine*

### Structure-property correlation in heterogeneous polymer systems

*Contact persons: Béla Pukánszky, Erika Fekete, János Móczó, Károly Renner*

Relationships among the type and amount of components, the component interactions and the properties of system are studied in different polymer blends and composites. The effects determining interactions, as well as their role in the characteristics of multicomponent systems are analyzed. The surface properties of polymers and fillers are investigated (contact angle measurement, inverse gas chromatography, FT-IR) to characterize interfacial interactions. The characteristics of composites are influenced by modification of filler surface.

The micro- and macromechanical deformations and the factors influencing them are investigated. The scale of polymers, as well as the type and size of fillers change in a wide range: from conventional fillers (e.g., talk, zeolite, $CaCO_3$) to nanosize particles (e.g., ZnO, $SiO_2$). Relationships between the structure of layered silicate nanocomposites and the competitive interactions are investigated. The study of biodegradable polymer (like PLA) composites containing natural fillers (like sawdust, cob dust) is also a part of the research. On the bases of general relationships obtained in basic research different compositions are developed for special purposes. Partners: TVK, Ongropack, Clopay, The University of Twente, Enschede, The Netherlands, Inha University, Inchon, Korea, Polymer Institute, Slovak Academy of Sciences, Dunastyr Zrt., Airsec-Süd Chemie, University of Mons-Hainaut, Mons, Belgium.

### Preparation of special polymers

*Contact persons: Béla Pukánszky*

The research can be divided into to parts: synthesis and chemical modification of polymers. In the field of polymer synthesis thermoplastic elastomers based on polyurethane are developed for medical purposes. The chemical modification of polymers ranges from polyolefin grafting with functional groups (e.g., modification with malein-anhydride) to modification of natural polymers (e.g., cellulose). Target applied research and development are based on basic research. Partners: The University of Twente, Enschede, The Netherlands.

### Crystallization and crystalline structure of polymers

*Contact persons: Béla Pukánszky*

Study of the crystallization of polyolefins and the effects influencing that has long tradition in the Joint Laboratory. Excellent results were achieved in the modification of the crystalline structure of isotactic polypropylene. Special additives are used to modify the morphology of polypropylene, which influence significantly the characteristics of polymer, e.g., transparency, mechanical strength, impact strength. Partners: InnoComp, TVK, Ciba Specialty Chemicals, Borealis.

### Special methods

- Contact angle measurement
- Inverse gas chromatography
- Investigation of the deformation processes of polymer based systems (acoustic emission, volume strain)
- Gas (oxygen, nitrogen) permeability measurement
- Thermal analysis (DSC, TGA, DMTA)
- Rheological investigation of polymers (dynamic, capillary and solution viscosity, MFI)
- Optical microscopy
- Instrumented impact testing





## ENVIRONMENTAL CHEMISTRY

### *Thermal Studies*

### Basic research on the utilization of biomass and on feedstock recycling of plastics waste

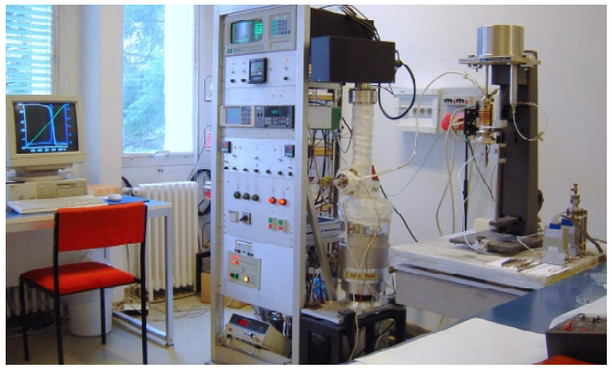
*Contact persons: Marianne Blazsó, Emma Jakab, Gábor Várhegyi*

The thermal decomposition and temperature-controlled combustion of plastics, plant materials and solid biomass fuels are studied.

### Areas of Investigations

- Examination of plastic wastes: composition analysis, thermal behavior, and ability for pyrolytic recycling
- Supporting the research and development of biomass utilization technologies by investigating their solid phase intermediates, products, and byproducts
- Studying biomass fuels and products of energy plantation for biomass-fired power stations
- Analyzing the chemical processes of charcoal production technologies. Study of the reactivity and self-ignition hazards of charcoals
- Study on upgrading pyrolysis oil of biomass and plastics waste over solid catalysts
- Reaction kinetic modeling of pyrolysis, gasification and combustion processes in the kinetic regime

*Study of the carbon deposition on catalysts*



*Thermobalance – mass spectrometer system (TG-MS)*

### Methods

- Thermogravimetry – mass spectrometry (TG-MS). The sample is heated by various temperature programs. The change of the sample mass is measured with high precisions during the experiments. The formed volatiles are analyzed simultaneously by a coupled mass spectrometer

- Pyrolysis – gas chromatography – mass spectrometry (Py-GC/MS). A fast heating of the sample is followed by an isotherm pyrolysis of 10 - 30 s. The volatile pyrolysis products are analyzed on-line by gas chromatography – mass spectrometry. The conversion of the thermal decomposition products over solid catalysts is also examined

## *Atmospheric Chemistry*

The main research area of our group is the study of the kinetics and molecular mechanism of elementary chemical and photochemical reactions. For the most part, we investigate such processes and phenomena that play an important role in the complex interplay between climate change and the chemistry of the environment. We apply mainly laser-based experimental techniques for the production and detection of reactive species (e.g., free radicals). The kinetic and photochemical data determined experimentally are being used as input parameters in atmospheric chemistry and combustion models. Following are the main research themes:

### Kinetics of gas-phase elementary reactions

*Contact person: Sándor Dóbé*

- Determination of kinetic parameters for the atmospheric reactions of Freon substitutes and other reactive greenhouse gases; effect of the formation of loose molecular complexes on the reactivity
- Combustion chemistry, kinetics and mechanism of alternative fuels (alcohols, ethers and esters); kinetics of multichannel radical-radical reactions

### Environmental photochemistry and photophysics

*Contact persons: Attila Demeter, Sándor Dóbé*

- Photochemistry of atmospheric carbonyls (aliphatic aldehydes and ketones): temperature- and pressure dependence of photodissociation quantum yields (contribution to the EU's atmospheric chemistry project SCOUT-O3)
- Investigations in liquid phase with relevance to environmental aquatic chemistry and air-born aerosols: relaxation kinetics of electronically excited molecules, effect of hydrogen-bonds on photophysical properties and photochemical processes

### Instrumentation

- Laser equipments: excimer lasers, Nd:YAG laser, dye lasers
- Discharge flow reaction kinetic apparatuses
- Laser photolysis equipments for kinetic and photochemical experiments
- Special light sources: mercury lamps, high-power and flash Xe lamps, resonance fluorescence lamps

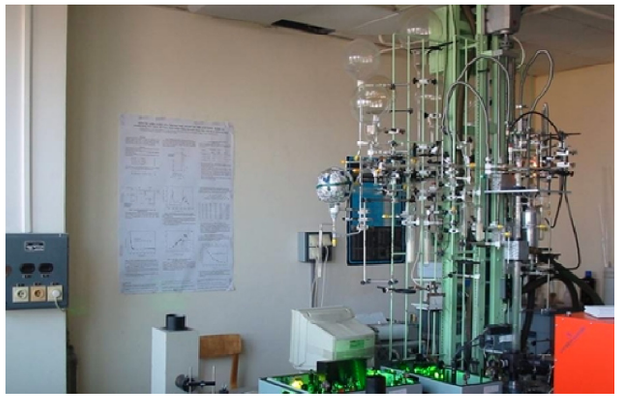
### Specialties

- Atmospheric chemistry, combustion chemistry, reaction kinetics, photochemistry, photophysics, spectroscopy

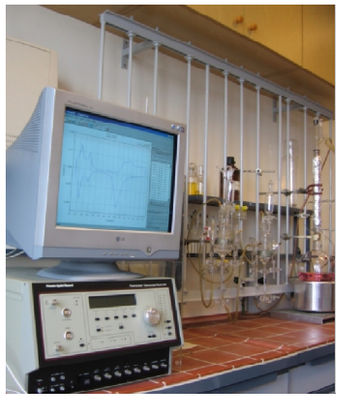




- Determination of kinetic parameters by using direct experimental methods, pulsed-laser photolysis and discharge flow
- Laser spectroscopy of atoms, free radicals and electronically excited molecules: luminescence, laser-induced fluorescence, UV-VIS transient absorption
- Photo-oxidation and relative-rate kinetic measurements in environmental photoreactors
- Thermodynamics and kinetics of hydrogen-bonded complexes
- Photophysical kinetics of organic molecules displaying dual luminescence
- Kinetics of photoreduction systems, applications in environmental chemistry
- Organic photochemical synthesis, industrial photochemistry
- Purification of water applying photochemical and photocatalytic methods
- Development of instrumentation and methods for the analysis of atmospheric organics



*Discharge flow reaction kinetic apparatus*



*Electrochemical measuring setup*

## *Electrochemistry*

In general, we are involved in electrochemistry projects of environmental protection significance: in particular, we study electrochemical processes being promising for removal of certain pollutants from groundwater. To this end we perform electrochemical kinetics measurement on various electrodes of electrocatalytic activity. Our related skills are as follows:

### Electrochemical impedance spectroscopy (EIS) and related methods

*Contact persons: Tamás Pajkossy, Gábor Mészáros, Gabriella Lendvay-Győrik*

- Dielectric spectroscopy, Faraday-distortion methods
- EIS for the study of various electrochemical kinetics problems (examples of the past five years: characterization of the electrochemical double layer and adsorption processes on the platinum-group metals; corrosion properties of metals; inhibitors; conversion layers; polymer coatings)

### Theories on electrochemical kinetics

*Contact persons: Tamás Pajkossy, Gábor Mészáros*

- Noise analysis and its application in electrochemical kinetics
- Relation of electrode geometry and electrode kinetics; calculation of current density distributions and diffusion fields at various geometries

### Electrocatalysis and corrosion

*Contact person: István Bakos*

- Developing metallic and bimetallic catalysts along with their characterization by electrochemical means; catalytic oxidation of chlorinated hydrocarbons; bimetallic corrosion; cathodic corrosion protection; connection between corrosion and catalytic properties of metals; metal adsorption and its role in soldering and welding technologies

### Development of instruments

*Contact persons: Gábor Mészáros, Tamás Pajkossy*

- Developing electrochemical instruments (examples of the past five years: bipotentiostat of femtoampere sensitivity for nanoelectrochemistry studies; development of various current meters for electrochemical scanning tunnelling microscopes, data aquisition systems)
- Construction of various industrial and/or laboratory measurement systems (examples of the past five years: measurement systems for electrical, optical, and spectroscopical quality control tests of metal-halide discharge lamps, for the GE Hungary)

## ENVIRONMENTAL PROTECTION

Within the analytical and technological research and development work we offer the clients a wide range of services. In this area the Laboratory has been authorized by the Hungarian Accreditation Board as Testing Laboratory that complies with the criteria of MSZ EN ISO/IEC 17025:2005 standard. **The No. of the accreditation certificate is NAT-1-1378/2009.** Accredited status is valid until February 24, 2013.

### Environmental protection analytics

*Contact persons: Tibor Horváth, Béla Lengyel, Zoltán Sándor*

The accredited testing fields of the Laboratory are as follows:

- Chemical analysis of different types of water including drinking water, surface water, groundwater, industrial water and sewage water





- Environmental protection analysis of sewage water sludge, soils, wastes, and their extractives, and the pre-treatment of these materials for testing
- Physicochemical and corrosion testing of anti-freeze engine coolants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VIZSGÁLÓLABORATÓRIUM
TESTING LABORATORY
NAT-1-1378/2009.
2008. október 24.
Budapest, 2008. október 24.

*Accreditation certificate*

The analytical methods applied:

- Potenciometry
- Gravimetry
- Corrosion tests
- UV-VIS spectrofotometry
- HPLC, LC-MS, GC, GC-MS
- ICP-OES

### Mitigation of harm, waste treatment, elaboration of cost-competitive new technologies

*Contact persons: György Mink, Tibor Horváth*

- Final disposal of polychlorinated biphenyls (PCB-s), polychlorinated dibenzo-p-dioxins and furans (PCDD-s, PCDF) by catalytic hydrogenation or moderate temperature thermal methods
- Processing of sewage water sludge with the utilization of its calorific value by a novel and dynamic method
- Design and construction of new, multi-channel cyanide monitoring systems for the continuous analysis of industrial water and the air space of huge workshops
- Solar desalination
- Solar assisted water purification

### Corrosion prevention

*Contact persons: Béla Lengyel, Tibor Horváth*

- Investigation of the physical and chemical properties of paint coatings
- Clearing up the cause of the corrosion damages and elaboration prevention methods
- Gravimetric and electrochemical corrosion tests
- Study and characterization of inhibitor effects
- Development of inhibitor compositions for anti-freeze and cooling water systems

## Department of Plasma Chemistry

- Atmospheric plasma spraying system (Metco gun and feeder)
- Automatic titrator (Titralab Tim 900)
- Centrifuge (SIGMA 4K10)
- Continuous fluidized bed drier and granulator (laboratory size)
- Continuous mechanically spouted bed dryer with inert packing (laboratory and big laboratory size)
- Contact angle measurement (SEE System)
- DC plasma furnace (40kW)
- ECWR plasma beam source (IPT PSQ100)
- Fast atom beam treatment facility (Ion Tech FAB 114)
- Freeze-dryer (Lyovac GT2, Leybold-Heraeus)
- High temperature reactors for gas-solid reactions
- Homogenizer (Braun)
- Microwave Digestion System (Anton Paar Multiwave 3000)
- Nanotribology tester (MicroMaterials Nanotest 600)
- Particle size analyzer (Malvern 2600 and Mastersizer)
- O/N Analyser in solid samples (Horiba/Jobin-Yvon, EMGA 620WC)
- Physi-and chemisorption measurements (AUTOSORB IC, Quantachrome)
- Plasma immersion ion implanter (ANSTO)
- Polarographic-voltammetric equipment
- RF and DC magnetron sputtering sources (AJA A315-UA, A320-UA)
- RF induction plasma systems (Linn, Tekna)
- Simultaneous ICP-AES (Spectro Genesis)
- Spark Plasma Sintering machine (SP D5, FCT GmbH)
- Spectrometer with CCD-3000 detector (Jobin-Yvon TRIAX 550)
- Surface resistance meter ($10^8$ – $10^{14}$ )
- Ultrasound homogenizer (Heat Systems-Ultrasonics W- 220 F )
- UV-VIS spectrophotometer (Biochrom 4060)
- Vibro Viscosimeter (SV-10)
- X-ray photoelectron spectrometers (Kratos XSAM 800, VG ESCALAB)
- X-ray fluorescence spectrometer, portable (Thermo Scientific NITON XL3t)
- Zeta potencial, particle size and molecular weight analyzer with MP-2 autotirator (Zetasizer Nano ZS)

## Department of Polymer Chemistry and Materials Science

- Gel permeation chromatograph (Waters 510)
- Laboratory ozonizer (Yanko Industry Ozone Services)
- Tester of PVC degradation (Donaulab)
- UV curing flood lamp system equipped with 400W standard UV lamp (UV-A and UV-B at 225mW/cm$^2$) and manual shutter (DYMAX 5000-PC)





## Department of Applied Polymer Chemistry and Physics

- Acoustic emission equipment (SENSOPOHONE AED 40/4)
- Contact angle goniometer (Rame-Hart 100-00-(115)-S Automated Goniometer)
- Fourier transform infrared spectrophotometer (Bruker Tensor 27)
- Gas chromatograph (Perkin Elmer XLGC)
- Gas permeation analyzers (Brugger GDPC, Systech 8000 Oxygen Permeation Analyzer)
- High pressure liquid chromatograph (Knauer HPLC 64)
- High-speed fluid mixer (Thyssen Henschel FM/A10)
- Impact testers (Ceast Charpy 6546, Ceast Resil 5.5, Zwick (Izod, Charpy))
- Injection molding machines (Demag Intelect 50/330-100, BA 200 CD)
- Internal mixer (Brabender, W 50EHTl)
- Laboratory press (Fontijne SRA 100, JBT Engineering, 25t)
- Laboratory rolling mill (Schwabentan Polimix L1010)
- Mechanical testing system (Zwick 1445, Instron 5566)
- Microtome (Reichert-Jung, Polycut)
- Optical instruments (Hot Stage Mettler FP 82 HT, Polaroid DMC1 digital camera, Hunterlab ColourQuest 45/0 Mathis Labomat BFA 12 colorimeter)
- Rheometry (Göttfert 2002 capillary viscometer, Göttfert MPS-D MFI tester, Brabender Rheotron rotational viscometer, Rheolab rheometer, Physica UDS 200 Universal dynamic spectrometer, Paar Physica MCR 301 rheometer)
- Single-screw extruder (Haake Rheomex S 3/4”, Brabender EXTRUSIOGRAPH)
- Textile chemical equipment: steaming frame (Werner-Mathis DHE), laboratory fular (Roachez)
- Thermal analyzers (Perkin Elmer DSC2, DSC7, TGA6, Mettler DSC30, TMA40, TG50, Perkin Elmer Diamond DSC, Perkin Elmer Diamond DMA)
- Thermomat Metrohm 763 PVC
- Thermomechanical analyzer (Polymer Labs, DMTA II)
- Twin-screw compounder (Brabender DSK 42/7)
- UV-VIS spectrophotometer (Hewlett Packard 8452A, Unicam UV 500 UV-VIS fotometer)
- Vacuum thermoforming machine (VFP 0505 1SL)

## Department of Environmental Chemistry

- Analytical pyrolyzer (CDS Pyroprobe 2000)
- Dielectric measurement device (in 5 Hz - 5 MHz range)
- Digital storage oscilloscopes
- Electrochemical measuring techniques (potentiostatic and galvanostatic, stationary and transient voltametric facilities, electrode impedance spectroscopy, noise spectroscopy, harmonic analysis)
- Excimer lasers

- Flash Xe lamp + power supply
- Gas chromatograph (HP 5880A)
- Gas chromatograph-mass spectrometer (Agilent 6890 GC / 5973 MSD)
- High pressure thermobalance (Hiden Hall IGA, high temperature furnace)
- High-pressure photolysis cell
- High-voltage power supplies
- Laser-diffraction particle size analyzer (Malvern 2600C)
- Microwave generators
- Monochromators
- Nanosecundum spectrometer + multichannel analyzer
- Nd:YAG laser + dye laser + frequence-doubling unit
- Pulsed laser spectrometer, consisting of: excimer laser, xenon lamp, oscilloscope, monochromator, deuterium lamp + power supply, circulator
- Quantum-photometer
- Thermobalance-mass spectrometer system (Hiden Hall 300 PCI, Perkin-Elmer TGS-2)
- UV-C spectrometer

### Laboratory of Environmental Protection

- Equipment for evaluating thin-layer chromatograms (Shimadzu)
- Finnigan MAT GC/MS instrument
- HPLC systems (Merck Hitachi, Waters 9110)
- HPLC/MS facility (Shimadzu LCMS 2010)
- ICP-OES spectrometer (Jobin-Yvon Ultrace 138)
- Methods for the evaluation of lifetime and paint properties of coatings
- Rapid corrosion resistance test equipments (salt-spray chamber, humidity chamber, hot-cold cyclic test)
- Reactive thermobalance (Mettler)
- Semi-preparative HPLC equipment (Waters LC-Module 1)
- Solar simulator
- Stone chipping equipment
- Two-column GC with automatic dosing system (Perkin-Elmer Autosystem XL)
- UV-VIS spectrophotometer (Unicam)
- UV-VIS-NIR spectrophotometer (Jasco)
- Volumetric adsorption system for studying adsorption and chemisorption





### Research projects financed by the Hungarian Research Fund

- Determination of provenance and fabricing technology of old, medieval Hungarian historical bricks with methods of modern analytical chemistry and physical sciences (PD 75740)
- Application of thermal analysis for studying thermal decomposition reactions of environmental interest (K 61504)
- Surface modification of engineering polymers by particle beams (K 67741)
- Environmental electrochemistry (K 67874)
- Surface and interfacial phenomena in heterogeneous polymer films and layers (K 67936)
- Investigation of structural and functional properties of complex surface nanolayers of polymers and their potential application as drug delivery systems (K 68120)
- Atmospheric kinetics and photochemistry of carbonyl molecules and carbonyl free radicals (K 68486)
- Study of micro- and macromechanical deformation processes in reinforced plastics (F 68579)
- Elimination of polluting components from pyrolysis oils of plastics wastes (K 68752)
- Study of the chemical processes of biomass utilization (K 72710)
- Study of the efficiency and mechanism of stabilizers in polyolefins under various conditions (K 77860)
- Amphiphilic polymer conetworks as templates and components of new nanohybrid materials (K 81592)
- The effect of physical and chemical pretreatments on the composition and thermal behavior of lignocelluloses (K 81959)
- Basic research for gamma-valerolactone economy (CNK 78079)
- Encapsulation of photochromic dye and its grafting to textile (MB08 A 80294)

### Research projects financed by various Hungarian agencies

- Production of nanostructured engineering ceramics by novel sintering methods (Gábor Baross Program REG KM 09)
- Development of high temperature radar absorbing materials by nanotechnology (OMFB 00252/2007)
- Destruction of polychlorinated aromatics (TECH_08-A462-2008-0160)

## Research projects financed by the European Union

- High added value materials from waste tyre gasification residues (Grant Agreement Number 226549)
- Stratosphere-climate links with emphasis on the UTLS (GOCE-CT-2004-505390-SCOUTO3)

## Research projects financed by various international or foreign resources

- Carbon-encapsulated magnetic nanoparticles were synthesized in RF plasma reactor in a common research with Department of Chemistry, Warsaw University.
- In the framework of the HUMAN MB08-A 80294 project, encapsulation of photochromic dye and its grafting to textile were studied in cooperation with researchers of the University of Maribor, Slovenia.
- In a bilateral agreement with the Laboratory of Biochemistry of the Stradins University of Riga (Latvia), free radicals and elements in tumour inflammatory diseases and tumours were studied.
- Nanophasic conetworks were jointly studied with the Institute for Macromolecular Chemistry and Material Research Center, University of Freiburg, Germany.
- The research on new type of multifunctional polymers was supported by DuPont (USA) Research Award.
- Together with the Department of Chemistry, University of Basel, Switzerland controlled polymerization with biomolecules was investigated.
- In a joint work with the Institute of Macromolecular Chemistry, Romanian Academy, Iasi, the thermal stability of polyimides was determined.
- The nucleation mechanism of a soluble additive in polypropylene was investigated for Ciba Company, Basel, Switzerland.
- The correlation between crystalline structure and properties in polypropylene were studied, and a method for the determination of nucleation efficiency in polypropylene was developed together with Borealis GmbH, Austria.
- The stabilizing mechanism of antioxidants was determined in a joint work with Clariant Huningue S.A., France, and Tisza Chemical Works.
- In a bilateral science and technology project with the University of Twente, The Netherlands, plastics for medical use were investigated.
- Micromechanical deformation processes in polypropylene composites were studied in cooperation with researchers of the University of Leoben, Austria.
- The deformation mechanism of polyamide6/montmorillonite nanocomposites were investigated with the University of Liege, Belgium.
- Polymer composites reinforced with natural fibers were studied with researchers of the University of Pisa, Italy.
- In a DFG-HAS cooperation with the University of Ulm, the electrochemical double layer of gold single crystals - ionic liquids systems were studied.
- Special electrochemical instruments have been developed for CEST Kompetenzzentrum für elektrochemische Oberflächentechnologie GmbH (Wiener-Neustadt, Austria).





- Instruments with improved noise levels for molecular conductivity measurements have been developed for the University of Bern, Switzerland.
- Electron transfer in new materials for molecular electronics was studied in cooperation with researchers of the Heyrovsky Institute in a Hungarian - Czech bilateral project.
- The pyrolysis and combustion of tobacco and the kinetics of the emission of nicotine and formaldehyde from aerosols was studied in cooperation with British American Tobacco R&D Centre (Southampton).
- In the field of physical chemistry of the atmosphere, a joint PhD work with University of Lille about kinetic and photochemical experiments is performed.
- The study of the photophysical properties of dual luminescent systems was the subject of the common work with the Max-Plack-Institute for biophysikaliskalische Chemie, Göttingen, Germany.
- The kinetics and mechanism of elementary reactions with relevance to tropospheric halogen chemistry were determined in a Hungarian–Polish intergovernmental cooperation with the University of Medicine in Wrocław.
- A new method for activated carbon preparation from cellulosic materials was jointly developed with researchers of the China University of Petroleum.
- In a common project with the Norwegian University of Science and Technology in Trondheim, biomass utilization possibilities and reliable kinetic description of the char gasification by carbon dioxide has been studied.

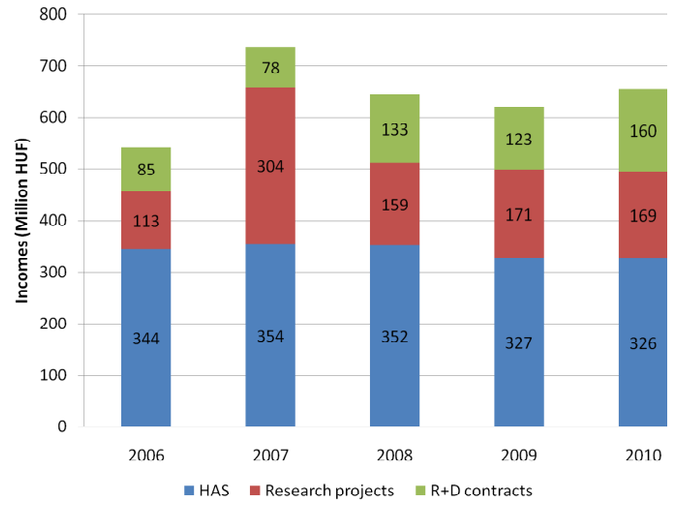
# 5 INDUSTRIAL R&D PROJECTS

- **AIRSEC SAS** - Development of advanced packaging materials
- **ALCOA KÖFÉM Ltd.** - Participation in solving R&D problems
- **Árnika Ltd.** - Participation in R&D projects
- **British American Shared Services Ltd, Southampton, UK** - Using a cylindrical denuder to sample formaldehyde in cigarette smoke
- **ERCOM Ltd.** - Analytical measurements
- **Feszo-Trade Ltd.** - Participation in solving R&D problems
- **GE Hungary Ltd.** - Participation in R&D projects
- **GEA EGI Contracting / Engineering Co.** - Corrosion and analytical investigations
- **Hungarian Indo-Chinese Society** - Characterisation of archaeological samples by portable XRF equipment
- **In Vitro R & D Ltd.** - Production of FERROCOMP pills
- **IVY Medical Ltd.** - Analytical measurements
- **Magyarlakk Paint Manufacturing and Trading Ltd.** - Participation in developing waterborne paints
- **MOL Co.** - Investigation, monitoring, and treatment of oil-contaminated soils
- **National Science and Technology Foundation** - Research on adhesive problems in plasma tv producing technologies
- **Peridox EU Ltd.** - Analytical investigations
- **Polinvent Ltd.** - Corrosion investigations
- **Swerea IVF AB** - Production of special ferrite powders in laboratory scale
- **Tisza Chemical Works TVK Co.** - Stabilization of polymers
- **Wessling Ltd.** - Analytical measurements

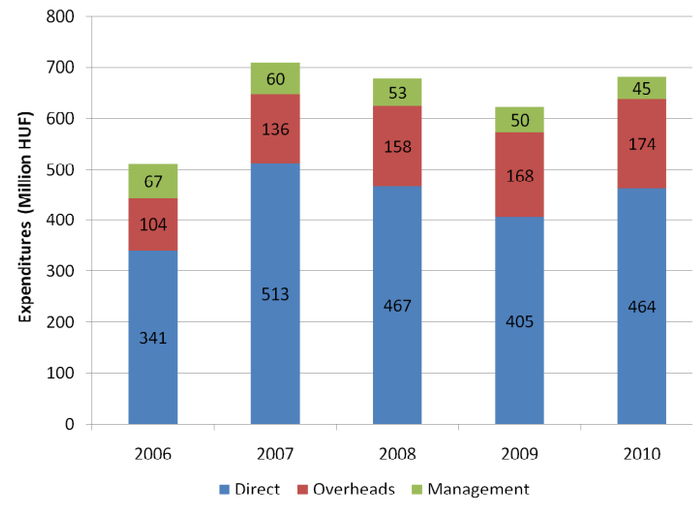


# 6 FINANCIAL DATA

The amount and the composition of our incomes in the last 5 years is to be seen in the following figure.




The amount and the composition of our expenditures in the last 5 years is to be seen in the following figure.

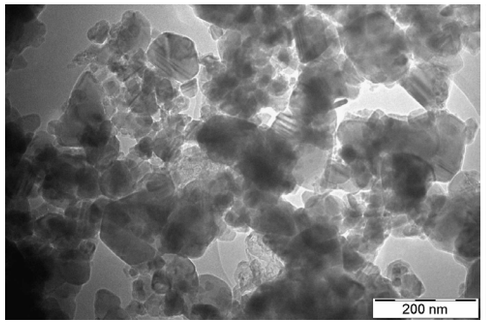


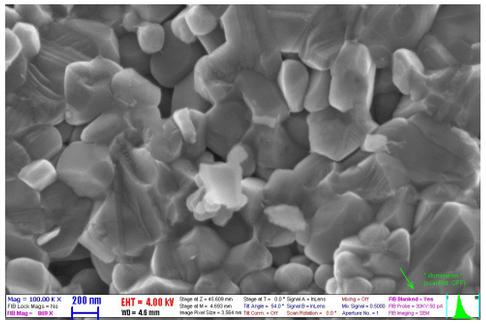
## 7.1 Synthesis of silicon carbide nanopowder in radiofrequency thermal plasma

*Anna Keszler, Szilvia Klébert, Zoltán Károly, Ilona Mohai, János Szépvölgyi*

Silicon carbide (SiC) nanopowders were synthesized in radiofrequency thermal plasma using various silicon and carbon sources. The study aims at the production of high added value ceramic row materials from waste materials. Experiments were performed with waste tyre gasification residues as carbon source and fly ash and quartz powders as silicon sources. Prior to the experimental work, thermodynamic calculations were performed to determine the optimal temperature conditions of carbothermal reduction and formation of carbide, and the composition of the gas and condensed phases at different temperatures. High surface area -SiC powders were synthesized with bimodal particle size distribution. The bigger portion of the powder consisted of 100-300 nm particles coming from gas phase reaction and condensation, while the smaller part of the powder was a 5-50 µm, porous fraction. The plasmathermal powder is peculiar due to its residual fine carbon and elemental silicon content. This carbon and silicon may react during the forthcoming sintering step, improving the mechanical properties of the ceramic body.

These laboratory experiments served as basis for the future installation of a pilot plasma plant that will be involved into a complete production line, realized in international cooperation and financed by the EU.




*Transmission electron micrograph (TEM) of the plasmathermal SiC powder (left) and scanning electron micrograph of the ceramic body sintered therefrom (right). Spark plasma sintering method allowed the preservation of the nanostructure of the starting nanopowder.*





## 7.2 Preparation, formulating and analysis of functional particulate materials

*Tivadar Feczkó, Andrea Fodor Kardos, Judit Tóth, Bence Németh** (**university student, Pannon University)*

The possibility of microencapsulation of functional materials has been investigated; biocompatible and biodegradable polylactic-glycolic acid – bovine serum albumin (model protein) composite nanocapsules have been formulated. These protein-containing drug formulas embody also magnetic iron oxide nanoparticles, thus, both controlled and targeted delivery of the medicine might be achieved.

Photochromic dyes have been incorporated into nanocapsules in cooperation with the Textile Department of University of Maribor in order to enlarge their lifetime and absorbance. As a further result, these microencapsulated dyes became suspendable in water phase. The textile printing paste, in which the nanoparticles have been dispersed, were used to coat fabrics. The durability tests of these coating are in progress.

A drying technology of a natural hydrocolloid in a spouted bed dryer was developed. The influence of operational parameters on the quality, as particle size, viscosity, optical rotation, of the product was investigated. The laboratory experiments were adapted to existing plant equipment. By now, on the basis of the developed method, the production has already been started at BUSZESZ Food Co.

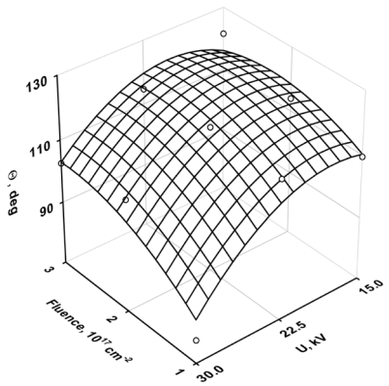
*Studies on particle size and zeta-potential of colloids*

*Determination of particle size by laser diffraction*

## 7.3 Synthesis and characterisation of nanolayers

*András Tóth, Klára Kereszturi, Miklós Mohai, Imre Bertóti*

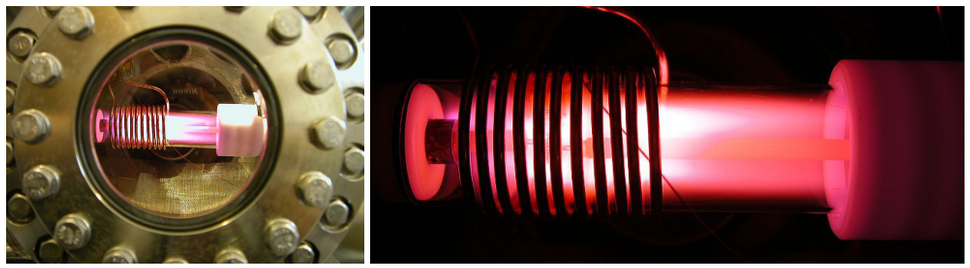
Poly(tetrafluoroethylene) (PTFE or Teflon) is a widely applied polymer in industry including micromechanics and biomaterials. The surface of PTFE was treated by nitrogen plasma-based ion implantation (PBII) and the induced changes were studied in surface properties like chemical composition, roughness, abrasive wear, wettability and surface electrical resistance. Extensive surface defluorination occurred, where the surface F/C atomic ratio correlated inversely with the acceleration voltage. The mean surface roughness increased, correlating directly with fluence and inversely with voltage. The wear volume increased after treatment due to the development of high surface roughness and post-treatment type surface oxidation. Water contact angle increased at low voltages and high fluences, due to preferential increase of roughness, and decreased at high voltages and low fluences, owing to intense defluorination and incorporation of N and O. The electrical resistance of the PBII-treated surfaces decreased by about five orders of magnitude, showing a significant inverse correlation with fluence. The described effects of the main parameters offer the possibility of purposefully altering the associated surface properties of PTFE by nitrogen PBII-treatment.




*Tuning the wettability of PTFE surface by changing the process parameters of N PIII treat-ment*

A review type article was accomplished on the synthesis and multisided characterization of Cr-, Si- and W- modified DLC coatings and has been accepted for publication in a special issue of the Surface and Coatings Technology.

A fast, efficient way of sidewall modification of multiwall carbon nanotubes was developed using RF- activated nitrogen plasma with appropriate DC bios, resulting in large amount of covalently built nitrogen into the outer 1-2 atomic layers of the CNTs. A model was developed for the quantitative evaluation of this modification taking into account the cilindrical geometry and the multi-stacked structure of the densely packed nanotubes.



*Surface modification of carbon nanotubes by nitrogen in a specially designed RF plasma reactor*





## 7.4 Nanostructured amphiphilic polymer conetworks

*Csaba Fodor*, Gábor Érsek**, Gergely Illés**, Béla Iván, Gergely Kali, Zsófia Osváth**, Szabolcs Pásztor**, Ákos Szabó*, Sándor Szabó, István Szanka* (* PhD student; ** university student, BME)*

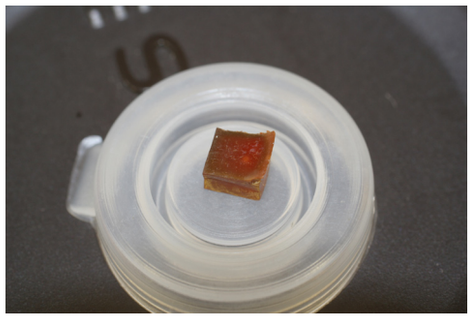
Poly(N,N-dimethylacrylamide)-l-polyisobutylene and poly(N-vinylimidazole)-l-poly(tetrahydrofuran) amphiphilic polymer conetworks were used to prepare nanohybrids containing various metal nanoparticles. The catalytic activity and the antimicrobial effect of these new materials were studied.

A modular synthetic method was developed to produce well-defined amphiphilic polymer conetworks by the combination of quasiliving atom transfer radical polymerization and click chemistry. In this process, propargyl telechelic macromolecules and azide-terminated star polymers were bonded by click reaction into a network structure.

*Preparation of a polymer conetwork gel*

The polymerizations of ethylene glycol dimethacrylate were performed with poly-(poly(ethylene oxide) methacrylate)-polyisobutylene triblock copolymers as macroinitiators, and in such a way amphiphilic conetworks were synthesized. The swelling and phase properties of these conetworks were investigated. Novel amphiphilic conetworks consisting of linear polyisobutylene and branched poly(di(ethylene oxide) methacrylate) segments have also been synthesized.

Conetworks based on N-isopropylacrylamide were synthesized using polyisobutylene-dimethacrylate and poly(ethylene glycol)-dimethacrylate cross-linkers. The thermal properties, as well as the amphiphilic and thermoresponsive swelling behaviour of these new materials were investigated. It was found that amphiphilic conetworks made of poly(N,N-diethyl acrylamide) as hydrophilic and polydimethylsiloxane, as well polyisobutylene as hydrophobic component possess lower critical solution temperature. The transition in these novel intelligent materials is immediate and reversible, and can be observed near to the body temperature.



*A polymer conetwork nanohybrid with silver nanoparticles: the „yellow silver”*

## 7.5 New type of polymers by quasiliving atom transfer radical polymerization

*Tamás Fekete**, Gergely Illés** Béla Iván, György Kasza*, Amália Soltész*, Ákos Szabó*, István Szanka, Klára Verebélyi* (* PhD student; ** university student, ELTE)*

Several synthetic methods have been developed to produce well-defined novel macromolecular architectures. The potential benefits of these new polymer systems include the unique and improved physical and chemical properties of the resulting polymers. Hyperbranched and star polymers were synthesized by quasiliving atom transfer radical polymerization (ATRP) in environmentally benign benzotrifluoride solvent with the use of commercially available monomers (styrene and (meth)acrylates). Several catalysts were tested to decrease the metal salt concentration. The produced multifunctional star and hyperbranched polymers with reactive functional groups are suitable for environmentally advantageous coatings and as starting materials for well-defined polymer network structures. They have also developed a new class of such materials capable of photocuring which can be applied as new dental filling materials.

*Quasiliving atom transfer radical polymerization (ATRP) systems*

The mechanical properties of poly(poly(ethylene oxide) methacrylate)-polyisobutylene triblock copolymers, investigated previously, were improved via coupling of poly(methyl methacrylate) segments to the triblock copolymers via ATRP. Flexible films were prepared from these new pentablock terpolymers.

## 7.6 Functional polymers by cationic polymerization

*Béla Iván, Brigitta Németh**, Viktória Pálfi, Ákos Szabó*, Klára Verebélyi* (* PhD student; ** university student, ELTE)*

*Preparations for the synthesis of a functional polymer*

The synthesis of unique macromolecular structures based on polyisobutylene and polystyrene with controlled structure and properties has been attempted via carbocationic polymerization studies. In order to easily synthesize functional polymers, studies were carried out on the reaction of polyisobutlyenes with olefinic chain end and various thiols to determine the optimal reaction conditions. This research resulted in various endfunctional polymer structures.

*A polymerization reaction system for obtaining highly functionalized polymers*

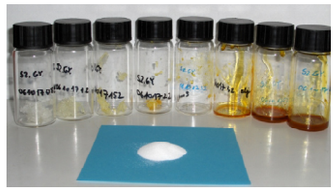
Polyisobutylene-poly(para-methylstyrene) block copolymers via quasiliving carbocationic polymerization were synthesized by sequential addition of monomers. The chemical modification of the poly(para-methylstyrene) blocks of these copolymers may open several ways to synthesize new, unique macromolecular structures with desired properties.

Styrene and divinylbenzne was copolymerized by carbocationic polymerization in an environmentally benign solvent with minimal amount of catalyst at room temperature. The reaction conditions were tuned in order to get polystyrene with hyperbranched structure bearing double bonds originating from the incorporated bifunctional monomer. As a result of these investigations, the preparation of such macromolecules capable to participate in further polymerization/functionalizing reactions can be achieved.

## 7.7 Environmentally advantageous degradation and transformation of polymers

*Márk Galát**, Béla Iván, Györgyi Szarka* (* PhD student; ** university student, ELTE)*

New processes, which may broaden the recycling possibilities of poly(vinyl chloride) (PVC), produced in the third largest amounts among polymers in the world, have been developed. Our research consisted of the degradative breakdown, transformation and polymer analogous reactions of PVC. Processes, which may lead to improved PVC products from the point of view of medicine and the environment, were also investigated. Thermooxidatively degraded PVC, obtained by a process based on their earlier results, was used to produce blends containing such PVC and biodegradable poly(lactic acid). Thus, new possibilities have been developed for the production of blends with biodegradable components.



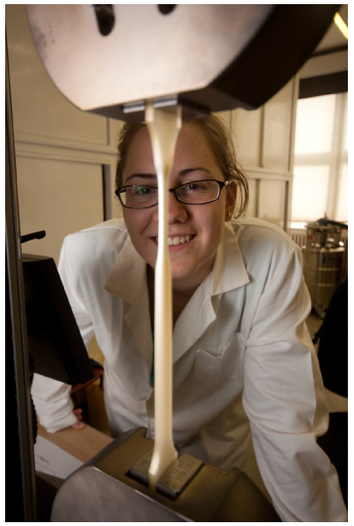
*Oil from PVC by mild, novel degradative process: a new recycling possibility*

PVC containing sequences of conjugated double bonds (polyenes) was prepared by thermal degradation, a process which is inevitable during industrial processing of this polymer. Subsequent modification of this polymer was investigated by thiol-polyene click reaction. Based on our results obtained during these studies, this process proved to be suitable for the saturation of the double bonds in the strongly colored PVC chain, and thus to produce new, modified PVC products. We have also developed an efficient method for azidation of PVC which may significantly broaden the modification possibilities of PVC via click chemistry.

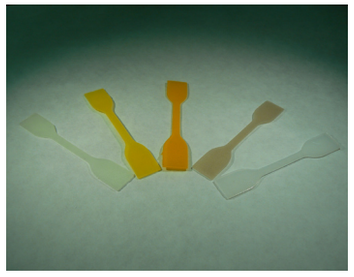
*Degradation apparatus for investigating environmentally benign degradation processes*

## 7.8 Determination of structure - property correlation in polyolefins and modification of properties

*Erika Fekete, Enikő Földes, Zsuzsanna Horváth*, Alfréd Kállay-Menyhárd (BME), Ildikó Kriston, János Móczó, Piroska Pataki*, Gábor Pénzes**, Béla Pukánszky, Károly Renner, Dóra Tátraaljai, József Varga (*PhD student)*



*Mechanical testing of samples made of natural antioxidants containing PE*



*Test samples of natural antioxidants containing PE*

The research in this area was further extended with academic, but even more with industrial partners. The questions indicated in the title were extensively investigated from the polymerization process to the interaction of additives and the modification of existing practice was suggested in several areas. The results are utilized directly in the development of additive packages of various polyolefin products, which increases the competitiveness of Tisza Chemical Works (TVK). Correlation was found between the chemical structure of phosphorous secondary antioxidants and their effect, and we proved that the exceptional stabilizing efficiency of phosphines is a consequence of their direct reaction with oxygen. Considering the expectations of the society against healthy food and its packaging materials, new research activities were launched to replace the presently used synthetic additives for natural antioxidants. The research is supported financially by the Hungarian Research Fund. The joint effort with Borealis, a multinational company producing polyolefins, led to correlations between the structure of various polypropilene polymers and copolymers as well as nucleating agents and the properties of the products. We found that the impact resistance of certain copolymers can be trebled by the addition of the proper type and amount of nucleating agent. The mechanism of nucleation was determined for a new soluble additive.

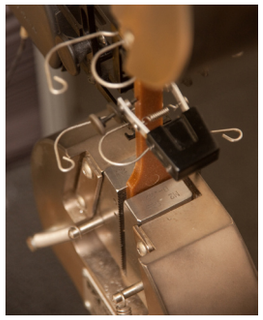




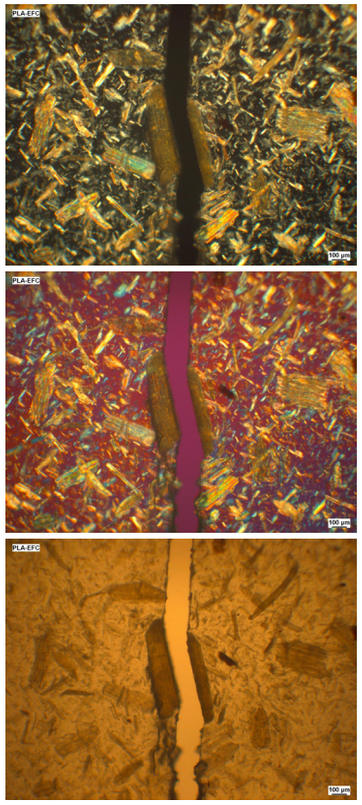
## 7.9 Natural and synthetic polymers and their compositions

*Kristóf Bagdi*, Zita Dominkovics*, Gábor Dora**, Gábor Faludi*, Erika Fekete, József Hári*, Balázs Imre*, Éva Kapin**, Gergely Keledi**, Csaba Kenyó*, János Kovács*, János Móczó, Kinga Molnár*, Péter Müller (BME), Béla Pukánszky, Károly Renner, András Sudár* (* PhD student; ** university student, BME)*

The study of traditional particulate filled composites yielded new information about the deformation mechanism of such materials. A novel method was developed for the quantitative determination of the strength of interfacial interactions in composites with strong adhesion. During the study of the deformation and failure mechanisms of polypropilene/lignocellulosic fiber composites, we came to the conclusion that composite properties are influenced mainly by the size and aspect ratio of the fibers. Failure of the product can be initiated by fiber fracture both in parallel and perpendicular directions, by debonding or fiber pull-out. It was also shown that the effect of surface modification of natural reinforcements depends on the character of the treatment and the improvement of all properties simultaneously is impossible. The study of the layered silicate/polyamide6 nanocomposites proved that although micromechanical deformation processes are influenced by the presence of the silicate, composite properties are mainly determined by the deformation of the matrix. Experience obtained during the study of polymer/layered silicate nanocomposites was summarized in several book chapters. More and more emphasis is put onto the study of biodegradable polymers and their composites. Nanocomposite films were successfully prepared from thermoplastic starch, the strength of which increased several folds as a result of reinforcement. Most of the above mentioned studies are connected to Hungarian or international coope-ration and research projects.



*Mechanical testing of wood flour containing polymer composites*



*The investigation of the degradation of a PLA/wood composite film by polarizing optical microscopy*

## 7.10 Fundamental research on biomass utilisation and on plastics recycling

*Marianne Blazsó, János Bozi*, Zsuzsanna Czégény, Emma Jakab, Zoltán Sebestyén*, Gábor Várhegyi (*PhD student)*

Catalytic conversion of the thermal decomposition products of halogen containing polymers has been investigated over zeolites in order to explore possible ways of catalytic dehalogenation of pyrolysis oils of plastics. It was revealed that chlorine bound to alkyl carbon atoms attached to an aromatic ring can be wholly eliminated from the molecule by sodium zeolites. However, chlorine atom is detached from an alkenyl chloride over sodium zeolite only if easily abstractable hydrogen atoms are available within the molecule. Chlorine atom attached to aromatic ring can be substituted by hydrogen merely over Na zeolite of high cracking activity. Nevertheless bromine atoms are partially eliminated from brominated aromatic hydrocarbons already over NaY zeolite of lower activity.

The alkaline pretreatment of the industrial hemp breaks up the strong fibers of hemp, which can be utilized as cellulosic fiber in composite materials as well as raw material for the second generation bioethanol production. The chemical composition and the thermal stability of the hemp samples undergone various alkaline treatments (NaOH, KOH) have been studied by thermogravimetry-mass spectrometry. It was concluded that the alkaline treatment removes certain functional groups of the hemicellulose component of hemp, while the residual alkali ion content has significant effect on the thermal decomposition mechanism. Correlations have been found between the thermal decomposition parameters, the altered composition of hemp, as well as the alkali ion content, by using principal component analysis.

The pyrolysis properties of agricultural by-products were studied from the aspects of bioenergy. A reaction kinetic evaluation strategy was developed that allowed reliable predictions outside of the given domain of experimental conditions.

*Evaluating gas-chromatograms*

*TG-MS measurement*

*Preparation of biomass samples*



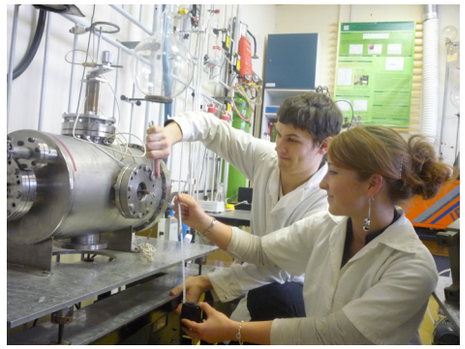


## 7.11 Atmospheric chemistry studies

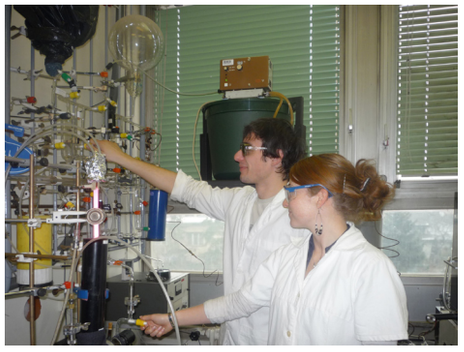
*Attila Demeter, Sándor Dóbé, Mária Farkas*, Ádám Illés**, Rebeka Nádasdi, Balázs Petri**, Emese Szabó*, István Szilágyi, Gábor László Zügner*, Dóra Zsibrita***
*(* PhD student; ** university student, BME)*

The photodissociation quantum yield ( ) of methyl ethyl ketone has been determined the first time under conditions relevant to the atmosphere by pulsed laser photolysis at 248 and 308 nm wavelengths coupled with gas-chromatographic analysis. was found to decrease with decreasing temperature and to decrease with increasing pressure. Kinetic analysis of the T- and P-dependent quantum yield data provided the experimental estimate of ES1 = 398 ± 9 kJmol–1 for the barrier on the first excited singlet state (S1). High-level quantum chemical computations carried out by the co-operating Japanese theoreticians have revealed that the photodecomposition undergoes by an unusual mechanism which involves a H-atom transfer on the S1 surface. The results of the authors have been featured on the cover page of the special issue of ChemPhysChem on atmospheric chemistry.

In our papers published last year, it was shown that N-(4-cyanophenyl)carbazole exhibits, contrary to N-phenylcarbazole, DMABN type dual luminescence, with ultrafast (fs scale) intramolecular charge transfer. The formation of the triplet excited species is an equally important energy consuming process for both molecules. Moreover, it was enlightened that pentacyano-N,N-dimethylaniline, in spite of the expectations, emits only from the locally excited state, which disappears in an exceptionally effective internal conversion reaction.



*Mounting of the vacuum chamber of the high-temperature photolysis reactor used for combustion kinetic studies*



*Alignment of the resonance-fluorescence detection line of the pulsed-laser photolysis apparatus used for atmospheric kinetic studies*

## 7.12 Environmental electrochemistry

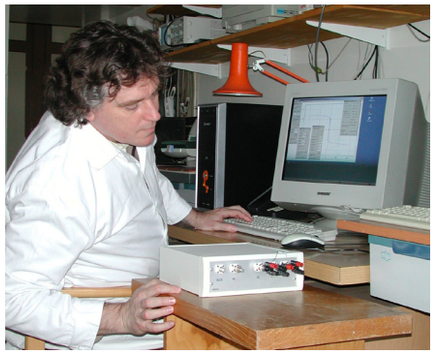
*István Bakos, Gabriella Lendvay-Győrik, Gábor Mészáros, Tamás Pajkossy, Sándor Szabó*

Ionic liquids - which are organic salts of fluid state even at room temperature – are regarded to be promising for modern, environmental-friendly electrochemical technologies; however, many fundamental property data and their theoretical analyses are still missing. To bridge the gap, electrochemistry studies have been done with the following results.

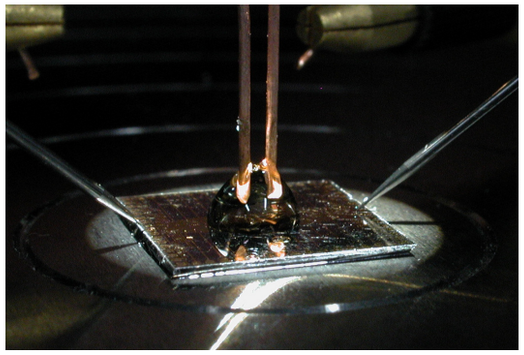
Au(100) single crystal electrode has been characterized in 1-butyl-3-metyl-imidazolium hexafluorophosphate electrolyte by voltammetry and impedance spectroscopy measurements. The potential of zero total charge has also been determined. By measuring temperature-dependence of double layer impedance parameters, data characterizing rearrangement kinetics have been obtained. The conclusion has been drawn that the current double layer theories are not applicable for treating metal / ionic liquid interfaces.

Quantized charge/discharge kinetics of electroactive monolayers formed by gold nanoparticles have been studied in four types of ionic liquids. These experiments lead to the conclusion that kinetic control varies with ionic liquid composition by about one order of magnitude. This can be attributed to the different chemical states of the ions in the electrolyte.

Various special electrochemical measurement systems have been developed: among others, three bipotentiostats of femtoampere resolution have been produced and installed for using with scanning probe microscopy experiments and single molecule conductance experiments in Austrian and Swiss laboratories, respectively.



*Instrument and software development*



*Electrochemical fabrication of nanocontacts on a silicon chip*





## 7.13 Destruction and energy utilisation of polychlorinated aromatics

*György Mink, Péter Szabó, Katalin Száraz*

The sized-up prototype plant belonging to the National Office for Research and Technology project entitled "Development of continuous operation technology for the dehalogenation of polychlorinated aromatic compounds" has been designed, and its working drawings have been elaborated. This activity also involved the selection of construction materials and the trial of their heat and corrosion resistance under real reaction conditions; the determination of the fluid mechanical characteristics of the system through theoretical calculations and by modelling the whole process in high laboratory scale, and the determination of the reaction heats of different feed stocks with different chlorine content by thermodynamical calculations.

*Laboratory size tube reactor*

*PCB dehalogenation and energy utilisation reactor under construction*

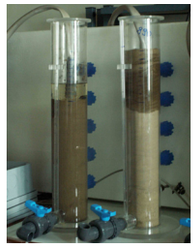
At present, the construction of the fully automated prototype of 100-200 t/y nominal capacity, depending on the exothermal heat of the overall reaction, is close to completion. The heat of the overall reaction will be utilised in two gas-gas and one water-gas heat exchangers. The trial and optimisation of the prototype plant will be done in March-April 2011. The work is going on in collaboration with members of the project consortium.

## 7.14 Monitoring and treatment of oil polluted soils

*Éva Fekete, Tibor Horváth, Béla Lengyel, György Mink*

A monitoring technology based on geoelectric measuring method has been applied to search oil contaminants in soils. During laboratory experiments, the resistance of different type of soils was measured, and the effect of various contaminants on the measured resistance was determined. The horizontal and vertical distribution and the migration of the oil were followed both in laboratory and in field.

Oxidizing treatment for oil contaminants was applied and its efficiency was measured indoor. Prior to the analytical measurements, oil had to be extracted from soil. An attempt to eliminate organic pollutants from soil by adsorption was made in a field experiment.



*Modeling the distribution of oil contaminants*

## 7.15 Participation in the activity of the Advisory Board of the red mud disaster Task Force

*László Kótai, Zoltán May, János Szépvölgyi*

Our institute played a major role in and carried out a significant part of surveying the environmental impacts caused by the red mud flood on October 4, 2010. Researchers of the institute communicated to government agencies and the society about the properties of the material, the risks of working with it, and the possible technologies of processing the high amount of stored red mud.

As members of the group of experts of the Hungarian Academy of Sciences, scientists of the institute participated in the activity of the Advisory Board of the Task Force of the Government, in cooperation with the National Directorate for Disaster Management.

The day after the disaster, samples were taken from the residue that spilled from the reservoir near settlements Kolontár and Devecser. After the first quick tests, the following measures were suggested to government agencies to contain and reduce the damage: the most urgent step was to decrease the basicity of the contaminant with e.g. gypsum, iron sulphate, magnesium sulphate, acetic acid or sulphuric acid. Application of gypsum has the further advantage that it can cover the red mud particles of a few micrometer sizes, preventing them from dusting after drying.

The basicity and the toxic heavy metal content of the soil were surveyed at different locations and at selected underground levels. According to the results, the soil of the fields covered by red mud have not been polluted by toxic metals, and the increase of the soil basicity of about three pH units was limited to the upper layer of about 10 cm thickness. For prevention of future disasters, our experts proposed the introduction of the technology they developed a few years earlier for processing the red mud with which all the valuable ingredients can be extracted in an economical way.

Appearing regularly in the broadcasted and printed media, scientists of the institute provided correct and up-to-date information to the domestic and international public about the consequences of the red mud flood and about the process of relief.

*View of the countryside after the red mud flood*

*Sampling the red mud covered soil*





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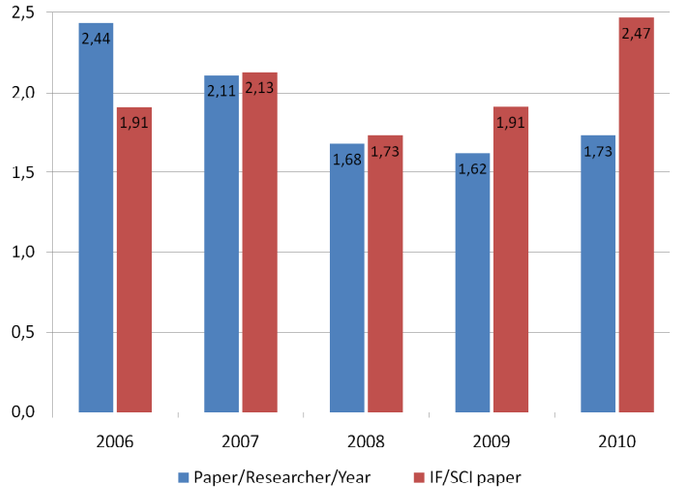
# 9 PUBLICATION DATA

Number of scientific publications by IMEC's co-workers and the mean impact factors of these publications changed in the following way in the last 5 years.






# 10 AWARDS

**János Szépvölgyi** was the recipient of the **Dénes Gábor Award** for his internationally recognized achievements in the fields of novel ceramic materials, plasma chemistry, and environmental and materials science.

**Béla Pukánszky** was awarded the **Leó Szilárd Professor Grant** for his excellent results in graduate, university, and rising generation education. By now, many of his former PhD students are leading experts and leaders of research institutes and companies. As a scientist, Béla Pukánszky got international recognition in the field of naturally reinforced and biodegradable plastics.

The **Hungarian Chemical Society Prize of Excellence** was awarded to **Szabolcs Pásztor** for his BSc thesis entitled "Synthesis of PMAA-l-PIB amphiphilic conetworks and investigation of their pH-dependent swelling properties". This work was supervised by **Professor Béla Iván** and **Gergely Kali, PhD**.

**Science Days** of the Chemical Research Center of the Hungarian Academy of Sciences:

- **György Kasza** won the Young Scientist Award for his talk entitled " Synthesis of hyperbranched polystyrene via carbocationic polymerization followed by Friedel-Crafts chain coupling". The coauthors of the paper were Gergely Kali, Márta Szesztay, and Béla Iván.

- **Mária Farkas** and **József Hári** got special honorable mention for their following excellent talks: M. Farkas, G.L. Zügner, I. Szilágyi, E. Szabó, D. Zsibrita, S. Dóbé: Kinetics of the elementary reaction of OH radicals with -valerolactone in the gas phase; E. Naveau, Z. Dominkovics, J. Hári, Ch. Jérôme, K. Renner, J. Móczó, M. Alexandre, B. Pukánszky: Effect of clay modification on the mechanism of local deformations in PA6 nanocomposites.

- The winning posters of the Poster Exhibition were: **I. Mohai, M. Mohai, I. Bertóti, Z. Sebestyén, P. Németh, A. Gergely, I.Z. Babievskaya, J. Szépvölgyi**: Formation of thin boron nitride coating on multiwall carbon nanotube surfaces and **S. Dóbé, R. Nádasdi, G.L. Zügner, M. Farkas, S. Maeda, K. Morokuma**: On the atmospheric photochemistry of methyl ethyl ketone.

## 11 CONFERENCES, PROGRAMS

The symposium on **„Free radicals and trace elements"** was instituted on 17th of September 2010, at the Chemical Research Center of the HAS in Budapest. The organizers were Klára Szentmihályi (IMEC CRC HAS) and Judit Jakus (IBC CRC HAS). The purpose of the symposium was to give an opportunity to the experts and students to present their works. The following topics were discussed: new results in the research of free radicals and trace elements, the role of free radicals and trace elements in the living organisms, connection of free radicals and trace elements. 59 active participants were present and 23 lectures were given.

The **"Hungarian-Romanian Workshop on Ceramic Coatings by Thermal Spraying"** was organized by Ilona Mohai (IMEC CRC HAS) and Réka Barabás (Babes-Bólyai University). The one-day-long workshop was held on 29th of April, 2010 with the aim of providing an opportunity for researchers working in the field of ceramic coating deposition to meet and consult. Several presentations were given from both Hungarian and Romanian sides in the morning session, while, in the afternoon the guests visited the laboratories of our institute. The workshop was sponsored by the Domus Hungarica Scientiarium et Artium Fund and the IMEC.

The **"Curious Chemist"** summer camp was organized by the institute the second time in 2010 with participants from 25 Hungarian and 2 Transylvanian towns and cities. By evaluating the students' grant proposals, the most talented 35 of them were chosen, and given the opportunity to work for one week on one of the 19 modern research projects. All four institutes of the Chemical Research Center contributed to the summer research camp with their subjects and researchers, served as supervisors. Twelve students worked for the Institute of Materials and Environmental Chemistry in the following fields: reaction kinetics investigations with lasers, the world of the lighting molecules, archaeometry studies, biomass materials, fullerenes and biodegradable polymer composites, synthesis of hiperbranched and linear polymers, biocompatible polymers.

*Participants of the summer research camp*



## 12 PARTICIPATION IN THE UNIVERSITY EDUCATION

Researchers of the institute delivered the following graduate and undergraduate lectures and laboratory courses:

### at the Budapest University of Technology and Economics (BME)

- Additives of plastics (lecture, János Móczó)
- Advanced ceramics (lecture, János Szépvölgyi)
- Application of plastics (lecture, Erika Fekete)
- Bioengineering processes (laboratory course, Zoltán Sebestyén)
- Bioreactors and engineering (laboratory course, Zoltán Sebestyén)
- Characterization of ceramic materials (laboratory course, Miklós Mohai, Zoltán Károly, Szilvia Klébert)
- Composites (laboratory course, János Móczó, Károly Renner)
- Deformation and break of polymers, Deformation of wood, Micromechanics (laboratory course, János Móczó, Károly Renner)
- Degradation and stabilization of polymers (lecture, Enik Földes)
- Drug formulation: surface modification and surface analysis (laboratory course, Ilona Mohai, András Tóth)
- Economic questions of plastics industry (lecture, Károly Renner)
- Identification of plastics (laboratory course, Erika Fekete, Dóra Tátraaljai)
- Injection molding (laboratory course, Károly Renner)
- Introduction to laboratory practice (laboratory course, Károly Renner)
- IR spectroscopic studies of polymers (laboratory course, Enik Földes, Piroska Pataki)
- Materials Science (lecture, Béla Pukánszky)
- Mechanical testing of polymers (laboratory course, János Móczó, Károly Renner)
- Physical chemistry (laboratory course, Gábor László Zügner)
- Physics of polymers (lecture, János Móczó)
- Plant projecting (laboratory course, Dóra Tátraaljai, János Móczó, Piroska Pataki, Károly Renner)
- Plastics (lecture, Béla Pukánszky)
- Plastics (lecture, János Móczó)
- Plastics and environmental protection (lecture, Enik Földes)
- Polymer blends (laboratory course, János Móczó)
- Polymer blends and composites (lecture, Béla Pukánszky)
- Polymer physics (lecture, Béla Pukánszky)
- Processing of plastics (lecture, Béla Pukánszky)
- Processing of PVC (laboratory course, Enik Földes)
- Rheology (laboratory course, Dóra Tátraaljai)
- Structure and properties of plastics – Rheology, Solidity of plastics, Polymer composites (lecture, Béla Pukánszky)
- Thermoforming (laboratory course, Károly Renner)

## at the Eötvös Loránd University (ELTE), Budapest

- Analytical chemistry (special laboratory course, Miklós Mohai)
- Designed syntheses of macromolecules (lecture, Béla Iván)
- Fundamentals of macromolecular chemical processes (lecture, Béla Iván)
- GC-MS (laboratory course, Marianne Blazsó, Emma Jakab, János Bozi)
- Molecular engineering of macromolecules (lecture, Béla Iván)
- Photochemistry (laboratory course, Attila Demeter)
- Photophysics and photochemical kinetics (lecture, Attila Demeter)
- Physical, organic and analytical chemistry principles of molecular engineering of macromolecules (lecture, Béla Iván)
- Polymer chemistry (laboratory course, Béla Iván)
- Polymer chemistry and technology (lecture, Béla Iván)
- Polymer chemistry and technology (special laboratory course, Béla Iván)
- Thermal treatment reactions for waste management (lecture, Marianne Blazsó)

## Ph.D. theses defended

- Péter Mezey: Synthesis and structural characterization of poly(N,N-dimethyl acrylamide)-l-polyisobutylene amphiphilic conetworks and nanohybrids therefrom, ELTE, supervisor: Béla Iván
- Viktória Pálfi: Synthesis of polyisobutylene with carboxylic chain end functionality and its reactions, ELTE, supervisor: Béla Iván
- Károly Renner: Micromechanical deformation processes in polymer composites, BME, supervisor: Béla Pukánszky

## M.Sc. theses supervised by researchers of the institute

- Ákos Hellner: Synthesis and analysis of hyperbranched poly(methyl methacrylate-co-ethylene glycol dimethacrylate) via quasiliving atom transfer radical polimerization, ELTE, supervisor: Béla Iván
- Gergely Keledi: Characterization of the miscibility of PVC/etylene copolymer blends, BME, supervisor: János Móczó
- Gábor Szabó: Effect of processing time and clay particle size on the structure and properties of polypropylene/clay nanocomposites, BME, supervisor: Erika Fekete

## B.Sc. theses supervised by researchers of the institute

- Péter Bak: Structure-property correlation in recycled polypropylene/wood composites, BME, supervisor: Béla Pukánszky, consultant: András Sudár
- Éva Bandi: Application of inverse gaschromatography for the characterization of the surface properties of cellulose substrates, BME, supervisors: Emília Csiszár, Erika Fekete
- József Bere: Development of multilayer packaging products containing recycled PET, BME, supervisor: Béla Pukánszky, consultant: Balázs Imre
- Lorántfy László: Synthesis of new functional polyizobutylenes via quasiliving carbocationic polymerization, ELTE, supervisor: Béla Iván





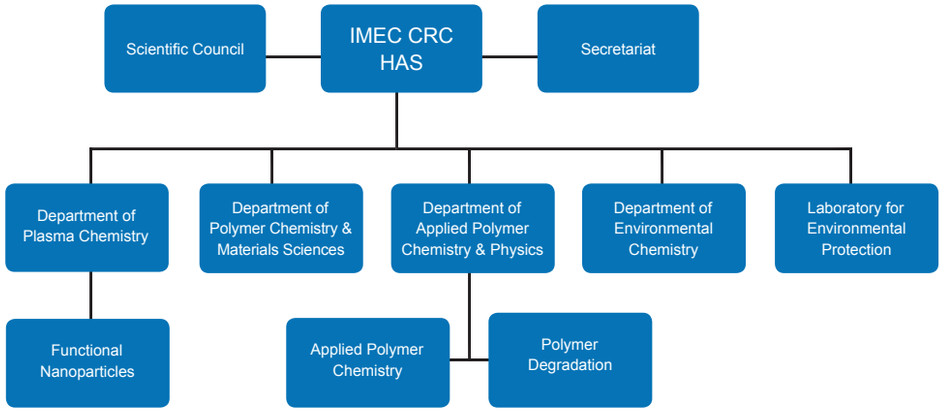
- Szabolcs Pásztor: Synthesis of PMAA-l-PIB amphiphilic conetworks and investigation of their pH-dependent swelling properties, ELTE, supervisors: Béla Iván, Gergely Kali
- Zsófia Péter: Modification of oxigen permeability of ethylene-vinylalcohol: interaction and structure, BME, supervisors: Béla Pukánszky, Károly Renner, consultant: Csaba Kenyó
- Péter Polyák: Synthesis of crosslinked PMMA particles by dispersion polymerization, BME, supervisor: Béla Pukánszky, consultant: József Hári
- Alekszandra Zsitkovszky: Effect of process conditions on the particle characteristics of wood flour filled PP composites, supervisor: János Móczó, consultant: Károly Renner

## Work, presented at the Scientific Students` Association Conference, supervised by researchers of the institute

- Éva Bandi: Application of inverse gas-chromatography for the characterization of the surface properties of cellulose substrates, Faculty 2nd Prize, BME, supervisors: Emília Csiszár, Erika Fekete
- Gábor Dora: Micromechanical deformation processes in PLA based biocomposites, Faculty 1st Prize, BME, supervisor: Béla Pukánszky, consultants: Gábor Faludi, Károly Renner
- Márk Galát: Modification reactions of poly(vinyl chloride) along the chain, ELTE, supervisors: Béla Iván, Györgyi Szarka
- Ádám Illés: Photochemical study of -valerolactone using pulsed-laser photolysis, BME, supervisors: Sándor Dóbé, Mária Farkas
- Gergely Illés: Synthesis of new polymer conetworks via a „click" coupling reaction, Eötvös Day Lecturer Award, ELTE, supervisors: Béla Iván, István Szanka
- Éva Kapin: Structure/property correlation in TPS/clay nanocomposite films, Faculty 3rd Prize, BME, supervisor: Erika Fekete
- Brigitta Németh: Synthesis of hyperbranched polystyrene via copolymerization of styrene and divinylbenzene under environmentally reaction conditions, ELTE, supervisors: Béla Iván, Klára Verebélyi
- Zsófia Osváth: Poly(N-isopropyl acrylamide) as intelligent material, Árpád Gerecs Prize, ELTE, supervisors: Béla Iván, Gergely Kali
- Szabolcs Pásztor: Synthesis of PMAA-l-PIB amphiphilic conetworks and investigation of their pH-dependent swelling properties, Alchemy Today Prize, ELTE, supervisors: Béla Iván, Gergely Kali
- Zsófia Péter: Modification of the gas permeability of polymers: interaction and structure, BME, supervisors: Béla Pukánszky, Károly Renner, consultant: Csaba Kenyó
- Balázs Petri: Kinetic study of the elementary reaction of OH radicals with ethyl-levulinate in the gas phase using the pulsed-laser photolysis technique, BME, supervisors: Sándor Dóbé, Gábor Zügner
- Dóra Zsibrita: Kinetic study of the elementary reaction of OH radicals with -valerolactone in the gas phase using the fast discharge flow technique, Faculty Distinguished 1st Prize, BME, supervisors: Sándor Dóbé, Mária Farkas

# 13 GENERAL INFORMATION

## Organization




## Staff

| | |
|---|---|
| 43 | scientists |
| 3 | engineers |
| 15 | PhD students |
| 19 | technicians |
| 5 | administrators |

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# 14 ORGANIZATION*

## Director

| | |
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| Szépvölgyi, János | DSc, science adviser |

## Secretariat

| | |
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| Beck, T. Mihály | emeritus professor, member of HAS |
| Babos, Gábor | technician |
| Kótai, László | PhD, senior research fellow |
| Kránicz, Andrea | secretary |
| Mezei-Seres, Ágota | financial manager |

## Department of Plasma Chemistry

| | | |
|---|---|---|
| **Head** | **Mohai Ilona** | PhD, senior research fellow |
| **Staff** | Ajler, László | technician |
| | Bertóti, Imre | DSc, emeritus science adviser |
| | Fazekas, Péter | PhD student, junior research fellow |
| | Feczkó, Tivadar** | PhD, senior research fellow |
| | Fodorné Kardos, Andrea** | junior research fellow |
| | Gulyás, László | technician |
| | Károly, Zoltán | PhD, senior research fellow |
| | Kereszturi, Klára | PhD, research fellow |
| | Keszler, Anna Mária | PhD, research fellow |
| | Klébert, Szilvia | PhD, research fellow |
| | Laczkó, Zsuzsa | technician |
| | May, Zoltán | PhD, senior research fellow |
| | Mohai, Miklós | PhD, senior research fellow |
| | Petrikowsky, Ottó | electrical engineer |
| | Szentmarjay, Erika** | technician |
| | Szentmihályi, Klára | PhD, senior research fellow |
| | Tóth, András | CSc, senior research fellow |
| | Tóth, Judit** | PhD, research fellow |

* As for March 1, 2011

** *A joint group with the Research Institute of Chemical and Process Engineering, Faculty of Information Technology, University of Pannonia*

## Department of Polymer Chemistry and Materials Science

| | | |
|---|---|---|
| **Head** | **Iván, Béla** | DSc, science adviser |
| **Staff** | Fodor, Csaba | PhD student, junior research fellow |
| | Haraszti, Márton | PhD, research fellow |
| | Kali, Gergely | PhD, research fellow |
| | Kasza, György | PhD student, junior research fellow |
| | Podlaviczki, Blanka | secretary, assistant |
| | Soltész, Amália | PhD student, junior research fellow |
| | Szabó, Ákos | PhD student, junior research fellow |
| | Szabó, L. Sándor | PhD, research fellow |
| | Szanka, István | PhD student, junior research fellow |
| | Szarka, Györgyi | PhD student, junior research fellow |
| | Verebélyi, Klára | PhD student, junior research fellow |

## Department of Applied Polymer Chemistry and Physics*

| | | |
|---|---|---|
| **Head** | **Pukánszky, Béla** | member of HAS, science adviser |
| **Staff** | Cseke, László | technician |
| | Erd -Fazekas, Ildikó | technician |
| | Fekete, Erika | PhD, senior research fellow |
| | Földes, Enik | DSc, science adviser |
| | Meskó, Mónika | technician |
| | Móczó, János | PhD, senior research fellow |
| | Pataki, Piroska | PhD student, junior research fellow |
| | Pénzes Gábor Pál | technician |
| | Renner, Károly | PhD, research fellow |
| | Selmeci, Erika | technician |
| | Szabó-Vers, Teréz | administrator |
| | Szauer, Judit | technician |
| | Tatay, Ede | technician |
| | Tátraaljai, Dóra | PhD student, junior research fellow |

* *A joint group with the Budapest University of Technology and Economics (BME), Department of Physical Chemistry and Material Science, Laboratory of Plastics and Rubber Technology*





## Department of Environmental Chemistry

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| **Head** | **Pajkossy, Tamás** | DSc, science adviser |
| **Staff** | Bakos, István | PhD, senior research fellow |
| | Blazsó, Marianne | DSc, emeritus science adviser |
| | Bozi, János | PhD student, junior research fellow |
| | Czégény, Zsuzsanna | PhD, research fellow |
| | Demeter, Attila | DSc, science adviser |
| | Dóbé, Sándor | DSc, science adviser |
| | Farkas, Mária | PhD student, junior research fellow |
| | Jakab, Emma | CSc, senior research fellow |
| | Lendvay-Gy rik, Gabriella | PhD, research fellow, science secretary |
| | Mészáros, Erika | PhD, research fellow |
| | Mészáros, Gábor | PhD, senior research fellow |
| | Metzger, Klára | administrator |
| | Sebestyén, József | technician |
| | Sebestyén, Zoltán | PhD student, junior research fellow |
| | Szabó, Emese | PhD student, junior research fellow |
| | Szabó, Sándor | DSc, science adviser |
| | Várhegyi, Gábor | DSc, science adviser |
| | Zügner, Gábor László | PhD student, junior research fellow |

## Laboratory for Environmental Protection

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| **Head** | **Horváth, Tibor** | PhD, senior research fellow |
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| | Fekete, Éva | research fellow |
| | Kéméndi-Fridrich, Erzsébet | technician |
| | Kiss, Mária | technician |
| | Lengyel, Béla | DSc, science adviser |
| | Lengyel, István | technician |
| | Mink, György | CSc, senior research fellow |
| | Prodán, Miklós | environmental engineer |
| | Sándor, Zoltán | research fellow |
| | Szabó, Péter | mechanical engineer |
| | Száraz, Katalin | junior research fellow |
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