INSTITUTE OF CATALYSIS AND SURFACE CHEMISTRY

POLISH ACADEMY OF SCIENCES

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CONTENTS

INSTITUTE OF CATALYSIS AND SURFACE CHEMISTRY

Polish Academy of Sciences

From theory to experiment and application

Institute of Catalysis and Surface Chemistry (ICSC) of the Polish Academy of Sciences in Krakow is the only scientific institution in Poland and one of eight in the world devoted entirely to research in catalysis and chemistry of interfaces. The Institute pursues interdisciplinary studies of the phenomena occurring at gas/solid, gas/liquid and liquid/solid interfaces, with emphasis on their significance in catalysis, materials engineering, adsorption, coating technologies and biomedical applications of dispersed systems,. ICSC integrates fundamental theoretical and experimental studies, and combines them with applied research so that the results obtained can be used directly to improve technological processes.

The number of employees is about 100, of which half are research staff. Over 20 PhD students are also involved in the research. ICSC is equipped with state-of-the-art research instrumentation, which serves not only Institute's employees but is also available to the whole scientific community.

Theory

An important aspect of the research carried out at ICSC is to provide the theoretical background for experimental studies. The methodologies employed involve quantum chemistry and solid state physics modelling methods, as well as molecular mechanics and Monte-Carlo simulation techniques. The field of expertise ranges from elucidating catalytic reaction mechanisms and modelling the structures of transition metal oxides, composite nanomaterials and enzyme active centres, to describing surfactant adsorption at liquid/gas and liquid/liquid interfaces, and simulating polymer particle adsorption on solid homogenous surfaces.

Experiment

The research activities of the Institute are very broad and versatile. The size of objects investigated ranges from 1 millimetre to less than 1 nanometre. The highest atomic resolution is available with the help of the Ultra High Vacuum Scanning Tunnelling Microscope. The time-scale of processes under study varies from centuries, as in the case of historical monument deterioration, to microseconds. The fastest recording equipment available is the High Speed Camera Speedcam, which can record pictures with more than 1000 Hz frequency.

The bulk of research is focused on the practical implementation of scientific results and encompasses design, synthesis, testing and practical verification of new, advanced materials and processes. In the area of heterogeneous catalysis, lots of effort is put into developing new, "intelligent" materials, with well-defined structure-property relations, tuneable to the requirements of a particular catalytic reaction. The materials under investigation include new types of oxidic structures and novel micro- and mesoporous inorganic solids. New magnetic materials and interactions between metallic nanoparticles deposited on single crystalline oxide surfaces are also investigated. The field of application encompasses selective oxidation, oxidative dehydrogenations, isomerization of hydrocarbons, end-of-pipe environmental catalysis, and green chemistry reactions. The work also involves the description of kinetic and mechanistic aspects of the studied processes. Research into homogeneous and enzymatic catalysis concentrates on bioactive and biomimicking systems. In the field of surface chemistry of dispersed systems, investigations are focused on understanding the mechanism of formation and stability of foams, nano- and colloid particle interactions, microencapsulation and biocompatible materials, as well as on description of adsorption phenomena. An important aspect of research is carried out by the culture heritage research group, whose work concentrates on the structure and properties of historic building and decorative materials, the deterioration mechanisms, as well as on the conservation and protection measures.

Application

Research carried out at ICSC is planned in such a way that the investigation outcomes can be turned into applications. In 1995, a spin-off company Katalizator Ltd. was created in order to promote the industrial implementation of catalytic materials designed at ICSC. This company, in which ICSC holds a control share packet, produces and sells catalysts synthesized according to ICSC-patented procedures to industrial partners in Europe and overseas.

Education

ICSC PAS is a parent institution for the International Postgraduate School, organised in cooperation with the Faculty of Engineering and Chemical Technology of the Krakow University of Technology, and the Faculty of Chemistry of the Rzeszów University of Technology. The School is attended by over 50 PhD students.

National cooperation

ICSC has a long-standing tradition of animating and coordinating research in the field of catalysis and surface science in Poland. For forty years the Institute has been organising the annual National Catalytic Colloquium, an extremely popular conference at which Polish scientists report their recent findings. The Institute is the coordinator of the National Catalytic Network “EKO-KAT Innovative catalytic materials in environmental protection”, National Network “SURUZ Surfactant and Dispersed Systems in Theory and Practice”, and newly established National Network "MANAR New Layered Materials with Controlled Architecture and Functionality", a member of the National Scientific Network „New Materials – Nanomaterials for Technical and Medical Applications”, the Polish Technology Platform of Sustainable Chemistry, the Regional Network of Centres of Excellence, the Regional Cluster of Information Technologies, the South Poland Regional Cluster of Clean Energy, the Consortium NANOTECH, the Consortium PAN-AKCENT, the Cluster Life Science, and the Polish Supramolecular Chemistry Network. In order to facilitate interdisciplinary research, a Joint Laboratory of Biotechnology and Enzymatic Catalysis (in cooperation with the Institute of Plant Physiology PAS) and a Centre for Surface and Nanostructures Research (in cooperation with the AGH-University of Science and Technology and the Krakow University of Technology) have been created. The Institute is also a co-founder of National Laboratory for Surface Studies.

International cooperation

ICSC PAN is widely involved in international cooperation. The activities include over 40 bilateral international collaboration schemes and participation in numerous EU scientific programmes. The bilateral collaboration with the Ukrainian Academy of Sciences led, in

1993, to the establishment of a Ukrainian-Polish Laboratory of Catalysis. In the years 2002-2006 the ICSC was granted the status of an EC Centre of Excellence “CATCOLL – the Krakow Research Centre of Molecular Catalysis and Soft Matter Chemistry”. CATCOLL activities contributed to the integration of the European scientific community through organising lectures by internationally renowned scientists, arranging study visits for researchers from different countries, and offering to young PhD students a unique opportunity to visit the leading European research laboratories.

Since 2005 ICSC is the host institution, responsible for the coordination of research and management of a Transfer of Knowledge project TOK-CATA. The project is implemented in collaboration with partner institutions (University of Nottingham, Consejo Superior de Investigaciones Cientificas, Stuttgart Universität, Humboldt Universität, Lunds Universitet.). The scientific program is carried out in the laboratories of ICSC by incoming foreign specialists and by outgoing selected staff members of ICSC in the laboratories of partner institutions. The principal overall objective of the project is the design and synthesis of porous catalysts with properties tuned to the requirement of a given catalytic reaction.

ICSC is also involved in the activities of two European catalysis networks: IDECAT and ACENET. IDECAT (Integrated Design of Catalytic Naomaterials for a Sustainable Production) is a Network of Excellence (NoE) launched in 2005 within 6th EU Framework Programme for Research and Technical Development. The Network is coordinated by the Consorzio Interuniversitario per la Scienza e Tecnologia dei Materiali, Italy and integrates 37 laboratories from 17 institutions in 11 countries (Italy, Belgium, Czech Republic, Finland, France, Poland, Spain, Sweden, Switzerland, The Netherlands, and The United Kingdom). The aim of IDECAT is to achieve a lasting integration between the main European Institutions in the area of heterogeneous, homogeneous and bio-catalysis via creating a coherent framework of research, know-how, training, promotion of science, spreading of excellence and technology transfer between the various catalysis communities. ACENET (Applied Catalysis European NETwork) ERA-NET network started in 2004 within 6th EU Framework Programme for Research and Technical Development and unites twelve research management and funding organisations from ten EU Member States: The Netherlands (Coordinator), France, Germany, Greece, Ireland, Italy, Poland, Portugal, Spain, and The United Kingdom. The aim of this ERA NET is to achieve coherence and cooperation between national research programmes and policies on applied catalysis. ICSC is responsible for the educational work package.

Currently ICSC is involved in 17 European projects of which 2 are financed by EEA financial mechanism and 2 are ERA-NETs projects. Additionally 3 projects of Sectorial Operational Programmes are carried out. In five projects ICSC PAS is the coordinating institution. Several 7th FP projects are being evaluated, 3 are in the negotiation phase.

Cultural Heritage and Environmental Protection

One of the focal points in the research carried out at ICSC PAS is the preservation of the natural environment and historical sites. Basic research is linked to practical conservation work. The culture heritage research group has animated a programme on the preservation of historic wooden churches, a unique heritage on the world scale. As a result of group activity the Roman cements, key materials for decorating facades of buildings during the nineteenth and early twentieth century, were re-established and used in renovation of several historic buildings in Europe, ensuring full compatibility between the historic substance and the repair technology. Recently, determination of the degradation mechanism of the early-Christian paintings in the St. Paulus Cave in the archaeological area of Epheus in Turkey and development of an action plan to mitigate the problems by controlling microclimate in the cave were successfully solved thank to the research and preservation programme coordinated by the Institute’s experts.

Moreover, the Institute has notable achievements in developing technologies for protecting the environment. One of them - SWINGTHERM - is a catalytic, low-energy-consumption process based on the Regenerative Catalytic Oxidation, targeted at the purification of waste gases from organic pollutants. It has already found its application in industry in Poland, Europe, Canada and Japan. In 2006 a new laboratory “Centre of Environmental Pollutants Analysis” was established, financed by the Sectorial Operational Programme grant.

Popularisation

It is our firm belief that making scientific research easily understandable to ordinary people is of immense importance for gaining public support in this area of human activities. Therefore, every year, ICSC PAS organizes Open Door Days, during which visitors may listen to popular lectures, participate in spectacular laboratory presentations and attend poster sessions depicting Institute’s research. The Open Door Days are aimed especially at young people from junior and senior high schools. They are very popular among students interested in science – every year ICSC receives ca. 1000 visitors. Institute participates also in the annual Science in Krakow Festival.

SCIENTIFIC TEAMS OF THE INSTITUTE

Research Groups

Adsorption

Professor Władysław Rudziński, DSc, PhD
Tomasz Pańczyk, PhD, Wojciech Piasecki, DSc, PhD, Piotr Zarzycki, PhD

Catalysis I

Professor Jerzy Haber, DSc, PhD, Dhc, PAN, PAU, AE, NANU member
Jan Połtowicz, PhD, Katarzyna Pamin, PhDEng, Erwin Lalik, PhDEng,
Edyta Tabor, MSc, PhD student, Robert Karcz, MScEng, PhD student

Catalysis II - Oxide Catalysts - Oxidation Reactions

Professor Barbara Grzybowska-Świerkosz, DSc. PhD
Marian Gąsior, PhDEng, Katarzyna Samson, PhDEng,
Małgorzata Ruszel-Kasza, PhD, Irena Gressel, technician

Catalysis III - Polymer Based Composites as Heterogeneous Catalysts

Associate Professor Alicja Drelinkiewicz, DSc, PhD
Anna Waksmundzka-Góra, PhD, Robert Kosydar PhD, Wojciech Stanuch, MSc,
Anna Knapik, MSc, PhD student, Adam Zięba, MSc, PhD student,

Colloids I

Professor Zbigniew Adamczyk, DSc, PhDEng, PAU member
Jakub Barbasz, PhDEng, Barbara Jachimska, PhDEng, Andrzej Kowal, PhD,
Małgorzata Nattich, PhDEng, Lilianna Szyk-Warszyńska, PhDEng.,
Paweł Weroński, PhD, Maria Zembala, DSc, PhD, Anna Bratek, MSc, PhD student,
Katarzyna Jaszczółt, PhDEng, Aneta Michna, MSc, PhD student,
Monika Wasilewska, MSc, PhD student, Elżbieta Porębska, technician

Colloids II - Colloid and Surfactant Systems

Associate Professor Piotr Warszyński, DSc, PhDEng
Grażyna Para, PhD, Ewelina Jarek, PhD, Marzena Noworyta, Eng,
Tomasz Jasiński, MSc PhD student, Jerzy Superata, MSc, PhD student,
Anna Trybała, MSc, PhD student, Magdalena Elżbiecik, MsC, PhD student, Dorota Dronka-Góra, MsC, PhD student, Krzysztof Szczepanowicz, MsC, PhD student

Cultural Heritage Research

Associate Professor Roman Kozłowski, DSc, PhD
Łukasz Bratasz, PhD, Grzegorz Adamski, PhD, Michał Łukomski, PhD,
Sławomir Jakieła, PhD, Anna Klisińska-Kopacz, PhD,
Łukasz Lasyk, M.Sc. Ph.D. student, Renata Tislova, M.Sc. Ph.D. student,
Dariusz Wilk, M.Sc. Ph.D. student, Bartosz Rachwał, M.Sc. Ph.D. student

Dispersed Systems

Professor Kazimierz Małysa, DSc, PhD
Marta Barańska, Eng, Wanda Barzyk, PhD, Marta Krasowska, PhD,
Marcel Krzan, PhD, Jan Zawała, MScEng, PhD student,
Anna Niecikowska, MSc, PhD student, Agnieszka Olszewska, MSc, PhD student

Electrochemistry of Mineral Systems

Associate Professor Paweł Nowak, DSc, PhDEng
Aleksandra Pacuła, PhD, Dawid Wodka, MSc, PhD student

Environmental Control

Tadeusz Machej, PhD
Janusz Janas, MSc, Robert Janik, MSc, Halina Piekarska-Sadowska, PhD,
Leszek Matachowski, MSc, Małgorzata Nattich, MScEng, PhD student

Heterogenous Reaction Kinetics

Associate Professor Ryszard Grabowski, DSc, PhD
Antonina Kozłowska, PhD, Piotr Olszewski, PhD, Michał Śliwa, MSc, PhD student,
Jan Mizera, MScEng, PhD student, Zofia Czuła, technician

Layered Minerals, Mesoporous Oxides, Nanostructures

Professor Ewa Serwicka-Bahranowska, DSc, PhD
Małgorzata Zimowska, PhD, Roman Dula, PhDEng, Alicja Michalik-Zym, PhDEng,
Dorota Duraczyńska, PhD, Daria Napruszewska, Eng, Jerzy Podobiński, MSc,
Wojciech Włodarczyk, PhDEng, Justyna Plona, MSc, PhD student

Polyoxometalates

Professor Adam Bielański, DSc, PhD, Dhc, PAN, PAU member
Anna Lubańska, PhD, Anna Micek-Ilnicka, PhD, Tomasz Kasza, PhDEng

Quantum Chemistry I

Professor Małgorzata Witko, DSc, PhD, PAN member
Renata Tokarz-Sobieraj, PhD, Robert Gryboś, PhD, Dorota Rutkowska-Żbik, PhD,
Maciej Szaleniec, PhD, Harry Kotsis, PhD, Paweł Hejduk, MSc, PhD student,
Jakub Goclon, MSc, PhD student

Quantum Chemistry II

Professor Ewa Brocławik, DSc, PhD
Tomasz Borowski, PhD, Artur Góra, PhD, Paweł Rejmak, MSc, PhD student

Surfaces, Thin films, Nanostructures

Professor Józef Korecki, DSc, PhDEng
Nika Spiridis, PhDEng, Jacek Gurgul, PhD, Robert P. Socha, PhD,
Dorota Wilgocka-Ślęzak, PhDEng, Kinga Freindl, MScEng, Ewa Zackiewicz MScEng

Zeolite Chemistry I

Professor Bogdan Sulikowski, DSc, PhDEng
Rafał Rachwalik, PhD, Ewa Włoch, PhD, Łukasz Mokrzycki, MSc, PhD student,
Urszula Filek, MScEng, PhD student, Dorota Walczyk, MscEng, PhD student

Zeolite Chemistry II

Associate Professor Mirosław Derewiński, DSc, PhDEng
Anita Burkat, MSc, PhD student, Veronika Pashkova, MSc, PhD student,
Adam Węgrzynowicz, M.Sc., Ph.D. student

Laboratories

AFM Laboratory
Jakub Barbasz, PhDEng, Andrzej Kowal, PhD, Małgorzata Nattich, PhDEng

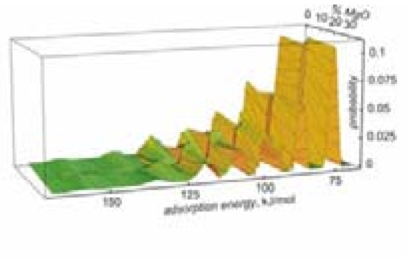
ESCA Laboratory
Jacek Gurgul, PhD, Robert P. Socha, PhD

X-Ray Diffraction and Thermoanalysis Laboratory
Professor Wiesław Łasocha, DSc, PhD
Maciej Grzywa, PhD, Dariusz Mucha, PhD

Microcalorimetry Laboratory
Erwin Lalik, PhDEng

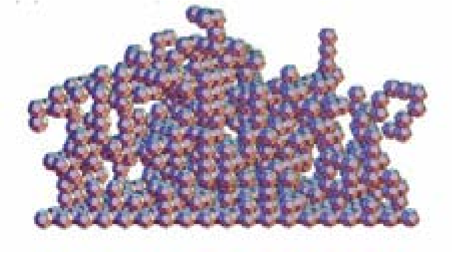
CEPA Centre for Environmental Pollution Analyses
Joanna Kryściak-Czerwenka, PhD, Janusz Janas, MSc

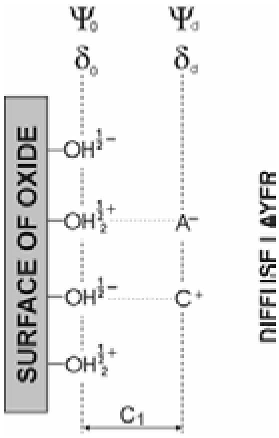
ADSORPTION



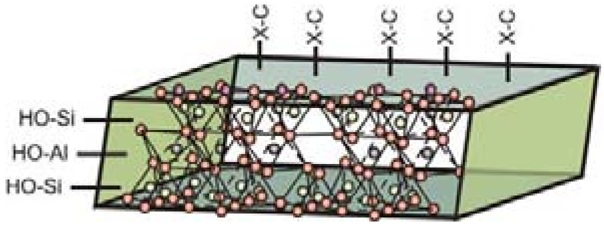
- application of the Statistical Rate Theory (SRT) for description of the adsorption kinetics
  - studies of fundamental features of the SRT approach
  - dissociatve adsorption on catalytically important surfaces
  - generalization of the SRT approach for the case of the energetically heterogeneous surfaces
  - theoretical origin of kinetic models of sorption used in environmental protection
- theoretical analysis of the temperature-programmed desorption spectra
  - determination of the adsorption energy distribution functions on catalysts surfaces

- studies of the transport processes in geometrically irregular/fractal structures
  - determination of the collision frequency factor on fractal surfaces





- application of the 1-pK Basic Stern Model of metal oxide/electrolyte interface to analyze ion adsorption from solution.
- theoretical interpretation of proton adsorption enthalpies.
- application of the Statistical Rate Theory (SRT) to investigate ion adsorption kinetics.

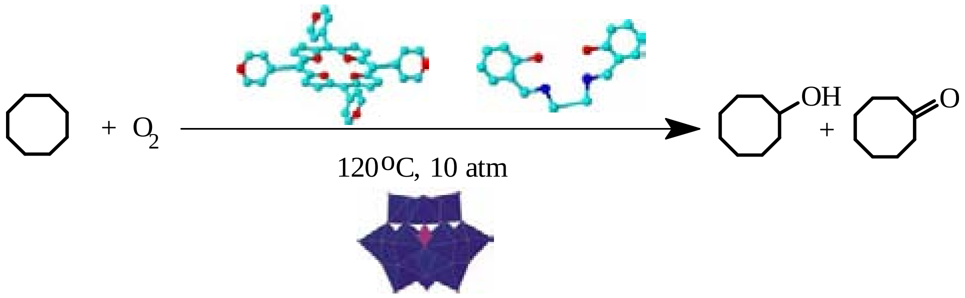


- ab-inito study of transition metal compounds
- quantum measurement along classical/quantum trajectory
- computational methods in geochemistry
- molecular modeling of complex systems (salvation, interfaces)
- new optimization schemes in the Density Functional Theory
- ab-initio molecular dynamics spectroscopy

CATALYSIS I

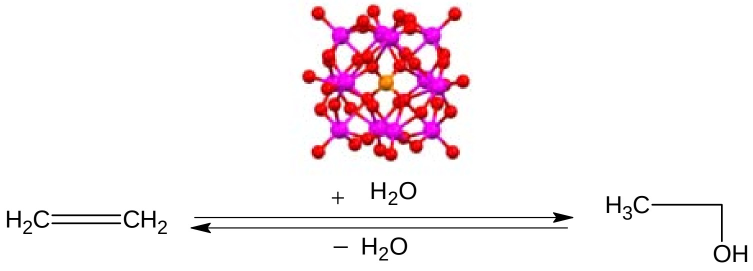
The unit "Catalysis I" addresses in its research the fundamental questions of the oxidation chemistry. It comprises 3 research groups:

- Oxidation of hydrocarbons in the liquid and gas phase
- Total oxidation of VOC in flue gases to prevent environmental pollution
- Influence of noble gases on heterogeneous catalytic oxidation

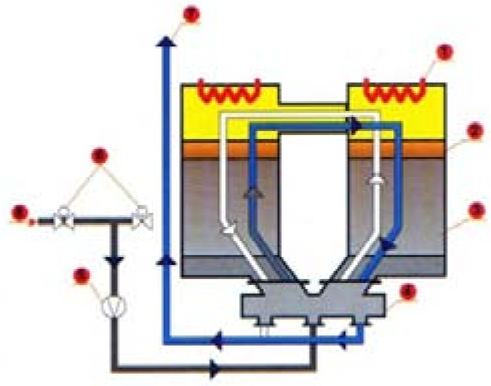


The mechanism operating in oxidation of cyclic alkanes in the liquid phase on metalloporphyrin has been elucidated, resulting in strong dependence of the rate on the type of axial ligand and the redox potential of the metalloporphyrin. The latter may be modified by electron donating substituents, which accelerate the chain initiation and electron accepting substituents, which accelerate chain propagation.

Keggin type polyoxometalates compounds of tungstophosphoric and molybdo phosphoric acids were also studied, for catalytic applications, due to their easy preparation, relatively high thermal stability and redox and acidic properties. These properties .were verified in the dehydration of ethanol or hydration of ethylene.



It was shown that catalytic propereties can be modyfied by changing central atom, atom addenda or compensation ion.



Regenerative catalytic oxidation system for volatile organic compounds (VOCs) was developed, which permits the destruction of pollutants from flow gases autothermally.

CATALYSIS II - Oxide Catalysts - Oxidation Reactions

I. Oxidative dehydrogenation of lower alkanes (ethane, propane, isobutane) on supported transition metal oxides, TMO (V_2O_5, MoO_3, Cr_2O_3)

- effect of additives (alkalis – mainly K, transition metals [Ni, Cr, Nb, Mo], P, W)
- active centres and mechanism in porous systems *(running)*

Main conclusions:
1. Effect of additives on catalytic performance depends on the nature of both active TMO and the support, as well as on the type of alkane.
2. **Potassium** additive to oxide catalysts of oxidation reactions modifies:
* acido-basic properties: decreases acidity, increases basicity,
* redox properties: decreases reducibility
* interaction of catalyst with oxygen: oxygen coverage, forms of oxygen

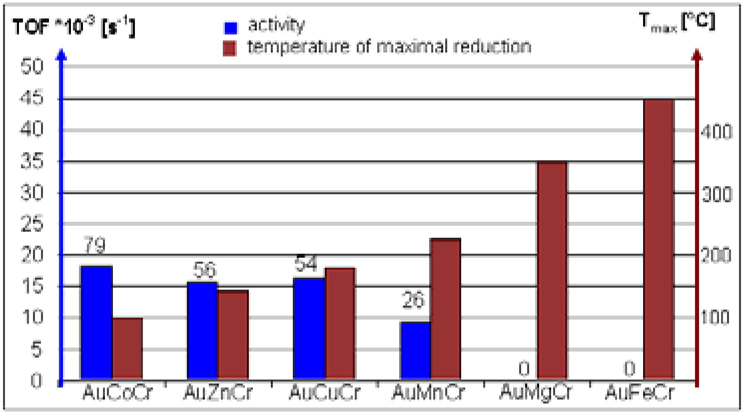
For catalysts of considerable acidity (high concentration of acidic centres), like VO_x/SiO_2, VO_x/TiO_2, the increase in the selectivity to olefins (for number of C atoms > 2) in the presence of **K** additive is due mainly to decrease in the acidity and increase in basicity: K facilitates desorption of olefins, thus preventing consecutive reactions of olefins total oxidation to CO_x

For catalysts of low acidity and dominating basic character (VO_x/MgO, CrO_x/oxide support) the effect of the **K** additive on the selectivity in ODH reactions is controlled by the changes in the catalyst-oxygen interaction (coverage of catalyst surface by oxygen θ)
* increase in θ (CrAl) – decrease in the olefin selectivity
* decrease in θ (CrTi) – increase in the selectivity

3. KVSi promising catalysts for ODH of propane and CrAl, CrTiK–for ODH of isobutane.

II. Au-nanoparticles on oxide supports as catalysts for oxidation of CO, preferential oxidation of CO (in the hydrogen presence, PROX) and of hydrocarbons

- Role of oxide support in oxidation reactions: oxides of main group elements [e.g. SiO_2, MgO], oxides of transition metals [e.g. TiO_2, FeO_x, MoO_3, V_2O_5], chromium spinels $M^{II}Cr_2O_4$ (M^{II}=Co,Zn,Mn,Mg,Fe), Au dispersed on Ti(Ce)–SBA-15 porous systems



Correlation of reducibility of the support and activity of the Au/$M^{II}Cr_2O_4$ catalyst in CO oxidation

Main conclusions:

* activity in CO oxidation and selectivity in oxidation of C_3 hydrocarbons is related to the reducibility of the oxide supports: activity increases with the reducibility
* the CO oxidation on the catalysts containing hardly reducible supports is more sensitive for Au particle size
* chromium spinels $M^{II}Cr_2O_4$ (M^{II} = Co, Mn, Zn) are promising supports for Au nanoparticles in CO oxidation and preferential CO oxidation

CATALYSIS III - Polymer Based Composites as Heterogeneous Catalysts

Research activities include the studies of polymers as catalysts and catalytic supports for the reaction performed in liquid phase. Nitrogen-containing polymers, electroactive such as polyaniline and electroinactive poly(4-vinylpyridine) as well as microporous and macroporous functionalized, crosslinked resins, derivatives of polyacrylic acid and styrene are studied. Polymers in the form of powder and film deposited onto various carriers (carbon, silica) are used. Role of specific properties of polymer matrix like hydrophobic character, swelling ability electroactive function in the activty/selectivity pattern of catalytic reaction is considered.

Main research topics :

A. Catalysts for hydrogenation reactions

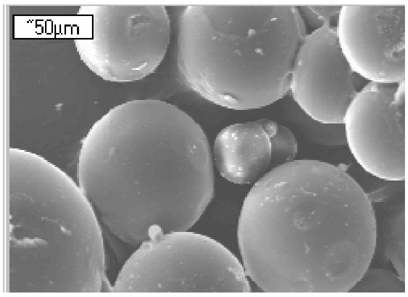
Preparation of metal - polymer nano-composites (Pd, Pt)

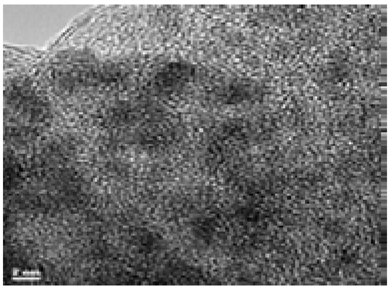
Incorporation of Pd, Pt to polymer matrix is carried out using $PdCl_2$, $Pd(OAc)_2$, $Pd(acac)_2$ and H_2PtCl_6 in aqueous and non-aqueous solutions.

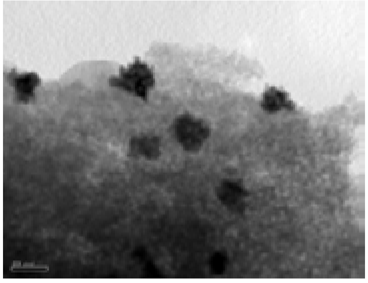
Characterization of Pd (Pt)-species in the metal-polymer catalysts
methods : BET, FTIR, UV-VIS, Raman, XPS, XRD, EXAFS, SEM, TEM, HRTEM

Catalytic tests; liquid phase hydrogenation of carbonyl compounds (acetophenone, 2-ethylanthraquinone), alkynes (2-butyne-1,4-diol, phenylacetylene, hexyne) and alkenes (unsaturated carboxylic acids). Reaction products control by GC analysis.

Main conclusions: Almost selective hydrogenation of alkyne to alkene (selectivity ~100%) is attained due to hydrophobic and electroactive function of polyaniline as well as when the resin-based catalysts are in expanded state under catalytic run.


Pd/microporous resin


Pd/poly(4-vinylpyridine)


Pd/polyaniline(SiO_2)

B. Bio-fuel synthesis in transesterification of castor oil by methanol (Biodiesel)

Preparation of acid catalysts by modification polymers by various acids (inorganic and organic). Polyaniline in the form of powder and films (10, 20, 30 wt % polymer) deposited onto carbon and SiO_2 carriers are used.

Catalytic tests; transesterification of castor oil by methanol (ethanol) in homogeneous and heterogeneous conditions, reaction products control by GC and HPLC methods. Two series of solid acid catalysts are studied. The first consists of heteropolyacid/ZrO_2 obtained by impregnation and sol-gel methods, the second is represented by polymer-based acid catalysts.

Main conclusions: activity of catalysts is determined by the leaching of "acid" function from the catalysts and oil-catalyst (support) interaction

COLLOIDS I

General

Understanding the dynamics of colloid and disperse systems is crucial for a quantitative prediction of such phenomena as aggregation, coagulation, flocculation, coalescence, membrane fouling, phase separation, foam formation and stability, rheology etc. being of fundamental importance for the electronic, pharmaceutical and cosmetic industries. Equally important role play interactions of colloid particles, bubbles, and bioparticles (proteins, viruses, bacteria) with interfaces leading to adsorption, deposition, and adhesion. A quantitative description of these processes has implications not only for polymer and colloid science, biophysics, and medicine but also for many modern technologies involving separation procedures, e.g. water and waste-water filtration, membrane filtration, food emulsion formulation, flotation, protein and cell separation, immobilization of enzymes in membranes, biosensors, immunological assays, etc.

On the other hand, by observing dynamic phenomena occurring in colloid system one can gain important clues on mechanisms and kinetics of processes appearing in molecular scale that cannot be studied by direct experimental methods. Especially attractive seems the possibility of exploiting colloids as reference systems for elucidating protein adsorption kinetics and to calibrate indirect methods of determining their concentration on surfaces (film thickness). Colloid particles of larger size also can be used for detecting adsorbed macromolecules and other surface features of nanometer size range.

Main Research Topics

- Convective diffusion of interacting colloid particles.
- Electrostatic double-layer interactions during particle adsorption
- Elecrokinetic phenomena and particle motion in electric fields
- Colloid (emulsion) dynamics and stability
- Electroviscous phenomena and suspension rheology
- Self assembling monolayers of colloids
- Mechanisms and kinetics of irreversible adsorption at solid/liquid interfaces
- Polyelectrolyte and protein adsorption
- Biocompatible coatings

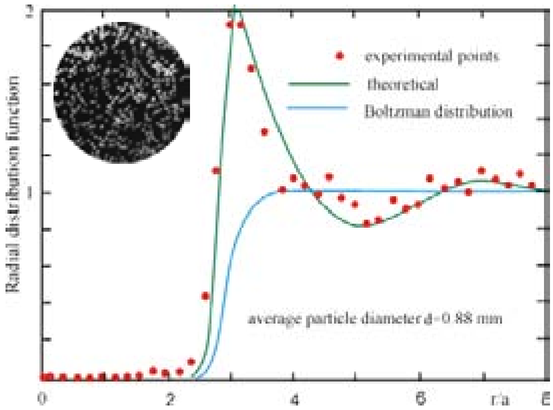


Fig.1. Distribution of latex particles on mica surface determined by direct microscope observations.

Main Achievements of the group

Generalization of Levich's convective diffusion theory,

Generalization of the Random Sequential Adsorption (RSA) model to polydisperse and nonspherical particles.

New theory of adsorption on heterogeneous surfaces.

Elaborating of a theory of electrokinetic phenomena for particle-covered surfaces.

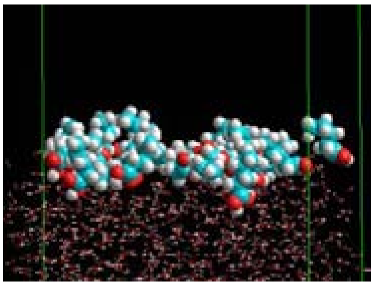
Discovery and experimental confirmation of the "inverse salt" effect.

First measurement of the 2D pair correlation function of adsorbed particles (see Fig. 1).

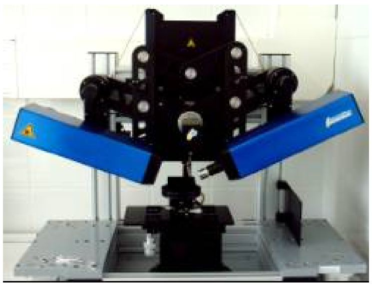
Experimental measurements of multilayer formation of polyelectrolytes.

Developing new experimental method of surface cluster formation of tergetd architecture.

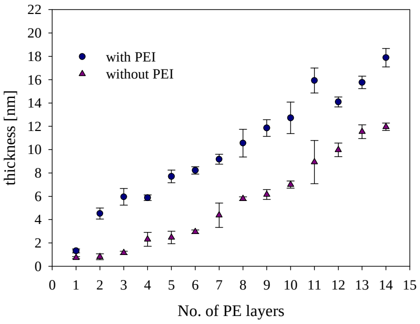
COLLOIDS II – Colloid and Surfactant Systems



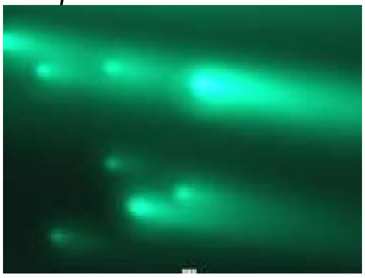
Simulation of adsorption of pentanoic acid at air/water interface



Imaging ellipsometer for thin layer thickness and topography measurements

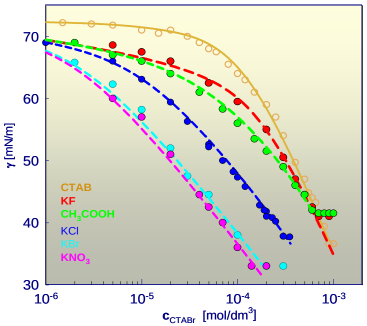


Thickness of PAH/PSS multilayer film with and without anchoring layer



Release of fluorescent dye from microcapsules attached to a surface

Profile of the pendant drop for surface tension measurements by drop shape analysis



Effect of type of anion on adsorption of cationic surfactant CTAB

RESEARCH TOPICS:

- *Thermodynamics and molecular mechanism of adsorption and self-organization of amphiphatic species at liquid/gas, liquid/liquid, liquid/solid interfaces;*
- *Experimental studies and molecular mechanics modeling of adsorption processes;*
- *Adsorption of polyelectrolytes, colloids, bio-colloid particles and microcapsules at solid/liquid interfaces in various flow regimes. Formation of nanostructured coatings;*
- *Structure and permeability of polyelectrolyte multilayers;*
- *Theoretical description of the structure of nonlinear double layer around single colloidal particle and for particle systems (including particle/interface case);*
- *Elektrokinetic phenomena with application to colloid and bio- colloid particles. Theory of electrophoretic mobility of complex systems. The electrokinetic phenomena for particles at interfaces and their role in adsorption;*
- *Colloidal hydrodynamics with application to adsorption, foam stability, etc.*

EXPERIMENTAL TECHNIQUES:

monochromatic imaging ellipsometry; fluorescent microscopy; surface tension/surface potential; drop shape analysis (surface&interfacial tension, contact angle);

MAIN ACHIEVEMENTS:

- *Description of electric double layer interactions for the charged spherical particles at charged interface and description of the fluid flow in the impinging jet and slot impinging jet cells;*
- *Theory of the transport of colloidal particles to the non-homogeneous interfaces and theory of the electrokinetic forces acting on the charged particle moving at the interface;*
- *Quantitative description of electro-hydrodynamic scattering effect;*
- *Theoretical model of the effect of deposited particles on the streaming potential of solid surfaces;*
- *Improved models of adsorption of nonionic and ionic surfactant and their mixtures at liquid/air interface;*
- *Explanation of pH dependent surface activity of alkanoic acids and explanation of the role of counterions in ionic surfactants adsorption;*
- *Determination of the role of PEI anchoring layer on the properties of polyelectrolyte multilayer films.*

CULTURAL HERITAGE RESEARCH

The research is focused on structure and properties of historic building and decorative materials, mechanisms of their deterioration, and measures to conserve and protect them. Special emphasis is laid on phenomena occurring at the material surfaces and direct tracing of physical change in historic materials using non-destructive methods. The basic research is linked to extensive case studies and practical conservation work.

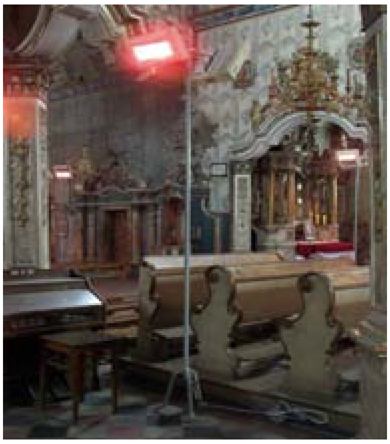
Our main research areas of expertise comprise:

Monitoring historic sites and objects using a range of physical sensors with a remote data recovery via the GMS transmission system.

Monitoring of acoustic emission to trace directly the evolution of fracturing in works of art at the micro-level.

Measuring water vapour adsorption and transport, and related dimensional change in historic materials, in response to microclimatic variations.

Re-establishing the production and use in conservation of Roman cements, the key materials for decorating the exterior of buildings during the nineteenth century.

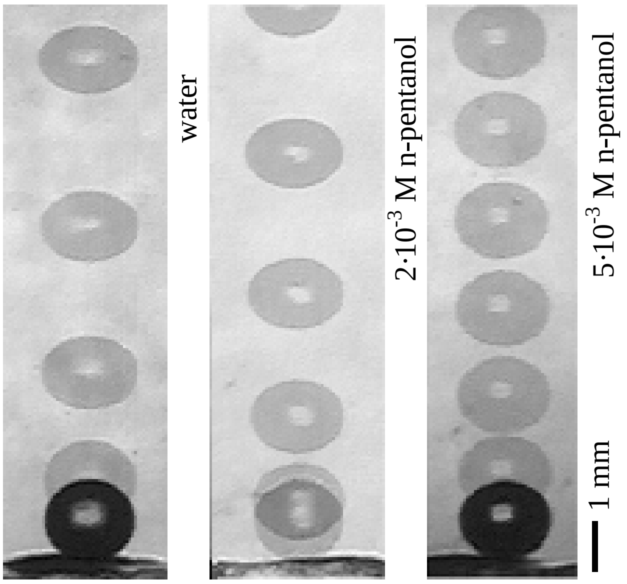


Investigating and optimising heating systems in historic churches.

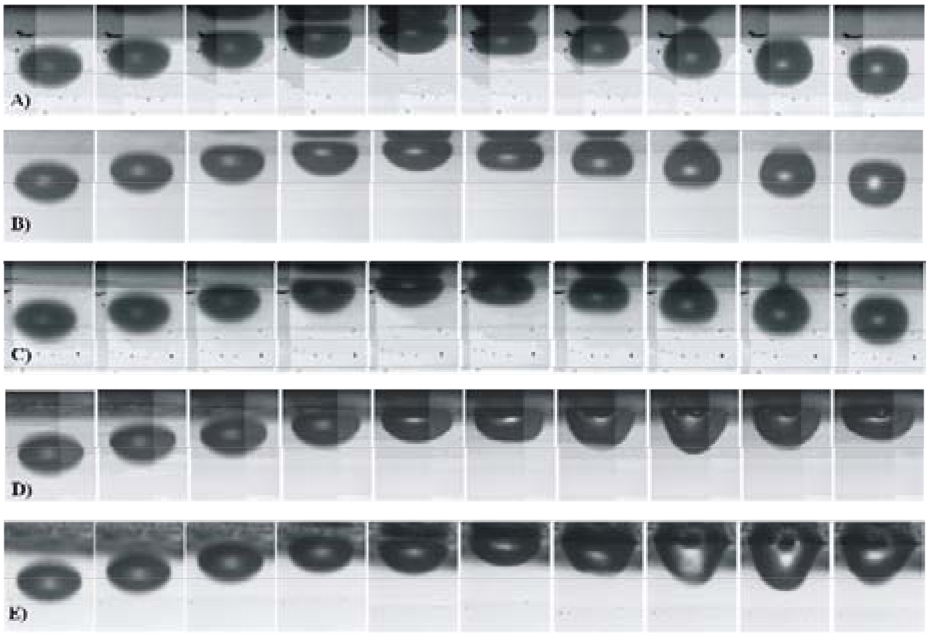
Using advanced laser techniques for monitoring damage areas in painted surfaces.

DISPERSED SYSTEMS

Research interest is focused on mechanism of formation and stability of dispersed systems, especially foams and flotation aggregates: bubble-grains. It has been showed that magnitude of forces, stabilizing foams formed under dynamic conditions, is determined by an actual often non-equilibrium adsorption coverage at liquid interfaces. Special interest is focused on the state of adsorption layer at gas/liquid interface under dynamic conditions and influence of the motion induced non-equilibrium adsorption coverage on stability of the thin liquid films formed (foam and wetting films). Influence of surfactant adsorption on local and terminal velocities of the bubbles, bubble bouncing and shape pulsations during collisions with various interfaces, dynamics and time-scale of the three phase contact formation (gas-liquid-solid), effect of surfactant, hydrophilic/ hydrophobic properties and roughness of solid surfaces on mechanism and time scale of the three phase contact formation have been studied. Equilibrium adsorption properties are measured and parameters characterizing the surfactant surface activity are evaluated by fitting the appropriate adsorption isotherms. Surface potential variations at air/liquid interface are determined, as well. The studies have an interdisciplinary character and have been carried out in co-operation with research teams from the Max-Planck-Institute for Colloid and Surface Chemistry in Golm/Potsdam, Institute of Physical Chemistry Bulgarian Academy of Sciences in Sofia, Universite Henri Poincare, Nancy and Université de Metz, France.

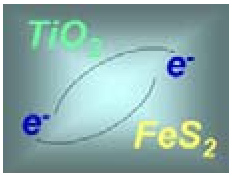


Images of the bubble departing from the capillary in water and n-pentanol solutions. Frequency of the stroboscopic lamp flashes – 100 Hz



Sequences of photos (time interval = 0.845 ms) illustrating phenomena occurring during the first collision of the bubble with Teflon plates having different surface roughness (distilled water). The roughness increases from the sequence A) to E).

ELECTROCHEMISTRY OF MINERAL SYSTEMS



The research activity of the laboratory concerns the properties of the solid-liquid interface and the electrochemical processes occurring at this interface (electrosorption, charge exchange, corrosion, dissolution, electrodeposition), with the special attention to the systems important in catalysis, hydrometallurgy, mineral processing and the protection of the environment.

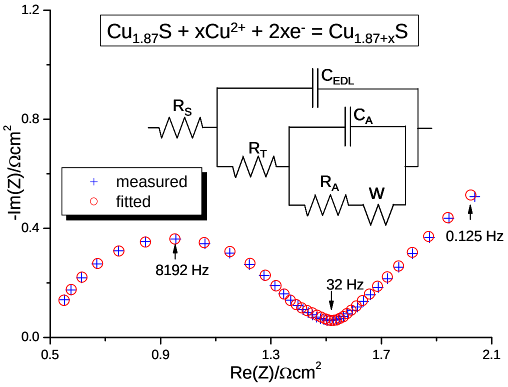
Main research topics/projects

- Contamination of the environment by the metal ions liberated during the oxidation of sulfide minerals in nature and at the waste depository places as well as mitigation of this process by controlled adsorption
- Surface doping of titanium dioxide by transition metal ions and the catalytic and photocatalytic properties of doped titanium dioxide
- Preparation of the metal/ceramic composites by electrolysis and their characterization by electrochemical and surface-science methods

Research methods : Electrochemical methods like cyclic voltammetry and impedance spectroscopy are used in the investigations. Those methods are frequently combined with other methods of surface characterization available at the Institute like X-ray diffraction, XPS, IR, and UV-VIS Spectroscopy and Scanning Probe Microscopy. The main apparatus used in the investigations is the measuring system for Electrochemical Impedance Spectroscopy consisting of FRA 1250 frequency response analyzer and ECI 1286 digital potentiostat (both Schlumberger-Solartron).

Main achievements

- The estimation of the exchange current density for the reaction of the exchange of metal ions between the crystal lattice of a metal sulfide and the aqueous solution of metal ions for many metal sulfides
- The estimation of the energy levels of the surface states at the interface TiO_2/aqueous solution , created by doping TiO_2 with transition metal ions
- Semi-quantitative description of the interaction between minerals in short-circuited galvanic cells
- Mechanism of the surface oxidation of sulfide minerals in air and in the aqueous solutions



Impedance spectrum of a non-stoichiometric copper (I) sulfide electrode in a solution of copper ions (0.1 mol dm^{-3} $CuSO_4$ + 0.9 mol dm^{-3} H_2SO_4) at the rest potential. The impedance spectrum reflects all features of the electrode reaction, namely the diffusion of copper ions, charge transfer resistance of the electrode reaction and the participation of the intermediate product (adsorbed copper (I) ion) in the reaction.

HETEROGENEOUS REACTION KINETICS

The research activities include the studies of kinetic of catalytic reactions, chemisorptions of the reactants on oxides as well as synthesis of mixed oxide catalysts.

Methods

- Kinetic steady state measurements with flow reactor, gravimetric analysis using microbalance
- TPD, TPR methods
- Computer simulations for modeling and reaction kinetics

Research topics

A. Catalysts of methanol synthesis

Catalyst: $Cu/ZnO/ZrO_2$

- Catalytic activity of M ($3\cdot ZnO\cdot ZrO_2$) system (M=Cu,Ag, Au) in the hydrogenation of CO_2 to methanol
- Effect of metal oxide additives on the activity and stability of $Cu/ZnO/ZrO_2$ catalysts in the synthesis of methanol from CO_2 and H_2
- Reduction kinetics of CuO in $CuO\text{-}ZnO\text{-}ZrO_2$ catalyst
- Kinetics of methanol decomposition on Cu-ZnO-ZrO2 catalysts

B. Kinetics of oxidative dehydrogenation of light alkanes on vanadia supported catalysts

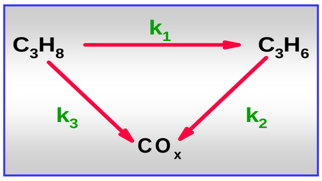
Catalytic network

$C_3H_{8(g)} + O_{(S)} \longrightarrow C_3H_{6(g)} + H_2O_{(g)} + V \qquad k_1$

$C_3H_{6(g)} + 3(1+x)\, O_{(S)} \longrightarrow 3CO_{x(g)} + 3H_2O_{(g)} + 3(1+x)\, V \qquad k_2$

$C_3H_{8(g)} + (4+3x)\, O_{(S)} \longrightarrow 3CO_{x(g)} + 4H_2O_{(g)} + (4+3x)V \qquad k_3$

$O_2 + 2V \longrightarrow 2O_{(S)} \qquad k_{OS}$



- Examination of different types of the kinetic models (power, Langmuir-Hinshelwood, Mars-Van Krevelen, Eley-Rideal-Steady State Adsorption Model).
- Development and improvement of calculation methods (analytical for simple models, numerical for complex models)
- Use of the obtained results for the analysis of the mechanism of ODH of alkanes

C. Adsorption - interaction of oxygen with vanadia catalysts

-In the vanadia phase both the hydrogen reduction and vacuum evacuation lead to the formation oxygen vacancies.

Quick process of the vanadia phase reoxidation is accompanied by slow oxygen uptake connected with the oxidation of the vacancies diffusing to the surface of the catalyst from the inside of TiO_2 bulk.

Reoxidation of the vacancies by the gaseous oxygen is associated with the oxygen dissociation and leads to the formation of nucleophyllic forms (O^{-2}) of oxygen.

Oxygen does not adsorb with the formation of ad-atoms on the oxidized surface of the catalyst. Two previous conclusions follow both from the theoretical and experimental results.

Surface nucleophyllic oxygen is responsible for the propene formation and the hydrocarbon combustion in the propane ODH reaction on the vanadia–titania catalyst.

LAYERED MINERALS, MESOPOROUS OXIDES, NANOSTRUCTURES

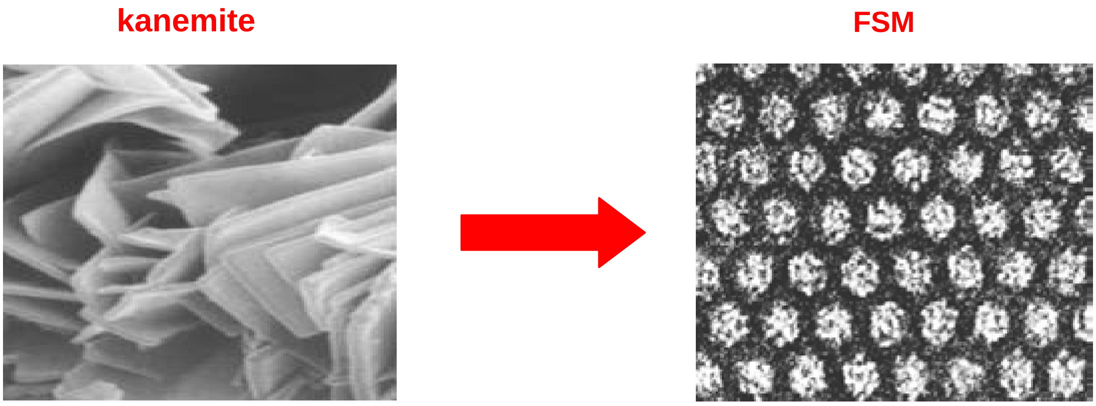
Research interests of our group include:

- application of natural and synthetic layered minerals in design and synthesis of solids with controlled catalytic and textural properties
- design and synthesis of hybrid materials based on nanoporous structures

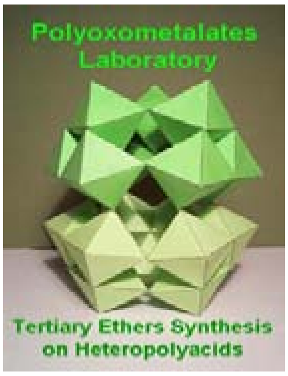
Layered minerals of interest include cationic and anionic clays, hydroxy double salts and oxides of manganese. Modification of cationic clays involves acid treatment, pillaring, doping with transition metal ions and formation of organo-clay composites. Anionic clays are synthesized using a variety of structure-forming elements and a number of compensating anions including isopoly- and heteropolyanions. Pillared clays and mesoporous oxides are used for synthesis of hybrid systems with redox functional components such as organometallic or transition metal species. The targeted catalytic reactions include abatement of nitrogen oxides, oxidative dehydrogenation of lower alkanes, combustion of volatile organic compounds, and green chemistry processes involving liquid phase oxidation of alkanes, olefins and aromatics.

Main research topics:

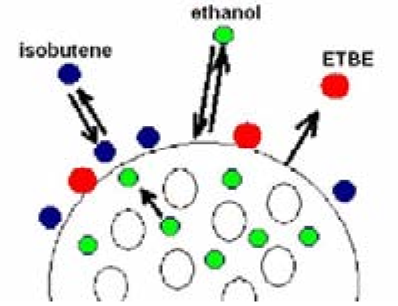
- Pillared clays as catalysts and catalyst supports
- Pillared clays with controlled textural properties
- Layered double hydroxides as hosts for isopoly- and heteropolyanions.
- Layered double hydroxides and hydroxy double salts as precursors of catalytically active mixed oxide phases.
- Layered manganese oxides as precursors of mixed oxide catalysts
- Mesoporous oxides as supports for transition metal ions and organometallic compounds.



POLYOXOMETALATES



The present interest of our team is connected with the physico-chemical and catalytic properties of heteropolyacids in acid-base type reactions. Synthesis of tertiary ethers (methyl-tert-butyl MTBE and ethyl-tert-butyl ETBE ethers) has been chosen as the reaction in which one reagent, methyl or ethyl alcohol is absorbed by the bulk of heteropolyacid crystallites and the other one, isobutene, remains only at the surface where it gets protonated. Basing on catalytic kinetic measurements supplemented by parallel sorption experiments, FTIR spectra of sorbed molecules, acidity characterisation by ammonia sorption calorimetry, a model could be proposed of the catalytic system according to which reaction occurs between protonated isobutene molecules and alcohol molecules supplied from the bulk of heteropolyacid crystallites as it is shown by the scheme.



The model assumes that there is in the bulk achieved equilibrium between non protonated alcohol molecules, protonated alcohol clusters and "free" protons, which are forming weak hydrogen bonds between heteropolyacid anions.

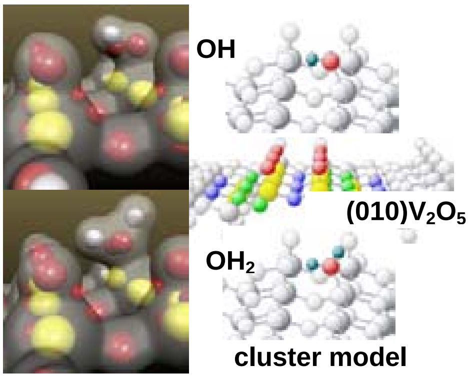
A system of kinetic equations has been proposed for the first time in the literature which, in accordance with the experimental results, shows that, depending on the pressure range, the reaction order with respect to alcohol can be either positive or negative while it is always positive with respect to isobutene.

In the last two years the effect of water on the catalytic ETBE formation was extensively studied as compared with catalytic system completely devoid of water. In the case of dehydrated catalyst and water vapour in the feed the mechanism of ETBE formation remains essentially not changed. However at high enough water vapour pressure the formation of tert-butyl alcohol (TBA) has to be taken into account. The study of different hydrates of $H_6P_2W_{18}O_{62}$ as catalysts enable to show the effect of HPA secondary structure.

The other problem studied in the last two years were the catalytic and physicochemical properties of silver salt of $Ag_6P_2W_{18}O_{62}$. In the last year the group undertook study of synthesis of zirconia based acid catalysts for transestrification of natural oils (biodiesel). The work in the collaboration of Metal-Polymer Systems in Catalytic Hydrogenation group carrying out catalytic measurements.

QUANTUM CHEMISTRY I

Modeling of Catalysts and Catalytic Reactions

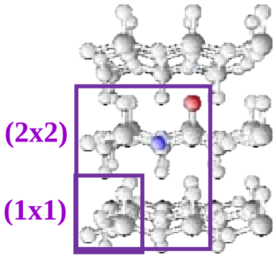


cluster model

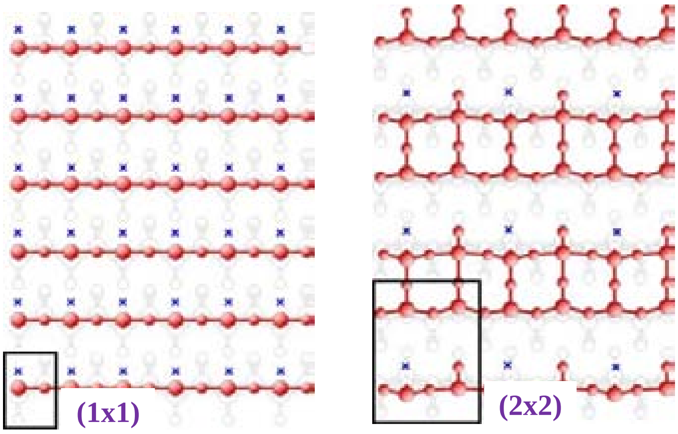
periodic model

Heterogeneous

- calculations by first-principles methods;
- identification of electronic / structural factors determining catalytic activity and selectivity;
- formulation of SAR for prediction of site reactivity and selectivity trends;
- interaction of molecules with the surface
- studies on mechanism of catalytic reactions.

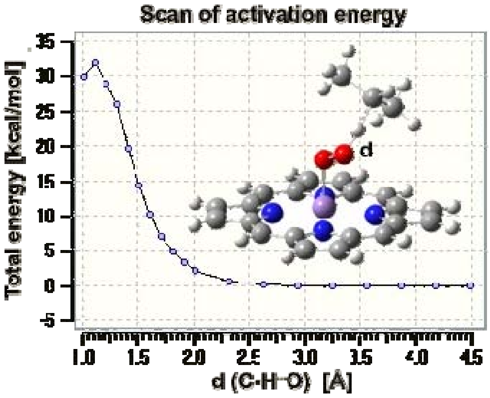


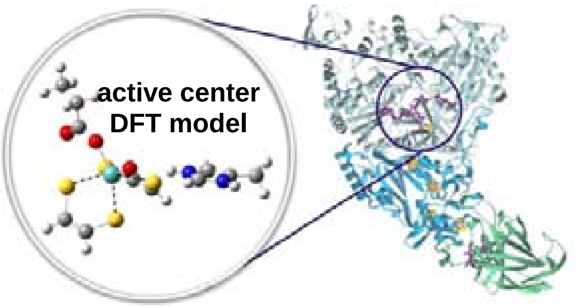
Coverage of oxygen vacancies at $(100)V_2O_5$



Homogeneous

- calculations by first-principles methods;
- modeling of transition metal complexes;
- structure-reactivity relationship studies;
- interactions of small, inorganic molecules with complexes;
- elucidation of reaction pathways and mechanisms.





EBDH crystallographic structure

Enzymatic

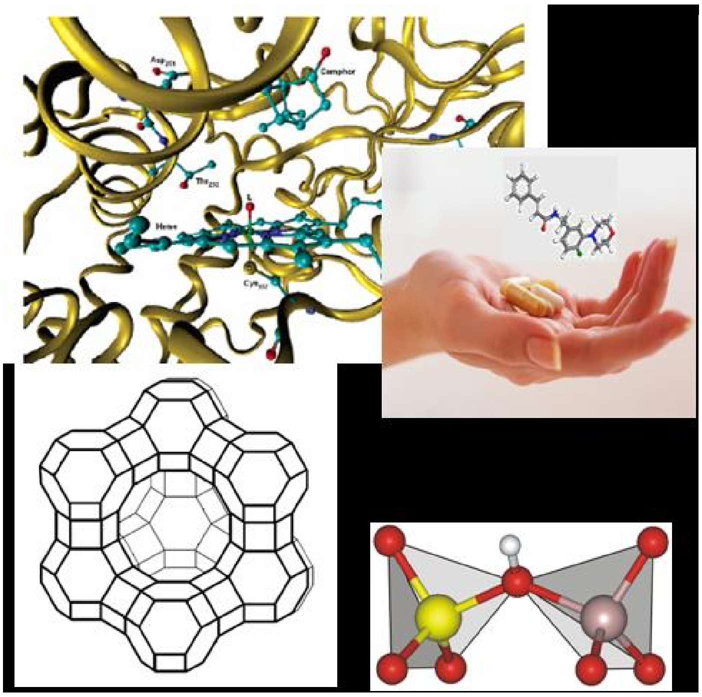
- experimental catalytic tests for ethylbenzene dehydrogenase (EBDH)
- calculations by first-principles methods;
- SAR analysis -– quantitative models describing variation in reaction kinetics;
- modeling of EBDH reaction pathway

QUANTUM CHEMISTRY II

RESEARCH FIELD:

Quantum chemistry as a tool for studying catalytic systems

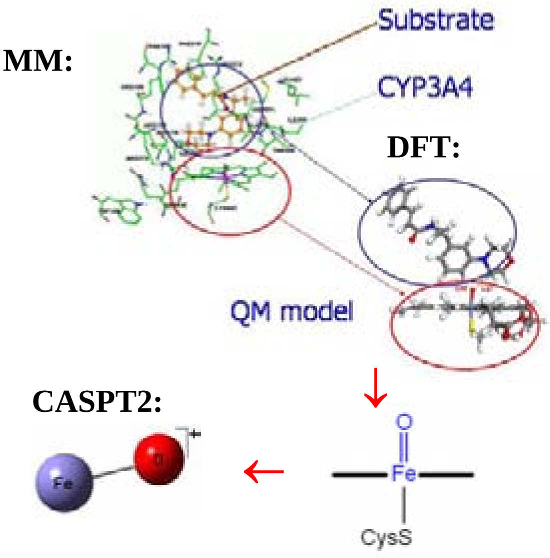
- advanced quantum methodologies (DFT, TDDFT, CASPT2) in revealing intricate electronic properties of active sites and their interaction complexes;
- adsorption and spectral properties in connection to experiment;
- catalytic reaction mechanisms



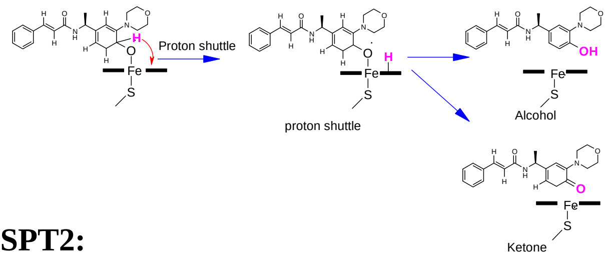
Selected topics:

- Properties of active centers in enzymes: structure, spectral properties and catalytic reaction mechanisms: iron centers in heme and non-heme enzymes
- Transition metal sites in zeolites: structure, adsorption and activation properties Copper and cobalt exchanged cations in MFI zeolite Properties of sorbed molecules - IR frequencies and EPR spectra

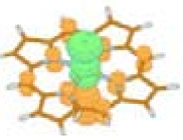
MODELING PROTOCOL:



MM/DFT:
successful design of the model for active site (Cpd I) in CYP 3A4 enzyme allowed for solving the mechanism of catalytic reaction of CYP 3A4: oxidation of arene ring in a drug molecule by proton-shuttle mechanism.

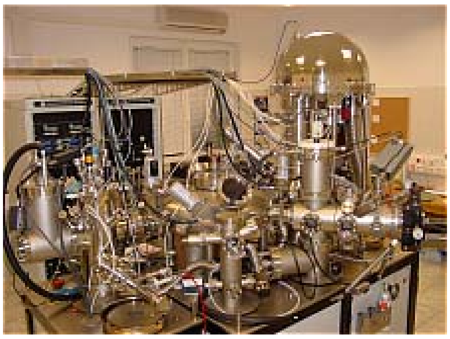


CASPT2:
calculations for idealized model of Cpd I with carefully designed active space allowed for solving peculiar electronic structure of Fe^{IV}-O core in cytochromes and for reproducing antirerromagnetically coupled spin density in low-spin state.



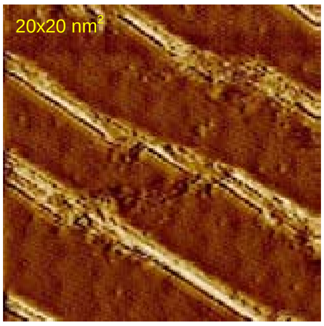
SURFACES, THIN FILMS, NANOSTRUCTURES

The research is focused on physics and chemistry of surfaces and nanostructures using modern surface science techniques. The investigated materials include metal and oxide single crystals, epitaxial thin films and nano-clusters.



Methods: surface techniques being used *in situ* include scanning probe microscopies (STM and AFM), X-ray photoemission spectroscopy, Auger electron spectroscopy, temperature programmed desorption, low energy electron diffraction (LEED) and conversion electron Mössbauer spectroscopy. Nuclear resonance scattering of synchrotron radiation (SR) experiments can be performed under UHV conditions at ID 18 at ESRF-Grenoble in a system developed during the EU 6FP project DYNASYNC.

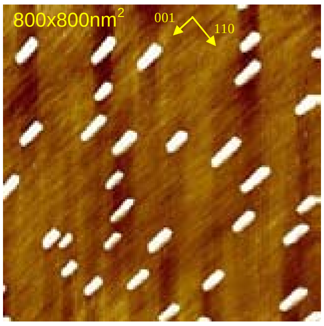
The most important ongoing activities are:

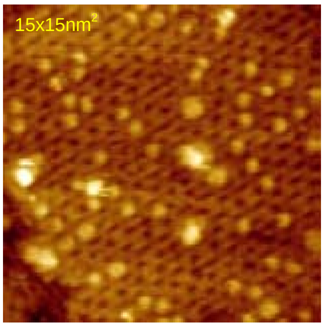


Metal and oxide nanostructures on vicinal surfaces – structure and reactivity

Epitaxial FeO monolayer grown on a vicinal Pt(997) surface (left). The substrate steps are reproduced in the oxide layer.

Uniformly magnetized ferromagnetic Fe nano-island on W(540) with potential storage density of 50 Gbit per square inch (right).



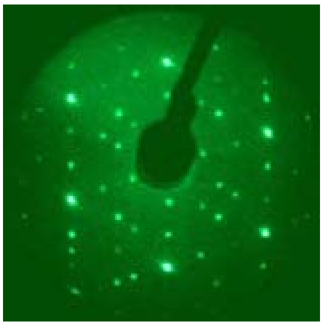


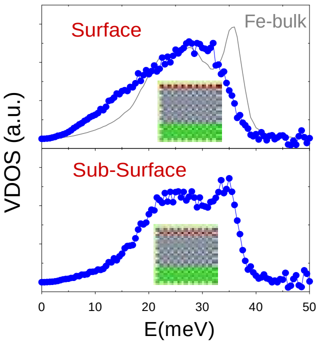
Mechanism of catalytic activity of "nano-Au/oxide" in oxidation of CO

Single Au atoms and clusters on Fe_3O_4 surface simulate a supported metal catalyst (left).

O_2 adsorption and oxidation of Fe surfaces

LEED pattern of a new (3x2) structure of oxygen adsorbed on Fe(110) (right).



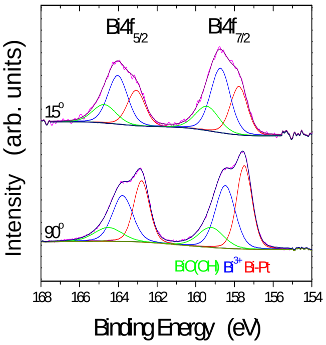


Phonons at surfaces and in nanostructures

Vibrational density of states at Fe(110) surface determined using the nuclear inelastic scattering of SR (left).

XPS analysis of complex materials

Deconvolution of angle-resolved photo-electron spectra for a PtBi electrode polarized at 0.8V vs. SCE in 0.5n H_2SO_4 (right).



ZEOLITE CHEMISTRY I

The molecular systems studied are diverse, and range from zeolites and mesoporous molecular sieves to mixed oxide catalysts. Our main interest is focused on synthetic molecular sieves, particularly crystalline aluminosilicates (zeolites), MCM and SBA type solids and related materials. We synthesize, modify and characterise zeolitic solids by IR, Raman, NMR and other techniques. The reactions we study comprise, *inter alia*, isomerization and transalkylation of hydrocarbons, de-NO_x in the presence of methane and surplus of oxygen, selective oxidation of various molecules in liquid phase, oxidative dehydrogenation of low molecular weight alkanes and transformations of terpenes.

MAIN RESEARCH TOPICS

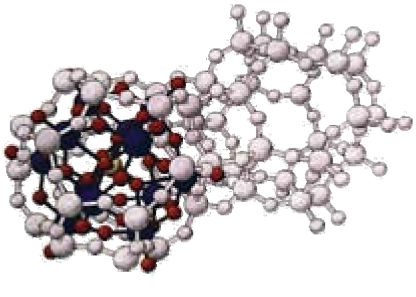
- Synthesis and properties of molecular sieves.
- Modification of molecular sieves with ions, metals and oxides. Contact-induced ion exchange.
- Dealumination and realumination of zeolites.
- Heterogenization and encapsulation of heteropoly acids and their salts in zeolites and mesoporous molecular sieves.
- Synthesis and properties of mixed oxide catalysts.
- Catalysis by zeolites, mesoporous materials and related solids, and by mixed oxides.

METHODS

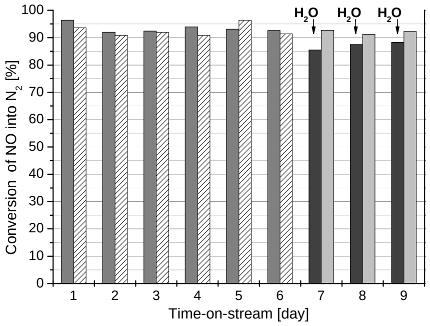
- Synthesis of zeolites, MCM, SBA and mixed oxide catalysts.
- X-ray diffraction, adsorption, FT IR and Raman.
- NMR studies in cooperation with the Institute of Nuclear Physics (Kraków) and University of Stuttgart (Germany).
- Catalytic tests in continuous flow, pulse and batch type microreactors.

MAIN ACHIEVEMENTS

- Dealumination and realumination of faujasite, ZSM-5, Silicalite-I, ferrierite and other zeolites.
- Catalytic properties of realuminated faujasite.
- Synthesis of MFI type zeolites isomorphously substituted with B and Al in the framework.
- Synthesis and characterisation of Ga-ferrierite.
- Selective transformation of methanol into hexamethylbenzene.
- NMR and catalytic studies of Ga_20_3 and Ga-containing zeolites.
- Contact-induced ion exchange in zeolites under anhydrous conditions.
- Measuring the fractal dimension of dealuminated and realuminated faujasites.
- Encapsulation of 12-tungstophosphoric acid in zeolite Y.
- Synthesis, characterisation and catalysis by heteropoly acid/faujasite & heteropoly acid/SBA-15 hybrid materials.
- Synthesis, characterisation and properties of VO_x/Ga_2O_3 and VO_x/In_2O_3 systems.
- Synthesis of highly active and selective ferrierite catalysts for the de-NO_x process in the presence of methane and surplus of oxygen.
- *In situ* and *ex situ* studies of vanadium-containing mixed oxide catalysts.
- Detailed dealumination route of ferrierite. Isomerization of α-pinene over ferrierite.
- Transformations of alkylaromatic and terpene hydrocarbons on various zeolitic solids.



Keggin unit encapsulated in zeolite Y



The CH_4-SCR NO process on the 0.6 In/0.5 Co-FER catalyst

ZEOLITE CHEMISTRY II

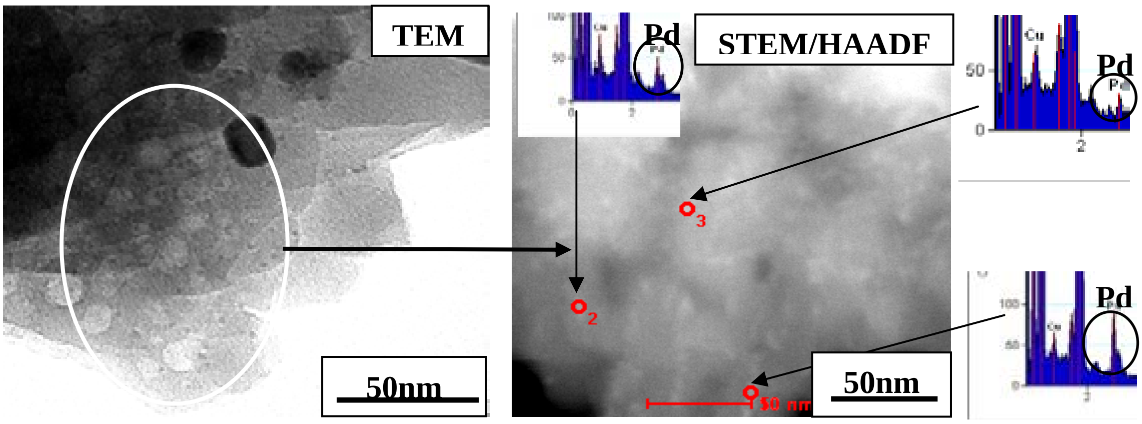
Research activity of the Group is focused on preparation and application in the different fields (catalysis, sorption) of porous solid systems which include molecular sieves, silica and alumina based mesoporous structures as well as nanomaterials with multimodal pore systems. We are also interested in the correlation between composition and texture of molecular sieve crystals or mesoporous particles and stability of the active centres. In addition, studies on the synthesis of zeolitic membranes on porous alumina supports are carried out.

MAIN RESEARCH TOPICS

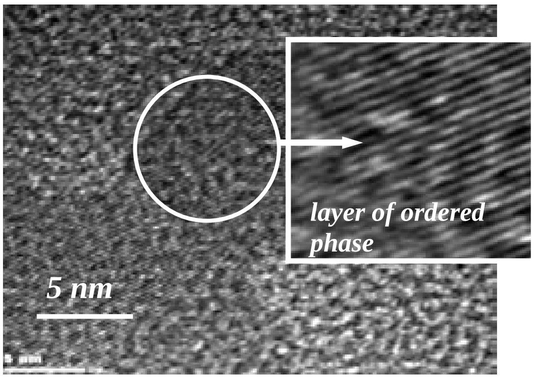
- Preparation of new systems with multimodal (micro/meso/macro) pore system
- Synthesis of crystalline, microporous materials (isomorphous substitution with different metals) and synthesis of silica and/or alumina based mesoporous materials
- Post-synthesis modification of micro- and mesoporous materials by thermal, hydrothermal and chemical treatments.
- Synthesis of zeolite membranes and their application in separation processes
- Application of FTIR spectroscopy for in-situ measurements (acidity, kinetic of sorption..)

MAIN ACHIEVEMENT

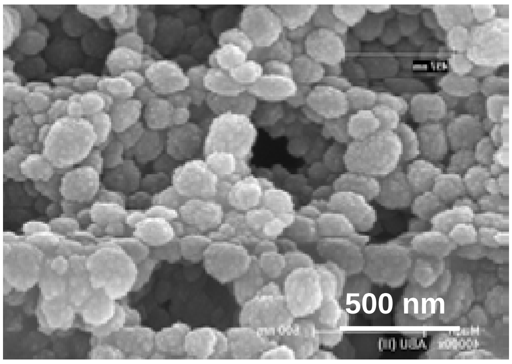
- Preparation of single zeolite crystals containing meso- and macrovoids and their use as supports for deposition of highly dispersed metal phase.
- Preparation of FAU- , BEA- and MFI-composite materials via partial recrystallization of amorphous aluminosilicates (SBA-15, MCM-41, porous monoliths).
- Synthesis of nanocrystals and protozeolitic species of high silica zeolites (MFI, BEA) and their application for preparation of nanomaterials of hierarchical pores structure.
- Preparation, characterization and use in mixture separation of MFI zeolite membranes
- Synthesis, characterization and application in catalysis of TON and BEA type zeolites isomorphously substituted with Al, B, Fe and Ga.
- The role of mobilization/immobilization processes in diffusion and low-temperature transformation of p-ethyltoluene over MFI zeolite.



TEM image (A) and STEM and EDX analysis (B) of small (2-4 nm) metal (Pd) clusters deposited inside meso-/macrovoids present in MFI crystal



TEM image of microporous BEA layer created during early stage of recrystallization.



Organized micro-/macroporous zeolite structure prepared from a mixture of monodysperse polystyrene particles and colloidal zeolite Beta nanoparticles

X-RAY DIFFRACTION AND THERMOANALYSIS LABORATORY

Our investigations concentrate on 'ab initio' crystal structure solution from powder data, and on monitoring of phase transitions and chemical reactions connected with catalytic processes.

Main research topics:

- Structural investigations on the basis of powder diffraction data
- Synthesis of amine penta- and heptamolybdate - layered materials
- Synthesis of new isopolycompounds of aliphatic and aromatic amines
- Synthesis of new peroxomolybdates, peroxovanadates and peroxotungstates
- Structure and phase transition investigations of heteropolyacids
- Phase analysis of complex phase systems (roman cements, historic binders etc.)

Main achievements:

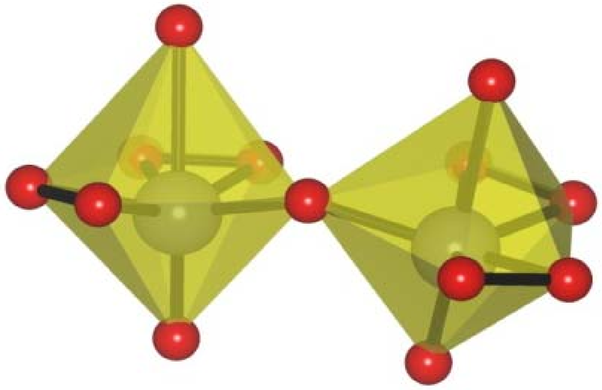
- Successful synthesis of several highly unstable, novel tetraperoxo compounds of Mo(VI), W(VI) and V(V) with Li, Na, K, Rb, Cs and ammonium cations.
- Successful synthesis of a rare family of new dinuclear diperoxocompounds. Crystal structure, spectroscopic characteristic and thermal stability were determined.
- Successful crystal structure solutions of several compounds from powder data by the global optimisation procedure and other modern powder diffraction structure solution methods (charge flipping etc).

X-Ray Powder Diffractometer
our basic experimental tool

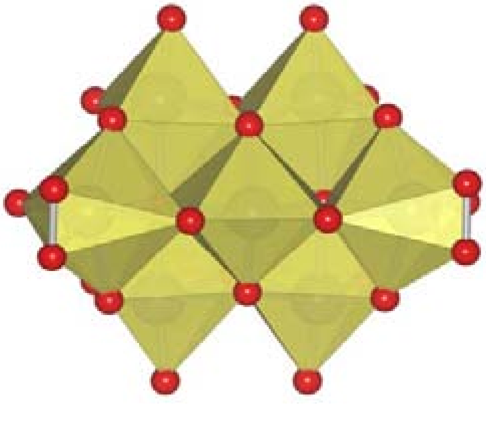
Examples of new compounds synthesised and investigated in our group.

anions of:

a) diperoxo-dimolybdate



b) diperoxo-heptamolybdate



RESEARCH SUBJECTS AND PROJECTS IN 2007

page

Statutory Research

Nanotechnology as the Basis of New Catalytic Materials

Catalytic Processes for Sustainable Development

Adsorption and Catalytic Processes Modeling

Dynamics of Nanoparticle and Colloid Systems

Self-Organized Structures and Functional Surface Layers

Physical Chemistry in the Protection of Cultural Heritage

Research projects of the Ministry of Science and Higher Education

PhD research projects of the Ministry of Science and Higher Education

Habilitation research projects of the Ministry of Science and Higher Education

Pol-PostDoc projects of the Ministry of Science and Higher Education

Scientific networks of the Ministry of Science and Higher Education

Commissioned research projects of the Ministry of Science and Higher Education

EU 6th Framework Programme projects

EU COST Actions projects

EEA Financial Mechanism projects

Projects of EU Sectorial Operational Programmes

Other international scientific projects

STATUTORY RESEARCH

Nanotechnology as the Basis of New Catalytic Materials

Nanostructured Carbon Materials of Graphitic Structure as Catalysts Supports in Electrocatalysis. Procedure of Catalysts Deposition and Testing of Their Catalytic Activity

(Assoc. Professor P. Nowak, A. Pacuła PhDEng)

The object of investigations was the characteristics of new nanostructured carbon materials of graphitic structure from the point of view of their possible application as catalysts supports, especially in fuel cells. Those materials were obtained by high temperature decomposition of volatile organic substances on the surface of SiO_2 matrix, which was later dissolved in HF solution. The characteristic features of the obtained materials were very high specific surface area (over 1000 $m^2 g^{-1}$, depending on the conditions of synthesis) as well as the presence of micro- and mesopores. Platinum was deposited on their surface using two methods: by reduction of the solutions of hexachloroplatinic acid at the surface of vitreous carbon electrode covered by the previously deposited carbon material or by the adsorption at the surface of carbon materials of platinum nanocrystals, formed previously in solution by chemical reduction (this material was subsequently deposited at the surface of vitreous carbon electrode). Activity of such obtained catalysts in the reactions of the reduction of dioxygen dissolved in the solution and in the reaction of the oxidation of methanol was investigated. Because investigated materials were obtained by the decomposition of nitrogen containing compounds (acetonitrile) they contained nitrogen in their structure. It follows from the literature data that iron on the surface of carbon materials may form complexes with nitrogen. Such complexes show catalytic activity in the reaction of dioxygen reduction. So, an attempt was undertaken to prepare the catalysts for that reaction by impregnation of the carbon materials by solutions of iron salts. Activity of prepared catalysts was investigated by cyclic voltammetry. Due to the very high specific surface area of investigated materials, high currents of electrical double layer charging were observed, which obscured the interpretation of results. The capacitance of the electrical double layer, estimated from the voltammetric data and referred to the specific surface area of the material measured by the BET method was relatively independent on material and amounted to approximately10 $\mu F\ cm^{-2}$. It was stated that the catalytic activity shows mainly the catalyst deposited on the external surface of the carbon material. Catalyst contained inside the pores practically does not participate in the reactions. Some of the catalysts obtained by impregnation of the carbon materials by iron salts showed high activity in the reaction of dioxygen reduction, comparable to the results published in the literature. The platinum catalyst obtained by the cathodic reduction of hexachloroplatinic acid on the surface of carbon material showed high activity in the reaction of the oxidation of methanol (see figure below).

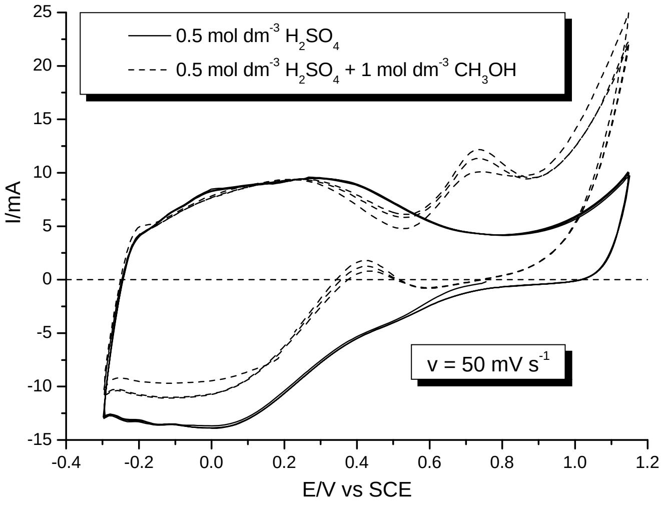


Fig.1. Methanol oxidation on the electrode made from vitreous carbon covered by the catalyst obtained by the cathodic reduction of H_2PtCl_6 on the surface of nanostructured carbon material (first three voltammetric cycles showed). Platinum content in the catalyst 30%. Surface of the electrode 0.8 cm^2, catalyst loading 0.5 mg. Microporous carbon material of the specific surface area 1720 $m^2 g^{-1}$.

Monodispersed, Colloidal Suspension of Zeolite Nanoparticles and Their Application in Preparation of New Systems for Catalytic and Sorption Processes

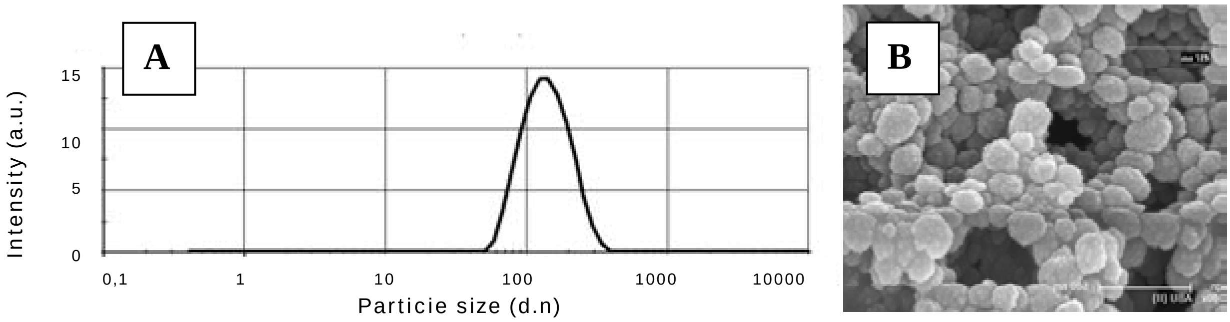
(Assoc. Professor M. Derewiński, A. Burkat-Dulak MSc, A. Węgrzynowicz MSc)

Development of nanotechnologies and their requirements for synthesizing nanoscale materials resulted in an extensive research on the preparation of nanosized porous systems. Nanosized-base sensing materials, low dielectric zeolite film which are among the major candidates for next generation of microprocessors, new devices for advanced medical diagnostics are examples of future applications of nanozeolites. Moreover, the nanosized zeolite-type materials or their precursors are widely used as building blocks for fabrication of thin film and layers and for preparation of complex hierarchical macrostructures. Nanocrystals with narrow particle size distribution are generally obtained from homogeneous so called *clear solution* where only subcolloidal or discrete amorphous particles are present and in conditions which favor nucleation over crystal growth.

The aim of the study was preparation of a stable nanosized MFI and BEA type zeolites particle suspensions and to use them for the preparation of zeolitic membranes as well as for preparation of multimodal porous materials

Discrete colloidal particles of MFI (silicalite-1) zeolite with an average particle size of ~100 nm and with a narrow particle size distribution (more than 90% of nanocrystals had a dimension in the range between 50 and 150 nm) have been synthesized from clear homogeneous solution. Low temperature of synthesis (below 90^{o}C) , high concentration of organic structure directing agent (tetrapropylammonium hydroxide) and use of silica source with a low degree of polymerization (tetraethoxysilane) favored formation of uniform in size and morphology nanozeolite particles. Nanosized BEA crystals with a narrow particle size distribution were also synthesized. A higher temperature (above 120^{o}C) and longer synthesis time were required to prepare nanoBEA particles. The XRD analysis provided evidence that BEA was the only crystalline phase present in the suspension and the main fraction of nanocrystals had a dimension of ~180 nm. The stability of obtained colloidal suspensions was determined by measuring of the zeta potential values at constant concentration. The pH values necessary to avoid agglomeration of nanoparticles were determined for both type of nanozeolites.

Prepared nanosized MFI particles were subsequently used as seeds for the preparation of thin zeolite film on the solid porous α-Al_2O_3 discs. Organized micro-/macroporous zeolite BEA structures were prepared by self-assembly procedure using a mixture of synthesized colloidal BEA nanocrystals and monodisperse polystyrene particles.



(A) Particle size distribution o fan aqueous suspension of nanoBEA determined by dynamic light scattering (DLS); (B) Hierarchical structure o micro-/macroporous material obtained from a mixture of nanoBEA and polystyrene particles

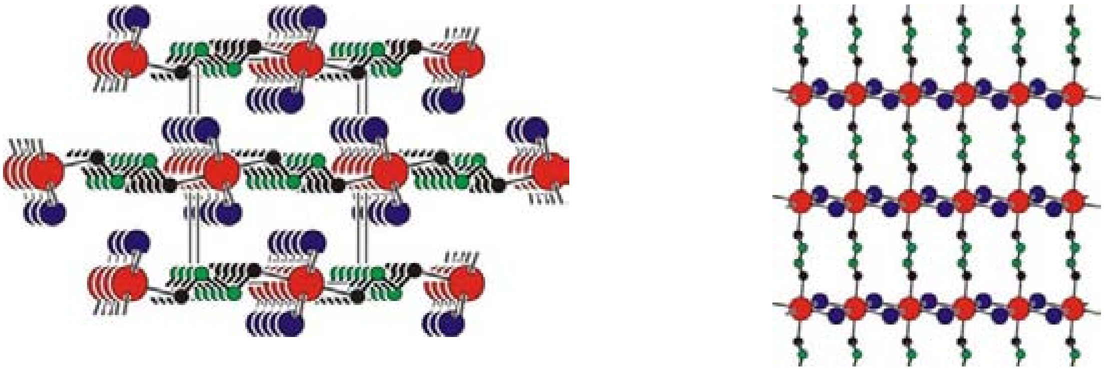
Hybrid Organic-Inorganic Layered Materials - Synthesis and Structural Investigations

(Professor W. Łasocha, M. Grzywa PhD, B. Gaweł MSc [Faculty of Chemistry Jagiellonian University])

New methods of synthesis of new hybrid layered compounds in which semiconducting monolayers Me(II)-X(VI) are separated by layers of diamines were elaborated. Such compounds are interesting materials for microelectronic and optic applications.

Performed tests indicate the possibility of synthesis of new layered compounds using aromatic diamines. For one such a compound - ZnSe(m-xylenediamine)$_{1/2}$, thermal decomposition process was studied in: He atmosphere, parafin oil, mixture of CH_3CN and CH_3COOH. In higher temperatures, decomposition of ZnSe(m-xylenediamine)$_{1/2}$ with loss of organic part, and formation of nanometric ZnSe was observed.

Within tests of synthesis conditions a few new compounds were obtained. The compounds turned out to be coordination polymers with a general formula {-MeX$_2$-NRN-}$_n$.



New coordination polymers obtained within this study. Red and blue circles represent metal and halogen atoms, green and black indicate carbon and nitrogen atoms respectively.

In the second group of activity, methods of synthesis of layered penta- and heptamolybdates were studied. This kind of compounds is built of molybdenum-oxygen layers separated by organic cations. Conditions of synthesis (pH and temperature) as well as an influence of the size of organic cation on a type of obtained compounds were also studied. Within this study p-bromoanilinum pentamolybdate (with the lattice parameters: 30.790(5), 5.6425(9) 14.252(3) Å, 106.88(1)^o , V= 2369.5(5)Å^3, SG; C2/c), and a few new molybdates with organic cations, such as: 2,6-dimethyloanilinium octamolybdate, 1-ammoniumnaphthale octamolybdate, 2-ammoniumnaphthale octamolybdate were obtained.

For the new compounds physicochemical investigations (spectroscopic, DSC and thermal decomposition investigations by XRPD methods) and crystal structure studies were carried out. Since in both groups of compounds polycrystalline materials prevail, the structure solution methods were based on powder diffraction measurements.

Oxide and Metal Nanostructures on Surfaces: Preparation, Structure and Dynamics, Electronic Properties, Reactivity

(Professor J. Korecki, N. Spiridis PhDEng, J. Gurgul PhD, R. Socha PhD, D. Wilgocka-Ślęzak PhDEng, K. Freindl MScEng, E. Zackiewicz MSc)

1. Oxygen adsorption on Fe(110)

Studies of oxygen adsorption on iron surface are of great importance for such processes as: oxidation, passivation, corrosion and, recently, also for spintronic application of metal-insulator systems. Our investigations are stimulated by a research program concerning metal-oxide bi-layers. We used epitaxial iron-oxides as model systems for studying dynamics in nanoscale with nuclear resonance scattering of synchrotron radiation. Despite numerous papers on initial oxidation of the Fe(110) surface, information on the adsorbate structure vs. oxygen coverage is incomplete and partially contradicting. For our studies we used the surface of epitaxial Fe films grown on W(110). The Fe(110) surfaces obtained in this way were of a perfect chemical purity and structural quality, which allowed high resolution low energy electron diffraction (LEED) analysis. Oxygen was adsorbed at room temperature in a wide exposure range from 0.5 to 500 L. We confirmed the (2x2) structure for low exposures from the range 0.5 - 5 L. In further adsorption stages (5 – 80 L), a structure described in literature as (3x1) we identified as a more complex with an oblique surface unit cell, containing three (coverage 0.375) oxygen atoms. We proposed several structural models, whose verification will request high resolution STM measurements or/and quantitative I-V LEED analysis. Furthermore, for coverage close to one, above 100 L exposures, we observed a well ordered (3x2) structure, which to our knowledge was not reported before. We believe that this phase precedes the onset of formation of an oxide that involves penetration of oxygen below the Fe surface. For selected stages of adsorption we performed hyperfine interaction spectroscopy studies using nuclear resonance scattering of synchrotron radiation. They revealed considerable changes of the Fe electronic structure upon oxygen exposures beyond 10 L. For the simplest (2x2) structure we performed test *ab initio* LDA calculations of hyperfine parameters using the Wien2k code.

2. Nanostructures and reactivity on vicinal surfaces

Ultrathin metallic films and nanostructures on vicinal surfaces are interesting for their special catalytic and magnetic features. We studied metal nanostructures (Fe, Au) on stepped metal and oxide surfaces. Using W(540) as a substrate we were able to optimize the growth conditions for reproducing the regular step stucture on Fe(110) and Au(111) surfaces. We compared the growth of Fe on a flat W(110) and vicinal W(540) surfaces revealing the influence of the regular steps of the vicinal substrate on structural and magnetic properties of Fe adsorbate. In particular, using LEED and STM we studied morphology of elongated Fe islands produced by a high temperature annealing with a high magnetic shape anisotropy. Changes of magnetic properties accompanying the island formation (in-plane spin reorientation transition) were monitored using magnetoopic Kerr effect and nuclear resonance scattering of synchrotron radiation.

Other studied system, important from the catalytic point of view, are gold nanostructures on a stepped iron oxide substrate. The ultrathin iron oxide layers grown on a vicinal Pt(997) surface were studied using STM . Depending on the growth temperature, the FeO layer displayed single or double atomic steps. A submonolayer gold adsorbate showed self-organization that corresponds both a modulation of the FeO atomic structure and the morphology of the vicinal substrate.

Using TPD, we studied also co-adsorption of CO and O_2 on Pt(997).

Physicochemical and catalytic properties of palladium – micro and maacro-porous resins

(Assoc. Professor A. Drelinkiewicz, A. Waksmundzka-Góra PhD, A. Knapik MSc)

The use of functional polymeric resins as supports for noble-metals catalysts is attractive owing to their specific properties that can essentially influence the course of catalytic reaction. These properties can be characterized as the presence of various functional groups (like ester, carbonyl, carboxyl, amine groups) the ability of polymer for swelling under reaction conditions and hydrophobic character of polymer. They can influence the accessibility of reagents to the metal centers located inside the polymer mass and in consequence the rate and selectivity of reaction. These effects are studied in the present work.
The role of polymer properties is studied in the hydrogenation of a series of unsaturated carboxylic acids, derivatives of acrylic acid. They differ with respect to the type, number and location of substituents (CH_3, C_6H_5, COOH) at the double bonded C=C carbon atoms (α-methyl-acrylic, crotonic, β-methyl-crotonic, cinnamic, α-methyl-cinnamic, maleic, fumaric). Hydrogenation is performed in the presence of palladium catalysts (0.25-4 wt % Pd) supported by functional resin (OFP). Polymer is composed of styrene (77mol %, 2-hydroxyethyl methacrylate 20 mol % and glutaric anhydride as the crosslinking agent 3-20 mol %). The samples used in studies are in the form of spherical beads (150-250 μm) of crosslinking degree 3%, 10% and 20%. Palladium catalysts are prepared using solution of $Pd(OAc)_2$ in THF, i.e. solvent leading to high expansion of polymer mass. They were reduced by $NaBH_4$ solution in THF-CH_3OH mixture. Swelling experiments showed that insertion of palladium as well as increase of crosslinking degree reduced expansion of polymer mass. Scanning electron microscopy (SEM) showed uniform distribution of Pd through the polymer mass. XRD and TEM techniques indicated the presence of Pd nano-particles of 2-5 nm in size. This shows high ability of OFP resin for stabilization well dispersed Pd-metal nanoparticles.

Hydrogenation tests are carried out in THF solvent, i.e. in conditions when the catalysts grains are in expanded state (temp. 22^0C, atmospheric pressure of H_2). It is observed that the extent of polymer swelling (determined by the loading of Pd and crosslinking degree of polymer) essentially influences the rate of unsaturated acids hydrogenation in the presence of Pd/OFP catalysts. For the comparison, hydrogenation tests are also performed for typical, 4%Pd/SiO_2 catalyst. From the obtained activity data substantial differences between performance of Pd/OFP and Pd/SiO_2 catalysts is established. To clarify the role of polymer matrix, theoretical modeling is undertaken. The correlation between experimentally determined rate of hydrogenation and the size of substrate molecule, its hydrophobicity and absolute hardness/polarizability is studied. For all studied catalysts, 4%Pd/SiO_2 and Pd/OFP, the rate of C=C bond hydrogenation is the highest for acrylic acid, a parent molecule of the smallest size. Generally, the rates for other reactants hydrogenation in which H-atoms are substituted by methyl (α-methylacrylic, crotonic, β-methylcrotonic) phenyl (cinnamic, α-methylcinnamic) or carboxylic (maleic, fumaric) groups are distinctly lower.

The rate of C=C hydrogenation was found to depend on the crosslinking degree of the resin and on the presence of steric hindrance around the C=C bond in substrates. It has been established that experimentally determined rate of hydrogenation on Pd/OFP catalysts correlates quite well with the size and hydrophobicity for reactants having the CH_3 groups as the only type of substituents. When there is a steric hindrance around the C=C bonds with phenyl ring or two carboxyl groups additional effects play a role in the rate of hydrogenation. They may be related to specific interactions between these substituents and the functional groups of polymer matrix.

Mesoporous materials as catalytic nanoreactors

*(Professor E. Serwicka-Bahranowska, D. Duraczyńska PhD, M. Zimowska PhDEng,
A. Michalik-Zym PhDEng, D. Napruszewska Eng, Z. Czuła, Z. Olejniczak PhD [Institute of Nuclear Physics PAS])*

Ordered mesoporous silicas, with their well developed specific surface and an array of uniform pores with dimensions over 2 nm, represent an attractive class of catalytic supports. Of particular interest is the use of these materials as carriers for catalytically active species, whose large dimensions preclude their location within the pore system of conventional microporous solids, such as zeolites or pillared clays. Among active centres of interest are numerous organometallic compounds, known for their catalytic activity in homogeneous systems. Encouraging results of our previous work on developing novel oxidation catalysts by immobilization of metalloporphyrins on the surface of different mesoporous silicas prompted us to continue the research with organometallic compounds capable of catalyzing hydrogenation reactions.

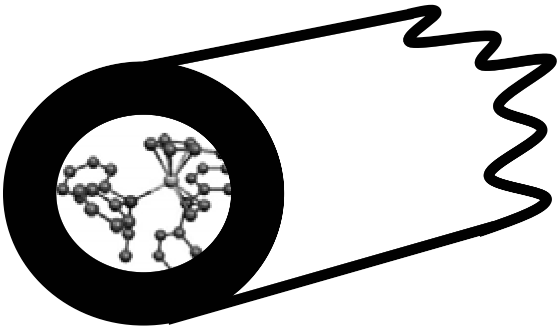


Fig. 1 Structural model of (**1**) immobilized on HMS(Si/Al=40)

A cationic ruthenium (II) complex (**1**) $[(\eta^5\text{-}MeC_5H_4)Ru(\eta^3\text{-}PPh_2CHCH_2)(\eta^1\text{-}PPh_2CHCH_2)]^+$ has been chosen as hydrogenation catalyst. It contains two different types of phosphine ligands, one of which (η^3- PPh_2CHCH_2), is labile, i.e. one of two bonds between the ligand and the metal centre “opens” while used in catalytic reaction, providing a coordination site for an incoming substrate, while the other group, (η^1- PPh_2CHCH_2), remains firmly bound to ruthenium center. The presence of such ligands in a complex may induce transformations that would not otherwise occur. Complex (**1**) has been immobilized inside the pores of aluminated hexagonal mesoporous silica HMS(Si/Al=40) by direct ion exchange method (Fig.1). Physicochemical characterization (XRD, TG/DTG, FTIR, ^{31}P NMR, ^{29}Si, ^{27}Al MAS NMR, UV-Vis, XPS, nitrogen adsorption at 77 K) confirmed that the ruthenium (II) cations are trapped within the support pore network, and that the immobilized complex retains its essential characteristics. The catalysts obtained this way were shown to be active and selective in the catalytic hydrogenation of phenylacetylene (Fig. 2). The activity of the supported catalyst represented ca. 2/3 of that observed for the homogeneous catalyst, with the selectivity to styrene remaining at the same, very high level (87% at 90% phenylacetylene conversion). The lower activity of heterogenized catalyst compared to that of the unsupported one is tentatively assigned to limited accessibility of some of the active ruthenium (II) sites localized within the mesopore system. Supported catalyst (**1**)/HMS(Si/Al=40) is stable under catalytic conditions and shows no leaching into the reaction medium, which renders the material ready for recycling and reuse.

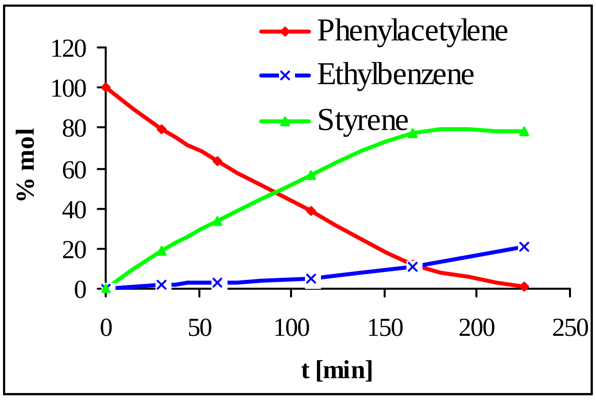


Fig. 2 Hydrogenation of phenylacetylene in the presence of 5.9 wt.% (**1**)/HMS(Si/Al=40).

Catalytic Processes for Sustainable Development

Optimization of Preparation Conditions of Supports Based on Chromium Spinels MCr_2O_4 and of Au Content in Au/ MCr_2O_4 Catalysts for Reaction Related to Protection of Environment

(Professor B. Grzybowska-Świerkosz, M. Ruszel PhD, I. Gressel, P. Olszewski PhD)

We have found in the last years that gold nanoparticles dispersed on spinels $M^{II}Cr_2O_4$, MCr, where M^{II} = Co, Fe, Mn, Mg, are promising catalysts in oxidation of CO and in preferential (selective) oxidation of CO in the presence of excess of hydrogen (PROX). The studies in 2007 have been concerned with optimization of the preparation conditions for the supports and optimization of the Au content in the catalysts. The studies comprised: (a) synthesis with a citrate method of CoCr, ZnCr oraz MgCr support precursors, and their calcination in the range 250-600°C, (b) characterization of the phase composition and sp. surface area of the obtained supports (XRD and BET techniques, (c) preparation by the deposition-precipitation (DP) method of catalysts: nano-Au on the supports, of different Au content (1, 2, 3wt%), and, for AuCoCr, of different calcination temperature of the support (350 and 500°C), d) catalytic tests in CO oxidation for fresh catalysts and after pre-activation in hydrogen, and in PROX CO reaction, at 35 and 60°C.

We have determined optimal calcination temperatures ensuring: a) homogenus phase composition (pure spinel chromites), b) comparable specific surface area (~60 m^2g^{-1}), suitable for nanoAu deposition, as 500°C for CoCr i ZnCr and 550°C for MgCr.

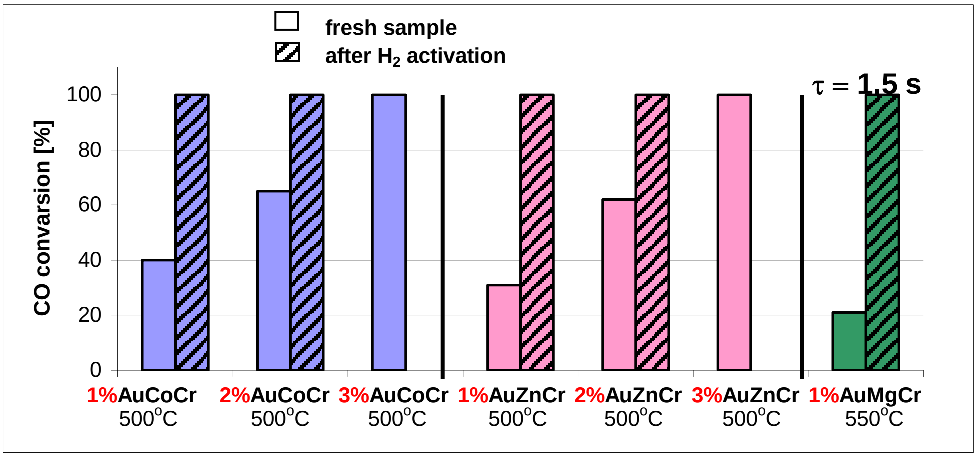


Fig. Effect of the Au content in AuMCr catalysts on activity in CO oxidation.

For catalysts containing the supports calcined in optimal conditions it has been found:

1. CO conversion in CO i PROX CO oxidation follows the sequence: Au/CoCr ≈ AuZn >> AuMg, and increases after the pre-activation in H_2.
2. For catalysts of the series AuCoCr and AuZnCr, conversion of the fresh catalysts in CO oxidation increases, and in the PROX Co decreases, with the increase in the Au content from 1-3 wt%.
3. After activation with hydrogen all catalysts show conversion of 100%, irrespectively of the Au content.
4. Selectivity to CO_2 in PROX reaction is high (> 90%) for all the studied catalysts: it decreases with the increase in the reaction temperature and with the increase in the Au content.

It should be also pointed out, that: a) conversion values are higher as compared with those obtained in our previous studies for catalysts, in which the supports were calcined at higher temperatures, and b) results for the PROX CO reactions are comparable with the best reported in the literature. Tests are being carried on application of the above catalysts in practice (in the group of dr Machej).

Oxidative Dehydrogenation (ODH) of Isobutane on CrO_x/Oxide Support (Al_2O_3, TiO_2) Catalysts: the Influence of Potassium on Oxygen Properties and Chemisorption of Molecular Oxygen

(Professor B. Grzybowska-Świerkosz, K. Samson PhD, Assoc. Professor R. Grabowski,
A. Kozłowska PhD, Assoc. ProfessorJ. Słoczyński)

Our previous results have shown the opposite effect of potassium on catalytic properties for CrO_x/Al_2O_3 (CrAl) and CrO_x/TiO_2 (CrTi) systems [atomic ratio K/Cr=0.1] in ODH of isobutane: the increase in selectivity to isobutene for CrTi and the decrease for CrAl system. The above differences cannot be explained by changes of acido-basic properties, since for both systems the potassium additive caused the decrease in acidity and increase in basicity.

In year 2007, to explain the opposite effect of potassium for CrAl and CrTi catalysts, the reducibility (by H_2-TPR method) and chemisorption of oxygen were studied.

Futhermore, to confirm the negative effect of potassium (unparalleled in the literature) the series of CrAl catalysts with different amount of potassium (Cr/Al=0.05-0.4) were obtained, characterized by XPS and in ODH of isobutane. The negative effect of potassium on selectivity to isobutene for CrAl catalysts in all the studied concentration range of potassium was confirmed.

For both studied systems the addition of potassium caused: a) the decrease of reducibility (T_{max} shifted to higher temperature, lower reduction rate, v_{red}), b) the decrease of activation energy of chemisorption of oxygen, c)chemisorption followed Elovich kinetic equation. On the other hand, potassium showed different influence on the rates of chemisorption of oxygen, v_{ox}, and surface oxygen coverage in reductant/oxidant mixture ($\theta = v_{ox}/v_{red}$). .

Table1. H_2 TPR and O_2 chemisorption data for CrAl and CrTi catalysts with and without K

Catalyst	Δm_∞ [μmol O m^{-2}]	% mnl	$\ln k_o$	α [kJ mol^{-1}]	$E_{act.ox}$ [$kJmol^{-1}$]	v_{ox} x10^{4*} [μmol O m^{-2} $s^{-1}kPa^{-1}$]	** T_{max} [°C]	v_{red} x 10^{5***} [μmol O $s^{-1}m^{-2}kP^{-1}$]	v_{ox}/v_{red} θ
CrAl	1.58	9.5	38.0	0.18	225.0	0.81	353	7.0	0.12
CrAlK K/Cr0.1	1.55	9.3	19.4	0.21	133.0	1.78	383	2.0	0.89
CrAlK K/Cr0.25	1.82	11.0	14.5	0.23	114.0	-	-	-	-
CrTi	0.98	5.9	2.9	0.59	44.0	147	335 435	20.0	7.4
CrTiK	0.73	4.4	-2.4	0.61	32.0	1.08	360 480	4.0	0.27

* from oxygen chemisorption (at 300°C) ** T_{max} of H_2 – TPR profile *** from H_2 – TPR measurements (up to 300°C)

The opposite effect of potassium on selectivity to isobutene in ODH of isobutane for CrTi and CrAl catalysts was explained by different influence on the above two parameters. For CrTi system potassium decreases the rate of chemisorption of oxygen and oxygen coverage θ, while for CrAl system the addition of potassium increases the rate of chermisorption of oxygen and oxygen coverage θ; the increase of θ causes the decrease in selectivity to isobutene, the decrease of θ – the increase in the selectivity.

Kinetics of Ethyl-*tert*-butyl Ether (ETBE) Formation from Ethanol and Isobutene. The Effect of Water in the Gas Phase

(Professor A. Bielański, A. Micek-Ilnicka PhDEng)

Ethyl-tert-butyl ether (ETBE) is frequently used as the only tertiary ether introduced into the automotive fuel. The later replaced methyl-tert-butyl ether (MTBE) considered being harmful for the environment.

The aim of the present research was to study the effect of water vapour on the kinetics of gas phase electrophilic addition of ethanol to isobutene. Reaction of etherification accompanied in water containing system by the formation of tert-butyl alcohol (TBA) was carried out at 40°C using Wells-Dawson type of heteropolyacid $H_6P_2W_{18}O_{62}$. The empirical rate orders with respect to ethanol (-2.0) and isobutene (1.7) are not influenced by the presence of water vapour. Both ethanol and water are inhibiting conversion of isobutene to ETBE (figure)

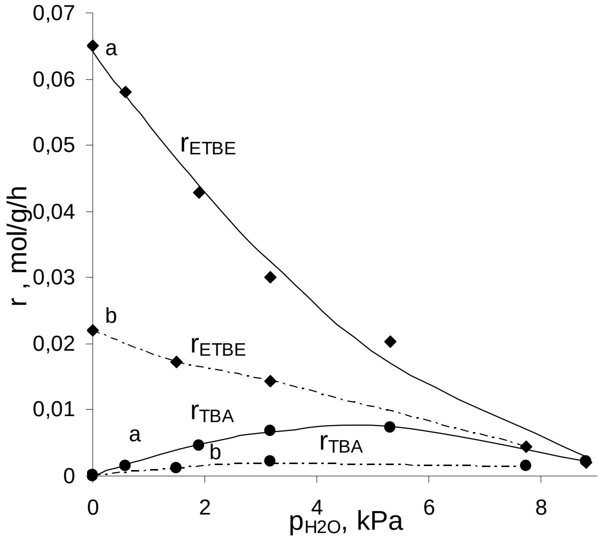


Fig. Formation rate of ETBE and TBA at 40°C as the function water vapour pressure ($p_{ethanol}$=17.2 kPa, and $p_{isobutene}$ 18.4 kPa (a), 10.3 kPa (b).

On the other hand the rate of TBA formation is non-monotonic function of water vapour pressure (figure). One may discriminate „catalysing" region of water vapour below ~4 kPa and „inhibiting" one above ~4 kPa.

Basing on kinetic measurements reaction mechanism was proposed taking into account the fact that polar molecules of ethanol and water penetrate the bulk of HPA crystallites while only very weakly polar isobutene remains chemisorbed on the surface possibly in the form of oligomers. Both ethanol and isobutene get protonated with the protons supplied from the bulk thus forming ethoxonium ions inside the crystallites or oligomeric carbocations at their surface. The ETBE formation occurs as the reaction between protonated carbocations and neutral ethanol molecules supplied from the bulk or from the gas phase. Similarly TBA formation occurs between surface carbocation and neutral water molecules. In the "catalysing" region of water partial pressure water is acting mainly as the reaction substrate forming TBA and not bonding protons of the acid. In the "inhibiting" region protonated water clusters $(H_2O)_mH^+$ formation predominates thus decreasing the concentration of loosely bonded protons in the bulk. Basing on such reaction mechanism of ETBE and TBA formation mathematical model of both processes has been formulated.

An Introductory Study of Bio-Fuel Synthesis in Transestrification of Natural Oil. The Choice of Catalysts

(Assoc. Professor A. Drelinkiewicz, T. Kasza PhD, A. Zięba MSc, Professor A. Bielański)

A microreactor for oil transesterification at temperature 60^0C and atmospheric pressure has been constructed and tested. The determination of the content of methyl-esters and conversion of natural oil is based on GC and HPLC analysis.

As the test reaction transesterification of castor oil with methanol has been carried out using both homogeneous and heterogeneous catalysts.

In the introductory experiments aiming to test the efficiency of our catalytic system KOH has been used acting as homogenous catalyst dissolve in alcohol phase. Another basic catalyst applied in studies was solid γ-Al_2O_3 impregnated with KOH from aqueous or ethanolic solutions.

Considering the fact that acid catalysts are perspective catalysts for the transesterification of waste oils produced by gastronomy (containing free organic acids) the further research concerned this type of catalysts. Two series of acid catalysts were prepared containing ZrO_2 gel obtained by standard and sol-gel methods. In the first series the gel was impregnated by the solution of H_2SO_4 (the catalysts were dried and calcined at different conditions). In the second series Keggin type heteropolyacid $H_3PW_{12}O_{40}$ (HPA) was introduced by impregnation and co-precipitation methods. The former one contained 9-40 wt % of HPA. All acid catalysts appeared to be active in the castor oil transesterification. They were also investigated using scanning microscopy and FTIR spectroscopy.

In the course of our investigations two problems for further studies were selected. First of them concern the problem of removing (leaching) the acid agent from solid support by the reaction mixture. In this situation catalyst acts partially in a homogeneous phase and can be used only in one run. The use of higher alcohols instead of methanol may be the solution of this problem. Important observation done during the present research was the statement that the order of contacting the catalyst with the reagents, oil or methanol, influences its activity. Catalyst contacted at first with the oil looses up to 30 % of its activity. This effect has not been signalled in the literature studied by us.

Catalytic Transformation of Glycerol, Byproduct of Bio-Diesel Fuel Production, for Its Utilization

(Professor J. Haber, K. Pamin PhDEng, J. Połtowicz PhD)

The production of diesel fuel from natural vegetable oils as a feedstock becomes increasingly popular in many countries. Such oils, although more expensive in production, guarantee lower emission of environmentally damaging compounds. So-called “biodiesel” fuel consists of fatty acids methyl esters (FAME) which form by transestrification of triglicerides present in the biosustainable sources. The transestrification proceeds between triglicerides and methanol in the presence of basic catalyst. Fatty acids methyl esters are the main products of transestrification while glycerol is a byproduct. However, as the demand for biodiesel fuel increases, the supply of glycerol becomes larger and finally one will end up with overproduction of glycerol that should be utilized..

Glycerol, $C_3H_8O_3$, is an aliphatic saturated tribasic alcohol, the main consumer of which is still cosmetic and food industry. The conversion of glycerol to propylene glycol might be a good idea for processing the increasing amount of glycerol (Fig. 1).

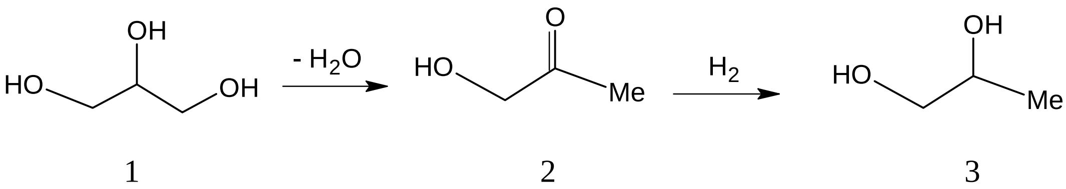


Fig. 1 Glycerol conversion to propylene glycol

Glycerol can be converted to propylene glycol in two steps. The first one is glycerol (1) dehydration to acetol (2), followed by hydrogenolysis to propylene glycol (3). Both reactions proceed in the presence of Cu-Cr catalyst, at higher pressure and temperature.

The first step of our study concerned the synthesis of selected catalysts, the acidic cesium salts of tungstophosphoric acid. They were synthesized in the reaction of stoichiometric amount of Cs_2CO_3 with an appropriate amount of heteropolyacid. The acidic cesium salts of tungstophosphoric acid are known as catalyst having strong acidic properties. The synthesized catalysts were characterized by means of thermal analysis, XRD, UV-Vis and FTIR spectroscopy.

Propylene glycol can be commercially used as automotive antifreeze and aircraft deicer.

Synthesis and Electrochemical Properties of Catalysts in Oxidation of Hydrocarbons

(Professor J. Haber, K. Pamin PhDEng)

Heteropolyacids of Keggin-type are widely employed as catalysts of acid-base and oxidation reaction. Their structure can easily be modified by alteration of molecule components like poltatom, heteroatom or counter-cation. Heteropoly compounds of transition metals are of scientific and practical interest. Introduction of a cation with variable oxidation state makes it possible to obtain new inorganic materials with charge transfer.

The first stage of my work consists of the introduction of transition metals into the counter cation position of the heteropolyacids. Cobalt cations were exchanged for protons into the $H_3PW_{12}O_{40}$ and $H_3PW_{12}O_{40}$ structures. Two series of heteropolyacids cobalt salts were synthesized: $H_2Co_{0.5}PM_{12}O_{40}$, $HCoPM_{12}O_{40}$ and $Co_3(PM_{12}O_{40})_2$, where M = Mo, W. Redox properties of the catalysts were characterized by means of cyclic voltamperometry and in the oxidation of cyclooctane with molecular oxygen. Oxidation of cyclooctane was performed at the temperature of 120^oC, for 6 hours and under the pressure of 10 atm. The reaction products are cyclooctanol and cyclooctanone. Introduction of these cations in the place of the charge balancing protons influences redox properties of the catalysts. The oxidation of cyclooctane in the presence of cobalt catalysts produced cyclooctanone as the main product and cyclooctanol in the small yield. Dodecamolybdophosphoric acid, which is known to possess redox properties, demonstrates high catalytic activity in the studied reaction. Incorporation of cobalt atoms to the HPMo structure improves only to some extent its catalytic activity. Parent HPW shows the lowest catalytic activity among the tested catalysts. Incorporation of cobalt atoms in the HPW structure has the major influence on their catalytic activity. Catalytic activity of neutral $Co_3(PW)_2$ salt is almost three times higher in comparison with 12-tungstophosphoric acid. Redox properties of the studied catalysts were verified by means of cyclic voltamperometry.

The determination of reduction potentials for the heteropolyacids and their cobalt salts by cyclic voltamperometry confirms the introduction of cobalt atoms into the Keggin structure. Moreover, the electrochemical study indicates that the exchange of the metal atom for proton brings about the changes of heteropoly compounds redox properties. It also results in the formation of additional active centers in the heteropolyacid molecules which probably causes the increase of its catalytic activity.

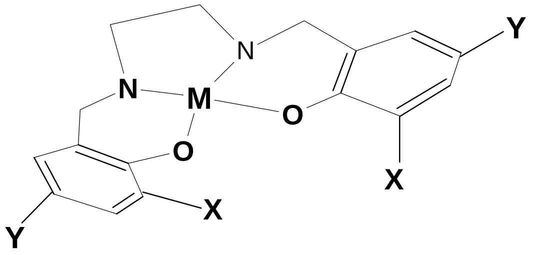
Synthesis and Investigation of Catalytic Properties of the Macrocyclic Salen Complexes in Oxidation of Hydrocarbons

(Professor J. Haber, J. Połtowicz PhD)

Oxidation of cycloalkanes with molecular oxygen is one of the most important large-scale processes in the chemical industry and one of the most attractive transformations in organic synthesis. Different kind of macrocyclic complexes like metalloporphyrins, metallophthalocyanines and metallosalens were applied as catalysts in these processes. The recycling and reuse of the expensive catalysts are the main drawbacks in oxidation reactions. Therefore, various methods have been developed to overcome this problem. One of them, fluorous catalysis without fluorous solvent, is easy to apply method for separation of catalysts from reaction mixture.

Manganese, iron and cobalt salen [N, N – bis (salicylidene) ethylenediamine] complexes and their perfluorous derivatives were synthesized and characterized by various techniques like FT-IR, UV-Vis, NMR and EPR spectroscopy.

We studied the catalytic activity of two series of catalysts in the oxidation of cyclooctane with oxygen: salen complexes with different metals and metallosalen complexes with different substituents (Fig.1). All catalysts were active in the oxidation reaction and the main products were cyclooctanone and cyclooctanol.



X	Y
H	H
H	C_8F_{17}
t-butyl	C_8F_{17}
t-butyl	t-butyl
C_8F_{17}	C_8F_{17}

Figure 1. Structures of the investigated salen metallocomplexes (where M = Mn, Fe, Co).

All complexes with electron-withdrawing or electron-donating substituents show higher catalytic activity than simple, unsubstituted MnSalen complex. The best studied catalyst was complex of MnSalen$(C_8F_{17})_4$ with four electron-withdrawing substituents. We have made a novel observation that perfluorous salen complexes exhibit temperature dependent solubility in reaction substrate. MnSalen and complexes with t-butyl substituents are well soluble at room temperature in substrate while complexes with perfluorous substituents are insoluble and become soluble only upon heating. MnSalen$(C_8F_{17})_4$ complex was recovered on cooling after the reaction and reused three times with only small decrease in catalytic activity. The similar tendency was observed for cobalt and iron complexes with the same perfluorous substituents.

Introduction of perfluorous substituents into salen rings enhances the catalytic activity of salen complexes. The use of a mixture of perfluorous metallosalen complex and organic phase, which turns into a homogeneous solution at elevated temperature, permits easy recovering of catalyst from reaction mixture after cooling to low temperature.

Catalytic Oxidation of Diesel Soot

(Professor J. Haber, T. Machej PhD, J. Janas MSc, R. Janik MScEng, W. Rojek MSc)

Diesel engine emission have gained considerable attention due to their health risk and environmental concerns, especially soot and NO_x.

The European Union limit to soot emission is becoming in increasingly severe. Starting from 2008 Euro V legislation puts into execution five times lower limits for soot emission comparing with Euro IV.

Application of catalyst for oxidation of soot particulates may by a great solution to meet the emission limit. The catalyst should lower the soot ignition temperature to the temperature of exhaust gases, 200-300°C. Moreover, highly reactive NO_2 present in exhaust gases may additionally decrease the oxidation temperature.

In 2006 preliminary catalytic testing catalyst samples, composed of vanadium and potassium oxides, was done by means of thermal analysis (TG-DTA). V_2O_5, KV-3 ($K_2O \cdot 3V_2O_5$), KV-4 ($K_2O \cdot 4V_2O_5$) and KV-5 ($K_2O \cdot 5V_2O_5$) were used as catalysts. The catalysts were mixed with synthetic soot Printex U (Degussa) which chemical compositions is close to this of diesel soot.

It was found that all catalysts are active in the soot oxidation and can be an object of further detailed investigation. The highest oxidation soot for all catalysts is in the temperature range 370–385°C. KV-5 ($K_2O \cdot 5V_2O_5$) is the most active catalyst.

The next step was experiments in a flow reactor. Honeycomb cordierite support covered with previously studied catalysts were used. The rate of the oxidation reaction as a function of the temperature (polythermic conditions) or time (isothermic conditions) was monitored by measuring the concentration of CO_2.

The flow of gas (10 w/w% O_2) was 10 dm^3/h in case of isothermic conditions (350°C). For the polythermic conditions the rate of the temperature increase was 10°C/min. and the gas flow 80 dm^3/h. The temperature was increased up to 700°C.

It was also studied an influence of NO on the soot oxidation. The NO content in feed was 1000 ppm. NO was oxidized to NO_2 on the Pt/Al_2O_3 catalyst before the honeycomb catalyst.

It was found that the results obtained in the flow reactor and by means of the thermal analysis are comparable. The highest rate of the soot oxidation fell in the temperature range 360-400°C. The temperature of the highest rate were additionally lower for KV-3, KV-4 and KV-5 by 20°C when NO was present in feed. This effect was not observed for V_2O_5 which points to essential role of potassium in oxidation reaction of soot.

Solid Superacids and New Peroxo-Compounds of Mo(VI), W(VI) and V(V). Synthesis, Crystal Structure and Physicichemical Investigations

(Professor W. Łasocha, M. Grzywa MSc)

New tetraperoxo-compounds: $Na_2[W(O_2)_4]{\cdot}4H_2O$, $Na_2[W(O_2)_4]{\cdot}5H_2O$ and (3,4-dimetylopyridyne)$_2$$[Mo(O_2)_4]$ were obtained. In these compounds the central W(VI) or Mo(VI) atom is surrounded by four O_2 groups. Approximate symmetry of the anions - 42m, is very close to a distorted dodecahedron.

Dinuclear-diperoxo complexes were the another group of the investigated compounds. Five new compounds were obtained: $(2\text{-}MepyH,NH_4)\{O[MoO(O_2)_2H_2O]_2\}$ (Mepy denotes methylo-pyridine), $(2\text{-}MepyH,Na)\{O[MoO(O_2)_2H_2O]_2\}$, $K_2\{O[MoO(O_2)_2H_2O]_2\}{\cdot}2H_2O$, $Rb_2\{O[MoO(O_2)_2H_2O]_2\}$, $Rb_2\{O[WO(O_2)_2H_2O]_2\}$. For the first three compounds the crystal structures were found. In the case of the rubidium compounds the lattice parameters, space groups and initial structure models were found using global optimization method.

A new diperoxo-heptmolybdate $(NH_4)_3(C_7NH_{10})_3[Mo_7O_{22}(O_2)_2]{\cdot}4H_2O$, in which two terminal oxygen atoms were replaced by two peroxo- groups, was also synthesized.

All the obtained compounds were characterized by chemical analysis and IR studies to confirm the presence of peroxo- groups. Stability of the compounds vs. time was tested by the series of XRPD measurements at room temperature and by thermograwimetric studies. Dinuclear diperoxo- compounds are more stable at room temperature than mononuclear tetraperoxo- complexes. During heating they are stable up to about 60°C. Only in the case of $(2\text{-}MepyH,NH_4)\{O[MoO(O_2)_2H_2O]_2\}$ was observed a very fast decomposition – (microscale explosion) at 100°C during DSC study.

In the table basic crystallographic data for the investigated compounds are presented.

Compound	**lattice parameters**	**Space group**	**V, Z**
$Na_2[W(O_2)_4]{\cdot}5H_2O$	a=6.9517(1), b=10.4832(2), c=14.0540(3), β=74.680(1)	$P2_1/c$ (14)	V=987.81(3) 4
$Na_2[W(O_2)_4]{\cdot}4H_2O$	a = 9.1180(2), b = 8.6230(1) c = 12.4000(2), β= 93.9040(8)	$P2_1/c$ (14)	972.68(3) 4
$K_2\{O[MoO(O_2)_2H_2O]_2\}{\cdot}2H_2O$	a=6.2745(2), b=9.7279(3), c=11.2976(3), α=78.7430(10), β=80.1900(10), γ=73.1300(10)	P-1 (2)	V=642.44(3) 2
$(2\text{-}MepyH,NH_4)\{O[MoO(O_2)_2H_2O]_2\}$	a=6.733(5), b=8.364(5), c=13.984(5), α=73.702(5), β=87.647(5), γ=85.216(5)	P-1 (2)	V=753.1(8) 2
$(2\text{-}MepyH,Na)\{O[MoO(O_2)_2H_2O]_2\}$	a=6.765(5), b=8.421(5), c=13.815(5), α=74.203(5), β=84.775(5), γ=71.371(5)	P-1 (2)	V=717.6(7) 2
$Rb_2\{O[MoO(O_2)_2H_2O]_2\}$	8.120(3), 12.547(3), 6.286(2), 93.31(2), 105.16(3), 105.34(2)	P-1 (2)	V=592.0(2) 2
$Rb_2\{O[WO(O_2)_2H_2O]_2\}$	8.145(2), 12.460(3), 6.348(2), 92.30(2), 104.98(2), 105.61(2)	P-1 (2)	V=595.2(2) 2
$(NH_4)_3(C_7NH_{10})_3[Mo_7O_{22}(O_2)_2]$ $\cdot 4H_2O$	a=14.0468(3), b=26.9834(6), c=11.7937(3), β=102.0397(10)°	C2/c (15)	V=4371.84(17) 4

Synthesis and Properties of Novel Zeolite Catalysts for Transformation of Aromatic and Terpene Hydrocarbons

(Professor B. Sulikowski, R.Rachwalik PhD, E. Włoch PhD, U. Filek MSc, Ł. Mokrzycki MSc)

The detailed pattern of dealumination of ferrierite-type zeolite has been studied, using ^{29}Si, ^{27}Al and ^{1}H MAS NMR *in tandem* with FT IR. We have developed a procedure for the dealumination of FER-type zeolite that allows removal of up to 53% of the framework aluminum atoms from the parent material. The procedure involves treatment of the ammonium form of FER (NH4-T) with aqueous solutions of hydrochloric acid of different concentrations. ^{29}Si MAS NMR spectroscopic studies indicated that the attack of HCl caused selective removal of aluminum atoms located at different crystallographic positions in the FER framework. The framework aluminum atoms were preferentially removed from their positions in the vicinity of silicon atoms occupying T_B sites. These aluminum atoms contributed to the 10-membered oxygen rings of the main channels. In contrast, aluminum atoms, bound via oxygen bridges to silicon atoms at the T_A positions, were much more resistant to dealumination. The latter are located exclusively in the five- and six-membered oxygen rings of the zeolite structure, which are less prone to attack by hydrochloric acid and possibly more stable. The dealuminated materials retain their crystallinity and good sorption properties, as demonstrated by nitrogen and α-pinene adsorption studies.

Subsequently, liquid phase isomerization of α-pinene was performed on a series of dealuminated materials. Even mild dealumination of FER led to an active catalyst containing both Brønsted and Lewis centers. It was shown that the initial rates of α-pinene transformations over FER-type materials exceeded those observed for other catalytic systems, comprising heteropoly acid HPW/SiO_2 and sulphated zirconia.

Novel MCM-41 modified catalytic materials were synthesized by impregnation of MCM-41 with niobium and gallium salts. A number of techniques, including nitrogen adsorption, X-ray diffraction, FT-IR and Raman spectroscopies, have been used to characterize a series of gallium and niobium-containing composite materials. Generally, the presence of highly dispersed NbO_x and GaO_x moieties in the mesoporous materials could be deduced from this approach. The deposition of Ga species on the matrix induces base/redox properties. It has been demonstrated that incorporation of gallium and niobium into the MCM-41 type silica matrix leads to formation of active and selective catalysts for the oxidation of cyclohexene. The highest selectivity to epoxide, for the same cyclohexene conversion, is observed on the bimetallic mesoporous system (Nb/Ga/MCM-41) indicating the promoting role of niobium–gallium interaction. It seems that the proper isolation of active species is required for the high activity in this process and this can be achieved using a high area support such as a mesoporous molecular sieve. The niobium impregnated samples based on the mesoporous MCM-41 matrix exhibit the much higher cyclohexene conversion than those prepared on the metal oxide supports, which is clearly due to the high surface areas of the former materials.

Cu-containing ZSM-5 materials were carefully prepared using a solid-state ion-exchange procedure to provide an outstanding performance in the direct gas-phase benzene oxidation to phenol using both oxygen and oxygen/hydrogen mixtures as oxidants. In particular, a ZSM-5 catalyst with a 100% modification level of copper showed a phenol yield increasing with temperature up to 400^{o}C and approaching a high value of ca. 10%, i.e. about 2-times more than described up to now in the literature. The study showed that optimization of the phenol yield in the Cu-ZSM-5 system appeared to be correlated with the appearance of size-limited Cu species, and that the presence of H_2 in the feed was either beneficial or detrimental for the catalytic performance, depending on the zeolite loading with copper.

Combustion of Volatile Organics over Catalysts Derived from Layered Minerals

*(Professor E. Serwicka-Bahranowska, M. Zimowska PhDEng, R. Dula PhDEng,
D. Napruszewska Eng, J. Plona MSc, J. Podobiński MSc, T. Machej PhD, R. Janik MSc)*

Catalytic combustion is one of the most attractive ways of controlling the emission of volatile organic compounds (VOCs). Both manganese- and copper-based mixed oxide systems serve as efficient catalysts in many industrially important oxidation processes, and proved also as highly active in the combustion of volatile organic compounds (VOCs). In view of the well known unique properties of mixed oxide phases prepared from the hydrotalcite-like precursors our intention was to use such precursors to develop Cu-Mn oxide catalysts for combustion of VOCs. Aluminium additive was used to promote the formation of a hydrotalcite structure. A series of precursors of intended Cu:Mn:Al atomic ratio equal 6:2:1 were obtained by coprecipitation at constant pH, which was varied the range 6-9. All materials, denoted CuMnAl(x), where x=pH of synthesis, possessed the hydrotalcite structure. The CuMnAl(6) sample contained additionally the layered double salt $Cu_2(OH)_3(NO_3)$. Chemical analysis showed that the solid precipitated at lowest pH retained only half of the intended amount of Mn. Mn content grew with increasing pH of precipitation. Mixed oxide catalysts were obtained by 3 h calcination at 723 K. Only reflexes due to CuO could be detected by XRD analysis, of intensity decreasing with increasing content of Mn. HRTEM analysis identified, additionally, nanocrystallites of spinel $Cu_{1.5}Mn_{1.5}O_4$ or $CuMn_2O_4$ (the former being more likely to occur in copper-rich system). Apparently, decrease of the CuO intensity was due to the growing involvement of copper in the formation of the nanocrystalline spinel phase. No separate Al-containing phase could be identified, but the EDX analysis suggested that Al may be present as an amorphous oxidic phase. All calcined materials possessed specific surface areas of ca. 80-90 m^2/g, with the exception of CuMnAl(6), whose BET specific surface was ca. 60 m^2/g.

Catalytic tests have shown that all samples were very active in the combustion of toluene, reaching 100% conversion in the range of 130-180^{o}C. The activity increased in the order CuMnAl(6)<CuMnAl(7)<CuMnAl(8)<CuMnAl(9) (Fig. 1). Since the best performance was achieved for sample with the highest amount of Mn and least intense CuO reflexes, the Cu-Mn spinel was thought to be the most active phase in the mixed oxide sytem studied. To verify this a hydrotalcite precursor was obtained at pH=9 with Cu:Mn:Al atomic ratio equal 4:4:1, i.e. with considerably higher amount of Mn and the Cu:Mn ratio corresponding to that of the $Cu_{1.5}Mn_{1.5}O_4$ spinel. The solid obtained by calcination of this precursor gave an XRD pattern of poorly crystalline spinel phase, with no evidence of copper (II) oxide. In the test of toluene oxidation the material proved most active of all tested catalysts, reaching 100% conversion at 110^{o}C, which supports the conclusion on the importance of the copper-manganese spinel in determining the activity of the investigated catalysts.

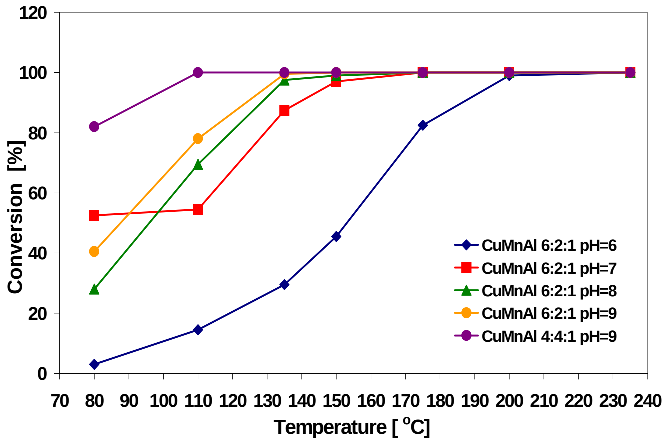


Fig. 1 Tempertaure dependence of toluene conversion over CuMnAl mixed oxide catalysts

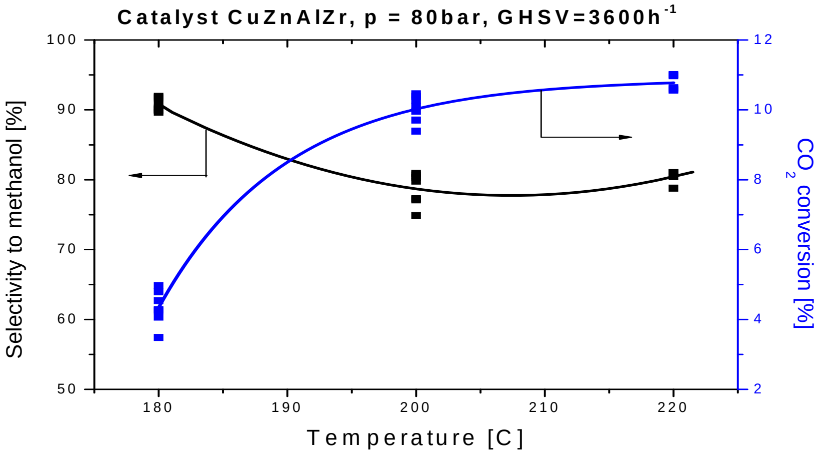
Start-up of High Pressure Reactor for Methanol Synthesis

(Assoc. Professor R. Grabowski, Proferssor E. Serwicka=Bahranowska, M. Śliwa MSc)

In 2007 the starting of high pressure reactor was accomplished and preliminary experiments concerning methanol synthesis and direct synthesis of dimethyl ether (DME) from syngas were carried out. The goal of these studies was to investigate whether the reactor works properly and to choose and fit the optimal parameters of the reaction.

Calibration of the substrates and products in methanol and DME synthesis was the first task to be completed.

The methanol synthesis from H_2/CO_2 mixture was performed at the temperature range 180 – 220^oC at pressure of 80 bars, GHSV = 3600 h^{-1}, over CuZnAl catalysts and CuZnAl containing zirconium. All catalysts were synthesized by hydrotalcite method but they differed in condition of the preparation. Temperature increasing up to 220^oC leads to the decrease in selectivity to methanol to 77% and 80% and to the increase of CO_2 conversion up to14% and 11% for CuZnAl and CuZnAlZr respectively. The results for the CuZnAl catalysts are in agreement with the results obtained in the Institute of Chemical Engineering PAS.



CuZnAl catalyst, characterized by the highest selectivity (94%) to methanol, synthesized at pH = 9, was chosen as metallic component. Commercial montomrilonite was selected as acidic component. Bifunctional catalyst was prepared by mechanic mixture of the grains of metallic and acidic components. The size of the grains was 0,64-1 mm. The volume ratio of the metallic component to acidic component was 2:1.

The one-step synthesis of DME direct from the syngas with 5% of CO_2 was performed at the temperature range between 250-280^oC and pressure 30-50 bars, GHSV=3600 h^{-1}. The increase of selectivity to DME was observed while temperature decreased. The highest recorded selectivity to DME was 83% and it was obtained in 280^oC at 50 bars. Additionally, it was determined that above 40 bars, the changes in the pressure have little effect on the increase of the selectivity to DME.

The preliminary results concerning methanol and one-step DME synthesis proves that high pressure reactor connected with chromatograph works correctly. The initial experimental data suggest that the optimal reaction conditions are 80 bars and 200^oC for methanol synthesis whereas optimal reaction conditions for DME synthesis are 40 bars and temperature ca. 270^0C.

Adsorption and Catalytic Processes Modeling

Porphyrin-Based Catalysts: Structure Activity Relationship

(Professor M. Witko, D. Rutkowska-Żbik PhD, M. Szaleniec PhD, R. Tokarz-Sobieraj PhD)

The aim of the research was to find a correlation between catalytic activity of manganese porphyrines (in the reaction cyclooctane oxidation to ketone and alcohol) and their electronic and geometrical structure. Theoretical investigation took into account variation in the type of the axial ligand (L=F, Cl, Br, I, OH, CH_3COO), structure of phenyl substituent (Z=H, Cl, CH_3, OCH_3CF_3, Z1=Cl, X=Cl) and modification of tetrapyrrole ring (Y=Cl, Br) in manganese (III) tetraphenylporphyrines – see Fig. 1. Moreover, research focused on the influence of metal oxidation state and presence of axial ligand on the process of adsorption of the molecular oxygen on MnP systems. The calculations were conducted in a gas-phase with DFT method with non-local B3LYP functional.

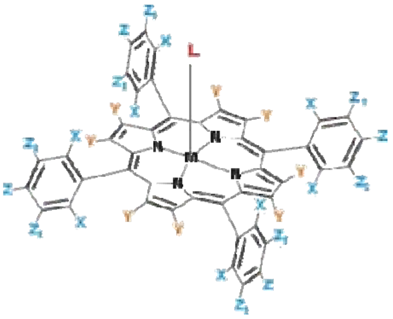
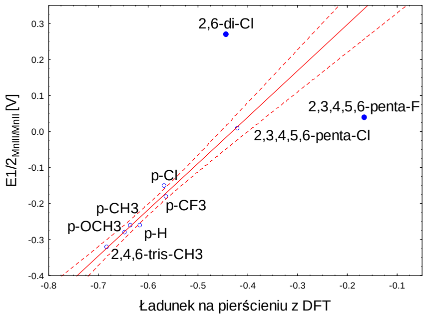
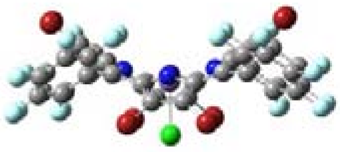


Fig.1 Structure of metalloporphyrin



Rys.2 Correlation of porphyrin ring charge with $E_{1/2}$



Rys3. Geometrical structure of halogenated porphyrin

For systems with different axial ligands the correlation was found between the catalytic activity and relative energy difference of molecular orbitals (HOMO and HOMO+1). This seems to suggest that initial reduction of porphyrines through C-H activation by axial ligand can take place. This process implies reduction of quintet $Mn^{III}PCl$ to sextet $Mn^{II}P$ + HCl).

The analysis of oxygen adsorption showed that O_2 spontaneously binds only to the reduced Mn^{II} porphyrines. For four coordinated systems it formed two stable structures: side-on (two Mn-O bonds) and end-on (one Mn-O bond) with binding energy of -43 kJ/mol and -34 kJ/mol, respectively. Introduction of axial Cl ligand resulted in weaker binding of O_2 (-15 kJ/mol). In addition only the side-on geometry was formed. The formation of complexes for system with Mn^{III} turned out to be thermodynamically unfavorable.

The calculations for systems with modification in phenyl substituents showed that charge of porphyrin ring is a good theoretical descriptor of inductive effect introduced by the substituent. This descriptor correlates with experimental value of redox potential Mn^{III}/Mn^{II} (Fig. 2).

Modeling of porphyrines with halogenated (Cl, Br) tetrapyrrole rings showed that significant geometrical changes take place i.e. the porphyrin ring is bent due to steric interactions (Fig.3) .

Adsorption of Atoms and Molecules at the Transition Metal Oxide Surfaces. Modeling by Theoretical Methods

(Professor M. Witko, P. Hejduk MSc, J. Goclon MSc)

The catalytic properties of active centers existing at the low-indices V_2O_5 surfaces were investigated. Theoretical calculations were performed in both, cluster and periodic approaches. The adsorption properties of surface O as well as V centers were tested in the probe reactions that were adsorption of one or two hydrogen atoms. Moreover, in the periodic approach the reducibility of the (010), (001) and (100) surfaces (Fig.1) was examined assuming the formation of oxygen vacancies. In addition surface relaxation due to oxygen vacancy formation was analyzed.

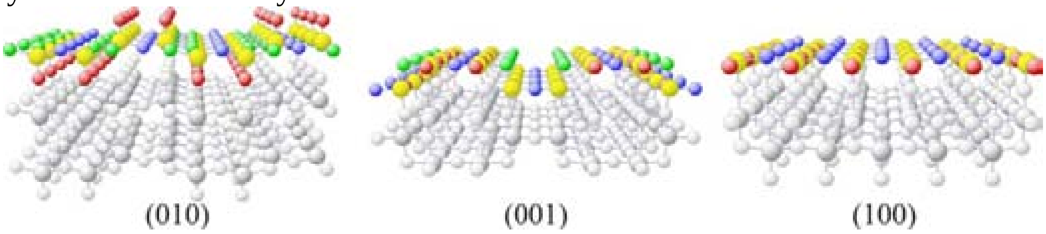


Figure 1. Three low-indices V_2O_5 surfaces.

The calculations were carried out by means of the DFT with generalized gradient approximation (GGA). The program package StoBe (cluster approach) as well as VASP code (periodic approach) was used. The energy of hydrogen adsorption or of vacancy formation was obtained from the differences of the total energies of appropriate systems.

The cluster calculations point out that hydrogen atom is stabilized stronger at unsaturated (001) and (100) surfaces (E_{ads} from -2.6 to -3.6 eV) than at the saturated (010) netplane (E_{ads} from -1.9 to -2.3 eV). The adsorption of second H atom is also more favorable at the under-coordinated surfaces (001) and (100) (E_{ads} from -5 to -6.3 eV) comparing to the most stable (010) netplane (E_{ads} from -2.9 to -3.9 eV). Therefore, the calculations indicate that the activity of the unsaturated (001) and (100) surfaces should be higher than the activity of (010) surface in the process of organic molecule activation.

The results of periodic calculations show that the surface oxygen atoms are strongly bounded to the surface. The bonding energies are larger for the fully saturated (010) surface (E_b in the range 5 to 7 eV) than for the unsaturated (001) and (100) netplanes (E_b in the range 3.5 to 4.2 eV). Moreover, for the (001) and (100) surfaces the values of vacancy formation energies decrease with increasing the size of supercell, another words when the density of the oxygen vacancies at the surface goes down. During vacancy formation process the strong geometry relaxation takes place, which for the unsaturated surfaces occurs in creation new bonds between adjacent atomic layers in the [010] direction. In addition, the surface relaxation for the large supercells, which follows due to oxygen vacancy creation, results in the formation of the amorphous-like bulk structure (see Fig.2).

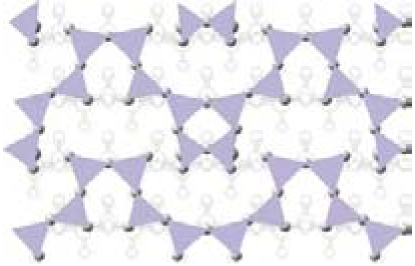


Figure 2. The amorphous-like bulk structure.

Kinetics of Oxidative Dehydrogenation of Propane at Steady State Conditions on V Mg O and K-V-Mg-O Catalysts

(Assoc. Professor R Grabowski, I. Gressel, M. Śliwa MSc)

Vanadium-containing oxide catalysts have interesting properties in various selective oxidation reactions including oxidative dehydrogenation (ODH) of lower alkanes, a reaction of considerable interest as a source of cheap olefins. Magnesium supported vanadia catalyst has exceptional properties, among these systems, because the distribution of the reaction products is different than in the case of the other vanadia supported catalysts.

The experimental data were obtained for the 1mnl VMgO and 1mnl KVMgO catalysts in the integral reactor for conversions (X_p) $0 < X_p < 0.3$. The obtained results were used for the calculations of the particular rate constants in a broad range of the independent variables (concentrations of propane, temperature of the reaction and contact time).

The LH (Langmuir-Hinshelwood), ER-SSAM (Eley-Rideal-Steady-State Adsorption Model) and MK (Mars van Krevelen) models have been applied to the description of the ODH. The results of these calculation showed that on this catalyst, reaction of propane ODH is the most appropriately described by the ER-SSAM-1 model.

In Table 1 the calculated values of the rate constants (pre-exponential factors and the activation energies) for ER-SSAM-1 (combustion propane/propene is second order reaction with respect to surface coverage by oxygen) and ER-SSAM-2 (combustion propane/propene is first order reaction with respect to surface coverage by oxygen) model are given. The differences between these two models are small and one must state, that is difficult to say, which of this models describes better this reaction.

Table 1.

Catalyst	$\mathbf{k_1}$		$\mathbf{k_2}$		$\mathbf{k_3}$		$\mathbf{k_{OS}}$		**Błąd [%]**
	$\mathbf{k_1^0}$	$\mathbf{E_1}$	$\mathbf{k_2^0}$	$\mathbf{E_2}$	$\mathbf{k_3^0}$	$\mathbf{E_3}$	$\mathbf{k_{OS}^0}$	$\mathbf{E_{OS}}$	
	PROPANE								
VMgO	140	13	380	9	230	12	13600	14	5.1
KVMgO	24	12	400	5	150	11	58000	17	6.8
VMgO	140	13	400	9	210	12	36550	12	5.1
KVMgO	50	13	41100	17	11	11	72150	17	7.2

*activation energy – kJ/mol

On the basis of the obtained results one can formulate the following conclusions concerning of propane ODH over VMgO and KVMgO catalysts.

1. Proposed model ER-SSAM described correctly of propane ODH on these catalysts in the studied temperature range and feed mixture composition.
2. Combustion products are formed mainly in the reaction of consecutive combustion of propene. The participation of parallel combustion of propane is small and depends on temperature and feed mixture composition.
3. Only one kind of oxygen (nucleophyllic oxygen) from vanadium oxide surface participates in selective (formation of propene) and non selective oxidation (parallel combustion of propane and consecutive combustion of propene).
4. Alkali additives (potassium) decrease the selectivity to propene, mainly by the increase of the participation of consecutive combustion path of propene.
5. It is not clear which of two models (1). formation of carbon oxides is second or (2). is first order reaction with respect to surface oxygen coverage) describe better this reaction.

Computer Simulations of Kinetics of Proton Adsorption on the Metal Oxide / Electrolyte Interface

(Professor W. Rudziński, P. Zarzycki PhD, W. Piasecki DSc)

Adsorption of hydrogen ions is basic mechanism of double layer formation on oxide/electrolyte solution interface. However very little is known about kinetics of proton adsorption in that system.

In our research we applied Kinetic Monte Carlo (KMC) simulations to investigate kinetics of hydrogen ion adsorption on metal oxides from solution. In particular the influence of the system properties (surface site density, interfacial dielectric constant, surface energetic heterogeneity) on the equilibrium and kinetic surface coverage was studied. It was shown that the kinetic properties were much more sensitive to lateral interactions than the equilibrium ones. Additionally, the assumption of surface energetic heterogeneity rapidly changes the time scale of the whole adsorption process as well as the time interval between two subsequent elementary processes.

To describe kinetic curves obtained from the simulations we applied two kinetic models: classical ART (Absolute Rate Theory) and new SRT (Statistical Rate Theory). Unfortunately none of them was able to correctly describe data obtained in the simulations. It can be explain as follows: Microscopic model of oxide/electrolyte solution interface applied in the simulations was simplified and could not take into account important phenomena for ion adsorption kinetics. On the other hand the applied kinetic models treat electrostatic interactions (which are very important in ion adsorption) in an approximate manner. Currently we would like to investigate the influence of the latter factor on the description of proton adsorption kinetics.

Sorption Processes Applied in the Environmental Protection: Theoretical Description of the Sorption Kinetics

(Professor W. Rudziński)

Adsorption at a solid/solution interface is probably the most commonly applied physical process in the industrial purification of waste waters. There the sorbent and the solution are brought into contact for a limited period of time. Thus, the kinetics of these processes is at least as much essential as their features at equilibrium.

The studies were focused on the theoretical description of adsorption kinetics at the solute/solution interfaces by using Statistical Rate Theory (SRT) approach. It has been shown that the popular pseudo-first order Lagergren equation can be applied to correlate kinetic adsorption data only in the adsorption systems which are not far from equilibrium. It has also been shown that the Lagergren equation is only the limiting form of the more sophisticated kinetic equations developed by assuming both diffusional and surface reaction kinetic models. The theoretical interpretation of the coefficients appearing in the linear form of the Lagergren equation is different for these two different kinetic models. The comparison of the theoretically predicted values of these coefficients with those determined experimentally creates a chance to conclude whether the diffusional or the surface reaction model should be assumed to represent the kinetics of adsorption in an investigated adsorption system. This possibility has been demonstrated by analyzing the behaviour of the two adsorption systems reported in literature, i.e. MCB/pine sawdust and Cd^{2+}/bone char.

Also, the problem of using proper theoretical expressions to represent the features of some kind of kinetics has been discussed. It has been shown how the technical conditions of adsorption system (mass of sorbent, volume of solution, initial sorbate concentration) may affect the kinetic isotherms in the systems in which kinetics is governed by the intraparticle diffusion, and that in which the surface reactions control the rate of sorption. The theory has been compared with the behaviour of two real adsorption systems.

Another problem which recently has been studied is the possibility of introducing some approximation into the basic SRT expression in order to obtain simple analytical equations describing sorption kinetics. Some simplified forms of the basic SRT expression for sorption kinetics has been derived and discussed from the point of view of their accuracy.

Influence of Fractal Structure of Surfaces on the Dynamics of Transport in Gas / Solid System

(*Professor W. Rudziński, T. Pańczyk PhD*)

Adsorption kinetics or surface reactions depend on many factors. One of them is the frequency of collisions of adsorbate/reactant particles with the surface. Real solid surfaces, from the point of view of their topography, are usually far from any deterministic structure. Therefore, it is difficult to predict any relation describing the actual flux of adsorbate particles to the surface under given conditions of pressure or temperature. This problem becomes more tractable when applying the fractal geometry concepts since the surface fractal dimension is the most general parameter defining the degree of surface irregularity.

The aim of the studies was to measure the collision frequency factors of ideal gas particles with rough surfaces and to correlate them with the fractal dimensions of surfaces. The studied surfaces have been created using two well-known surface growth models, namely: *random deposition* and *ballistic deposition*. The most important differences between them can be easily recognized while looking at the two samples, shown in Figure 1.

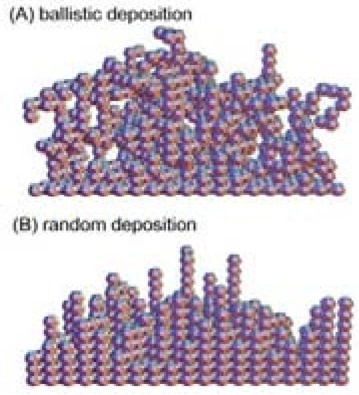


Figure 1: Samples of studied surfaces

Fractal dimensions have been determined for surfaces obtained after deposition of various amounts of atoms on an initially perfect surface. Next, using the self-designed molecular dynamic simulation code, the frequencies of collisions of ideal gas atoms with those surfaces have been measured. Studies were carried out for various ratios of gas atom diameter to the surface building ball diameter, σ.

The most important results of calculations are shown in Figures 2 and 3, where the determined values of collision frequency factor versus surface fractal dimension are plotted for both growth models and various ratios of gas atom diameter to surface building ball diameter. Dashed lines represent the predictions given by the Hertz-Langmuir equation, valid for ideally flat and smooth surfaces:

$\phi = 1/\sqrt{2\pi mkT}$, where *m* – mass of gas atom.

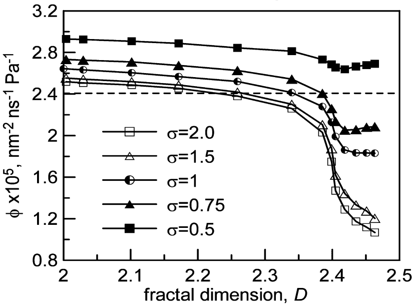


Figure 2: Random deposition

The most important conclusion, which can be drawn from the studies, is the statement that the collision frequency does not differ dramatically from the Hertz-Langmuir prediction even for surfaces representing strongly irregular nature. It is however valid only for the case when the collision frequency is calculated in reference to the actual surface area of the fractal object. Thus, it is often possible to apply the Hertz-Langmuir equation in microkinetic modeling of surface reactions on catalysts surfaces. Although such a treatment introduces some errors to the pre-exponential factor, their limiting values can be approximately estimated from the results shown in Figs. 2 and 3.

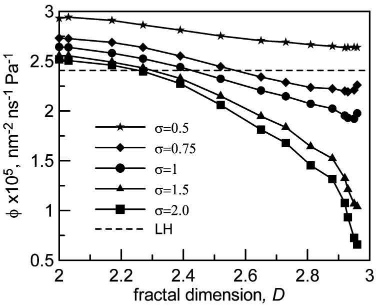


Figure 3: Ballistic deposition

Structural and Electronic Properties of Enzymes' Active Sites Hosting Transition Metals - Theoretical Studies

(Professor E. Brocławik, T. Borowski PhD)

Within the scope of this task there are theoretical investigations of electronic structure and reaction mechanisms for metallic centres in selected enzymes. Work done during the last year involves the following subtopics.

Investigations of cyclization reaction mechanism catalysed by clavaminic acid synthase (CAS) (one paper published). Results obtained with classical dynamics simulations and DFT (B3LYP) methods suggest that this reaction may follow an unprecedented mechanism involving fragmentation of the substrate into aldehyde and ylide and their subsequent cyclization.

Molecular dynamics simulations for enzyme-substrate complex for histone demethylase JMJD2A (one paper published). Computational studies confirmed the stability of the structures observed in the crystals and provided insights into the dynamics of the active site region.

Quantum-chemical (DFT: B3LYP) studies on the mechanism of oxidative cleavage of polyene chain by apocarotenoid oxygenase (ACO) (one paper in print). Computational results suggest that two mechanisms involve comparable barriers, yet one of them explains the observed product specificity in a more elegant way.

Studies on aromatic oxidation reaction for molecules modeling drugs with aromatic fragment, catalyzed by the active oxyferyl sites in CYP 3A4 cytochrome and by FeO^+ molekule (two papers published, one submitted). Results of DFT calculation indicate at low-spin state of iron as the active form and allow for discriminating electronic and steric effects in reaction mechanism. Substituents responsible for the lowering of the activation barrier for oxygen insertion into C-H bond and the role of protein environment in ligand orientation are described. Low-spin state and peculiar antiferromagnetically coupled electronic structure of Fe^{IV}-O core w is confirmed by correlated CASPT2 calculations; CASPT2 results validated reliability of DFT methodology for intricate electronic structures of iron sites in enzymes.

Electronic and Structural Properties of Metallic Active Sites in Nanoporous Materials

(Professor E. Brocławik, P. Rejmak MSc)

The main goal of this task in 2007 was DFT modeling of proerties of Cu^+, Ag^+ AND Na^+ cationic sites in ZSM-5 zeolite and their interaction with benzene molecule. The present work concerns the activation of benzene by Cu^+, Ag^+ and Na^+ ions in zeolites. DFT cluster calculations have been carried out to obtain geometric structure and electronic properties of the cluster models of the three systems to analyze differences and their impact on the activation of adsorbed benzene. NOCV (Natural Orbitals for Chemical Valence) has been used to estimate components of differential electron density: donation and back-donation. Zeolite framework is shown to enhance the latter one and to influence strongly benzene activation for Cu^+ and Ag^+ sites.

DFT modeling performed for Cu^+, Ag^+ and Na^+ sites in zeolite framework interacting with benzene molecule aided by the analysis of natural orbitals for chemical valence allow for better understanding of charge flow processes and their influence on benzene activation. NOCV may be used to separate donation and back donation contributions what enables the discussion of effective charge flow in terms of increasing/decreasing electron population on particular molecular fragments. This in turn leads to better description of benzene activation after adsorption.

For Cu^+ sites π-back donation prevails over donation; for Ag^+ the two processes are comparable while for sodium they are negligible. The comparison with bare cations shows that the framework enhances π-back donation ability of Cu^+ while for Ag^+ π-back donation, which is not effective for bare cation, is triggered by the zeolite framework. Therefore activation of benzene by Ag^+ is significantly weaker than by Cu^+ site what follows as well from experimental IR spectra as theoretical results such as geometrical parameters or the analysis of charge flow after adsorption.

Dynamics of Nanoparticle and Colloid Systems

Influence of Angle of Collision and Roughness of the Hydrophobic Surface on the Three Phase Contract Formation

(Professor K. Małysa, M. Barańska Eng, M. Krzan PhD, J. Zawała MScEng,
A. Niecikowska MSc, A. Olszewska MSc)

The aim of the studies was to determine the influence of the angle of collision and the surface roughness on the TPC formation during the bubble collision with the model hydrophobic solid samples. Phenomena occurring during the collisions of the rising bubble with hydrophobic surfaces (Teflon) plates in distilled water were recorded using high speed camera. The time of TPC formation, i.e. the time period form the bubble first collision to the TPC formation and bubble attachment were determined for the Teflon plates of different surface roughness and oriented at various angles in respect to the trajectory of the rising bubble. The velocity variations and bubble shape pulsations during the collision were determined, as well. The roughness of the Teflon plate was modified by the abrasive paper of different grid numbers and the following samples were prepared – “Teflon I” and “Teflon II” (scratches’ dimensions below 1μm), “Teflon III” (30 –60 μm), “Teflon IV” (50-80 μm), “Teflon V” (80-100 μm).

It was found that roughness of the hydrophobic solid surface (Teflon) was of crucial importance for kinetics of the bubble attachment (time of TPC formation – t_{TPC}). Depending on degree of the surface roughness the time of the three phase contact formation varied by over an order of magnitude (from 3 - in the case of Teflon IV and V, to over 80 ms - in the case of Teflon I and II). In the case the Teflon surfaces having roughness below 1μm there were recorded four to five “approach-bounce” cycles prior to the bubble attachment. Simultaneously, after the first collision the bubble shape started to pulsate rapidly within time intervals of an order of fraction of millisecond. In the case of the Teflon plates having surface roughness of ca. 50 μm and larger the attachment always occurred during the first collision – there was no bouncing observed and the time of the attachment was below 3ms. Moreover, during the first collision with the “Teflon III” surface a small satellite-bubble was left and the stable attachment was observed during the second collision, when the bubble "hit" the spot with the satellite-bubble left.

The crucial influence of the surface roughness on the time of the colliding bubble attachment was attributed to the following mechanism: i) higher roughness means larger asperices (pillars) at the surface and higher probability that rupture thickness of the thinning liquid film is locally faster attained, and/or ii) there are larger cavities at rougher surface and larger amount of gas (air) can be present there, what leads to a faster formation of long enough perimeter of the TPC for the bubble attachment. The experiments with the different angle of collision supplied additional evidences confirming importance of the entrapped air presence. When the Teflon plate having roughness comparable to “Teflon III” was mounted in such a way, that the angle between the bubble trajectory and the Teflon surface was 80°, then a significant scatter of the result was observed - in 50% measurements the bubble was attached to the Teflon plate during the second collision, i.e. the t_{TPC} was ca. 40 ms. This value was practically identical with the t_{TPC} obtained for 90°. Lowering the collision angle to 60° caused prolongation the t_{TPC} to 83 ms (4 collisions of the bubble with the Teflon surface was observed prior to the TPC formation). The t_{TPC} prolongation with the collision angle decrease can be attributed to an increased probability that the bubble “hit” different “spot” (local area) of the solid surface. When the collision angle was large enough for the bubble to bounce practically perpendicular to the surface then the probability that it hits this same “spot” (the satellite bubble left) at the surface was much higher.

Determination of the Formation Kinetics and the Structure of Particle Monolayers Interacting via a Short-Range Potential

*(Professor Z. Adamczyk, J Barbasz PhD, A. Bratek MSc, A. Michna MSc, M. Nattich PhD,
P. Weroński PhD)*

Interactions of colloid and biocolloid particles with interfaces leading to adsorption, deposition (irreversible adsorption) and adhesion have major significance enabling one to optimize new processes aimed at selective separation of DNA, proteins, viruses, pathological cells, bacteria and so forth. etc. The efficiency of separation processes is often enhanced by modification of substrate surfaces, most often realized by pre-adsorption of polymers, especially polyelectrolytes. Thus, the main goal of this work was determination of the kinetics and structure of particle monolayers formed at heterogeneous surfaces, created by polyelectrolyte adsorption.

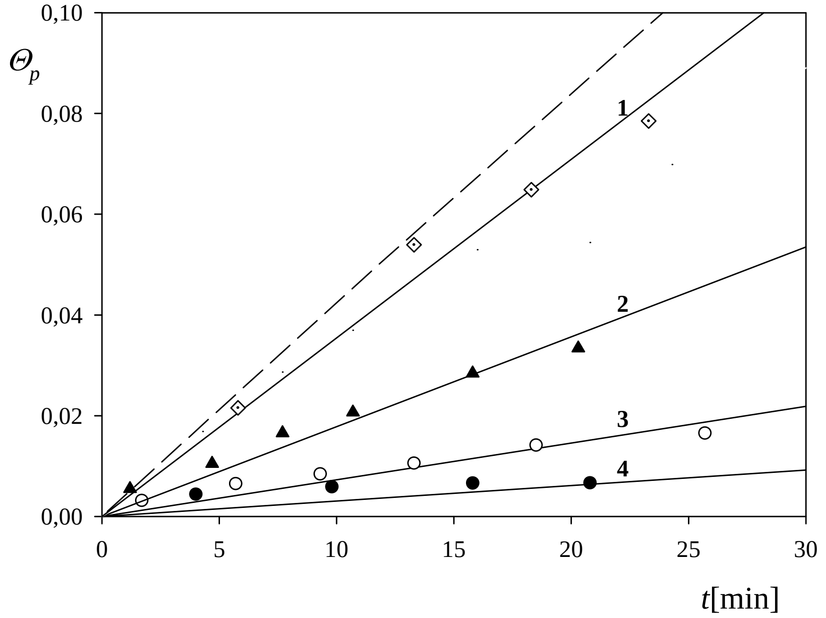


Fig. 1. The dependence of the latex particle coverage Θ_p at mica surface covered by various amounts of adsorbed PEI on the deposition time t. Particle deposition performed at $Re = 2$, $I = 10^{-3}$ M, PEI adsorption at pH 6.1–6.4, $I = 10^{-3}$ M. PEI coverages are as follows: (1) (◇) $\Theta_{PEI} = 0.116$; (2) (.▲ $\Theta_{PEI} = 0.074$; (3) (○) $\Theta_{PEI} = 0.055$; (4) (●) $\Theta_{PEI} = 0.042$. The solid lines represent linear fits and the dashed line denotes limiting results for continuous surfaces.

Experimental measurements have been carried out for freshly cleaved mica surface modified by adsorption of a cationic polyelectrolyte: polyethylene imine (PEI) having a well-controlled coverage. Deposition of polystyrene latex (having an average particle size of 660 nm) have been carried out under convection-controlled transport conditions using the radial impinging-jet cell. In Fig. 1 the kinetics of latex particle deposition is show for the linear deposition range as a function of the PEI coverage. The dependence of the initial deposition rate on PEI coverage determined from these experiments was interpreted in terms of a new theoretical model based on the charge fluctuation concept. It was also demonstrated that the widely used DLVO theory postulating a homogeneous charge distribution was inadequate. This enabled one to elaborate a precise experimental method of determining the bulk concentration of polyelectrolytes and biopolymers in aqueous solutions.

Self-Organized Structures and Nanoparticles Monolayers

Determination of the Correlation between the Shape on Nanoparticle Shape at Surfaces and the Electrokinetic Potential

(Professor Z. Adamczyk, M. Zembala DSc, B. Jachimska PhDEng, E. Porębska)

Deposition of cationic and anionic polyelectrolyte layers on solid supports proved to be an efficient method of creating substrates of targeted functionality, which allows one to selectively attach proteins and other biopolymers from their mixtures. Despite a major significance of these processes, few systematic works have been undertaken aimed at determining mechanisms and kinetics of polyelectrolyte adsorption at solid/liquid interfaces. Therefore, the basic goal of this work was elaborating a new experimental method, allowing one at a precise determination of the polyelectrolyte coverage and the shape of the macromolecules adsorbed at surfaces. This method is based on measurements of the streaming potential carried out in the parallel-plate channel, under controlled hydrostatic pressure difference. The measurements have been carried out for the anionic polyelctrolyte: polyethylene imine (PEI).

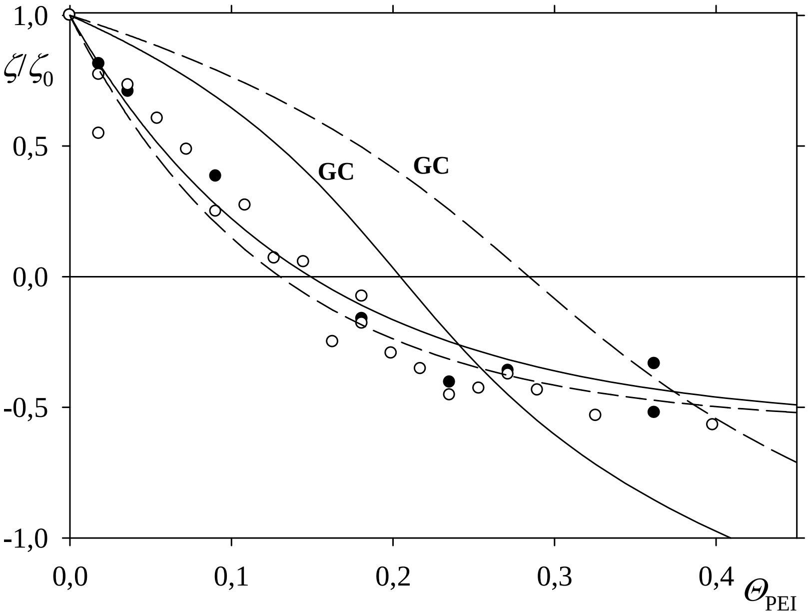


Fig. 1. The dependence of the relative zeta potential ζ/ζ_0 of mica on the coverage of PEI Θ_{PEI}, full and empty circles correspond to adsorption performed from PEI solutions of the ionic strength of 10^{-3} and 10^{-2} M, respectively, *pH* = 6.1-6.4. The dashed and solid line denotes the theoretical results calculated for the ionic strength of 10^{-2} and 10^{-3} M, respectively. The curves calculated from the Gouy-Chapman model are denoted by GC.

The physicochemical characteristics of PEI were determined from the PCS measurements of the diffusion coefficient (hydrodynamic radius) and the microelectrophoretic mobility. The dependence of the reduced zeta potential of PEI layer on mica on its coverage, obtained in these experiments, is shown in Fig. 1. As can be seen, the experimental results are quantitatively reflected by our theoretical model. On the contrary, the commonly used in the literature, Gouy-Chapman model (denoted by GC in Fig. 1) proved inadequate. This agreement showed that PEI molecules adsorbed at mica surface preserve to a considerable extent their spheroidal shape, characteristic for the bulk.

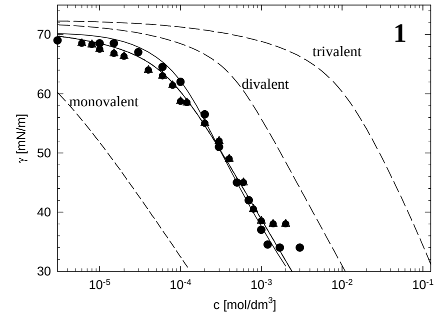
Adsorption of Ionic Surfactans at Luquid Interfaces

(Assoc. Professor P. Warszyński, G. Para PhD, E. Jarek PhD, M. Noworyta Eng)

Influence of multiple charge on surfactant adsorption, namely an effect of divalent sulphate SO_4^{2-} anions and monovalent hydrosulphate HSO_4^- anions, on the surface tension of cethyltrimethyl ammonium salts (C_{16}TABr (CTABr) and $C_{16}TAHSO_4$ (CTAHSO$_4$)) and the adsorption of multivalent bis and tris ammonium salts (i.e. bis[2-hydroxy-3-(dodecyldimethylammonio)propyl]alkylamine dichlorides, and bis[2-hydroxy-3-(dodecyldimethylammonio) propyl]dialkylammmonium trichlorides,) was analyzed, both experimentally and theoretically. The dynamic and equilibrium surface tension was determined by the pendant drop-shape analysis method. The previously proposed "surface quasi two-dimensional electrolyte" (STDE) model of ionic surfactant adsorption, based on the assumption that the surfactant ions and counterions can undergo non-equivalent adsorption within the Stern layer, was extended for the description of ionic surfactant adsorption in presence of multivalent electrolytes. The results indicate that a very good description of experimental data by the developed model can be achieved. They show that monovalent anions like Br^-, Cl^- or HSO_4^- decrease more effectively the surface tension of investigated surfactant than SO_4^{2-} ions if the solutions of the same ionic strength are compared. That can be explained in terms of low ability of divalent SO_4^{2-} ions to penetrate the surface layer due to their strong hydration.

In the case of multivalent ammonium salts the determined surface tension isotherms indicate on the lack of significant differences in surface activity between bis and tris ammonium salts, i.e., for divalent and trivalent surfactant ions (Fig.1). That effect was explained by the formation of multiple surfactant ion - counterion associates. The calculated surface tension isotherms described well our experimental results assuming that at surfactant concentration close to c.m.c. presence of 10-20% of $Surf^{2+}Cl^-$ associates in solutions of bis ammonium salts and c.a. 50% $Surf^{3+}Cl^-$ and 10% $Surf^{3+}Cl_2^-$ associates in solutions of tris ammonium salts (Fig.1). For lower surfactant concentrations the amount of associates in the solution decreases, and for concentrations below 10^{-5} M only fully dissociated surfactant ions are present in the solutions.

The degree of association necessary to explain the lack of difference in surface activity between bis and tris ammonium salts was in quantitative agreement with the results of measurements of concentration of free chloride anions in the surfactant solution (Fig.2).



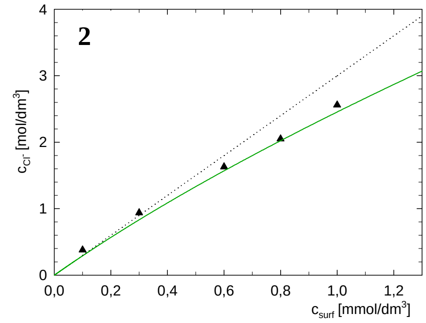


Fig. 1. Experimental adsorption isotherm of (bisAmC_{12})C_2 (triangels) and (trisAmbisC_{12})bisC_2 (circles) described with theoretical isotherms assuming the formation of multiple surfactant ion - counterion associates. We presented also theoretical isotherms calculated for hypothetical monovalent, divalent and trivalent surfactant salts with the same molecular structure .

Fig. 2. The concentration of chloride ions in the solution of (trisAmbisC_{12})bisC_6 as a function of surfactant contents; symbols denote experimental data, dotted lines - chloride ions concentration for fully dissociated surfactants, solid lines – chloride ions concentration calculated from mass action law taking into account the formation of surfactant-chloride associates.

Electroactive Thin Polymer Layers with Incorporated Carbon Nanostructures

(Assoc. Professor P. Warszyński, J. Superata MSc)

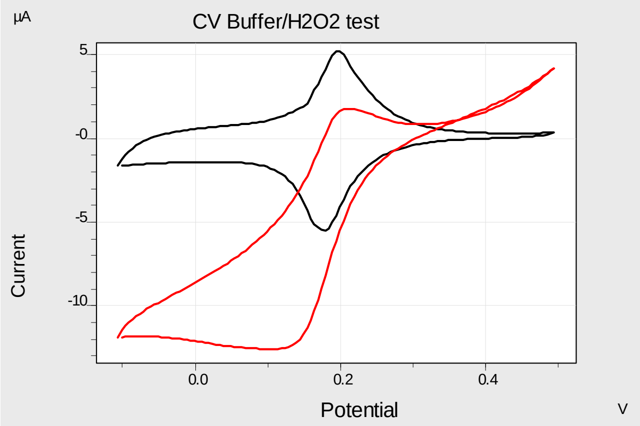
The experimental work performed in this task in 2007 was devoted mainly to the preparation of hybrid biomimetic surface layers on metallic fibres followed by characterization of their electrochemical properties in the perspective of future applications in bio- or chemical sensors. Complex surface structures were formed by implementation of chemical, electrochemical or physical surface modification techniques. Innovative procedures were developed for convenient work with microelectrodes, their handling and storage.

Surfaces of thin metallic substrates were modified applying a number of alternative preparation procedures, regarding not only variation of materials and reagent composition but also different processing steps such as pretreatment, synthesis, polymerization and deposition of the sensing system constituents. Multiple-wall carbon nanotubes and carbon black nanoparticles were used; combined with polymers and - essentially - with the Prussian Blue (PB) redox system, thus completing a hybrid layer structure. Various deposition techniques were employed: chemical, electrochemical (electropolymerization) or physical coating. Electrocatalytic properties of the obtained microelectrodes were assessed by comparison of the cyclic voltammetry (CV) scans performed in physiological buffer solution alone or with hydrogen peroxide added as the analyte. The following structures were investigated:

- composite layers containing carbon nanoparticles or nanotubes within the polymer network synthesized in-situ (polyaniline, polyindole derivatives, polyphenylenediamine, polyethylenedioxythiophene);
- surface layers consisting of aligned carbon nanofibres.

In another series of experiments the microelectrode surfaces were modified using the Layer-by-Layer technique of alternating deposition of oppositely charged nanoparticles. Prussian Blue nanoparticles and polyelectrolytes (polyvinylpyridine, chitosan and poly(diallyl-dimethyldiammonium) chloride were used for building the multilayers. The experimental results showed correlations between observable electrocatalytic effects and structural properties of the composite layers resulting from their fabrication process.

The figure below illustrates the example of voltamgrams received for the system of platinium wire electrode modified by chitosan/Prussian Blue multilayers in phosphate buffer at pH 7.2 (black line) and in the same buffer in presence of 2 mM H_2O_2 (red line). The results presented indicate on the possibility of application of that type of multilayer electrode structure in hydrogen peroxide sensors.



Physical Chemistry in the Protection of Cultural Heritage

Establishing Risk of Wood Degradation in Historic Structures Exposed to Infiltration of Rain Water

(Assoc. Professor R. Kozłowski, Ł. Bratasz PhD, S. Jakieła PhD)

Growth of wood-degrading fungi, when the availability of the moisture necessary for their life functions has exceeded critical levels, constitute the principal damage mechanism of historic wooden structures exposed to the outdoor weather. It was assumed that precipitation and temperature would overshadow other elements of climate that might influence attack by wood-destroying fungi and that the relation between the growth rate to temperature was linear above the low temperature limit of 2 ^{o}C. A final form of the risk index was developed which took into account the real moisture penetration depth and resulting real infestation volumes. The water transport into 3 species of wood – oak, spruce and pine, favoured in the past by builders and artists in Europe, was measured using a scanning Nuclear Magnetic Resonance (NMR) technique. Moisture content profiles across wood were determined as a function of duration of the precipitation wetting the external surface. A model of two-stage infiltration, interpretable in terms of very rapid transport through the vessels with a simultaneous slower infiltration into the denser material surrounding them was used to interpret the results. The model has allowed simulating numerically a profile of moisture penetration into wood for any precipitation event. Following the fungal growth models available in the literature, the moisture content of 20% was assumed as a threshold level above which the fungal growth occurs. Further, 48 hours were assumed as the required “exposure time” to initiate fungal growth after a period of dry conditions preventing growth. Taking into account these two conditions, the moisture penetration profiles could be recalculated into “events of fungal growth risk”. The profiles corresponding to single events were agglomerated into the quarterly “time of fungal growth risk” profile, since the climatic data were available for for quarterly time intervals. Therefore, the final form of the Climate Risk Index for Wood (CRI_{CH}) was therefore:

$$CRI_{CH}^{Q} = (T_Q - 2)\int_0^{D_{\max}} t_{Qcrit}(D)\ \sigma(D)\ dD$$

where : T_Q is the mean quarterly temperature in ^{o}C, $t_{Qcrit}(D)$ is quarterly time of fungal growth risk in the σ(D) percent of the wood’s cross-section at distance D from the external wood surface, D_{max} is the maximum distance at which infiltration of water produces moisture contents above the critical level; D_{max} is specific for each species of wood and is determined experimentally.

RESEARCH PROJECTS

of the Ministry of Science and Higher Education

Influence of Position of Transition Metal in Heteropoly Compound Structure on Catalytic Activity and on Reaction Mechanism of Oxidation of Cyclic Hydrocarbons

Research project 3 T09A 092 29 [2005-2009]
(priject leader: K. Pamin PhDEng)

The incorporation of transition metal ions into heteropolyacid structure influences the oxidation properties of the metal. Heteropolyacids modified by transition metal ions are known as effective catalysts of the oxidation reaction. Due to their multifunctionality, which join acidic and redox properties, heteropolyacids can be useful in those reactions where different kind of synthetic steps are needed like oxidation of saturated organic substrates.

The immobilization of heteropolyacids on supports like polysaccharides results in the formation of self-assembly systems. The properties of immobilized metallocomplexes are governed by the properties of both the heteropolyacid and the carrier. Chitosan, which is natural cationic polysaccharide with amino groups, was selected as the universal carrier.

Heteropoly compounds having strong acidity were immobilized on the surface of chitosan layer forming catalytically active systems. The subject of this project was the synthesis of $H_3PW_{12}O_{40}$ and $H_3PMo_{12}O_{40}$ and their cobalt salts $Co_3(PW_{12}O40)_2$, $HCoPW_{12}O_{40}$, $H_2Co_{0.5}PW_{12}O_{40}$, $Co_3(PMo_{12}O_{40})_2$, $HCoPMo_{12}O_{40}$, $H_2Co_{0.5}PMo_{12}O_{40}$ immobilized on chitosan and the characterization of their catalytic properties in the oxidation of cyclooctane. Catalytic activity of the synthesized catalysts was compared with the activity of unsupported heteropoly compounds in the tested reaction. The liquid-phase oxidation of cyclooctane was performed at the optimum temperature of 120 ^{o}C, for 6 hours and under the pressure of 10 atm..The reaction products are cyclooctanol and cyclooctanone. In the presence of chitosan alone the reaction does not occurs. Catalytic activity of the tungstophosphoric acid upon deposition on chitosan increases while for the $H_3PW_{12}O_{40}$/chitosan catalyst catalytic activity practically does not change. However, catalytic activity of the cobalt salts of tungstophosphoric acid decreases upon immobilization on the chitosan carrier.

Application of Macrocyclic Complexes of Transition Metals: Metalloporphyrins, Metallophthalocyanines and Metallosalens for Catalytic Oxidation of Propylene

Research project 3 T09B 091 29 [2005-2008]
(project leader: J. Połtowicz PhD)

Macrocyclic complexes of the transition metals: metalloporphyrins, metallophthalocyanine and metallosalens are known as effective and selective catalysts of the reaction epoxidation of olefins in liquid phase. Process epoxidation of propylene in mild conditions with molecular oxygen and aldehyde as co-reductant and with metalloporphyrins as catalysts was investigated in our Institute through many years. Propylene oxide is an important intermediate product in industry and substrate to obtain for example the polypropylene glycol or polyglicolicethers for production of polyurethanes.The demand for propylene oxide increasingly grows with the increase simultanies of its price.Propylene oxide is not yet produced in Poland. The technologies which are in use nowadays demonstates comperatively low yield to propylene oxide and the presence of unwanted byproducts. Increasingly growing regulations of environment protection pose an additional motivation.

In our work the results of propylene oxidation in the presence of phthalocyanine complexes of transition metals presented. Their catalytic activity can be easily modified by the change of active center as well as introduction of electron-withdrowing substituents into phthalocyanine ring. Epoxidation of propylene was performed at ambient by molecular oxygen and in the presence of isobuteraldehyde as co-reductant. The main product of the reaction was propylene oxide. Three types of metallophthalocyanines (Fig. 1) were used as catalysts; simple metallocomplexes MnPc, FePc, CoPc, NiPc, CuPc; complexes with nitro groups $MnPc(NO_2)_4$, $CoPc(NO_2)_4$, $FePc(NO_2)_4$; complex with chloride substituents $FePcCl_{16}$ and complex with fluoro substituents $CoPcF_{16}$.

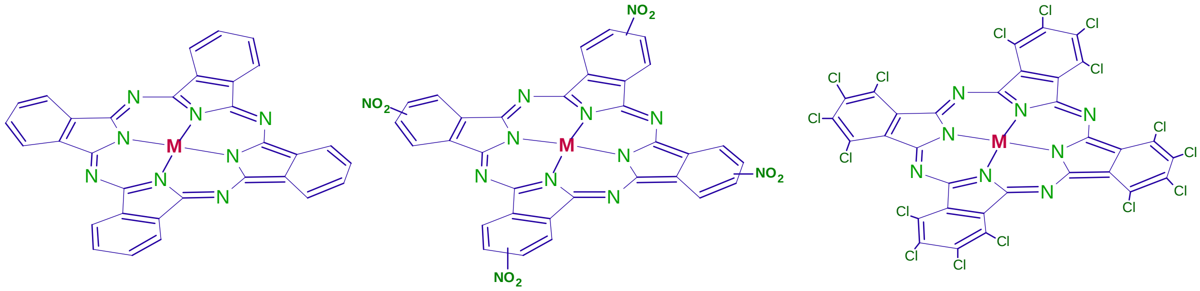


Fig. 1. Structure of the investigated catalysts

All the macrocylic metallocomplexes used as catalysts are active in the studied process and their activity depend on the type of active center, number and type of substituents introduced into the phthalocyanine ring. Between the simple phthalocyanines the best catalyst was cobalt complex. The following order of catalytic activities was obtained for these catalysts: CoPc > MnPc > FePc > NiPc > CuPc. Among the all catalysts with substituents the most active was also cobalt complex $CoPcF_{16}$. The difference in catalytic activity of phthalocyanine complexes is probably connected with different mechanism of activation of the molecular oxygen.

Mesoporous Silica Supports as a Tool for Controlling the Course of Catalytic Reaction over Macrocyclic Metallocomplexes

Research project 3 T09B 066 26 [2004-2007]
(project leader: Professor E. Serwicka-Bahranowska)

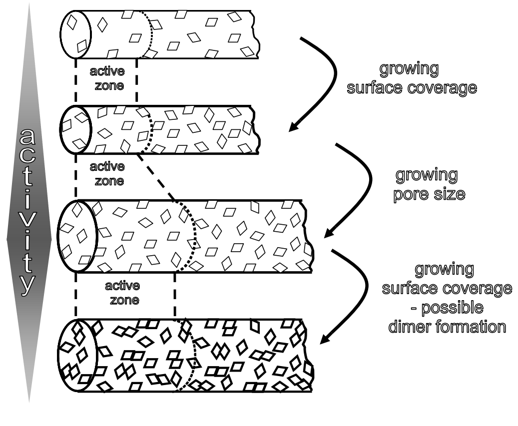
The project aimed at development preparation procedures for hybrid catalysts consisting of catalytically active metallocomplexes and mesoporous silica matrices, in such a way as to allow for control of the selectivity pattern of a catalytic reaction. The project was completed in April 2007. Aluminated HMS, MCM-41, FSM-16 and SBA-15 mesoporous solids were used in the capacity of silica carriers. MTMPyP and MTAPP (M=Mn, Co lub Fe) metalloporphyrins were deposited onto these supports by means of cation exchange. Oxidation of cyclohexene with single oxygen donor (iodosobenzene) and oxidation of cyclooctane with molecular oxygen from air were chosen as test reactions.

The most important conclusions resulting from the research are:

1. Deposition of catalytically active site within the mesoporous network modifies the spectrum of products in the tested reactions.
2. Extent of the effect depends on the distribution of the active metalocomplex sites in the support lattice: the more is located inside nanotubes (as opposed to the external grain surface) and the narrower their dimension, the higher is the observed steric effect.
3. Cyclohexene oxidation is a sensitive test allowing for determination of Al sites distribution in the mesoporous support (between the internal pore walls and the external grain surface).
4. Low temeparture liquid phase reactions carried out on catalysts derived from mesoporous solids experience diffusional limitations within the pore network.
5. Catalytic activity of supported metallocomplexes decreases when the coverage is sufficiently high to enable formation of less active dimers.
6. Deposition of metalloporphyrins onto mesoporous silica supports lengthens the catalyst lifetime.
7. Alumination procedures have been developed allowing for control of the distribution of organometallic cation within the mesoporous silica matrix.

Results of the research have been published in 4 papers.

Factors influencing the catalytic activity of metalloporphyrin located in the pores of a mesoporous support



Determination of Physicochemical Mechanisms of Formation of Multilayer Ceramic Nanomaterials with Higher Biocompatibility

Research project 3T08D 045 29 [2005-2007]
(project leader: B. Jachimska PhD)

The development of self- and directed-assembly techniques is key for the formation of molecularly determined structures for applications ranging between biocompatible and bioactive materials. The polyelectrolyte adsorption depends strongly on many parameters such as surface charge density, fraction of charged monomers on the polymer backbone, polymer-solvent and polymer-surface affinity, pH and ionic strength of the solutions. The combined effect of these factors can lead to specific behavior of the adsorbed polymers. Preparation of the multilayer films on solid substrates is an important field of polyelectrolyte applications of the desired composition and functionality. This is often realized by layer-by-layer (LbL) deposition of anionic and cationic polyelectrolytes. The simplicity of this procedure, feasibility of embedding of various molecules, proteins and colloid particles into the polymeric layer opens a broad spectrum of possibilities to produce films of designed architecture. The controlled formation of polymeric film requires a throughout knowledge of the structure of the polyelectolyte molecules in relation to its molecular weight, ionic strength and pH of the solutions.

The bulk characteristics of polyelectrolytes were determined by measuring of their viscosity in various pH and ionic strength. The dynamic viscosity of polyelectrolyte solutions as a function of its volume concentration was measured using a capillary viscometer. This allowed one to calculate the specific conformation of polyelectrolyte chains in the suspension, approximated by prolate and oblate spheroid shape. The conformation of the molecules is strongly influenced by the ionic strength and pH of the solution. Because of the lack of universal theory the true structure of polyelectrolytes in solutions cannot be unequivocally determined only from the viscosity measurements. Complementary data, such as the hydrodynamic radius of molecules (containing shape information), their electrophoretic mobility, and enabling estimations of the true ion condensation degree are necessary. Additionally, the interpretation of experimental data was facilitated by comparison with theoretical simulations, based on the molecular dynamic approach, which furnish the necessary shape information.

This versatile methodology enables facile evaluation of self –assembly conditions and demonstrates the potential of this bottom-up approach to prepare organized bioactive materials. The present original project enters totally in to the new objectives, which develop a new approach to design functional interfaces of the molecular structure. It is thus directly related to the creating advanced functional materials.

Structure and Enzymatic Activity of Clavamic Acid Synthase: Theoretical Studies of the Catalytic Reaction Mechanism

Research project 2 P04A 042 26 [2004-2007]
(project leader: Professor E. Brocławik)

Project was aimed at molecular mechanism of biosynthesis by clavulanic acid synthase, tri-functional enzyme from the group of non-heme, α-ketoglutarate dependent enzymes. Clavulanic acid synthase catalyses synthesis of clavulanic acid, an inhibitor of β-laktamase and thus important factor for β-laktame antibiotics.

Multi-directional research comprised:

- modeling of general properties of iron centres in monooxygenases both non-heme centres analogous to clavulanic acid synthase and iron heme centres;
- methodological research on electronic structure f iron sites in enzymes that requires both advanced quantum chemistry and novel methods to include environment (protein and water molecules) modeling protocol;
- a proposal of new route of clavulanic acid synthase catalytic mechanism.

The purpose of project research was fully reached. The results may have potential influence on rational drug design for β-laktame antibiotics.

Dynamic Adsorption Layer – the Influence of Surface Active Substance on Interfacial Mobility

Research project 3 T09A 164 27 [2004-2007]
(project leader: Professor K. Małysa)

A mechanism and most important factors deciding about formation of dynamic structure of adsorption layer, which caused the immobilization of liquid/gas interface, were determined as a result of investigation carried out during realization the research project 3 T09A 164 27 entitled: "Dynamic structure of adsorption layer – influence of surface active substance on interfacial mobility. It was showed that as a consequence of formation of dynamic structure adsorption layer i.e. steady state non-uniform distribution of the surfactant molecules over the surface of the rising bubble the hydrodynamic resistance for its motion was increased. The increased hydrodynamic resistance caused by immobilization of the liquid/gas interface, due to the induced dynamic structure of the adsorption layer, resulted in significant reduction of the terminal velocity of the rising bubble.

The local velocities and the bubble shape deformation were determined as a function of the distance from a point of the bubble formation (capillary orifice), for different concentrations of solutions of the surface active substances (SPA) studied. The influence of the SPA solution concentration on size of bubble formed at the capillary orifice was also determined. The measurements were carried out for three representatives of homologous series of n-alkyltrimethylammonium bromides (C8, C12, C16) and five surface active substances having different head groups but eight hydrocarbon chains in their molecules (n-octyl acid in 0.001 M HCl, n-octanol, n-octyl-β-D-glucopyranoside, n-octyldimethyl-phosphine oxide, n–octanol, sodium n-octylsulfate) as well as the proteins Lysozyme and Bovine Serum Albimine (BSA at various conditions - pH 4.8 and 5.9). Influence of the SPA solution concentration on the maximum and terminal velocities of the bubbles were determined, as well. The bubbles terminal velocity was 34.7±0.3 cm/s in distilled water and decreased to ca. 15 cm/s at high concentration of the surfactants solutions.

For all surfactants studied the values of a critical concentration, i.e. the solution concentration above which the terminal velocity stopped to decrease rapidly, were determined. Above the critical concentration there was observed only small variations in terminal velocities, which were related rather to the bubble size decrease (surface tension decrease – Tate law) than to changes in the bubble surface mobility. It was evaluated that these critical concentrations assured the adsorption coverage at liquid/gas interface of an order: 3% for n-octyl acid, 4% for n-octyl-β-D-glucopyranoside, 3% for n-octyldimethyl-phosphine oxide, 2% for n-octanol, 5% for n-cetyltrimethylammonium bromide, 9% for dodecyltrimethylammonium bromide, 25% for n – octyltrimethylammonium bromide and 32% for sodium n-octylsulfate. In the case of the proteins studied the adsorption coverage needed were ca. 5% for BSA and 98% for Lysozyme. It was found that variations in profiles of the bubble velocities are well correlated with the bubble shape deformations. Highest degree of the bubble shape deformations, of an order of 50%, was observed in distilled water. With increasing concentration of the surfactants studied the degree of the bubble shape deformation was decreasing and at the highest concentrations the deformation was very small only, χ<1.03-1.05, where χ is a ratio of of the horizontal to vertical diameters of the rising bubble.

Zeolite Membranes as New Nanomaterials for Separation Processes

Research project Nr 3 T09A 029 29 [2005-2008]
(project leader: Assoc. Professor M. Derewinski)

Molecular-sieve thin films have drawn great attention over last years, due to their molecular sieving properties, high thermal stability and resistance to harsh environment. Their possible applications, ranging from selective molecular separation, chemical sensing, catalysis and use as new optoelectronic materials have provided additional interest for synthesis of the zeolite films. Membranes formed with a thin continuous layer of MFI crystals (silicalite-1 and ZSM-5) are among the most frequently studied, because MFI zeolite has a channel system with pore openings similar to the critical diameter of many industrially important organic molecules like xylenes, cyclohexane, butane isomers etc. Therefore, they could be used as highly effective systems for the separation of hydrocarbon mixtures.

Secondary growth is a mostly used method of zeolite thin films synthesis. It consists of the deposition of nanosized seed crystals on the support, followed by a hydrothermal growth of the seed crystals to form zeolite film. Elimination of the nucleation step provides more flexibility for the crystal growth and enables a better control of the membrane formation and its microstructure. The purpose of the work was to study the formation of the zeolite membranes on a porous alumina support using the *secondary growth* method and to evaluate the influence of synthesis parameters on the quality of the membrane, its structure and surface morphology.

Continuous films of ZSM-5 (MFI type, Si/Al = 30÷70) having a thickness of 2-5 μm were synthesized on home-made polished α-Al_2O_3 discs seeded with colloidal silicalite-1 nanocrystals (diamention of ~100 nm). The film morphology was characterized with SEM and the Al- and Si distribution profile were determined by EDX analysis of the cross-sections of the films. The dominating orientation of the crystals was determined by XRD. The obtained thin films have a columnar grain microstructure and depending on the growth conditions exhibit [00l] or [h0h] orientation. The film formed during shorter time (below 15h) had the poor columnar morphology in comparison to that obtained after 30 h of growth. The analysis of the XRD pattern indicated that obtained film is mainly [h0h] oriented i.e. {101} phase of crystals is exposed at the surface of membrane. The experimental data recorded for the film obtained after 30 h of secondary growth showed more pronounced the *c*-oriented layer formation. The orientation of zeolite film depended also on the growth temperature. The SEM images of the top-view and cross-section of membrane and analysis of the XRD patterns clearly evidenced [h0h] orientation of membrane obtained at 130^o for synthesis time ranging from12 h to 24 h. The increase of the temperature of secondary growth above 150^{o}C resulted in formation of the *c*-out-of-plane oriented zeolite films. The syntheses of the MFI film on the rotated discs were also carried out. It was proved that the applied method did not influence significantly orientation of the MFI crystals in the film.

In order to examine the quality of the membranes permeation fluxes of single gas (H_2 and CO_2) were measured and the Ideal Selectivity (I.S.) (ratio of H_2 flux over the CO_2 flux) was calculated. The membranes showed the highest I.S. were selected for the separation of hydrocarbons (n-/i-butane) mixtures.

Research of Effectiveness of Hydrogen Activation of the Supported Catalysts Based on the Au Nanoparticles

Research project 1 T09A 094 30 [2006-2009]
(project leader: E. Lalik PhD)

The project seeks to investigate an effect of small amount of argon increasing the effectiveness of the hydrogen activation in Au supported catalysts for the reaction of the low temperature oxidation of CO to CO_2. The part scheduled for 2007 included (1) the catalytic tests in CO oxidation on the catalyst containing Au supported on TiO_2+SiO_2; (2) the synthesis of a series of Au catalysts supported on the chromium spinels (Co, Zn and Mg); (3) setting up the mass spectrometer as a down stream detector for the flow microcalorimeter and preliminary test of this modification.

(1) The effect of a sequential treatment with Ar and H_2 of two catalysts (**A**) 1%Au/75%$TiO_2$25%SiO_2 and (**B**) 1%Au/50%$TiO_2$50%SiO_2 in the CO oxidation have been measured. Attempts to obtain an active catalyst containing 1%Au/25%$TiO_2$75%SiO_2 turned out to be unsuccessful. The results are summarized in Table 1. It is clear the material (**A**) alone shows significant increase of effectiveness of hydrogen activation as a result of Ar treatment. Additional experiments consisted of measuring the activity of catalyst after a double treatment with H_2, however without the intermittent contact with Ar. Here the conversion of CO for a sample activated twice with H_2 was the same as that activated only once and was 13%. Any potential effect of either an increased activation period, or a sequence of $H_2/O_2/H_2$ treatment on the catalytic activity can therefore be excluded. Thus the increase in activity can be solely attributed to the presence of Ar between the two H_2 treatments. The experiments were repeated twice, each yielding the same (within 0.5% error) activity values.

Table 1. The effect of H_2 and Ar on the activity of samples (A) and (B) in CO oxidation.

State of catalyst	**Conversion of CO [%] on catalyst (A) 1%Au/75%$TiO_2$25%SiO_2**	**Conversion of CO [%] on catalyst (B) 1%Au/50%$TiO_2$50%SiO_2**
Fresh sample	7.9	1.6
After treatment in H_2 at 150°C for 30 minutes	12.6	7.4
After contact with Ar (50°C, 5 minutes) and repeated treatment in H_2 (150°C, 30 minutes)	27.3	6.7

(2) Table 2 shows the results of testing of mass spectrometer (MS) combined with flow microcalorimeter (FM) used in the reaction of oxidation of H_2 in a mixture with synthetic air (20%O_2+80%N_2) as a function of both the H_2 content and the flow rate. The test was intended to establish agreement between the O_2 consumption measured with MS, and the amount of heat observed with FM. In the Table 2, the observed thermal effects of H_2 oxidation have been expressed as a fraction of a possible total heat evolution that could be observed if a total conversion of O_2 occurred, calculated for the heat of water formation of 500 kJ/mol O_2. It can be seen that such a fraction remains in good agreement with the actual consumption of O_2.

Table 2. The heats of oxidation of H_2 compared to the corresponding oxygen consumption.

Contents of H_2 in synt. air	**Flow rate of 1cm^3/min**		**Flow rate of 2cm^3/min**	
	O_2 consumption	Fraction of heat	O_2 consumption	Fraction of heat
25%	0.61	0.66	0.51	0.51
50%	0.66	0.71	0.56	0.54
75%	0.63	1.3	0.92	1.1

The Mechanism of Formation of Polyelectrolyte Multilayer Films with Controlled Microarchitecture on Metallic Surfaces

Research project 1 T09A 123 30 [2006-2009]
(project leader: L. Szyk-Warszyńska PhD)

The aim of the project is to investigate the adsorption mechanism of the polyelectrolyte, colloidal particles and microcapsules on heterogeneous surfaces in presence of hydrodynamic and external forces.

The objectives of our studies performed up to now were as following:

- formation by ‘layer by layer’ (LbL) method of multilayers composed of polyelectrolytes (polycations - PAH* poly(allylamine hydrochloride) fluorescein labeled, PEI poly(ethyleneimine), polyanion PSS poly(sodium 4-styrenesulfonate)) on mica and silicon waffers;
- characterization of PE multilayers deposited in various conditions by elipsometric film thickness and fluorescence intensity measurements.

To investigate the effect of PEI first layer on the thickness of polyelectrolyte multilayers we prepared films (PAH*/ PSS)$_n$, PEI(PSS/PAH*)$_n$ of various thickness. The results presented in Fig.1 indicate that films with given number of layers built up on PEI anchoring layer were thicker than structures having the same number of PE layers but consisting of PAH/PSS only. Branched PEI used as a first layer acts as an anchoring network for the consecutive layers’ formation. We also investigated the effect of ionic strength of PE solution on film thickness. For that purpose polyelectrolytes were deposited from the solutions of various ionic strength: 1.5M, 0.15M, 0.015M regulated by addition of NaCl. PE concentration was 100 ppm in all experiments. The results depicted in Fig.2 show that film thickness is growing with increasing the ionic strength of PE solution. For high ionic strength of the solution, the electric charges along PE chains are screened, therefore, chains can assume more coiled conformation. This conformation is preserved during PA adsorption and that favors thicker layers. Moreover, as a result of stronger screening the electrostatic repulsions between adsorbing PE molecules are diminished. The results of measurements of fluorescent intensity, which is proportional to the amount of adsorbed polycation indicated on similar effect of PEI and ionic strength of the PE solution.

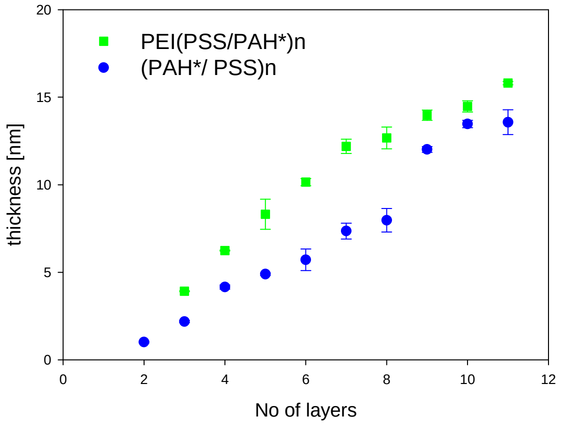


Fig. 1 Ellipsometric thickness of (PAH/PSS) and PEI(PSS/PAH) multilayer films deposited from solutions of I=0,15M.

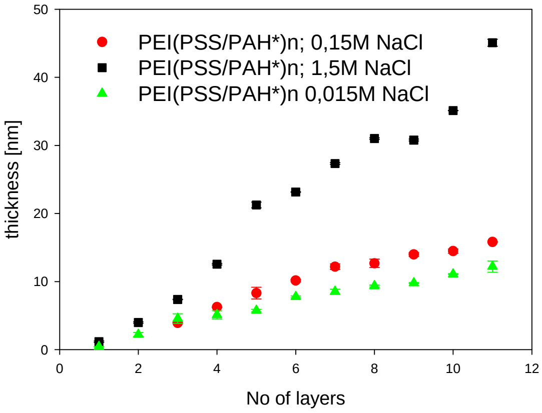


Fig. 2. Ellipsometric thickness of PEI(PSS/PAH) multilayer films deposited from solutions of various ionic strength.

The Effect of Cadmium and Selenium onto Surface Properties of Model Lipid Layers Formed on the Basis of Material Obtained from Natural Cell Membranes

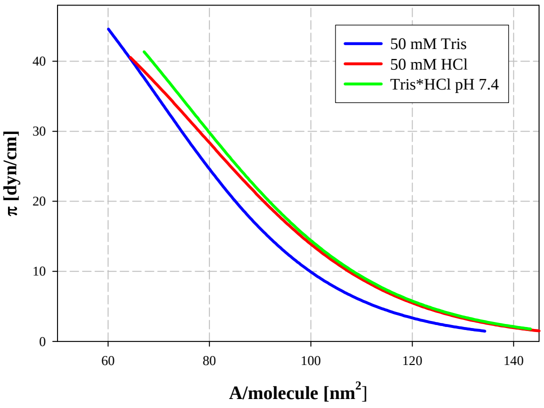
Research project 1 T09A 122 30 [2006-2009]
(project leader: M. Zembala DSc)

The aim of studies planned in the frames of the grant is to determine the changes of properties of galactolipid layers due to a contact with cadmium and selenium ions. Chloroplasts of wheat are the natural source of galactolipids. Cadmium is considered as one of the most toxic agents causing meaningful damages of plant tissues, dimishing drops, photosynthesis inhibition, reduction of chlorophyll content in leaves as well as disturbing water relations and taking nutritive components from a soil. On the other hand, Se ions may inhibit the tonic effects caused by other metals.

The material under study are galactolipids: mono- (MGDG) and di-galactosyldiacylglycerol bounded to two saturated and/or unsaturated fatty acids present in chloroplasts. This particular composition of chloroplasts` lipid membranes distinguishes them from other membranes and probably plays an essential role in their functioning. The cell cultivation, isolation, purification and chemical analysis of galactolipids obtained from wheat chloroplasts represents an important part of the work.

Parallely to accumulation of material of natural origin, the surface properties of monolayers of commercial galactolipids was determined. MGDG layers was deposited using the Langmuir through onto aqueous subphase containing either Tris buffer of pH 7.3 and 10 or HCl. All solutions have constant concentration equal to 50mM. As surface pressure isotherms were very weakly pH dependent in further experiments only solutions of pH 7.3 were used.

The method of MGDG monolayer deposition onto solid supports (mica modified on various ways) was work-out. The most stable covering layers were obtained for mica modified by chemisorbed cationic silane (APTES). The zeta potential of the support covered by MGDG monolayer was determined by the streaming potential technique using Tris buffer solution as an electrolyte.



Unfortunately, results obtained this way were rather scattered due to, as it was proven in further measurements, non-reproducible properties of mica modified by silane. Thus, in next measurements we will try to deposit 3 layers of lipid for better screening of support electric field.

Preliminary determination of characteristics of reference material i.e. properties of layers of pure lipids is crucial for further studies of the influence of of ions onto lipid membrane properties.

Theoretical Studies on Surface Heterogeneity of Catalysts Based upon Vanadium Pentoxide

Research project N 204 024 31/0475 [2006-2008]
(project leader: Professor M. Witko)

Catalysts based upon vanadium pentoxide are widely used in different industrial processes belonging to chemical reactions of various characters. This is due to the appearance of different active centers (metallic and oxygen) at catalyst surfaces both chemically saturated (010) and chemically unsaturated (100) and (001). Addition source of catalytic activity follows from the possibility of reduction of vanadium centers during the reaction, which leads to the formation of lower vanadium oxides ($V_2O_5 \rightarrow VO_2 \rightarrow V_2O_3$), as well as the possibility of introducing the different chemical elements such as for example phosphorus. Periodic studies on the thermodynamic stability of different low-indices V2O5 surfaces show that unsaturated surfaces participate in almost 15% in the crystal morphology. Therefore, in the following the electronic structure of three low-indices (010), (100) and (001) surface of V_2O_5 is reported. In addition the electronic analysis of different cutting of (0001)V_2O_3 is given.

Calculations are performed by means of DFT method (StoBe program) using non-local RPBE functional for electronic and energetic parameters and local LDA functional for geometry optimization. Clusters of different geometries model surfaces of oxides. Charge distribution (Mulliken analysis), bond orders (Mayer analysis), total and partial atom-projected densities of states (DOS, pDOS) are analyzed.

Results of calculations give for all (010), (100) and (001) low-indices V_2O_5 surfaces similar electronic structure with V-O bonds of mixed covalent-ionic character. Charge on oxygen centers scales with the coordination number of center, whereas charge on vanadium sites are lower for unsaturated (100) and (001) surfaces in comparison to saturate (010) surface. Densities of states structure are similar for all three surfaces both for valence and conduction regions. Vanadium cations form centers of electron-acceptor properties, whereas oxygen centers have Lewis-base character.

Thermodynamic analysis of the stability of different possible cutting of (0001)V_2O_3 surface points out the V'OV plane as the most stable. All V-O bonds are characterized by mixed ionic-covalent properties. Nucleophilic character of oxygen surface sites increases in order O(1)<O(2)<O(3)<O(4). Charge distribution existing in studies systems results in the strong electrostatic field operating between layers and leads to the relaxation of few layers near the surface. The relaxation effect is different for different cutting. Density of states in conduction region as well as position of HOMO level in this region indicates that surfaces of studied systems can undergo both electrophilic and nucleophilic attack.

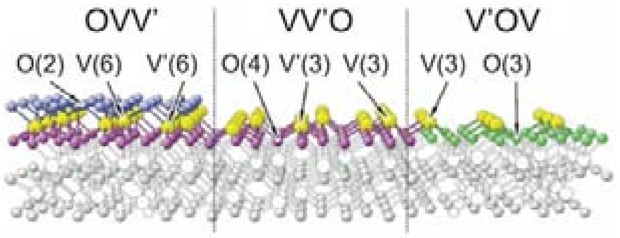


Figure 1. Possible atomic terminations of the (0001) V_2O_3 surface.

Structure, Interfacial Properties and Permeability of Multilayer Polyelectrolyte Films for Surface Modification and Encapsulation of Chemicals

Research project N 204 166 31/3734 [2006-2009]
(project leader: Assoc. Professor P. Warszyński)

The layer by layer (LbL) sequential adsorption of oppositely charged polyelectrolytes multilayers (PEM) is a method for forming ultrathin membrane shells with controlled thickness. Combination of different polyelectrolytes opens a wide range of applications, where PEM's can be used. Multilayers are used to modify surfaces of various materials improving their interfacial properties. They are of special importance in biomaterial area such as contact lens production or modification of surface of titanium implants. Coating of colloidal particles by polyelectrolyte multilayers and formation of hollow shell structures are of importance in case of encapsulation applications, e.g: in drug carrier systems or microreactors.

The aim of the project is to determine the effect of type of polyelectrolyte and conditions of PEM formation on their structure, stability and permeability. In particular, in the previous project phase, we determined the effect of pH on the properties of PEM films formed of weak polyelectrolytes - PAH/PAA. Multilayer films were formed in the following conditions: both polyelectrolytes strongly charged (PAH – pH 3, PAA – pH 11), both polyelectrolytes weakly charged (PAH – pH 11, PAA – pH 3) and in mixed conditions (PAH, PAA – pH 3), (PAH, PAA – pH 11). Films were formed by LbL technique on silicon wafers Si/SiO_2. Since the p.z.c. for silica is around pH 3 – 3.5, first four layers of films were adsorbed from PE solutions having pH 7. Thickness PEM films were measured by ellipsometry. All films were dried prior to measurements. Results for the adsorbed film thickness were confronted with ones concerning mass of the films obtained with Crystal Microbalance (QCM). The QCM measurements were obtained in collaboration with Max-Plack Institute in Potsdam. The exemplary results are depicted in the figure.

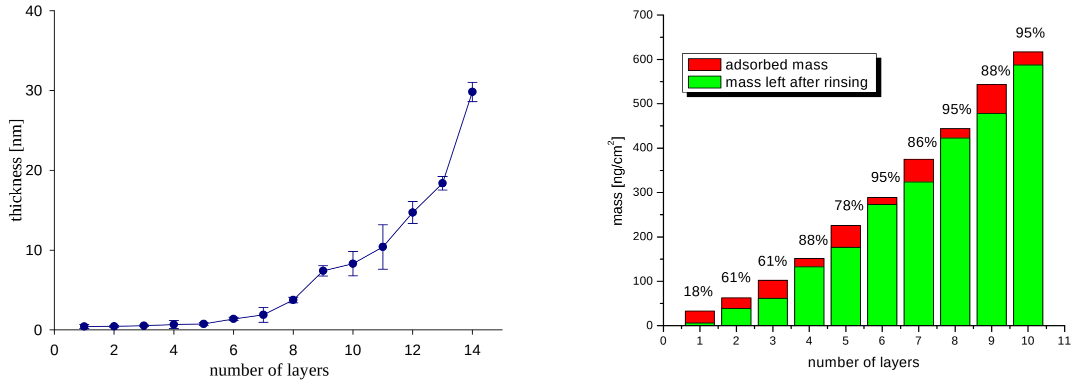


Fig. 1. Thickness and mass of PAH/PAA multilayer film adsorbed at silicon wafer surface at pH 7 for layer 1-4 and pH 3 for layers >4.

The thickest layers were observed in the conditions when both PE were weakly charged and the thinnest for strongly charged PAH and PAA. Thick films were very heterogeneous and unstable, which was evidenced by irregular layer to layer oscillations of their thickness. It can be explained by formation of PE complexes (size of c.a. 70 nm) weakly attached to film surface.

Heteropolyacids (HPA) as he Catalysts in Gas Phase Ethyl-*tert*-butyl Ether (ETBE) Synthesis

Research project N 204 64 31/3689 [2006-2009]
(project leader: A. Micek-Ilnicka PhDEng)

Ethyl-tert-butyl ether (ETBE) is now used as an antiknocking additive to the automotive fuel. It is obtained from ethanol and isobutene using acid catalysts. According to the plan of the project synthesis of ETBE has been studied in a catalytic system not containing water in gas phase. Solid Wells-Dawson type heteropolyacid $H_6P_2W_{18}O_{62}$ as catalyst and absolute alcohol as reagent in gas phase were used. In a differential microreactor a series of kinetic experiments has been carried out. ETBE synthesis rate was measured at 40°C at different partial pressures of reagents: C_2H_5OH and C_4H_8 at the conditions when the system was far from reaction equilibrium conditions (figure).

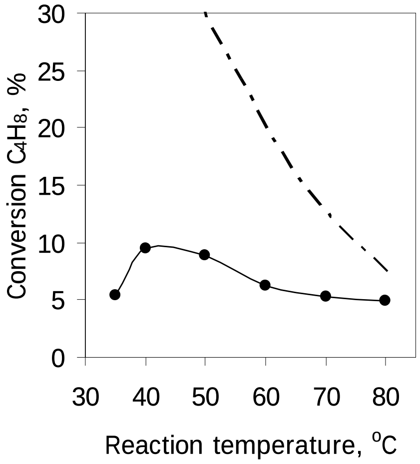


Fig. 1. Dependence of isobutene conversion on temperature (dotted line corresponds to the equilibrium conversion).

Empirical reaction order with respect to isobutene (1.6) and ethanol (-2.0) were determined. Negative reaction order with respect to ethanol was explained basing on the mechanism of catalytic reaction proposed on the basis of physicochemical characterization of the catalytic system. It has been shown that methanol penetrates the bulk of HPA crystallites while isobutene remains chemisorbed at the external surface possibly forming oligomers. Both ethanol and isobutene are bonding protons supplied by HPA thus forming ethoxonium ions in the bulk and protonated isobutene oligomers at the surface.

Catalytic reaction occurs at the surface between isobutene carbocation and neutral ethanol molecules supplied from the bulk. Basing on such assumption mathematical model of the investigated process was proposed. This model assumes the formation of protonated ethanol clusters (protonated oligomers). Assuming on that carbocation formation is the rate determining step and comparing the calculated theoretical rate equation with an empirical one it was possible to conclude that the predominant form of ethanol in the next-to-surface layer is protonated dimer $(C_2H_5OH)_2H^+$. On the other hand if ETBE formation would be the rate determining step the formation of ethanol trimers $(C_2H_5OH)_3H^+$ would be rather expected. The possibility of ethanol dimers and trimers was confirmed by ethanol sorption experiments.

Theoretical Description of Oxygen Activation Process and Reactivity of Different Oxygen Centers in Hetero- and Homo- Molybdena Catalysts

Research project: N 204 034 31/0795 [2006-2008]
(project leader: R.Tokarz-Sobieraj PhD)

Molecular oxygen, which plays a fundamental role in catalytic oxidation processes of many organic substrates, as a stable paramagnetic species, has to be activated in order to make the reaction possible. The activation may be caused by bonding of O_2 to the metal center, either in the coordination compound (homogeneous catalysis) or at the surface of a solid (heterogeneous catalysis). The reactivity of bonded molecular oxygen depends on the type of bond that is defined by the properties of metal (its oxidation state and coordination number) and by the surrounding ligands or surface neighbor atoms.

In this paper ab initio quantum chemical DFT method within GGA functional is used to study bonding and further transformations of O_2 molecule into the MoP complex (where P=porphyrin ligand) and (010) surface of MoO_3 that model homo- and heterogeneous systems, respectively. A common block for both homo and hetero processes includes adsorption of molecular oxygen, formation of differently bonded oxygen and hydroperoxo species and their transformation into oxo species (Fig.1.). The obtained results are discussed in terms of geometric (distances and angles), electronic (atomic charges, bond orders, charge transfers) and energetic (bonding energies) parameters.

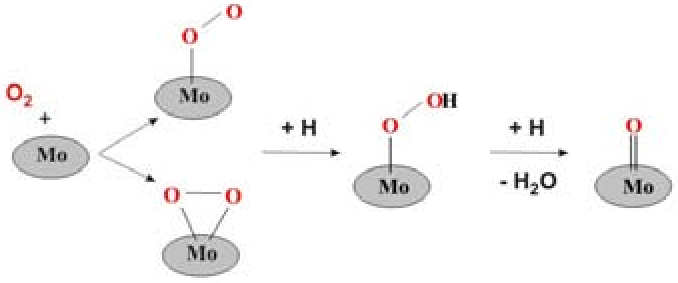


Fig. 1. Scheme of adsorption and transformation of O_2 molecule to oxo species

Results of performed calculations allow one to show differences and similarities in oxygen activation in the course of homo and hetero processes. In all studied systems dioxygen is bonded to Mo preferentially in side-on geometry (formation of two Mo-O bonds). It is found that in any system the direct consequence of O_2 binding to the Mo ions is the O_2 activation that is expressed by the elongation (from 1.2Å to ~1.4Å) and weakening of the O-O bond (bond order changes from 1.8 to ~1.0). In majority of cases (except the porphyrin complexes with Mo^{2+}) hydrogen adsorption leads to the formation of OOH group bonded to the metal center. Adsorption of second hydrogen results in water species that can be removed both from homogeneous and heterogeneous systems. Activation of oxygen causes of formation of oxo species that are different depending on the system. The differences concern charges on Mo and O, bond orders describing Mo-O bond and energies needed to form this bond, thus influencing the properties of oxo species and determining the type of catalytic reaction.

New Method of Producing Nano- and Microcapsular Systems Characterized by Targeted Functionality for a Selective Drug Delivery

Research project N 205 022 31/1112 [2007-2010]
(project leader: Professor Z. Adamczyk)

Mono- and multilayers of nanoparticles having a controlled architecture and functionality have a growing significance because of a wide range of practical applications, mainly in medicine, pharmaceutical, cosmetics, food and electronic industries, investment casting, as well in processes connected with environment protection. Multilayers of polyelectrolyts formed on particulate templates having colloidal dimensions can be exploited for production of nano- an microcapsular systems having potential applications as selective drug delivery systems. Despite major significance for basic science and for practice, formation mechanisms of layered nanometerials have not been studied quantitatively. Thus, the scientific goal of this research project was developing an unified, quantitative description, both theoretical and experimental, of multilayer formation of nanoparticles of various shape, including polyelectrolytes and proteins. The first stage of theoretical studies were numerical calculations of the structure of selected, model polyelectrolytes, used often for preparation of shells of nanaocapsules. These calculations were conducted using the molecular dynamic method using the HYPERCHEM software, exploiting the AMBER procedure for describing the force field. The solvent was treated implicitly as a continuous phase, characterized by a given dielectric constant. However, the motion of the supporting electrolyte was considered explicitly, using the Lanegevin dynamic method. These calculations carried out for the polyallyl amine (PAH) and polyacryclic acid (PAA) enabled one to determine basic parameters, characterizing polyelectrolyte behavior in solution, and their adsorption ability, especially the effective chain diameter, effective length of the macromolecule, and the ionization degree. It was demonstrated that by changing the ionization degree one can controls, to a large extent, the size and shape of macromolecules In solutions. The second stage of the quantitative description of nanoparticle multilayer formation were the Monte Carlo–RSA (random sequential adsorption) calculations expoilting original algorithms written in our group. In these calculations, the two- and threedimensional density distribution of particles was determined, pair correlation functions, averaged layer thickness and the multilayer roughness, as a function of the density of the first (precursor) layer, and the number of layers forming the structure. It was shown, that for low covarge of the precursor layer, a very homogeneous distribution of particle density within the film can be obtained. Using results of these calculations the so called exponential growth of polyelectrolyte multilayers was quantitatively explained, which was interpreted before in a qualitative way only, as an effect of nanoparticle aggregation.

Mechanism of Catalytic Activity of "Nano-Au/Oxide" in Oxidation of CO

Research Project N 204 089 32/2633 [2007-2010]
(project leader: Professor J. Korecki)

Tasks for 2007 included:

1. Preparation and characterization oxide supports and catalysts (real and model)

Powder catalysts nano-Au/ FeO_x (nominal 1 wt.%Au) were obtained using commercially available Fe_3O_4 from Cerac. The catalysts were prepared to determine the influence of the defect density (oxide stoichimetry) on their properties. For this purpose the catalysts were calcinated in a stream of different gases (dry air, argon) at various temperatures. Chemical and electronic properties of the catalysts were checked using XPS and the Mössbauer spectroscopy. Preliminary catalytic test of CO oxidation for the catalyst calcinated at 350^oC i 450^oC indicated that a higher conversion is favored by the higher calcination temperature and the oxygen-free atmosphere

Single crystalline $Fe_3O_4(001)$ film substrates with different surface stoichiometries were prepared by reactive molecular beam epitaxy on MgO(001). The substrates were characterized using XPS. For a series of model $Au/Fe_3O_4(001)$ catalysts, Au and Fe fotoemission spectra were measured as a function of nominal Au coverage and thermal annealing.

2. Development of catalytic measurements in a high pressure reactor connected to the ultrahigh vacuum system.

A system for observation of catalytic reactions in a high pressure reactor, connected to the ultrahigh vacuum system, has been constructed. The system is based on a quadrupole mass spectrometer and includes a set of valves for probing reaction gases at the outlet of the reactor. The system is controlled by a software developed using the LabView platform and enables the temperature programming and control and acquisition up to sixteen mass signals. The system was successfully tested for CO oxidation on the Au/FeO_x catalyst.

Synthesis of the Mesoporous Structures of the SBA-15 Type with Hierarchical Pore Distribution with the Use of Carbon or Latex Nanoparticles as a Hard Templates

Research project N 204 166 32/4313 [2007-2009]
(project leader: M. Zimowska PhD)

Hierarchical pore distribution in heterogeneous catalysis is important for the optimization of mass and heat transfer. Ordered mesoporous sieves represent a class of materials, whose pore structure can be tailored in a controlled manner. A characteristic feature of SBA-15, which belongs to the most commonly studied mesoporous solids, is the simultaneous occurrence of meso- and microporosity. Mesopores form hexagonal array of one-dimensional straight pores, while micropores, whose contribution depends on the synthetic procedure, exist within the mesopore walls. The present work reports our attempt at developing in the SBA-15 material yet another type of porosity, by addition of carbon black nano-particles to the synthesis mixture. In this approach carbon black serves as a hard template, which, when removed after synthesis by means of calcination, leaves empty voids in the material, in which it was embedded. The following samples were obtained: SBA-15/s (SBA-15 prepared according to the standard procedure), SBA-15/CB (SBA-15 prepared with addition of carbon black), SBA-15/2xCB (SBA-15 prepared with addition of double amount of carbon black). The materials were characterized with XRD, SEM, HRTEM, and N_2 adsorption/desorption isotherms.

The HRTEM image of SBA-15/s material shows well-ordered hexagonal arrays of mesopores (Fig. 1a). The distance between the parallel rows of channels corresponding to d_{100}, estimated from the HRTEM images, is ca. 80.0 Å, and agrees well with the XRD result. The average thickness of the wall is ca. 38 Å, and the pore diameter is around 54 Å, in agreement with the N_2 adsorption measurement. HRTEM investigation of SBA-15/CB shows the areas with regular arrangement of the uniform channels as in SBA-15 and disordered areas showing formation of carbon templated domains intergrown with the SBA-15 framework (Fig. 1b). HRTEM images of SBA-15/2xCB show only structureless foam-like material associated with carbon templated silica (Fig. 1c).

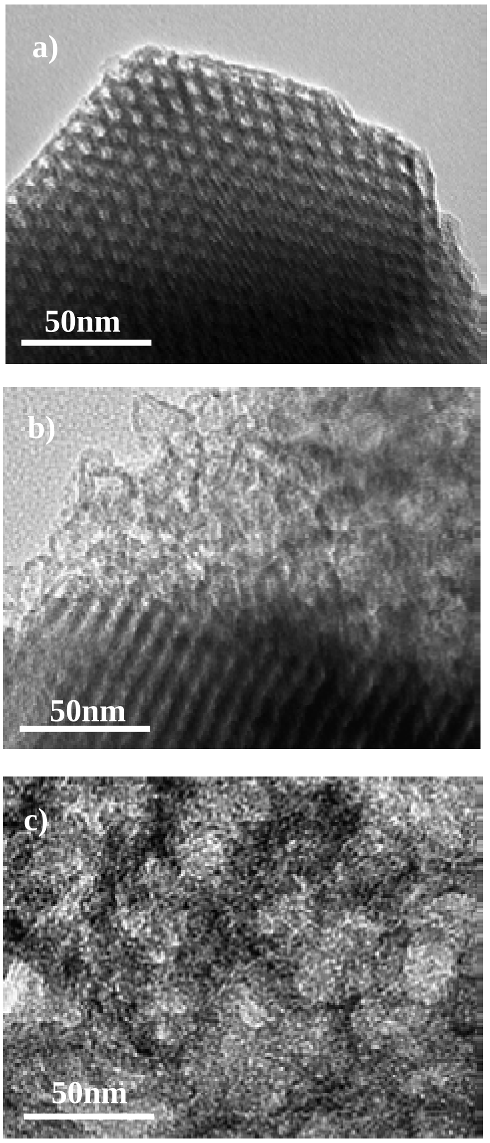


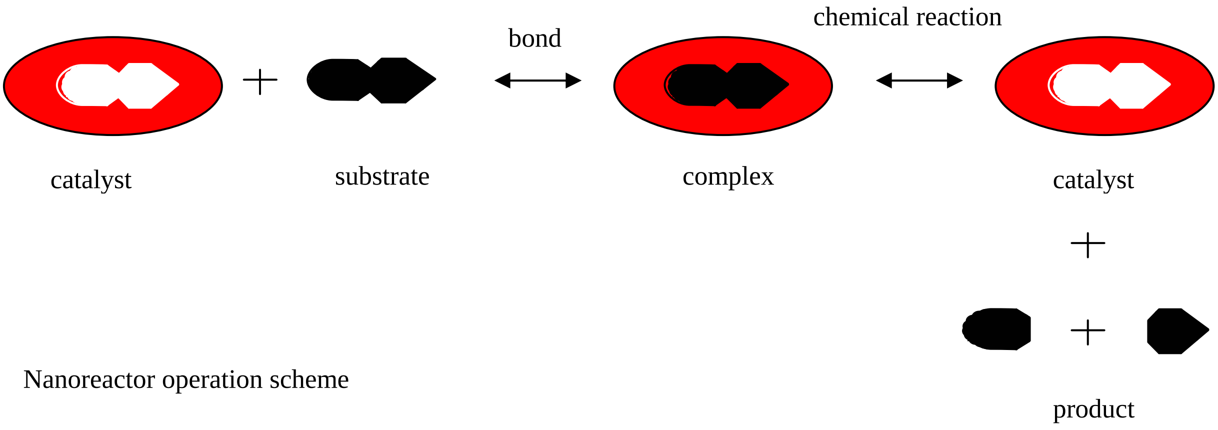
Fig. 1 HRTEM of a) SBA-15/s,
b) SBA-15/CB, c) SBA-15/2xCB

It may be concluded that addition of carbon black particles during the synthesis of SBA-15 results in the formation of mesoporous silica, whose porosity, specific surface area and morphology depends on the amount of hard template. Moderate quantity of carbon black leads to the solid containing SBA-15 domains intergrown with foam-like amorphous silica generated by the hard template. In the presence of large quantity of carbon black the nucleation of SBA-15 component is hindered in favour of the formation of foamy amorphous silica.

Employment of Macrocyclic Metallocomplexes of Transition Metal ions in Self-Assembling Systems for Catalytic Oxidation of Hydrocarbons

Research project N 204 122 32/3142 [2007-2010]
(project leader: Assoc. Professor R. Grabowski)

Metallocomplexes are known as active and selective catalysts of the oxidation of organic compounds in mild conditions. The use of suitable polielectrolite, surfactant or fosfolipid and suitable macrocyclic complexes of transition metals results in the formation of a specific type of nano-reactor. Its properties and architecture substantially influence the environment in which the catalytic reaction occurs. For oxidation, the reaction of nonpolar substrates occurs in the center, while hydrophilic products are transformed outside the reaction zone. This type of catalytic system is environment-friendly because the reaction is performed in an aqueous medium. The employment of self-assembling systems like polysaccharides or liposomes in catalysis results in an easy and fast separation of the catalyst from the reaction products, which influences the yield and reaction selectivity and prevents the formation of unwanted by-products.



Nanoreactor operation scheme

The main aim of this project was to study the synthesis and characterization of metallocomplexes like metalloporphyrins, metallophthalocyanines and heteropoly compounds immobilized in self-assembling systems, i.e. polyelectrolytes. Polyelectrolytes like chitosan (Mw 390kDa) or alginine (Mw 100kDa) were used as matrices for a nano-catalytic reactor. In order to establish optimum conditions for polyelectrolyte-metallocomplex system, the measurements of zeta potential for the solutions of chitosan and alginine as the function of pH and ionic strength were performed. The isoelectric point for tested polyelectrolytes was established at 8.0 and 2.0 for chitosan and alginine, respectively. The immobilization of metallocomplexes on polyelectrolytes was performed at optimum pH conditions, which for chitosan were in the range 3-6 and for alginine between 4-10. Using aqueous solutions of polyelectrolytes the synthesis of the series of polyelectrolyte-metallocomplex systems was performed. The following catalytic systems containing metalloporphyrins: CoTPPS, MnTPPS, FeTPPS, metallophthalocyanines: CoPcS, MnPcS, FePcS and heteropoly compounds: $H_3PW_{12}O_{40}$, $H_3PMo_{12}O_{40}$, $Co_3(PW_{12}O40)_2$, $HCoPW_{12}O_{40}$, $H_2Co_{0.5}PW_{12}O_{40}$, $Co_3(PMo_{12}O_{40})_2$, $HCoPMo_{12}O_{40}$, $H_2Co_{0.5}PMo_{12}O_{40}$ were prepared.

The metallocomplexes immobilized on polyelectrolytes were applied as catalysts of the oxidation of hydrocarbons.

The Influence of Kind of Central (P, Si) and Addenda Atoms (W, Mo) in the Silver Salts of Heteropolyacid with Keggin Structure on Direct Decomposition f Nitrogen Oxide NO_x

Research project N 204 1494 33 [2007-2010]
(projects leader: T. Machej PhD)

The project was started in september 2007 and only a few tasks were done. The contents of crystallization water and water solvating protons in tungstophosphoric, molybdophosphoric, tungstosilicic and molybdosilicic acids were determined. The factors influencing the precipitation of neutral silver salts of heteropolyacids (HPA) were studied. It was found out that the mixing, pH and temperature of the solution affect the specific surface area of silver salts which was checked with BET method. The contents of water in silver salts of HPA were determined using thermogravimetric method. It was shown that $Ag_3PW_{12}O_{40}$ salt apart from crystallization water contains also water solvating silver cations. The thermal stability of silver salts of HPA was examined in the range of 20-1000°C with DSC method. It was demonstrated that among silver salts of HPA the neutral silver salt of tungstophosphoric acid is the most stable and the strong exothermic effect visible at about 600°C is connected with its decomposition. The phase transformations appearing in other salts require additionally measurements by means of high temperature XRD.

On the basis of XRD measurements carried out at ambient temeperature the Rietveld refinements were performed. In the case of $Ag_3PW_{12}O_{40}$ salt it was determined that silver ions exist in its structure as a single cations Ag^+ and also in the dimeric form $(Ag\text{-}Ag)^+$. This important observation will be verified in future by means of XPS spectroscopy. Moreover, the structure of this salt will be check out *in situ* after the reduction performed with hydrogen by means of XRD and XPS methods. These results will indicate which form of silver cations is easy to reduce. It also seems possible that unusual structure of $Ag_3PW_{12}O_{40}$ salt inluences its catalytic activity in the decomposition of nitrogen oxide. On the basis of obtained results the poster will be prepared and presented on „XL Annual Polish Conference on Catalysis" in 2008.

PhD RESEARCH PROJECTS
of the Ministry of Science and Higher Education

Comparison of Catalytic Properties of Metalloporphyrins and Their μ-Oxo Complexes in Hydrocarbons Oxidation

PhD research project 3 T09A 167 29 [2005-2007]
(Professor J. Haber, E. Tabor MSc)

Metalloporphyrins play an important role in both biocatalytic an catalytic processes. Their catalytic properties depend on the type of metal centre, structure of macrocycle ring and substituents in this ring as well as the type of axial ligand. It is possible to tune the catalytic properties to the requirements f different reactions by changing these elements.

A series f iron, manganese and cobalt porphyrins which contain in their *meso* position phenyl rings with electron-donating (TMP, T(p-CH_3)PP, T(p-OCH_3)PP, TTP) or electron-withdrawing (T(p-Cl)PP, T(p-CF_3)PP, TPFPP) substituents were synthesized, In the process of catalytic reaction the porphyrins undergo oxidation and dimerization to μ-oxo species which are considered as a main cause of deactivation. To verify this hypothesis μ-oxo porphyrins with electron-donating or electron-withdrawing substituents were synthesized and their catalytic activity was determined. All synthesized metalloporphyrins were used as the catalysts in oxidation of cyclooctane to cyclooctanol and cyclooctanone. The reaction was carried out at 120 ^{o}C and under the air pressure of 10 atm.

Axial ligand influences catalytic activity on metalloporphyrins especially in the first step of oxidation reaction. Role of axial ligands was determined for iron or cobalt *terakis*(toluiolo) porphyrins with different axial ligands (F, Cl, Ch_3COO_2, OH, Br)in oxidation of cyclooctane with oxygen.

All synthesized metalloporphyrins are active in investigated reaction. It was found that the μ-oxo porphyrins show a certain catalytic activity which is lower then the one of monomeric species. This activity can be enhanced by introduction of electron-donating as well as electron-withdrawing substituents to the porphyrin ring. During the catalytic reaction μ-oxo adducts of metalloporphyrins disintegrate into two simple metalloporphyrins. One of them possesses a hydroxyl group as an axial ligand, while the metal centre of the second metalloporphyrin is reduced from III to II oxidation state.

For metalloporphyrins with different axial ligands the linear relationship between the yields of products in oxidation reaction and the half-wave potentials were found. The higher the catalytic activity the lower the redox potential is observed. Axial ligands effectively modulate the behavoiour of the metalloporphyrins in the cyclooctane oxidation with dioxygen. They initiate the chain reaction by generating the radicals with simultaneous reduction of metal centre in metalloporphyrin.

Mechanism of Interaction of Colloid Particles with Heterogeneous Surfaces Determined by Adsorption and Electrokinetic Measurements

PhD research project 3 T09A 145 29 [2005-2008]
(Professor Z. Adamczyk, A. Michna MSc)

The aim of this grant was to determine the kinetics of colloid particles deposition with regulated surface potential (positive and negative) on surfaces covered by polyelectrolyte multilayers. The influences of: the ionic strength, the type of used polyelectrolyte and the molecular weight the first polyelectrolyte layer were studied.

The experimental results of initial deposition rate of particles deposited onto mica covered by pre-adsorbed PE multilayers as a function of layer number were presented in Fig. 1.

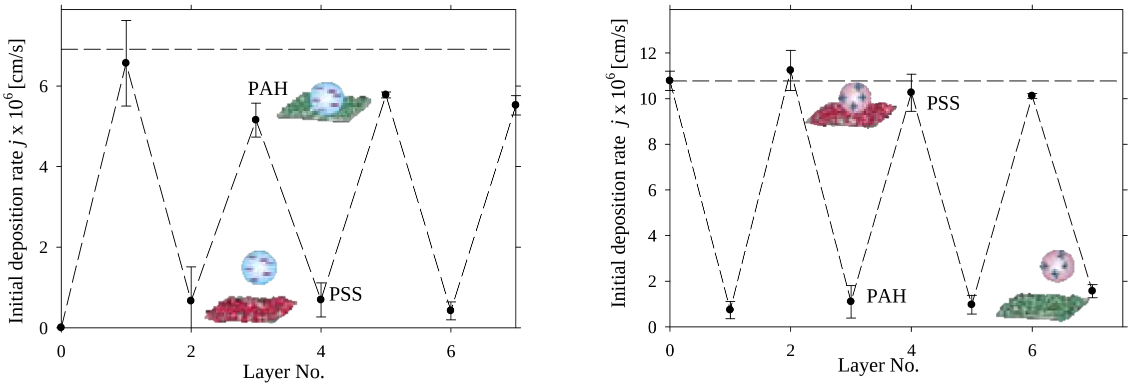


Fig.1 The dependence of the initial deposition rate j_0 on the number of polyelectrolyte layers adsorbed on mica: a) negative latex and b)positive latex.

It was proven that deposition of polystyrene particles on polyelectrolyte multilayers is strictly correlated with the charge of the outermost layer. The deposition of colloid particles on oppositely charged layers of higher polyelectrolyte coverage proceeds with the maximum initial rate corresponding to barrier less conditions observed for homogeneous surfaces. On the other hand, deposition rate was negligible for latex particles bearing surface charge of the same sign as the charge of polyelectrolyte layers. The deposition of colloid particles on polyelectrolyte PAH/PSS multilayer built up on first PEI layer with molecular weight 750 kDa was determined as well. The influence ionic strength of polyelectrolyte adsorbing bath on structure of polyelectrolyte layer was studied. It was found that initial deposition flux increased rapidly with increasing ionic strength of PE adsorbing bath. This effect was accounted for by increased density of the PEI layer, which caused the increase in its charge, and thereby on increase in the density of PSS and PAH layers. Molecular mass of the PEI film used as precursor layer can influence the structure of formed multilayers. It was found that initial flux of particles deposited on PEI layer increased with molecular weight of adsorbed PEI. It was observed that the oscillatory changes in the particle flux are strictly correlated with oscillations in zeta potential of multilayers (measured by using the streaming potential method) and periodic variations in the contact angle of water drops on dried multilayers.

The Mechanism of Rhodium Catalyst Operation for Nitrous Oxide Decomposition in the Gases Emitted to the Environment

PhD research project 3 T09D 010 28 [2005-2007]
(Professor J. Haber, M. Nattich MScEng)

The aim of the PhD thesis was to determine the dependence of the activity of the rhodium on alumina catalyst in the decomposition of nitrous oxide (N_2O) on: the nanoparticles structure, the method of rhodium deposition on the support surface, the presence of alkali metal ions (lithium, sodium, potassium and cesium) as additives to the γ-Al_2O_3 support. Different physicochemical methods gave the information about the structure of the catalyst surface and its proprieties. Following methods have been used: IR spectroscopy of adsorbed molecules, transmission electron microscopy (TEM) and scanning electron microscopy (SEM), BET, hydrogen titration of catalyst samples for determination of rhodium dispersion.

The catalytic activity of catalyst samples as a function of temperature, gas phase composition and GHSV has been determined by measurements of the decomposition of nitrous oxide.

The thesis comprise three experimental parts:

- the synthesis of catalysts by deposition of rhodium as well as promotors on the γ- Al_2O_3 support ,
- physicochemical characterization of synthesized catalysts,
- the study of catalytic activity in the decomposition of N_2O.

The experiments enable to determine the parameters, which could influence the catalytic activity of rhodium supported on alumina in the reaction of nitrous oxide decomposition as well as elucidation of mechanism of influence of these parameters.

Acoustic Emission of Wood in Historic Objects in Response to Microclimatic Fluctuations

PhD research project 1 H01E 010 30 [2006-2007]
(Assoc. Professor R. Kozłowski, S. Jakieła MSc)

A systematic numerical modelling of the mechanical damage of wood in response to variations in microclimatic parameters in its environment allowed determining quantitatively gradients of moisture across wooden elements, subjected to various variations of air temperature and relative humidity (RH), corresponding to real-world conditions in the environment of historic objects. The obtained results allowed determining the threshold levels of variations in the environmental parameters above which damage of wooden works of art would occur. The maximum changes in RH, engendering critical elastic stress, were derived as functions of the amplitude, time period and starting RH level of the variation. In this way domains of reversible and irreversible response of wood could be determined as well as the domain of risk of total mechanical damage.

Acoustic emission (AE) monitoring of wooden cylinders, subjected to variations of microclimatic parameters in the laboratory conditions, allowed tracing of microfracturing which resulted from the stress fields developing in the investigated samples. The distribution of the EA events recorded has revealed a negative impact on the fast microclimatic changes on wood. The non-invasive monitoring of damage has confirmed allowable levels of RH variations, obtained earlier from the numerical modelling.

The application of the AE technique to the monitoring of wooden elements of the historic organs in the church in Olkusz, Poland, in the course of heating cycles, proved a useful tool for the detection of stresses leading to damage.

The obtained results were used in the doctoral thesis which was defended with distinction in March 2007.

Synthesis of High Silica Zeolite Crystals (MFI, BEA) with Multimodal Pore System and Their Application for New Catalysts Preparation

PhD research project N 204 162 31/3659 [2006-2008]
(Assoc. Professor M. Derewiński, A. Burkat-Dulak MSc)

Molecular sieves (zeolites) are solid/acid catalysts widely used in many industrial processes, among others for the preparation of the bifunctional acid/redox catalysts. In spite of a unique pore architecture and high acidity of the zeolite components, the deposition of metal clusters is often limited by the size of cages and channels. As a result, the deposition of nanoclusters usually takes place on an external surface of the crystals. This significantly influences the amount of the deposited dispersed metal phase and the catalytic activity of the catalyst. One of the ways to overcome these limitations and improve the catalytic performance would be preparation of zeolite materials with isolated meso- and macrovoids, when metal clusters could be located. Such materials could be used for the preparation of a more efficient bifunctional catalyst, e.g. containing a higher number of deposited metal clusters accessible by the channels, with strong acid sites present, which interconnect meso-/macrovoids. The aim of our study was the preparation of high-silica zeolites with a secondary system of the meso-/macrovoids, and their use as new supports for the deposition of highly dispersed metal phase.

The MFI type zeolites of different Si/Al ratio, containing meso-macrovoids, were synthesized hydrothermally in basic media. Mono- and polydispersed suspensions of carbon and organic (polystyrene latex) particles were used as templates to generate the secondary pore system. A high crystallinity and phase purity of the obtained MFI type zeolites was proved with the XRD analysis. A high thermal stability of the new material was confirmed by the ^{27}Al MAS NMR data. In spite of high organic template content, the applied calcination procedure enabled avoiding the dealumination of the crystals. Presence of the meso-/macrovoids of varying size inside the crystals were directly proved with the TEM analysis. Impregnation of the modified crystals with a metal salt solution ($PdCl_2$) (the incipient wetness technique) followed by the reduction in an H_2/N_2 stream led to the deposition of metal clusters/nanoparticles not only at the outer surface but also inside the crystals. Size of the clusters located in the meso-/macrovoids was significantly smaller (2-5 nm) than that of the clusters formed after the reduction at the outer surface (10-25 nm). Moreover, the deposition of Pd in the voids inside the zeolite crystals considerably limited the size and number of bigger Pd nanoparticles deposited outside.

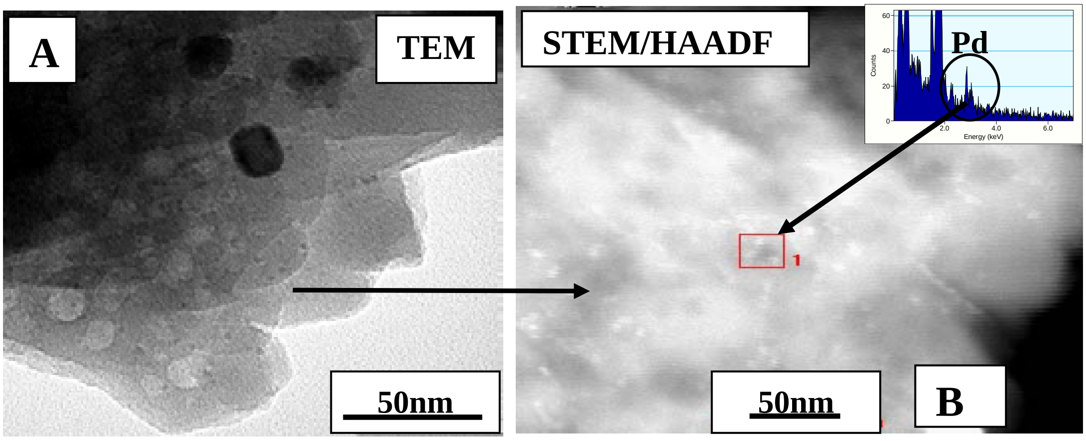


Figure 1. TEM image (A) and STEM and EDX analysis (B) of containing meso-/macrovoids MFI crystal after deposition of metal (Pd) clusters.

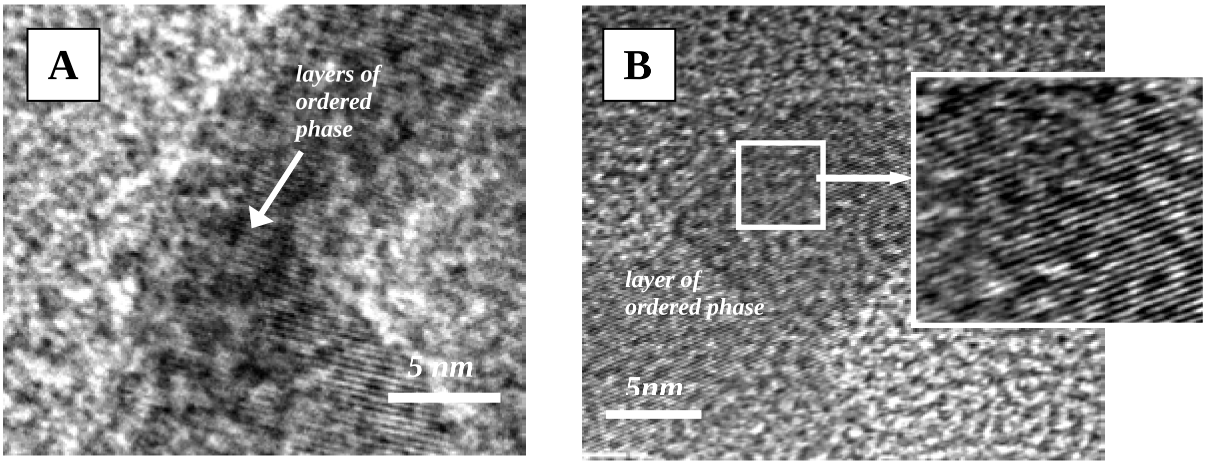
New Systems of Hierarchical Pore Structure and High Acid Properties Containing Dispersed Zeolitic Phase

PhD research project N 205 048 31/2120 [2006-2008]
(Assoc. Professor M. Derewiński, V. Pashkova, MSc)

Composite materials of hierarchical pore structure (micro-/meso-/macroporous) and containing dispersed zeolite nanodomains constitute a new group of solids, which could be successfully used as catalysts, especially in processes where larger molecules should be transformed. One of the ways to prepare this type of material is impregnation of the parent solid with concentrated template solution followed by hydrothermal, partial recrystallization of meso-/macroporous amorphous aluminosilicates into the zeolitic phase. The main goal of the undertaken studies was to investigate whether the proposed metod allows obtain micro/meso/macroporous composite materials containing zeolitic (FAU, BEA) nanodomains and how varying the synthesis parameters affects the transformation process and properties of the prepared materials.

The composite materials containing FAU and BEA nanodomains were prepared hydrothermally using amorphous aluminosilicates of Si/Al ratios of 3.3 and 7.8 respectively. ^{27}Al MAS NMR technique was used to follow changes in the state of Al atoms during the synthesis of the FAU- and BEA-composites. The process of formation of the zeolitic nanodamains in amorphous matrices was monitored with TEM (Figure 1). Characteristic of new acid sites present in the obtained composites was determined by the adsorption of pyridine and carbon monoxide, monitored with IR spectroscopy.

The optimal synthesis conditions for the preparation of the FAU and BEA zeolite composites were established. Similar results of the investigations carried out using different methods, obtained for composite materials with either FAU or BEA domains suggest similarity in the process of the formation of the microporous phases of a different structure. Chemical composition of the aluminosilicate used as well as amount of the template had a decisive effect on the crystalline phase formed. The sorption experiments showed that the obtained composite contained the microcrystalline phase and retained – at least partially - the meso/macroporosity of the parent aluminosilicate. The IR spectroscopy data (CO sorption) proved a high acidity of the FAU and BEA composites, attributed to the formation of the Brønsted acid sites of the zeolitic character.



TEM images of microporous FAU (A) and BEA (B) layers formed during early stage of recrystallization of parent amorphous aluminosilicates (Si/Al ratios 3.3 and 7.8 respectively)

Properties of Cu(I) Centres in Faujasite and MFI Zeolites and Their Interaction with Molecules Studied by Quantum Chemical and Hybrid Methods

PhD research project N 204 180 31/3999 [2006-2008]
(Professor E. Brocławik, P. Rejmak, MSc)

The main goal of this task in 2007 was the investigation of the activation mechanism of NO adsorbed on Cu(I) active sites in faujasites (FAU) and MFI zeolites in the context of the framework structure and aluminum content (Si/Al ratio). Earlier calculations for CO adsorption on copper sites in faujasites have been published in one paper in Physical Chemistry Chemical Physics journal.

The calculations were carried out by combined quantum mechanics – molecular mechanics (QM/MM) methodology with the use of QMPOT software, combining Turbomole (QM part) and Gulp (MM part) programs. The investigations involved geometry optimization, calculations of adsorption heats and vibrational analysis for harmonic frequencies.

In order to model NO adsorption in high aluminum FAU zeolites the models were constructed for the framework with various aluminum content (MM part) and clusters (in QM part) with varying sizes and number of Al atoms. Low-aluminum MFI was modeled by the elementary unit cell and clusters with one Al atom.

The research on mononitrozyl systems has been completed by testing larger QM clusters such as 16T model for site II and 20-22T model for site III (*n*T denotes number of atoms tetrahedrally coordinated, Si or Al, in the cluster) for selected structures in FAU zeolites. Extension of the cluster size (from 12T and 8T for sites II and III, respectively) does not influence the results, calculated NO stretching frequencies become uniformly blue-shifted by ca 10 cm^{-1} for bigger clusters.

Modeling of dinitrozyl complexes NO on Cu(I) in FAU and MFI zeolites has been accomplished. The most stable dinitrozyl forms appeared to be singlets with π bonds formed between the two NO ligands. Dinitrozyl complexes have comparable stabilities for site II and III whereas the adsorption energy of single NO ligand was nearly two times higher for site III than for site II. On the basis of results for mononitrozyl complexes on Cu(I) in FAU the interpretation of experimental IR spectra has been proposed. One paper is in preparation on NO adsorbed on copper sites in FAU zeolites.

Evaluation of the Parameters Determining the Three-Phase Contact Formation in the Time-Scale of Miliseconds

PhD research project N204 012 31/0279 [2006-2008]
(Professor K.Małysa, J. Zawała MSc)

The aim of this project is to determine the influence of the bubble velocity (kinetic energy) and dynamic structure of adsorption layer induced over interface of the bubble rising in surfactant solutions on a course of the collision and kinetic three-phase contact formation at various solid surfaces. The importance of the electrical charge of the interacting liquid/gas and liquid/solid interfaces on the three-phase contact formation during the bubble collision was studied, as well.

In the reporting period the accelerations, profiles of the local velocities, i.e. the bubble velocities at different distances from the capillary, and degrees of deformation of the rising bubble shape were measured. The measurements were carried out for distilled water, in electrolyte solutions and in solutions of ionic (cationic and ionic) and non-ionic surfactants. The profiles of the bubble local velocities and values of the terminal velocities were determined. It was found that the profiles of the bubble local velocities and the bubble shape deformations in various electrolytes solutions were similar as in distilled water. In the surfactant solutions the initial accelerations of the bubbles was decreasing with the solution concentration from ca.930 cm/s^2 in distilled water to ca. 500 cm/s^2 in the highest surfactant concentrations. For all surfactants studied it was observed that the bubble terminal velocities were decreasing from 34.7 cm/s in distilled water to ca. 15 cm/s at the concentrations of the surfactants studied. At low surfactants concentration a maximum on the bubble local velocities profiles was observed, what was the evidence that the dynamic structure of the adsorption layer was not established yet over surface of the rising bubble. There was no maximum at high surfactants concentration, what was the consequence of establishment of the dynamic adsorption layer immediately after the bubble detachment from the capillary orifice.

It was showed, that the state of the adsorption layer and type of the surface active substance had a crucial influence on the kinetics of the three phase contact formation during the bubble collisions with solid surfaces, bearing a definite electical surface charge. In these series of experiments two different surfactants, having identical length of the hydrocarbon chain – n-octanol (non-ionic) and n-octyl-trimethylammonium bromide (cationic) – were used and their concentrations were chosen in such way that the bubble adsorption coverage at the moment of detachment from the capillary was practically identical (ca. 2%). The bubble collisions and the three phase contact (TPC) formation at negatively charged mica surface were investigated. The three phase contact formation was observed only in n-octyl-trimethylammonium bromide (OTABr) solutions – the OTABr adsorption caused recharging of the bubble surface. There was no TPC formation in distilled water and in the solution of non-ionic surfactant because the bubble surface was negatively charged, similarly like the mica surface. The wetting film at the mica surface was stable due to the repulsive electrostatic interaction between similarly charged the solid/liquid and liquid/gas interfaces. In the case of the n-octyltrimethylammonium bromide solutions the bubble surface was positively charged and the film was not stable. The TPC was formed because there were attractive electrostatic interactions between the bubble and the mica surfaces.

Determination of the Influence of Adsorbed Polyelectrolytes on the Kinetics of Deposition and Topology of Particle Monolayers

PhD research project N 204 150 32/3822 [2007-2009]
(Professor Z. Adamczyk, A. Bratek MSc)

The dynamic viscosity of polyelectrolyte (PE) solutions was measured using a home made capillary viscometer. For these measurements we used a poly(acrylic acid) PAA of average molecular weights of 12 000, 70 000 and 145 000. Dynamic viscosity was measured using the three molecular weights of PAA as a function of concentration, ionic sength and pH. These results were interpreted in terms of the hydrodynamic model, which describes the physical and chemical properties of polyelectrolytes much better than other models used in the literature. This model enables one to determine the hydrodynamic radius of the macromolecules. This parameter is very useful for the further interpretation of the macromolecule structures in aqueous solutions.

Subsequently, the bulk characteristic of PAA, PAH poly(allylamine), PEI poly(ethylene imine) was performed by measuring of diffusion coefficients (PCS method), and electrophoretic mobility as a function of PE concentration, ionic strength and pH using a modern apparatus from Malvern called Zetasizer Nano ZS. This device allows one to characterize subjects of the nanoscale-size range such as polyelectrolytes. The hydrodynamic radii of PAA obtained from the PSC measurements corroborate with the data calculated using the hydrodynamic model. It means that viscosity measurements are a sensitive tool for determining the conformation of polyelectrolyte molecules. Simultaneously, measuring electrophoretic mobility allows one to determine the effective ionization degree of macromolecules. In our case this value is much lower than the nominal ionization degree widely used in the literature. It causes different bahaviour of PE in aqueous solutions.

The next task was modeling the conformations of PE molecules. Calculations of PE structures were performed according to the molecular dynamic simulations. The structures of poly(acrylic acid), of an average molecular weight of 12 000, were determined as a function of ionic strength and ionization degree. This method permits one to determine important parameters such as the effective cross-section of the chain, the shape of a molecule (see Fig. 1), the effective ionization degree (uncompansated charge) and the critical concentration of an electrolyte which causes the condensation of charges on a molecule.

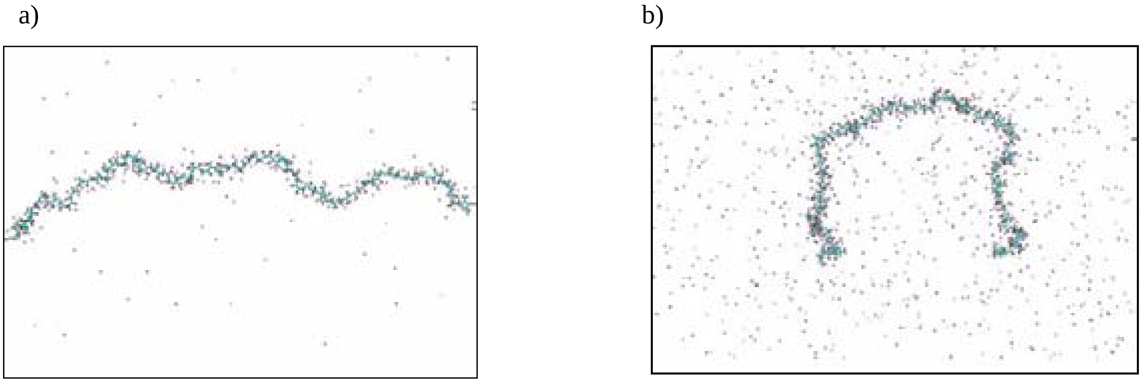


Fig.1. Snapshots of PAA molecule (M_w= 12 000)conformations derived from numerical simulations in aqueous solutions :a) I = 10^{-3} M, α_i = 1.0, b) I = 10^{-1} M, α_i = 1.0.

Deposition of Model Microcapsules on Metallic Surfaces Modified by Adsorption of Polyelectrolyte Mulitayers

PhD research project N 204 2145 33 [2007-2009]
(Assoc. Professor P. Warszyńsk,; A. Trybała MSc)

Modification of metallic surfaces by adhesion of nano- or microcapsules can be of importance for biomedical applications (e.g. bone implants or stents covered with capsules containing anti inflammation drugs) or corrosion prevention. Therefore, the aim of the project is to investigate the deposition of model microcapsules at bare metallic surface and ones modified with polyelectrolyte multilayers (PEM). PEM films are often used for surface modification and as adhesion promoters. The objectives of our studies performed in 2007 were as following:

- formation by 'layer by layer' (LbL) method of multilayers composed of natural polyelectrolytes (polycations - Chitosan - CHIT, poly(ethyleneimine) - PEI and polyanion - polyalginic acid sodium salt –ALG, on silicon waffers;
- characterization of PE multilayers deposited in various conditions by elipsometric film thickness and fluorescence intensity measurements.

To investigate the effect of PEI first layer on the thickness of polyelectrolyte multilayers we prepared films $(CHIT/ALG)_n$, $PEI(CHIT/ALG)_n$ of various thickness.

In Fig.1 the results obtained for ellipsometric thickness of these multilayers are presented. They indicate that films with given number of layers built up on PEI anchoring layer were thicker than structures having the same number of PE layers but consisting of (CHIT/ALG) only. Branched PEI anchors the structure to the substrate and probably acts as a scaffold for the buildup of next layers. This effect is observed for untreated films and ones exposed to various pH conditions too. As far as stability of multilayers is concerned one can observe (Figs. 2) that acidic or basic treatment leads to the thinning of studied films (CHIT/ALG), which is extremely significant for basic treatment - about 60% decrease of initial thickness of untreated films can be noted. As chitosan is practically uncharged at pH = 11 the film can be peeled off. The same effect of basic solution can be observed for structures with PEI anchoring layer. The neutral and acidic treatment don't influence PEI(ALG/CHIT) thickness.

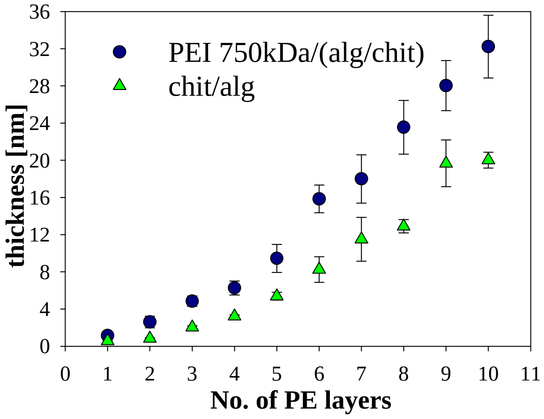


Fig. 1. Thickness of (CHIT/ALG) and PEI/(ALG/CHIT) films as a function of a number of layers.

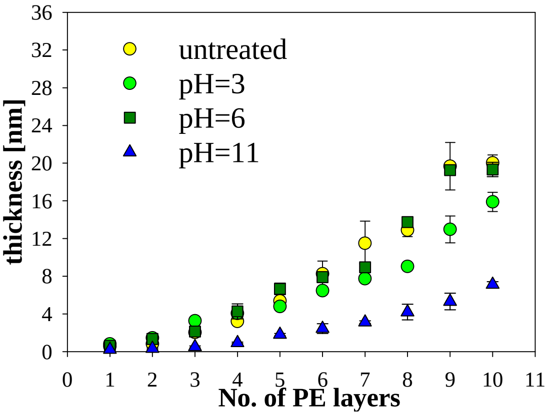


Fig. 2. Thickness of CHIT/ALG films as a function of a number of layers for untreated, pH=3, pH=6 and pH=11 treatment

Transformations of Terpene Hydrocarbons over Zeolite Catalysts

PhD research project N 204 1240 33 [2007-2009]
(Professor B. Sulikowski, Ł. Mokrzycki MSc)

Growing contamination of our environment and essentially restricted amounts of available standard resources used in chemical industry (crude oil) are behind the current trends which put more accents on *renewable natural resources* and developing of related technologies for production of higher value added chemicals. The terpene hydrocarbons are of major importance for chemical, pharmaceutical, and food industry. One of the most available hydrocarbons is α-pinene.

Isomerization of α-pinene is an important industrial process. The acid-impregnated TiO_2 is currently used as an industrial catalyst in batch reactors, but because of the low rate of the industrial process and corrosion problems, there is a great interest in finding new catalysts exhibiting higher activity and selectivity towards camphene (camphor production), limonene (solvent) and *p*-cymene (PET production).

Application of zeolite catalysts can commence new opportunities in of α-pinene isomerization. This is due to tunable, in a broad range, acidity of zeolites. The objective of this project is to study behaviour of zeolites: ZSM-5, ZSM-12 and MCM-22, as well as their modified forms, in isomerization of α-pinene. Desilication of zeolites will be one of the method used for tailoring of catalytic properties.

Within the frame of the project, introductory synthesis of zeolite ZSM-12 with the Si/Al ratio of 40 to 75 was carried out in 2007. Some preliminary works aimed at the synthesis of MCM-22 materials (precursors and zeolite) were also performed. The materials were characterised by XRD, SEM, NMR and nitrogen sorption. The parameters of gas chromatography analysis of α-pinene and isomerization products were established.

HABILITATION RESEARCH PROJECTS

of the Ministry of Science and Higher Education

Reaction Mechanisms of Nonheme Iron and Manganese Enzymes Activating Dioxygen

Habilitation research project N 204 173 31/3823 [2006-2008]
(T. Borowski PhD, Professor E. Brocławik)

The scope of this research project involves quantum chemical investigations of reaction mechanisms for three metalloenzymes: two mononuclear nonheme iron enzymes (PCD – protocatechuate 3,4-dioxygenase, ACO – apocarotenoid oxygenase) and one manganese (OxDC – oxalate decarboxylase). For activity, these enzymes require dioxygen, either as one of the substrates (PCD, ACO) or as an activator (OxDC), and they catalyse the following chemical reactions: oxidative cleavage of aromatic rings in 3,4-dihydroxybenzoate (PCD), oxidative cleavage of carotenoid (polyene) chain (ACO), and dismutation of oxalate into formate and CO_2 (OxDC).

Since the commencement of the project, the following goals have been achieved:

- a computer server has been purchased,
- a licence for quantum chemical program Jaguar has been purchased,
- investigations on the reaction mechanism of PCD has been done, the results have been published [1],
- the mechanism of oxidative cleavage of apocarotenoids by ACO has been investigated, the results are being published [2]

POL-POSTDOC PROJECTS

of the Ministry of Science and Higher Education

Epitaxial Oxide Nanostructures on Metallic Single Crystalline Substrates

(D. Wilgocka-Ślęzak, PhDEng)

As a first project task preparation of an iron oxide on a vicinal Pt(997) surface has been developed at ultrahigh vacuum conditions. The Pt(997) surface was prepared to atomic purity and a high degree of the structural order by numerous cycles of argon ion bombardment and annealing in oxygen and high temperature flashing. LEED and STM measurements confirmed the well ordered structure of steps spaced by 2.1 nm. On the substrate prepared in this way Fe ultrathin films were deposited at room temperature from a thermal source. Then the films were annealed and oxidized at optimized oxygen exposures and temperatures. The Fe thickness was selected to obtain the FeO films of a nominal thickness between 0.5 and 1.5 monolayer (ML). The best structural quality and the homogeneity of the oxide films was obtained for the nominal thickness not exceeding 1 ML. Examples of LEED and STM results are shown in Figs 1 and 2. The six-fold symmetry of the diffraction pattern indicates the (111) orientation, while the satellites are due modulation of the oxide structure resulting from the lattice misfit between the FeO monolayer and the Pt(111)-like terraces (the misfit amounts to 11 %). The substrate step structure is not well visible in the complex diffraction patterns. The atomic resolution STM pictures fully confirmed the presence of the superstructure and they reveal a high degree of the surface structural order. Moreover, which is important for the surface engineering, the monoatomic steps of the substrate are perfectly reproduced on the surface of the oxide. For the oxide layers beyond 1 ML, basing on the STM measurements a Stranski-Krastanov growth mode was found: on the first modulated FeO layer elongated disordered 3-d islands were formed.

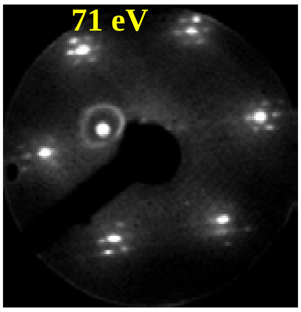


Fig. 1.

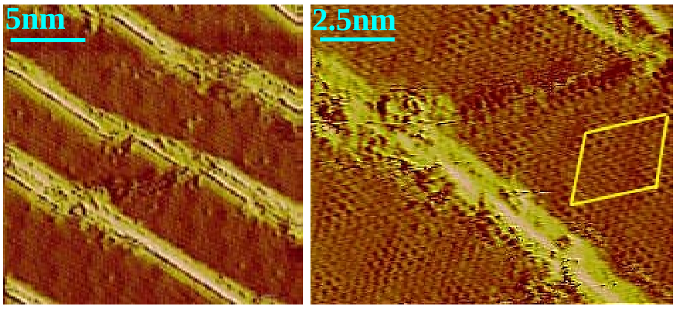


Fig. 2.

Establishing Standards for Allowable Microclimatic Variations for Polychrome Wood

(M. Łukomski, PhD)

The main aim of the project has been establishing precisely and quantitatively the variations of air parameters that are safe for the painted wood surfaces. During the first year of the project the emphasis was laid on preparation of samples mirroring medieval panel paintings for future tests and analysis. Ground layer (or gesso), which is a mixture of animal glue and chalk, is the most fragile part of the entire painting which is subjected to biggest stresses during the microclimatic fluctuations. The preparation procedure for the gesso of mechanical parameters similar to those of the historic materials was elaborated.

Within the confines of the project, historic technologies applied in panel painting were identified and analyzed. Samples of gesso with varying pigment-to-binder ratio were prepared on the basis of recipes recommended in the literature. Ultimately, gesso with pigment volume concentration of approximately 95% was chosen as the best material for further work; the preparation procedure and the structure of such gesso material were very similar to those found in paintings and used in the conservation practice. Thin layers of gesso were prepared and used to produce specimens suitable for measuring the tensile properties.

To mimic the historic materials, artificial ageing of the gesso specimens at the conditions of increased temperature and relative humidity was carried out in a climatic chamber. Basing on the literature survey, 70^{o}C and 80% RH were selected. Analysis of the tensile properties of the gesso specimens aged between 1 – 6 weeks to identify optimal conditions and time of ageing is under way. It is also planned to collect as many samples of historic gesso as possible to analyze their tensile properties for comparison.

All mechanical tests of samples (stress/strain relationships, swelling isotherms, creep) are carried out with the help of a Tritec 2000 Dynamic Mechanical Analyser. The measurement procedures (number of specimens, initial strain rate, interpretation of the results) were elaborated by modifying the ASTM and CEN standards. Construction of a temperature and humidity controller necessary for the main body of testing has been advanced.

Parallel to the technological and mechanical study of materials, optical methods for direct monitoring of delamination of the decorative layers from the wooden support and their mechanical damage were developed. An Electron Speckle Pattern Interferometer was built using the resources of this project and those of the PL0086 Grant of the EEA Financial Mechanism.

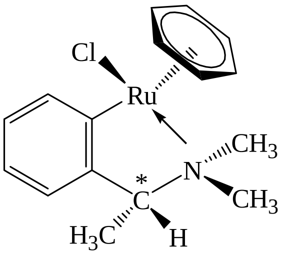
Synthesis and Immobilization of New Chiral Ru(II) Complexes onto Mesoporous Supports. Application in Asymmetric Catalysis

(D. Duraczyńska, PhD)

The goal of this project is:

- the determination of the method of the chiral Ru(+2) complexes preparation,
- the determination of the immobilization method of the chiral Ru(+2) compounds onto mesoporous silicas,
- the application of the supported catalysts in asymmetric catalysis.

We synthesized and characterized Ru(+2) complex containing chiral amine ligand TMBA whose structure is shown below. Moreover we obtained the starting materials such as $[(\eta^5\text{-}C_5H_5)Ru(CH_3CN)_3]PF_6$ and $[(\eta^5\text{-}C_5Me_5)Ru(CH_3CN)_3]PF_6$ for the preparation of ruthenium complexes with chiral phosphine DuPhos.



Furthermore, we were able to determine the immobilization method of cationic Ru(+2) complexes onto mesoporous supports such as HMS, FSM and SBA. Heterogenized catalysts were obtained by immobilization of $[(\eta^5\text{-}MeC_5H_4)Ru(\eta^3\text{-}PPh_2CHCH_2)(\eta^1\text{-}PPh_2CHCH_2)]^+$ onto aluminated hexagonal mesoporous silicas by direct ion exchange method. Mesoporous silicas can acquire cation exchange properties by partial substitution of Si^{4+} ions with Al^{3+} in the framework.

Immobilized catalysts were found to be catalytically active in the hydrogenation of phenylacetylene.

SCIENTIFIC NETWORKS
of the Ministry of Science and Higher Education

EKO-KAT Innovative Catalytic Materials in Environmental Protection

(network coordinator: Professor E. Serwicka-Bahranowska)

The man goal of research carried out in the frame of scientific network EKOKAT is the development of interdisciplinary collaboration aimed at design and synthesis of novel catalytic materials for processes important for the protection of environment. All institutes of Polish Acedemy of Sciences involved in the network activities belong obtained top ranks in the last classification carried out by the Ministry of Science and Higher Education. The list of partners includes:

1. Institute of Catalysis and Surface Chemistry PAS, Krakow (ICSC - coordination)
2. Institute of Physical Chemistry PAS, Warsaw (IPC)
3. Institute of Industrial Chemistry, Warsaw (IIC)
4. Institute of Plant Physiology PAS, Krakow (IPP)
5. Institute of Nuclear Physics PAS, Krakow (INP)
6. Institute of Chemical Engineering PAS, Gliwice (ICE)
7. Institute of Metallurgy and Material Chemistry PAS, Krakow (IMMC)
8. Institute of Low Temperatures and Structure Research PAS, Wroclaw (ILTSR)

Research is divided into 6 thematic groups dealing with materials chemistry issues of current interest:

a) Catalysts based on supported noble metals nanoparticles for removal of atmospheric pollutants (ICSC, IPC, ILTSR). Topic of research carried out in 2007: Noble metal catalysts (*Au/chromium spinels* MCr_2O_4 *[M=Co,Mn,Fe], Au/*MgF_2*, Au/MgO, and PtAu/γ-*Al_2O_3*) for hydrodechlorination and oxidation of CO and hydrocarbons.*

b) Layered silicates as precursors of nanostructures designed for application in green chemistry processes (ICSC, IIC, INP, IMMC). Topic of research carried out in 2007: *Synthesis and physico-chemical characterization of polymer composites based on polyethylene and hydrotalcite or polyethylene and halloysite.*

c) Functionalized multimodal materials for selective catalytic processes and sorption (ICSC, IIC, IMMC). Topic of research carried out in 2007: *Synthesis of materials with hierarchical pore structure (micro-/meso-/macro) derived from meso-macroporous silica monoliths.*

d) Novel mixed oxide catalysts for utilization of CO_2 (ICSC, IIC, IMMC). Topic of research carried out in 2007: *Optimization of a synthetic procedure of CuZnAl-O mixed oxide catalysts for* CO_2 *hydrogenation, derived from hydrotalcite-like precursors.*

e) Enzymatic biocatalytic processes – theory and practice (ICSC, IPP). Topic of research carried out in 2007: *Biocatalysts in application for stereoselective hydroxylation of hydrocarbons - investigation of EBDH substrate spectrum, modeling of electronic structure of EBDH, modeling of reaction mechanism.*

f) Model metal catalysts on monocrystalline oxide supports - theory and experiment (ICSC, INP, IPC). Topic of research carried out in 2007: *Investigation of size effects in electronic structure of metal-metal and metal-oxide systems Fe/W(110) and Au/*Fe_3O_4*.*

Results of the EKOKAT activities have been presented during the reporting seminar organized in ICSC PAS on 7th September 2007.

COMMISSIONED
RESEARCH PROJECTS
of the Ministry of Science and Higher Education

New Catalytic Materials as a Basis of Environment Friendly Chemical Processes

Commissioned research project PBZ-KBN-116/TO9/2004
(project coordinator: Professor M. Witko)

Project is divided into 13 tasks, three of them are carried out in the Institute:

1e - Pd-Nanoparticles in Polymeric Matrices – Novel Catalytic Systems for Hydrogenation of Unsaturated Hydrocarbons
(task leader: A. Drelinkiewicz, DSc)

Physicochemical characterization of Pd-polymers
Physicochemical characterization was performed (FTIR, XPS, XRD, SEM, TEM, HRTEM, swelling experiments) for catalysts basing on microporous resin (FCN), poly(4-vinylpyridine) (PVP) and polyaniline (PANI)
Pd/FCN: insertion of palladium into FCN resin with $–NH_2$ groups resulted in gradual decrease in swelling ability of polymer mass in THF. Expansion of polymer decreased especially strongly for the catalysts Pd(VOL) in which Pd was located throughout the bulk of polymer. This was ascribed to crosslinking of polymer by the palladium ions. In reduced catalysts the presence of Pd-nanoclusters was observed by HRTEM.
Pd/PVP: Catalysts (1 wt %Pd) were prepared using aqueous solutions of $PdCl_2$ containing HCl, CsCl and LiCl. The type of Pd-species and the size of Pd-particles in reduced catalysts were found to depend on method of preparation. Dispersion of Pd was the highest in 1%Pd-Li catalyst (nano-clusters of size below XRD limit), whereas the Pd-crystallites of diameter 4.2 nm and 5.7 nm were present in 1%Pd-H and 1%Pd-Cs catalysts, respectively
Pd/PANI: two polymer samples PANI-DL (m_w=100 000) and PANI-Kr (m_w=10 000) differing in molecular weight of PANI were used. Pd^{2+} ions were reduced to Pd-metal under insertion to both polymers (FTIR, XPS). The size of Pd-particles formed was found to depend on molecular weight of PANI. Nano-clusters of Pd were present in 2% Pd/PANI-DL, whereas the size of Pd-particles was distinctly higher (15.6 nm) in 2%Pd/PANI-Kr catalyst.

Hydrogenation of 2-butyne-1,4-diol (B3-D) in the presence of Pd/FCN, Pd/PVP and Pd/PANI
Catalytic tests were carried out in :batch" type reactor, at 22^0C and atmospheric pressure of H_2. Reaction was followed by hydrogen consumption of GC analysis.
Pd/FCN: At the same Pd loading (0.125 – 0.5 wt %Pd) much higher activity in hydrogenation of B3-D was offered by Pd/FCN catalysts having Pd within the surface layer of catalysts grain. They were prepared using aqueous $PdCl_2$ solution. For all studied catalysts, selectivity to alkene (2-butene-1,4-diol) was very high (ca. 95%) and only low content of by-products was formed(10-20 %). This advantageous performance of Pd/FCN catalysts was ascribed to the influence of amine groups of polymer.
Pd/PVP: hydrogenation of B3-D was carried out in the presence of Pd-H, Pd-Li and Pd-Cs catalysts in solvents of various polarities (pentanol, water, ethyl acetate). In all systems studied the highest activity was exhibited by Pd-H, the lowest by Pd-Cs catalyst. Selectivity to alkene (B2-D) was high (ca. 90 %) in water and ethyl acetate solvents. Polarity of solvents influenced the content of by-products formed via isomerization and hydrogenolysis of B2-D. The highest content of by-products was formed in aqueous conditions. The observed performance of catalysts was correlated not only with the size of Pd-particles but also with accessibility of reactant to Pd-centres located inside the polymer mass.

2c - Development of Technological Procedure for Preparation of Nanostructural Oxide Catalysts with Controlled Properties for Destruction of Toxic Solvent Vapours

(task leader: T. Machej, PhD)

A relation between the chemical composition and physicochemical properties of MnAl-O, CuAl-O and CuMn-O pure active phases and their catalytic activity in the test reaction of toluene combustion has been determined. The activity increased with the materials reducibility, the Cu-Mn mixed oxides representing the most active group. Comparison of the surface composition determined by means of XPS spoectroscopy with that of bulk led to the conclusion that the calcined CuMn-O and CuAl-O solids are composed of CuO crystallites coated with an amorphous Mn-rich or Al-rich layer, respectively, while MnAl-O materials represent amorphous structures, with Mn-enriched surface. Preliminary tests show that the order of activity changes upon preparation of a washcoat for the monolithic support. The effect is assigned to the modification of mixed oxide phase composition due to the interaction of the precursor slurry with the colloidal alumina used for washcoat preparation.

3a - Synthesis, Spectroscopic and Catalytic Studies, and Quantum-Chemical Calculations on Novel Zeolite Catalysts for the Environment Friendly Reactions

(task leader: Professor B. Sulikowski)

In 2007, delamination of the precursor of MCM-22 zeolite was studied in details. First, the influence of parameters on hydrothermal synthesis was checked. Then synthesis of MCM-22 precursors with the Si/A=15 and Si/Al=40 was carried out under dynamic conditions at 157 °C. Hexamethyleneimine (HMI) was used as a structure-directing agent. The samples obtained were characterised by XRD and sorption. By applying the procedure of preparation, delaminated matrices were obtained, onto which heteropoly acid and its salt was deposited.

Reduction of Co^{3+} i Co^{2+} by H_2, CO and formaldehyde was studied, revealing that HCHO was the most effective reductor, which was oxidised towards formic ions. The influence of initial acidity of H-FER zeolite onto the status of Co^{3+} and Co^{2+} ions and catalytic activity of the samples in the Selective Catalytic Reduction of NO (SCR) was tested. The status of the Co^{3+} i Co^{2+} ion in the Co-ZSM-5 and Co-FER zeolites was studied by IR using CO and NO as probe molecules. Three types of Co^{3+} ion exhibiting various electron-acceptor properties were found, as well as Co^{2+} in the cationic positions, oxide-like-clusters and bulk CoO.

The relative amounts of the different cobalt forms are a function of zeolite composition (Si/Al and Co/Al ratios) and the particular route of its treatment. Experiments with *coadsorption* of pivalonitrile and CO brought about information on the localisation of oxide clusters.

New batches of ferrierite catalysts were obtained, taking into account our earlier experience in the procedure of zeolite modification. The ferrierite matrix was treated in a different way before introduction of metal ions (cobalt and indium). The samples were tested in SCR of NO, in the presence of methane as a reducing agent.

In 2007, parameterization was carried out and theoretical calculations were performed using the DFT method (quantum chemistry) *in tandem* with molecular mechanics (force fields) for the description of properties and stability of different cobalt(II) centres, i.e. potential centres for adsorption and catalytic reactions. It was demonstrated that parameterization of force fields taking into account *oxide* parameters for cobalt led to better description of metal centres in zeolite. Cobalt(I) ions occupying β positions were more stable, in comparison to those located at the α sites.

Finally, it was found that distribution of the Al pairs at the given framework crystallographic position affected stability of cobalt(II) ions. The structures with the symmetric location of the Al pairs were the most stable ones.

Chemistry of Perspective Carbon Transformation. Multifunctional Catalysts Derived from Layered Minerals for Single Stage Process Syngas→Methanol→Dimethyether

Commissioned research project PBZ-MEiN-2/2/2006 [2006-2010]
(project leader: Professor E. Serwicka-Bahranowska)

Project aims at development of novel catalyst formulations for direct transformation of syngas to dimethylether (STD), via methanol as an intermediate:

$$\begin{array}{lll}
(1) & 2CO+4H_2 \longrightarrow 2CH_3OH & \Delta H=-182,06\ kJ \\
(2) & 2CH_3OH \longrightarrow CH_3OCH_3+H_2O & \Delta H=\ -22,67\ kJ \\
(3) & H_2O+CO \longrightarrow H_2+CO_2 & \Delta H=\ -41,12\ kJ \\
\hline
\text{Sumarycznie} & 3H_2+3CO \longrightarrow CH_3OCH_3+CO_2 & \Delta H=-245,85\ kJ
\end{array}$$

Synthesis and optimisation of a multifunctional catalyst for STD process is foreseen, the design being based on the use of natural and synthetic layered minerals. Hydrotalcite-like precursors will serve for the development of the mixed oxide component for methanol synthesis and modified layered silicates will be used as acidic component responsible for methanol to DME transformation. In the reporting period a series of Cu-Zn-Al hydrotalcites with various additives have been synthesized. The investigated synthesis parameters included the method of reagents addition, synthesis pH, ageing, and thermal decomposition program. Tests of methanol synthesis have been carried out.

EU 6th FRAMEWORK PROGRAMME PROJECTS

Dynamics in Nano-scale Materials Studied with Synchrotron Radiation

UE STREP Research Project DYNASYNC NMP4-CT-2003-001516
[2004-2007]
(project coordinator: Professor J. Korecki)

The Dynasync project was running from March 1, 2004 to February 28, 2007. According to the project time frame most of the tasks were accomplished in years 2004-2006. During the last two months of the project duration the ICSC Partner finished the following tasks:

1. Comparison of theoretical and experimental VDOS in selected multilayer systems

The task combines the theoretical calculations of the vibrational properties of multilayer systems with the measurements of their phonon densities of states by nuclear inelastic scattering (NIS) of synchrotron radiation. In the frame of this task our group studied structural and magnetic properties of the Fe_n/Au_n multilayers composed of n Fe(001) and Au(001) atomic monolayers. In this way we obtained an ordered alloy, which does not occur in the bulk Fe-Au phase diagram. The comparison of the experimental NIS data with the theoretical first principles calculations indicates stabilization of the ordered structure of the $L1_0$ type.

2. The magnetization dynamics during the growth of Fe nanostructures on W(110).

The nuclear resonance scattering of the synchrotron radiation has been used to study the evolution of the chemical, structural and magnetic properties during the Fe film growth on W(110). The method has resolution of a single atomic layer and is sensitive also to buried layers. Using these features, we studied the dynamics of the spin reorientation transition in the ultrathin iron films as a function of temperature, layer thickness and chemical state of the surface.

Along with the research tasks during the last two months of the project duration our group realized also important management tasks:

1. Preparation of the annual and final activity and management reports.
2. Preparation, organization and participation in the final workshop of the Dynasync project: “Workshop on Nano-Scale Materials: Growth-Dynamics-Magnetism” taking place at ESRF Grenoble, Feb. 6-8, 2007.

The Dynasync project has been accomplished in perfect agreement with the time schedule. In the frame of the project 35 deliverables were realized; several tens scientific papers have been published, many others are in preparation; over hundred twenty conference contributions have been presented. The project remarkably increased the European Research Area giving the international scientific community the unique and proved equipment in several scientific centers. The European Commission approved the project scientifically and formally without any reservations.

Scientific Network – Surfactants and Dispersed Systems in Theory and Practise

EU SSA Project SURUZ INCO-CT-2003-003355 [2004-2007]
(project coordinator: Professor K. Małysa)

The main objective of the “SURUZ” project was to build a network of scientific institutions in Poland involved in research on surfactant and dispersed systems. The network brings together 24 research groups from 14 various scientific institutions (universities, research institutes) in Poland. The project was coordinated by the Institute of Catalysis and Surface Chemistry Polish Academy of Sciences (Coordinator- K.Małysa) and have got a special website www.cyf-kr.edu.pl/~ncmalysa/ on server ICSC PAS.

During the third, last year of the project realization the research teams of the network continued realization of their tasks and activities via mutual contacts and collaboration, via human mobility, via participations in network conferences, meetings and workshops for young scientists. Within the reporting period 110 scientists visited, got familiar with Labs and equipment available in institutions of the SURUZ Network Partners and carried out some experiments. Thanks to networking activities there was 6 lectures presented by visiting scientists on seminars in partner institutions. Total number of employees and PhD Students visits in the partners labs., attending workshops, conferences and cluster meetings organized and/or co-organized by SURUZ Network was ca. 394.

Two major scientific conferences were organized with financial support of the project. Large scale (117 participants) network “SURUZ” conference was organized in Książ on May 22-24, 2007, where 35 lectures and 80 posters were presented. The second major conference: “XI International Conference of Mineral Processing”.coupled with “XLIII Symposium on Physicochemical Problems of Mineral Processing” (68 participants) was held in Zakopane, September 18-21, 2006. Moreover, the Microsympozjum SURUZ coupled with V Kongres Technologii Chem., was organized in Poznań, September 11-15, 2006 and the II Ogólnopolska Konferencja Gospodarka Osadami „OSAD 2006” (150 participants) was organized in Gdańsk, September 25-28, 2006.

Five workshops and meetings for young scientists were organized during the third reporting period. „Pro-ecological aspects of surfactant research” was organized in Sarbinowo, September 20-22, 2006, (attendance 11), “Electrokinetic Phenomena in Dispersed Systems” was organized in Lublin, January 24-25, 2007 (attendance 21). SURUZ Workshop on “*Surfactants and Dispersed System*” coupled with COST D43 Meeting: ”*Functional Interfaces – Theory and Experiment*” was organized in Cracow by Institute of Catalysis and Surface Chemistry PAS , March 19 - 21, 2007 by ICSC (attendance 59) *and* SURUZ Workshop Wetting and Surface Modification” was organized in Sudomie, June 15-21, 2007 (attendance 34).

Several new research topics were proposed and some common studies have been carried out within the frame of the SURUZ Network. These common studies already resulted in 22 common papers. Majority of theses papers have been already published or accepted for publication in international journals of wide circulation. Moreover there was many common presentation at various international conferences. There are also a few papers being in preparation. Especially encouraging and promising for the future are close contacts, discussions and interactions between young scientists and Ph.D. students.

Transfer of Knowledge in Design of Porous Catalysts

EU ToK Project TOK-CATA MTKDCT-2004-509832 [2004-2008]
(project coorditator: Professor E. Serwicka-Bahranowska)

TOK-CATA is a Transfer of Knowledge project, in which Institute of Catalysis and Surface Chemistry PAS is the host institution, responsible for the coordination of research and management. The project is implemented in collaboration with partner institutions (University of Nottingham, Consejo Superior de Investigaciones Cientificas, Stuttgart Universität, Humboldt Universität, Lunds Universitet.). The scientific program is carried out in the laboratories of ICSC by incoming foreign specialists and by selected staff members of ICSC in the laboratories of partner institutions. The outgoing fellows implement the newly acquired expertise during the reintegration periods, of duration equal to the time spent abroad. The principal overall objective of the project is the design and synthesis of porous catalysts with properties tuned to the requirement of a given catalytic reaction.

The research has been divided into three general scientific tasks:

- design, synthesis and optimisation of porous materials based on zeolites, modified layered silicates and ordered mesoporous structures
- control of the catalyst texture, grain morphology and insertion of active sites, targeted at application in processes of fine chemicals synthesis and abatement of air pollutants
- creation of a progressive connection between theoretical simulation modelling of porous structures and catalyst design.

The selected topics of research include:

- Mesoporous silicas with controlled morphology
- Porous clay heterostructures
- Zeolite membranes and membrane microreactors
- Nanoporous carbons for application as sustainable energy materials.
- Implementation of advanced NMR methodology for investigation of zeolitic structures
- Catalytic alkylation and isomerization
- Selective hydrogenation of unsaturated hydrocarbons.
- Applications of combined Quantum Chemical – Force Fidel (QM/MM) methods (DFT/AMBER) to transition metal sites in enzymes.
- Theoretical modelling of SiO_2 surfaces

The scientific results of the project were disseminated through publications in scientific journals and conference presentations. 5 papers have been published in 2007 as a result of TOK-CATA activities,1 is in press. 13 conference presentations included one invited lecture, 4 oral communications and 8 posters. The highlights of the reporting period were following:

- the porous graphitic carbon with enhanced (and reversible) hydrogen storage capacity was obtained by CVD deposition using zeolite β as template
- it was demonstrated that the PCH solids can be efficiently aluminated by means of post synthesis alumination, and become excellent hosts for cationic organometallic complexes.
- structured silicalite-I/ZSM-5 composites were obtained, in which large crystals of ZSM-5 were successfully coated with thin silicalite-I films by using a self-assembly method. The ZSM-5 crystals were coated with small silicalite-I crystals aligned with their (0 1 0) faces parallel to the faces of large ZSM-5 crystals.

Annual Polish Conferences Are Setting Up a New Platform for Dissemination of Knowledge in the Field of Catalysis

EU SSA Project POL-CAT NMP3-CT-2004-510318 [2004-2007]
(project coordinator: Professor B. Sulikowski)

A 3-year project POL-CAT was carried out at the Institute of Catalysis and Surface Chemistry, in the period of 1 March, 2004 until 28 February, 2007. Three conferences on catalysis have been organised in 2004, 2005, and 2006, respectively.

The 36th Annual Polish Conference on Catalysis was held at the Institute of Catalysis and Surface Chemistry (Kraków, Poland) on 17-19 March, 2004. The 36th conference hosted 186 scientists, and the program obeyed:

- 5 plenary lectures
- 20 oral communications
- 2 poster sessions (186 posters).

The *Book of Abstracts* comprising 350 pages (A-4 format) was published before the event.

The 37th Annual Polish Conference on Catalysis was held at the Institute of Catalysis and Surface Chemistry (Kraków, Poland) on 15-18 March, 2005. The program obeyed:

- 8 plenary lectures
- 1 Key-note Lecture
- 23 oral communications
- 2 poster sessions (194 posters)
- moreover, the EU officer responsible for the project, Mr. Soren Bowadt, has delivered a special lecture ”Opportunities for Research within the NMP priority of FP6”.

All the contributions presented at the meeting were printed in *The Book of Abstracts* (394 pages).

The 38th Annual Polish Conference on Catalysis was held at the Institute of Catalysis and Surface Chemistry (Kraków, Poland) on 15-18 March, 2006, and gathered 241 registered scientists. The program consisted of:

- 4 plenary lectures of foreign speakers
- 6 plenary lectures of Polish speakers
- 7 invited lectures
- 8 flash oral presentations
- 2 poster sessions (205 posters).

All the contributions presented at the meeting were printed as ***The Book of Abstracts*** (406 pages).

In 2005, a special issue of *Catalysis Today “Oxide-Based Materials in Catalysis”*, vol. 101, (2), pp. 51 – 184, 30 March, 2005, (ISSN 0920-5861), was published.

Guest Editor: B. Sulikowski.

In 2006, a special issue of ***Catalysis Today “Nano-Structured Materials for Catalysis”,*** vol. 114, (2-3), pp. 125-332, 15 May 2006, (ISSN 0920-5861), was published. *Guest Editor:* B. Sulikowski.

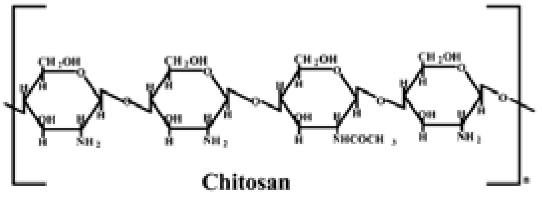
Nanocapsules for Targeted Controlled Delivery of Chemical
Optimization of Microcapsule Shells

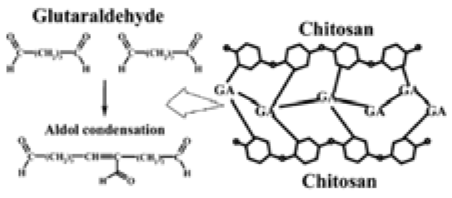
UE STREP Research Project NANOCAPS NMP4-CT-2003-001428
[2004-2007]
(project leader: Assoc. Professor P. Warszyński)

The main aim of the “NANOCAPS” project was to develop new technologies based on micro-encapsulation to solve industrial problems related to controlled release of chemicals. The technical objectives are to develop nano-materials and nano-composite coatings for cost-efficient production of nano-capsules and to validate the technical and economical feasibility of the knowledge acquired in the fields of biomedical (anti-proliferating and anti-allergic agents) and metal plating (self-healing) applications.

The PEI polycation was used so far as a first layer for polyelectrolyte multilayer film construction. However, properties of films having PEI as polycation were not investigated. The ellipsometric thickness of $(PEI/PSS)_n$ films was measured and the non-monotonic growth of PE multilayer film containing PEI/PSS was observed suggesting partial removal of polyelectrolyte upon adsorption of consecutive layer of PEI, however, very regular changes of wettability seemed to contradict that hypothesis. Similar (yet unexplained) behavior was observed, when the polyelectrolyte film was constructed with weak polyelectrolyte pair PAH/PAA in the conditions when the polyelectrolytes were weakly charged. Layers 1-4 were deposited at pH = 7, from 5th layer: PAH at pH=11 PAA at pH=3 (weakly charged PE) or PAH at pH=3 PAA at pH=11 (fully charged PE). Further investigation of adsorption process, preferably with QCM, are necessary to resolve this problem.

It was shown previously by streaming potential measurements, deposition experiments and capsule stability that uppermost layer of chitosan in the chitosan/alginate shells were unstable. Therefore, to resolve the problem of instability of chitosan shells we decided to make an attempt of chemical modification of chitosan to improve that stability. The chitosan/alginate films were prepared by normal LbL technique. Such prepared multilayers were cross-linked using glutaraldehyde.





The results of electrokinetic experiments indicated that layers of crosslinked chitosan were more stable for the prolonged washing (in pH 4). However, the decrease of absolute value of zeta potential (up to 75% of value of zeta potential for untreated chitosan) was observed due to loss of charged groups in the crosslinking process. We also measured ellipsometric thickness of CHIT/ALG polyelectrolytes mulitayers before and after they were cross-linked with various addition of crosslinking agent. We found that the crosslinking seems not to influence considerably thickness of chitosan/alginate films.

To test the adhesion properties of Allergoff Bio capsules (with bimodal distribution) at biomimetic surface, they were deposited at the chitosan modified silica surface (positively charged). The diffusion driven deposition of capsules from the 10x diluted stock suspension was observed for 1 hour and c.a. full coverage was obtained. It was observed that c.a. 10% of the surface was covered by microcapsules (d = 2µm). The rest of the surface is covered by nanocapsules (d = 50 nm), which is therefore blocked for the further deposition of microcapsules.

Global Climate Change Impact on Built Heritage and Cultural Landscapes

EU STREP Research Project NOAH’S ARK SSP1-CT-2003-501837
[2004-2008]
(project leader: Assoc. Professor R. Kozłowski)

The aim of the project has been establishing meteorological parameters and variations which will affect in a critical way the material heritage environment in the coming 100 years, as well as development and dissemination of strategies mitigating the resulting threats. These strategies will be used by broadly defined community of heritage administrators and curators. The activities of the research team of the institute has focused on development of risk indices for historic materials sensitive to moisture and temperature, like wood or clay containing sandstones, which would describe relative potential of a climate to promote the material decay.

The tasks implemented during the reporting period covering the last five months of the project aimed at dissemination of the project’s results among representatives of the administrative authorities and conservation communities responsible for the protection of museum collections and historic buildings in Europe. The tasks encompassed:

- final edition and publication of atlas containing maps of changes in climatic parameters relevant for the protection of historic materials and objects, maps of risks to these materials induced by climate change, description of threats resulting form the intensification of extreme climatic events like intense rainfalls, flooding or landslide;
- final edition and publication of Guidelines containing adaptation strategies to risks induced by the climate change, addressed to cultural heritage managers in Europe - owners and curators of historic buildings and collections, conservation and administrative authorities and policy-makers;
- co-organising a two-day international workshop in London on January 18-19, 2007 ‘Climate change vulnerability: Maps and guidance for cultural heritage protection, 18-19 January. The workshop attracted the attention of 70 specialists from 16 countries;
- co-organising an international workshop in Rome on May 30, 2007 ‘Climate change and protection of cultural heritage in Europe: research, evidence and policy’. 70 specialists and politicians participated. A panel discussion with the participation of 2 Members of the European Parliament and the representatives of the European Commission constituted a part of the workshop.

ERA-NET for Applied Catalysis in Europe

EU ERA-NET Project ACENET ERAC-011784
[2004-2008]
(project leader: Professor E. Serwicka-Bahranowska)

The ACENET (Applied Catalysis European NETwork) ERA-NET network started in 2004 within 6th EU Framework Programme for Research and Technical Development and unites twelve research management and funding organisations from ten EU Member States: Netherlands Organisation for Scientific Research, the Netharlands; Bundesministerium für Bildung und Forschung, Germany; Centre National de la Recherche Scientifique, France; Fundação para a Ciência e a Tecnologia, Portugal; Ministero dell'Istruzione della Università e della Ricerca and Consorzio Reattivita e Catalisi, Italy; General Secretariat for Research & Technology, Ministry of Development, Greece; Ministerio de Educación y Tecnologa, Spain; Forschungszentrum Jülich GmbH, Germany; Engineering and Physical Sciences Research Council, UK, Ministerstwo Nauki i Szkolnictwa Wyższego, Polska, Instytut Katalizy i Fizykochemii Powierzchni PAN, Polska and The Irish Research Council for Science, Engineering and Technology, Irland. The aim of this ERA NET is to achieve coherence and cooperation between national research programmes and policies on applied catalysis.

In Spring 2007 ACENET has launched Europe's first jointly coordinated, transnational call for project proposals in Applied Catalysis, entitled:

"Innovative, Sustainable Catalytic Processes with Improved Energy and Carbon Efficiency". The theme of the call focuses on the scientific and technical basis for innovative processes with reduced intensity in both energy and fossil carbon, important requirements for tomorrow's sustainable economy. It is thus closely aligned with the aims of the strategic research agenda developed by SusChem, the European Technology Platform for Sustainable Chemistry. This call is aimed at stimulating European public–private collaborate research in the field of Applied Catalysis and will encourage national organisations to work together in key areas of science and technology, thus enabling ambitious transnational projects to be developed whilst still retaining sensitivity to national programme policies and constraints. It also aims to create partnerships between researchers with the complementary expertises essential for success in Applied Catalysis research.

All researchers in Applied Catalysis based in France, Germany, Greece, Ireland, Poland, Portugal, Spain and The Netherlands, who are eligible to apply for funding to the ministries and funding agencies in their countries were eligible to apply for ACENET research grants.

Moreover, within ACENET a uniform European Joint Education and Training Programme has been developed addressing strategic needs in the area of applied catalysis.

These needs comprise boosting the standards of professionals, improving the fit between employer demand and job market supply, and enhancing student, researcher and job market mobility. The Programme is divided into four modules: Integrated Course on Catalysis, Excellence Training in Applied Catalysis, School on Catalysis Continuous Professional Development. In the Spring time of 2007 three educational pilot events were organized under auspices of ACENET: Integrated Course in Kraków in Poland, The Industrial Catalytic Processes course in Bath in The United Kingdom and School on Catalysis in Bari in Italy.

Integrated Design of Catalytic Materials for a Sustainable Production

UE NoE Project IDECAT NMP2-011730-2 [2005-2008]
(project leader: Professor M. Witko)

IDECAT is a Network of Excellence launched in 2005 within 6th EU FP. The Network is coordinated by the Consorzio Interuniversitario per la Scienza e Tecnologia dei Materiali, Italy and integrates 37 laboratories from 17 institutions: Consorzio Interuniversitario per la Scienza e Tecnologia dei Materiali, Italy; Ghent University, Belgium; Katholieke University Leuven, Belgium; J. Heyrovsky Institute of Physical Chemistry, Czech Republic; Helsinki University of Technology, Finland; Centre Nationale de la Recherche Scientifique, France; Max-Planck-Gesellschaft, Germany; Leibnitz Institute of Organic Catalysis, Germany; Technische University Munchen, Germany; Consiglio Nazionale delle Ricerche, Italy; NRSC-Catalysis, Tha Netherlands; Instytut Katalizy i Fizykochemii Powierzchni, Poland; Consejo Superior de Investigaciones Cientificas, Spain; Stockholm University, Sweden; University St. Andrews, The United Kingdom; University of Southampton, The United Kingdom; Ecole Polytechnique Federale de Lausanne, Switzerland.

The aim of the IDECAT NoE is to achieve a lasting integration between the main European Institutions in the area of heterogeneous, homogeneous and bio-catalysis via creating a coherent framework of research, know-how, training, promotion of science, spreading of excellence and technology transfer between those various catalysis communities.

The Network is divided into 5 joint programmes (Integration, Research, Spreading Excellence, Science and Technology Transfer, and Management) and 13 Workpackages.

Joint Programme of Integration is aimed to achieve long-term integration within European Research Institute of Catalysis (ERIC) to be established as a legal entity under the Law of Belgium in the form of a non profit association - A.I.S.B.L (Association International Sans Bout Lucratif). ERIC will gather leading European institutions in the field of catalysis, such as but without limitation universities, research institutes, SMEs and industrial companies. Main activities in 2007 were concentrated on creating legal documents necessary to start the process of the formal incorporation of ERIC, i.e. Statute, Internal Regulations and Framework Agreement. Moreover, electronic tools to facilitate the gathering of information and allow better communication between the integrated groups were improved. Within JPI also encouragement activities to increase women participation in research were continued.

The Joint Programme of Research focuses on four research tasks: 1) creating and mastering nano-objects and nano-organisation, 2) creating and designing new multifunctional and nano-structured materials, 3) bridging the gap in multi-disciplinary approaches, 4) eco-processes and sustainable energy and production. Activities within these tasks have been continued by the ICSC research groups in the frames of collaborations started within the project.

In the frames of The Joint Programme of Spreading Excellence ICSC was actively involved in the Festival of Science and The Open Door of the Institute was organised. Moreover, the Institute’s research staff actively participated in the workshops and conferences organized within the Network as well as in the Integrated Course on Applied Catalysis organized in the ICSC in March 2007.

The objective of the Joint Programme of Science and Technology Transfer is to transfer to the industrial sectors and in general terms to Society of the scientific results and breakthrough arising from the network. To achieve this aim the Industrial Liaison Office was established. The ILO organized two IDECAT Industrial Board meeting whose outcome was the preparation of two large Collaborative Projects to be submitted in the FP7 Calls. ICSC was actively participating in the vast majority of the Network activities and tasks.

Sensor System for Detection of Harmful Environments for Pipe Organ

EC 6th FP SSP-4 SSPI-CT-2004-022695 SENSORGAN (STREP) [2006-2008]
(project leader: Ł. Bratasz PhD)

Last year was the second of three years planned for the implementation of the project which aims at a development of the sensor system for detection of harmful environment for pipe organs. The main research tasks of the institute in the project are divided into three packages from which first two were started already in 2006.

The first task has been focused on the development of a simple and economic acoustic emission sensor (AE) which would allow monitoring fracturing in wooden parts of pipe organs and other wooden works of art. The investigations, which started in the last year, were focused on the adaptation of the AE method to the specific requirements of the cultural heritage field and particularly to pipe organs. They have resulted in identifying a group of critical parameters, which would allow detecting and tracing fracturing development in wooden objects independently of the environmental noise in their vicinity. The parameters encompass characteristic frequency and AE event and the environmental noise, energy of the event and correlation between events in characteristic band and below it. Their determination made it possible to build an AE sensor prototype which possessed features necessary for its commercialization. Efforts of the research team concentrated on a maximal simplification of the electronic circuits and maintenance. A particular stress was laid on such configuration of the communication which would enable a maximally broad application of the EA sensor both in museums and in the field work also by personnel without full research qualifications. The activities have led to signing a license agreement between the Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences and Hanwell Instruments Ltd from the UK which is one of the world leaders in the production of equipment for monitoring preservation conditions for of works of art.

In the second package, the institute is responsible for measurement and analysis of the microclimatic situation in the reference object – the historic church in Olkusz, Poland. The measurements are carried out continuously, and were combined with a simultaneous recording of AE events, which allowed identifying very precisely the microclimatic fluctuations causing episodes of fracturing in wooden parts of historic organs preserved in the church.

Multifunctional Particulate System for Nanomedicine

NANOMEDPART [2007-2010] in frameworks of ERA-NET MATERA project
(project leader: Assoc. Professor P. Warszyński)

The objective of the project is to develop effective methods for preparation of nanoparticles/nanocapsules and modification of their surfaces for targeted drug delivery (anticancereous, antimicrobial). Various methodologies of capsule core and shell formation and surface modification will be investigated and optimised for selected applications.

The main scientific and technical challenges of the project are the formation of stable particles and capsules in the nanosized range (preferably 20-50 nm) containing active compounds with shells tailored for cancer therapy and antimicrobial applications. For the formation of functionalised shells various adsorption or polymerisation techniques will be used, combined with surface modification. The project is realized by the consortium consisting of: Institute of Catalysis and Surface Chemistry PAS, SINTEF Materials and Chemistry Oslo, Hebrew University Jerusalem, Institute for Cancer Research at the Norwegian Radium Hospital Oslo and Chemistry Dept. of Wrocław University of Technology.

In 2007 we concentrated on preparation of various size, dye containing capsules by microemulsification. The dye containing capsules will be used in the later phase of the project as marker particles to asses penetration of cellular membranes by nanoparticles. Microemulsions, which contained as oil soluble fluorescent dye (Cumarine -green) in decane or octane, stabilized by Tween80 and butanol as co-surfactant were preapared. Emulsions were obtained with average droplets size 10nm. For water soluble dye rhodamine B, stable microemulsion of water in oil (toluen, decan, octan, cycloheksan) were prepared, stabilized by AOT. The average droplets size was 4nm. The example of size distribution of droplets of emulsions are illustrated in Figure 1

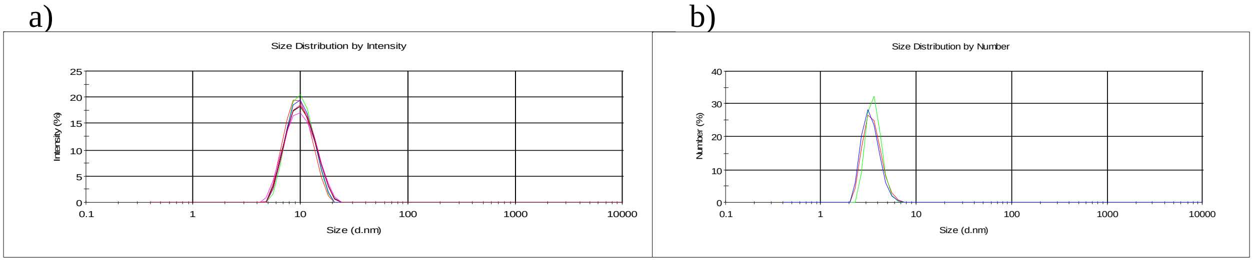


Fig 1. Size distribution of droplets of emulsions a) cycloheksan/T80/water, b) water/AOT/octan

Since silver nanoparticles have proven antibacterial and antifungal properties, in this phase of the project we concentrated on the development of various procedures of preparation of these nanoparticles by reduction of silver ions. Complex of silver ions with ammonia were reducted by hydrazine, ascorbic acid or formaldehyde. The example of size distribution of silver nanoparticles are ilustrated in Figure 2. Bimodal distribution 4nm with small fraction of 50nm was obtained, when nanoparticles were prepared by reduction with formaldehyde.

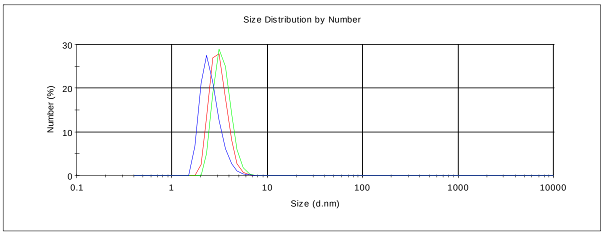


Fig 2. Size distribution of silver nanoparticles obtained by reduction of silver ions with formaldehyde.

EU COST ACTIONS PROJECTS

Colloid and Interface Chemistry for Nanotechnology

EU COST Action D43 research project [2006-2011]
(Polish representative: Professor Z. Adamczyk)

Deposition (irreversible adsorption) of colloid and bioparticles on solid/liquid interfaces is of major significance for predicting the efficiency and kinetics of many processes such as self assembly, filtration, separation by affinity chromatography, immobilization at interfaces, removal of pathological cells, immunological assays, biofouling of transplants and artificial organs, etc. From a practical point of view, especially interesting seems the problem of particle deposition at patterned surfaces, bearing surface features of regular shapes. The growing interest in such surface architecture stems from their practical significance as antireflecting and self cleaning surfaces, biosensors (protein arrays) optical filters, masks, photonic crystals, microfluidic and microelectronic devices. This concerns for example the problem of particle deposition on stripes pertinent to microcirciutry. Despite a considerable significance for basic science and practice, the problem of particle deposition at surface features of various shape, e.g., stripes, has not been systematically studied theoretically or experimentally. Therefore, the main goal of this research project is to develop efficient methods of a quantitative, theoretical and experimental analysis of these phenomena with the emphasis focused on the jamming limit and the structure of various particle monolayers. The first stage of these works was preparing a critical review on the particle deposition at heterogeneous surfaces. In the first section various theoretical models, based on the random sequential adsorption (RSA) approach were discussed, whose range of validity was assessed using existing analytical solutions. Three main particle deposition regimes were distinguished: (i) the quasi continuous surface regime, (ii) the random site surface (RSS) regime and (iii) the patterned surface regime. Theoretical results pertinent to the RSS and the patterned surface regime were presented, in particular the topology of particle monolayers, the jamming (maximum) coverage, the averaged number of particles adsorbed and particle distribution density over various surface patterns. Special attention was focused on rectangular surface features (stripes). These theoretical predictions were see for interpretation of experimental results obtained mostly for monodisperse latex particles adsorbing on random site surfaces created by controlled colloid particle or polyelectrolyte adsorption. The structure of monolayers in terms of pair correlation function was analysed, as well as adsorption probability as a function of site coverage and the jamming coverage limit for various particle to site size ratio. Finally, recent results were discussed, obtained for surface features of regular shape like circles and rectangles. It was shown that these experimental data confirmed the validity of the RSA model for describing particle deposition at heterogeneous and patterned surfaces. It was also concluded that theoretical and experimental results obtained for model colloid systems can be effectively used as useful reference states for analyzing protein and macromolecule adsorption at heterogeneous surfaces.

Wood Science for Conservation of Cultural Heritage

EU COST Action IE0601 research project [2006-2011]
(Polish representative: Assoc. Professor R. Kozłowski)

The action started on April 18, 2007. Its planned duration is four years. By November 2007 the number of countries who have signed the Memorandum of Understanding was 24. Three working groups have been activated within the Action: WG1 – Wood properties, WG2 – Assessment and diagnosis, and WG3 – Conservation and restoration. Dr Roman Kozlowski of the Institute, representing Poland in the Action's Management Committee, has been elected to the eight-person Steering Committee and to the position of a leader of WG2. He participated in all three Management or Steering Committee meetings organized in 2007 as well as represented Action at the 5th Meeting of the COST Domain Committee Materials, Physics and Nanosciences.

The action organised in 2007 two workshop meetings in Tervuren (Belgium) and in Florence. During the meetings, members of staff of the institute presented altogether 3 oral presentations and 2 posters.

Physics of Droplets

UE COST Action P21 research project [2006-2010]
(Polish representative: Professor K. Małysa)

The aim of the project COST P21 “Physics of droplets” is a deeper understanding and description of the processes related to the motion and interactions of droplets and bubbles with various interfaces, as well as an importance of thin fluid layers for these processes. The COST project duration is 4 years and its official starting date was July 27, 2006. Professor N.Vandewalle, GRASP, Institut de Physique, Université de Liège, Belgium is the project coordinator. In 2007 the Ian Wark Research Institute of University of South Australia joined the project and currently there are 27 research teams from various scientific institutions of 16 European countries (+ Australia).

From Poland, besides Institute of Catalysis and Surface Chemistry Polish Academy of Sciences (ICSC PAS), there are also involved research teams from Institute of Fundamental Technological Research Polish Academy of Sciences (IFTR PAS) and the Warsaw University of Technology, Department of Chemical and Process Engineering (WUT-CPE). Professor K. Malysa from ICSC PAS is the polish representative in the Management Committee. In 2007 there were held two official meetings of the Management Committee (MC) and K. Malysa attended the both meetings. The Third MC Meeting (two meetings were in 2006) was held in Granada, Spain on March 28, 2007 and the Fourth Meeting took place in Marne-la-vallée, France on November 13, 2007. The both meetings were dedicated to analysis of the project performance and the funds available for different activities, especially for Short Technical Scientific Missions (STSM) and the working groups (WG) meetings. During the Marne-la-Vallée Meeting it was decided that a summer school (3 days) will be organized in Capri, Italy in May 2008. The topics of the school will be focused on physicochemistry of droplets and the school will be coupled with joint meeting of the Working Groups (1 day) and the Managment Committee Meeting (1 day). Professor S. Guido of University of Napoli is going to organize the event.

The research teams taking part in the COST P21 project are divided in three Working Groups (WG); WG1: “Formation, transport and manipulation of a droplet”, WG2: “Coating and protecting droplets”, WG3: “Applications and devices”. The scientists and PhD Students of the ICSC PAS are taing part mainly in activities of the WG2. In 2007 there were two workshops of the WG2 – in Granada, March 29, 2007 and in Liege, June 12, 2007. The workshops were by scientists from ICSC PAS and the following oral presentation were delivered: i) in Granada - J. Zawala, M. Krasowska, K.Malysa, “Influence of the bubble kinetic energy on rupture of liquid films at liquid/gas and liquid/solid interfaces”, and ii) in Liege - J. Zawala, K. Malysa “Does and how the collision angle can affects kinetics of TPC formation?”.

Within the frame of the COST P21 project M.Sc. Jan Zawala from ICSC PAS applied and obtained financing – STSM grant – for 3 weeks research stay in Max Planck Institut fur Kolloid- und Grenzflachenforschung (dr R. Miller group), Golm/Potsdam, Germany. During the visit he carried out the measurements of dynamic surface tensions of n-octyl-trimethylammonium (OTAB) and n-dodecyltrimethylammonium (DDTAB) bromides solutions, using the Maximum Bubble Pressure Tensiometry (MBP) and Pendant Drop Technique (PDT). He determined the dynamic and equilibrium surface tension values for the following ranges of concentrations: $5*10^{-4}$ - $1*10^{-1}$ M (OTAB) and $1*10^{-5}$ - $2*10^{-2}$ M (DDTAB). The Frumkin isotherm was fitted to the experiomental data and the diffusion coefficient for the DDTAB was calculated on the basis of the numerical solution of the Ward-Tordai equation.

EEA FINANCIAL MECHANISM PROJECTS

Effective Photocatalytic-Membrane Methods of Removal of Organic Contaminants for Water Treatment

EEA PL0084 NOMRemove [2007-2010]
(project leader: Assoc. Professor P. Warszyński)

The aim of the project is the elaboration of the new, highly effective method of the removal of natural organic matter (NOM) from potable water. Although by themselves the substances composing NOM are not dangerous contaminants of drinking water, they favor the growth of bacteria, creating substantial problems in the water supply systems. NOM, especially those parts of them that appear in the form of real solutions, are very difficult to be removed from water and the compounds being NOM products after chlorination of water are toxic. The main objective of the project is to develop technology of the simultaneous application of the four methods of water purification: nanofiltration, photocatalytic oxidation on the surface of a semiconductor, sterilization by UV radiation and chemical oxidation by the substances released from the nanocapsules. Project is realized by the consortium formed by two partners: Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences and The Foundation for Scientific and Industrial Research at the Norwegian Institute of Technology, SINTEF - Material Science and Chemistry, Oslo, Norway. The works conducted in the Institute of Catalysis during this year concerned the construction of the equipment for the illumination of solutions and suspensions by visible light and by UV radiation. Apparatus for the illumination of the solutions and suspension by the visible light has been constructed and tested (one for the illumination by the UV radiation is under construction). The activity of the TiO_2 photocatalyst (Degusa P25 and P90) in the process of two model organic substances (Rhodamine B and commercial humic acid) decomposition on its surface under the illumination by visible light was investigated. In the case of Rhodamine B significant degree of decomposition under the influence of visible light was observed (see figure). In the case of humic acid photocatalitic activity achieved by visible light illumination appeared insufficient. The works on the preparation of new catalysts based on TiO_2 doped with silver nanoparticles were also conducted.

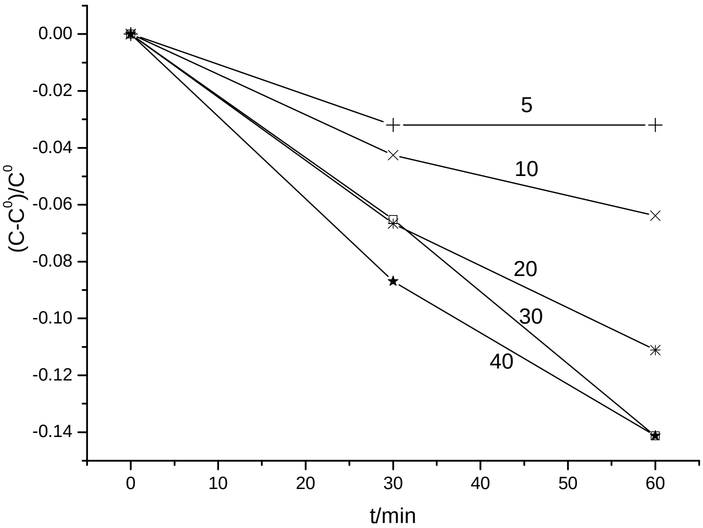


Figure 1. Rate of Rhodamine B decomposition in the suspension of TiO_2 (Degusa P25) illuminated by visible light for different concentrations of TiO_2 in suspension. Initial concentration of Rhodamine B: $1x10^{-5}$ mol dm^{-3}. Numbers at the lines denote the concentration of TiO_2 in suspension in mg dm^{-3}.

Establishing Standards for Allowable Microclimatic Variations for Polychrome Wood

EEA PL0086 [2007-2010]
(project leader: Assoc. Professor R. Kozłowski)

Panel paintings, polychrome wooden sculpture and paintings decorating wooden architectural surfaces are an important part of the artistic heritage. The protection of this heritage is particularly important for Poland and Norway in which a group of polychrome wooden churches, unique on a world scale, has been preserved. The most valuable of them are inscribed on the UNESCO World Heritage List.

Uncontrolled variations of the air parameters in the environment of polychrome surfaces, leading to deformation and mechanical damage of wood, gesso and paint layer, are principal hazards to their preservation. The most severe disturbance of the climate results from introducing heating systems inappropriate for the historic interiors. The main aim of the project is establishing precisely and quantitatively the variations of air parameters that are safe for the painted wooden surfaces. The main research tool is direct monitoring of the climate-induced delamination of the decorative layers from the wooden support and their mechanical damage using optical methods, acoustic emission and computer modelling.

During first several months of the project duration all equipment was built or installed and made operational. An Electron Speckle Pattern Interferometer was built and calibrated for the measurements using wooden panels coated with gesso layers, in which an isolating layer of cyclododecan was laid on parts of a panel to weaken the adhesion of the gesso to the wood. Sound-induced vibration of the surface has been successfully used to make the delaminated areas visible in the interferograms. FLIR ThermoVision A40 Series Infrared Camera has been tested as an additional method, especially suitable for the work in real-world conditions of museums or historic buildings. The surface was heated slightly for a period of time of around 10 s and the temperature distribution on the surface and various cooling rates characteristic of sound or delaminated areas were followed with the camera.

Panel deformation caused by RH changes was analysed. One surface and all edges of panel of varying thickness were covered with a silicone sealant to enforce a completely asymmetrical diffusion of the water vapour from the panel and thus to produce the most pronounced deformation. In a series of tests, the relative humidity was rapidly reduced by a varying magnitude and scanning of the curvature of the panel surface was performed using a laser scanner. The measurement was repeated every 5 minutes. As a result, information on the dynamic response of wooden panels of varying thickness with asymmetric water vapour diffusion was obtained. The information gained will support the computer simulation and the main testing programme in which dimensional changes of painted wood induced by various repetitive fluctuations in RH will be mechanically simulated by compressing and stretching, or bending, the specimens imitating the paintings.

PROJECTS OF SECTORIAL OPERATIONAL PROGRAMMES OF EU STRUCTURAL FUNDS

Implementation of the Roman Cement Technology into the Practical Conservation of Historic Buildings

SPO WKP_1/1.4.1/1/2005/8/8/222/2005/U TECHKON [2005-2009]
(project leader: G. Adamski PhD)

The aim of the project is to introduce novel materials into the conservation practice which would possess characteristics of Roman cements originally used during the nineteenth and early twentieth centuries for the economic and easy manufacture of stuccoes for the exterior of buildings. This will make possible a proper conservation of the vast urban built heritage of the period. The technology of manufacturing these materials was re-established within the ROCEM project supported by the European Commission 5th Framework Programme. The present project is implemented by a consortium of the conservation enterprise AC Konserwacja Zabytków Piotrowski, Kosakowski Spółka Jawna and the institute.

The pore structure is one of the main properties of mortars, influencing greatly their permeability to water and water vapour, and strength. Similarity of the pore structures of the historic and repair mortars is a vital criterion of their compatibility i.e. ability to interact without inducing any decay. Pore structures of historic Roman cement mortars collected from buildings across Europe and for repair mortars formulated from the Roman cements presently available were compared within this project. The pore structure was determined with the use of mercury porosimetry. Three categories of pores were found to coexist in the historic mortars: fine pores with the diameter below 0.2 μm, characteristic of fully hydrated Roman cement pastes, larger ‘air-pores’ with the diameters between 0.2 – 5 μm due to the evaporation of water during the hydration process, and large pores of the diameter exceeding 5 μm due to a secondary mortar weathering. The volume of air-pores was found to depend on the water-to-cement ratio (w/c) used originally and their formation was enhanced at the surface of the stucco elements exposed to the external environment favouring drying. To reproduce historic mortars, repair mortars were produced at the w/c ratio varying from 0.6 to 1.0. The mortars were cured under 100% relative humidity and the samples were collected after hydration time varying between 1 day and 3 months. In the repair mortars, a unimodal distribution of pore sizes was observed for low w/c ratios with the pore width decreasing with increasing hydration time. With an increase in the w/c ratio, a development of a bimodal pore structure was noticed. The formation of larger pores is the result of the evaporation of water unbound during the hydration. In this way, repair mortars with controlled pore structure could be easily obtained by changing the w/c ratio during the preparation process.

The investigations of the durability of the repair mortars using salt crystallization and freeze-thaw cycles indicated that it increases with an increase of the hydration time and with a decrease of the w/c ratio. The strength of adhesion between repair mortar and historic substrate also increases with an increase of the hydration time. The highest values of strength of adhesion were obtained for completely wet substrate, while very weak strength of adhesion was observed for a dry one.

Centre for Environmental Pollution Analyses

SPO WKP_1/1.4.2/2/2005/9/90/294/2006/U CeZaŚ (CEPA) [2006-2009]
(project leader: J. Janas MSc)

In the course of second year of CEPA project accomplishment a new deliveries of analytical instruments and accessories were realized propitiously.
The supply list comprises:

- stationary GC/MS Polaris-DSQ chromatograph with the DANI thermodesorber,
- mobile FT-IR multichannel analyzer GASMET DX-4000,
- laboratory FT-IR Nicolet spectrometer with gas and liquid phases analysis countershafts,
- fluorescence EDXRF spectrometer Epsilon 5,
- stationary LC/MS (UV) Shimadzu chromatograph,
- mobile laboratory for environmental analyses based on Fiat Doblo and specially adapted for the CEPA Laboratory purposes,
- necessary equipments and stock for analytical laboratory (furniture, UPS devices, glassware, chemicals and EPA standards).

In the reported period promotional and advertising activity were realized by advertising campaign in biweekly magazine "Środowisko" ("Environment") three times in row, preparation of internet page presenting CEPA Laboratory, printing advertising leaflets, visit cards and firm's ball pens with CEPA Laboratory overprint.

In the reported period the CEPA Laboratory activity was realized by realization of the 6 outer and 7 inner orders. The first group of orders comprised of VOC emission measurements in the industry, measurements of organic and inorganic (eg. NO_x, CO) substances in the industrial waste gases, measurements of the micro concentration of cancerogenic and/or highly dangerous substances emitted in some branches of industry (epichlorohydrine, fluoric acid). The another type of measurements was based on determination of the different types of RCO reactors efficiency.

Into the second group of orders we can put the investigations of the catalytic activity of materials synthesized in our Institute, IR measurements of these catalysts and activity testing of the monolithic catalyst for the NO SCR with ammonia.

Apart from analytic and/or scientific activity in CEPA Laboratory a set of office and administrative work was done. They comprised of preparation of technical specification support to put the purchase of analytical devices for open tender, work out planes of car adaptation for the Mobile Laboratory purposes, and elaboration of the documentation necessary for the QMS system implementation in the CEPA laboratory. The latter consist of Standard Operating Procedures elaboration, including general procedures and method procedures along with LOG operation manuals preparation for every analytical devices.

Last year the CEPA Laboratory was registered as the full member of POLLAB organization (a member of EUROLAB – European Federation of National Associations of Measurement, Testing and Analytical Laboratories).

Conservation Heating Systems for Historic Churches

SPO WKP_1/1.4.1/1/2006/93/93/648/2007/U IGNIS [2007-2008]
(project leader: Ł. Bratasz PhD)

The main objective of the project has been to implement into the conservation practice a heating system for historic churches, which, on one hand, would provide heat to people visiting them, and, on the other, would help in preservation of buildings and their furnishings. Such system should supply heat:

- locally to zones in which people congregate with a minimum disturbance of the microclimate in the rest of the interior,
- selectively, using infrared radiation, to architectural surfaces endangered by moisture condensation.

The project is implemented by a consortium of the conservation enterprise Monument Service – Marcin Kozarzewski and the Institute.

The work of the research team, in the first phase of the project, was focused on the development of the *modus operandi* of the new system and on investigations determining its work parameters, which would eliminate possible negative impacts of the system developed on the objects preserved in the historic interiors. Therefore, characteristics of various heating elements were determined in the context of their interaction with historic materials, the impact of the radiation emitted on historic objects was established, the tolerable range of microclimatic fluctuations was determined numerically and experimentally, as well as natural climate and existing hazards in the reference object - a Church of the Annunciation in Skepe - were surveyed. The walls and ceiling of the church are covered by valuable fresco paintings dated to 1750-1753. The research carried out has confirmed that the most important condition for a proper preservation of historic objects consists in limiting the fluctuations of relative humidity caused by the heating so that they do not exceed natural fluctuations. The acceptance of such criterion has allowed developing a suitable heating system, together with the steering and control units.

Localized pew heating was selected to provide an acceptable comfort for those using the church. A further heating module was designed consisting of electric radiant heaters positioned to provide a short-term warming of the painted ceiling, cold during winter and endangered by condensation when large number of people gathers in a church for a short period of a service. Both systems are activated or deactivated by a programmable logic controller which receives, stores and processes signals from sensors measuring temperatures of the air and the ceiling surface, and the relative humidity in the church. The control is based on keeping the disturbance of relative humidity induced by heating within a safe band determined by 84th percentile of natural fluctuations recorded in course of long-term climate monitoring in the church. Additionally, the same unit activates the radiant heaters countering condensation when only temperature difference between the ceiling and the dew point temperatures is smaller than 0.5^{o}C. The supplied heat increases then slightly the ceiling temperature and thus protects the paintings from the episodes of condensation.

OTHER INTERNATIONAL PROJECTS

Enzymes as Nanotools - Development of a New, Enzyme-Based Technology for Engineering Selectivity Permeable, Nano-Structured Membranes

GRDE France [2007-2010]
(project leader: Assoc. Professor P. Warszyński)

Lipases and phospholipases play a key role in living organisms and biotechnological processes, therefore, their properties are widely investigated. However, some of their properties have not yet been fully understood due to difficulties in analyzing of complex processes occurring in these multicomponent and multiphase systems. One has to use various experimental characterization techniques to achieve reliable description of these processes. Therefore, any project, which concerns characterization of lipases and phospholipases and their effect on lipid (phospholipids) films, has to be realized by the consortium of research groups specializing in various experimental and theoretical techniques. The GDRE project is realized by the consortium of five French and four Polish scientific institutions with complementary expertise. The aim of the project is to acquire new results and knowledge, which allow application of enzymes as "nanotools" for obtaining new materials with nanostructured surfaces for biomedical and/or sensor applications. In particular the enzymes will be applied to modify lipid or phospholipids layers in order to prepare selectively permeable, nanostructured membranes. Polish partners participating in the consortium represent: Chemistry Dept. of Warsaw University (Polish coordinator), Institute of Physical Chemistry PAS, Chemistry Dept. of Jagiellonian University and Institute of Catalysis and Surface Chemistry PAS.

The research task of ICSC in the project (the project started in November 2007) include:

1. Analysis of structure, thickness and homogeneity of lipid films at solid surfaces by ellipsometry and fluorescent microscopy TIRF;
2. Electrokinetic measurements of surface potential of lipid films and determination of its effect on the kinetics of the three-phase-contact formation and dynamic contact angle;
3. Determination of degree and kinetics of binding of enzymes to lipid layers by SPR and TIRF;
4. Assessment of the effect of enzymes on structure, thickness, surface potential and homogeneity of lipid films and formation of the three-phase-contact.

At the initial stage of the project, preliminary selection of lipids was made. Lipid films will be transferred onto solid support (mica, silicon wafers) using Langmuir-Blodgett technique. Imaging spectroscopic ellipsometry will be used to determine thickness of transferred films their structure, optical properties and their changes induced by enzymes. Surface potential of solid surfaces modified by lipid layers will be determined by streaming potential measurements. The surface potential will be correlated with wetting of lipid films determined by "captive bubble" method allowing measurements of contact angle in aqueous environment. Measurements of the kinetics of formation of the three-phase-contact at surface modified by lipid films will be also performed.

Casein Polyelectrolyte Multilayer Films

ECO-NET France IUP [2007-2008]
(project leader: Assoc. Professor P. Warszyński)

The objective of the project is to elaborate the technology of formation of polyelectrolyte multilayer (PEM) films containing casein. Casein belongs to the group of proteins, which were lately distinguished as intrinsically unstructured proteins – IUP. They are characterized by open structure, which can be preserved even after ligand binding. The open structure allows relatively large surface area for binding between protein and ligands, which is favorable for prospective applications due to strong interactions with polyelectrolyte film. Therefore, PEM films can be used as scaffold or matrix for adsorption of proteins and their properties should allow for maintaining of their biological activity. The research on biological activity of IUP is rapidly progressing, due to their importance in biological processes. However, there is still not enough data concerning adsorption and selforganisation of IUP. Understanding of these processes is essential for their practical applications in biotechnology. One of the basic properties of casein is its ability to bind calcium that opens many potential fields for its application. For instance polyelectrolyte multilayer films containing casein can be used to cover dentine in order to avoid formation of caries. Casein films can also play an important role in diary industry. They can be used to prevent formation of calcium deposit on milk processing vessels.

The project is realized by the consortium of French (University of Montpellier I – coordinator), Hungarian (Institute of Center for Biological Research of Hungarian Academy of Sciences and Polish (Institute of Catalysis and Surface Chemistry PAS) scientific institutions. In 2007 we concentrated on characterization of β-casein, which was used for the construction of PEM films. We determined surface activity, size and zeta potential of casein as a function of pH of the solution. We concluded that in neutral and alkaline conditions β-casein is negatively charged. Therefore, for the formation of multilayer films at silicon waffer surface polycations, PAH, PDADMAC and MADQUAD were used. Thickness of the films was determined by ellipsometry. We found that the thickest films were formed by the pair MADQUAD/β-casein (c.a 15 nm for 10 layer film – see figure 1), while in the case of the pair PAH/β-casein multilayer system were not formed. When PDADMAC is used as a polycation the situation was intermediate. Growth of the film was observed, however, accompanied with some formation of complexes, which can be removed in the consecutive dipping cycle.

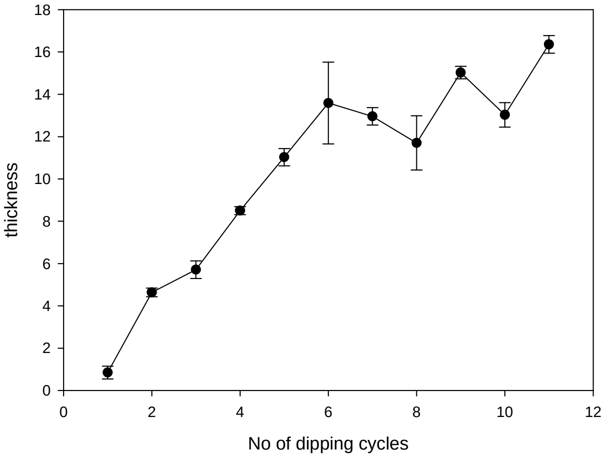


Fig. 1. Ellipsometric thickness of MADQUAD/β-casein films

Catalysis for Environment Depollutation, Renewable Energy and Clean Fuels

GDRI France [2007-2010]
(project leader: Professor J. Haber)

Nowadays, the catalytic treatment of global or local pollution and the renewable energies are research topics that need to be developed due to environmental concerns. The International Research Network has begun on 1st January 2007.

The research topics are following:

- reduction of nitrogen oxide compounds (SCR, TWC, deN_2O);
- oil valorization;
- isomerisation and ring opening;
- clean fuel (reforming, FT, Biomass valorization);
- catalytic oxidation of soot;
- volatile organic compounds catalytic treatment;
- catalytic water treatment.

In the frames of the network these is a mutual research between the Institute of Catalysis and Surface Chemistry of the Polish Academy of Science and Laboratoire de Reactivite de Surface of the Université Pierre et Marie Curie regarding SCR of nitrogen oxides with alcohols on zeolite catalyst. The catalyst samples are prepared in UPMC and the catalyst activity tests are performed in ICSC PAS.

Nanostructural Micro/Mesoporous Materials as New Catalysts for the Production of Environmentally Friendly Diesel Fuel

Intergovernmental Polish-Spanish project [2007-2009]
(project leader: Assoc. Professor M. Derewiński)

Liquid fuels obtained from natural gas through the well-known Fischer-Tropsch synthesis (FTS) offer significant advantages over those derived from crude oil. In particular, FTS diesel fuels have high cetane values and are almost free of contaminants such as sulfur, nitrogen, and (poly)aromatics. In order to produce higher yields of the desired product, the heavy n-paraffins (waxes) formed during FTS are separated from the rest of hydrocarbons and subjected to a selective hydrocracking step in the presence of a bifunctional (metal-acid) catalyst. In the project we propose to use new nanostructured materials with combined micro- and mesoporosity and controlled pore size distribution as the acidic component of bifunctional hydrocracking catalysts. The new zeolite/mesoporous composites were obtained by the controlled transformation of aluminosilicates with regular mesopores (SBA-15 type) into composite materials which retain the original porosity, while at least part of starting material was converted into nanocrystalline zeolites (MFI structures).

SBA-15 material (prepared at the first step of the study) is a member of the family of mesoporous solids synthesized in the presence of nonionic triblock copolymers as a template. It is characterized by the hexagonal pore ordering, pore walls thickness between 3 and 6.4 nm, adjustable pore size and high hydrothermal stability. Before recrystallizaton the calcined pure silica SBA-15 samples were impregnated with $Al(NO_3)_3{\cdot}9H_2O$ to deposit aluminum in the mesopores. The amount of aluminum source used was adjusted to obtain 1 mol% and 2 mol% of Al (in relation to the mass of Si). Although aluminum containing mesoporous SBA-15 material possesses an open structure and high thermal stability it could not be used as a catalyst because of lack of the strongly acidic active sites. Thus, partial recrystallization of the amorphous walls of mesopores into crystalline microporous domains of the MFI type could be an effective functionalization of the Al-SBA-15 material. The recrystallization of the pore walls of SBA-15 was carried out hydrothermally in a vapor phase.

The parent SBA-15 material had a BET surface area of 578 m^2/g and the hexagonally ordered mesopores of 4.3 nm in diameter The deposition of 1÷2 mol% of aluminum on the walls of SBA-15 followed by a heating at 200^oC for 18 h did not influence the mesoporosity of the solid. The presence of the broad peak with maximum at ~25^oC, in the XRD pattern of the recrystallized material, confirmed low extent of transformation into microcrystalline phase and retaining the amorphous character of the obtained samples. The analysis of the SEM micrographs revealed that the applied procedure of recrystallization did not change the size and morphology of SBA-15 grains. Moreover, no separated MFI crystals were detected. These observations supported conclusion that the partial recrystallization of the walls of the mesopores into the MFI domains was the only process occurred during hydrothermal treatment. This was directly proved with the TEM analysis of the partially recrystallized samples Whereas, a high regularity of the hexagonally ordered mesopores could be seen in the parent Al-SBA-15, the partial recrystallization into the MFI nanodomains resulted in changes of the walls thickness (HRTEM data). However, irrespectively of a small decrease in the pores regularity, the obtained new materials retained the mesoporous character.

Thus, the new multimodal porous system was obtained in which an open porosity, unrestricted transport of the reactant molecules and easy access to the new active sites present in the nanodomains of the MFI phase are combined.

The Development of a Substitute Ru Catalyst Based on Ni Catalyst by Improving Resistance for Carbon Deposition and Ni Sintering

NANO Japan research project[2007-2008]
(project leader: Professor E. Brocławik)

Ru catalyst is the standard catalyst used in steam-reforming process and in the fuel cell field. However, Ru metal is a by-product of Pt or nickel production, there are limited resources, and also the area of its production is limited, thus securing its sources will be of great concern in the future. Therefore, it is necessary to consider the substitute for Ru metal from the earliest possible stage. The man objective of the project was the development of Ni-substituted catalysts by improving its properties against coking and sintering

Because Ni metal has a lower melting point than Ru metal, Ni catalyst has poor property against sintering at about 800°C, which is required for steam reforming reaction of hydrocarbons. In this development, the particle growth of nickel catalyst is controlled by improvement of the chemical interaction between support surface and nickel particulates, and/or optimization of support surface and structure.

The interaction of the active metal and the catalyst support was analyzed theoretically. The modeling of supports with various shapes such as sphere, stick and plane was performed, and it was found that the simulation, which takes account of diffusion coefficient, could be performed.

The second goal of the project was to promote international cooperation in the field of catalyst development. Here the activity comprised business trip carried out within the NEDO project to China and Japan to discuss the most recent developments in the field of mesoporous materials and exchange information on catalyst design

SCIENTIFIC OUTPUT OF THE INSTITUTE IN 2007

PRINTED SCIENTIFIC PUBLICATIONS

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124. W. Rudziński, T. Pańczyk, T. P. Warzocha, Collision Frequency of Ideal Gas Particles with Irregular Surfaces as a Function of Their Fractal Dimension. Molecular Dynamic Studies", 11th Polish-Ukrainian Symp. on Theoretical and Experimental Studies of Interface Phenomena and Their Technological Applications, Zamość 2007

125. M. Ruszel, B. Grzybowska, M. Łaniecki, M. Wójtowski "Au Nanoparticles Dispersed on Ti-SBA-15 Supports as the Catalysts in Oxidation of CO and of C_3 Hydrocarbons", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

126. D. Rutkowska-Żbik, T. H. Rod, U. Ryde "Opracowanie metodologii teoretycznego wyznaczania wartości pKa i potencjału redox w proteinach", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

127. D. Rutkowska-Żbik, M. Witko, G. Stochel "Pochodne chlorofilu – badania właściwości katalitycznych i przydatności do terapii fotodynamicznej", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

128. K. Samson, I. Gressel, B. Grzybowska-Świerkosz, A. Kotarba, M. Hermanowska "Utleniające odwodornienie izobutanu na domieszkowanych potasem układach tlenków chromu i wanadu na nośnikach tlenkowych", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

129. J. Słoczyński, R. Grabowski, A. Kozłowska, M. Śliwa "Interaction of Oxygen with the Surface of Vanadia Catalysts", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

130. R. P. Socha, A. V. Tripković, P. Nowak, A. Kowal "Surface Composition of PtBi Electrode Cycled in Sulfuric Acid", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

131. N. Spiridis, K. Freindl, T. Ślęzak, M. Ślęzak, M. Zając, J. Korecki "Fe Nanostructures on W(110) and W(540)", Workshop on Nano-Scale Materials: Growth-Dynamics-Magnetism, Grenoble 2007

132. J. Stawowska, W. M. Bartczak, A. Drelinkiewicz "Investigation of the Palladium-polyaniline System with the Methods of Computational Chemistry", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

133. J. Stawowska, W. M. Bartczak, A. Drelinkiewicz "Investigation of the Palladium-4-vinylpyridine and Palladium-poly(4-vinylpyridine) Systems with the Methods of Computational Chemistry", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

134. A. Struska, D. Wodka, P. Nowak "Electrocatalytic Properties of Titanium Dioxide Gels Doped with Nickel Ions. Comparison with Nickel Hydroxide", COST D43 Workshop Functional Interfaces – Theory and Experiment & SURUZ Workshop Surfactants and Dispersed Systems, Kraków 2007

135. J. Superata, I. Janowska, P. Warszyński "Microelectrode Surface Modification with Carbonaceous Nanostructured Hybrid Composite Sensing Layers", EMRS Fall Meeting, Warszawa 2007

136. M. Szaleniec, M. Witko, J. Heider "Ethybenzene Dehydrogenase – Biosynthesis of Secondary Alkylaromatic and Alkylheterocyclic Alcohols", Int. Symp. on Relation between Homogeneous and Heterogeneous Catalysis ISHHC XIII, Berkeley 2007

137. M. Szaleniec, M. Witko, J. Heider "Ethybenzene Dehydrogenase – Biosynthesis of Secondary Alkylaromatic and Alkylheterocyclic Alcohols", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

138. K. Szczepanowicz, D. Dronka-Góra, G. Para, A. M. Bouzga, C. Simon, P. Warszyński, "Emulsion Containing Silica Sources as a Cores for Microencapsulation", ECIS 2007, 21st Conf. of the European Colloid and Interface Society, Geneve 2007

139. L. Szyk-Warszyńska, A. Trybała, P. Warszyński "Permeability of Polyelectrolyte Shells for Fluorescein Containing Microcapsules Suspended in Solution and Attached to a Surface", 9th Conf. on Colloid Chemistry, Siofok 2007

140. L. Szyk-Warszyńska, A. Trybała, P. Warszyński "Deposition of Fluorescently Labelled Model Microcapsules at Steel Surface", Int. SURUZ Conf. Surfactants and Dispersed Systems in Theory and Practice, Książ 2007

141. M. Śliwa, R. Grabowski " Synthesis and Physico-chemical Properties of Bifunctional Catalysts for Direct Syngas-to-dimethylether Process" Industrial Catalytic Processes Course, Bath 2007

142. E. Tabor, K. Pamin, J. Połtowicz, J. Haber "Comparison of Catalytic Activity of Monomeric Metallorphyrins, Their μ-Oxo Analogues and Supported Complexes in Oxidation of Cyclooctane", Int. Symp. on Relation between Homogeneous and Heterogeneous Catalysis ISHHC XIII, Berkeley 2007

143. E. Tabor, J. Połtowicz, K. Pamin, P. Nowak, J. Haber "Wpływ struktury i właściwości elektrochemicznych metaloporfiryn na ich właściwości katalityczne w reakcji utleniania cyklooktanu", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

144. E. Tabor, J. Połtowicz, K. Pamin, G. Pozzi, J. Haber "Synthesis and Physico-chemical Characterization of Perfluoroalkylated Salen Complexes", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

145. R. Todorov, J. Zawała, K. Małysa, D. Exerowa "Foam Films from Serum Albumine", Conf. NPCIS 2007 Nanoscale Phenomena in Colloid and Interface Science, Plovdiv 2007

146. R. Tokarz-Sobieraj "Theoretical Description of Molybdena Based Catalysts; DFT Cluster Model Study", 20th North American Catalysis Society Meeting, Houston 2007

147. R. Tokarz-Sobieraj, R. Gryboś, M. Witko "Electronic Structure of MoO_2. DFT Periodic and Cluster Studies", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

148. R. Tokarz-Sobieraj, M. Witko "Wpływ liganda i stopnia utlenienia Mo na proces aktywacji tlenu na porfirynach molibdenowych", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

149. R. Tokarz-Sobieraj, M. Witko "DFT Cluster Model Studies of Oxygen Activation at Molybdenum Porphyrins and Molybdenum Trioxide", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

150. A. Trybała, D. Dronka-Góra, K. Szczepanowicz, P. Warszyński "Co to są nanokapsułki ?", Int. Conf. on Chemistry at the Service of Society "Why Chemistry ?!", Kraków 2007

151. A. Trybała, L. Szyk-Warszyńska, P. Warszyński "Permeability of Polyelectrolyte Shells for Fluorescein Containing Microcapsules Suspended in Solution and Attached to a Surface", ECIS 2007, 21st Conf. of the European Colloid and Interface Society, Geneve 2007

152. A. Trybała, L. Szyk-Warszyńska, K. Szczepanowicz, P. Warszyński "Permeability of Polyelectrolyte Shells of Fluorescein Containing Microcapsules Suspended in Solution and Attached to a Surface", COST D43 Workshop Functional Interfaces – Theory and Experiment & SURUZ Workshop Surfactants and Dispersed Systems, Kraków 2007

153. A. Trybała, L. Szyk-Warszyńska, K. Szczepanowicz, P. Warszyński "Permeability of Polyelectrolyte Shells for Fluorescein Containing Microcapsules Suspended in Solution and Attached to a Surface", Int. SURUZ Conf. Surfactants and Dispersed Systems in Theory and Practice, Książ 2007

154. A. Waksmundzka-Góra, A. Drelinkiewicz, J. W. Sobczak, J. Stejskal "Hydrogenation of 2-Ethylanthraquinone on Pd-Polyaniline (SiO_2)-Composites", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

155. A. Waksmundzka-Góra, A. Zięba, A. Knapik, J. W. Sobczak, A. Drelinkiewicz "Fizykochemiczne i katalityczne właściwości układów Pt-polianilina i Pt-poli(4-winylopirydyna)", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

156. E. Wenda, A. Bielański "Diagram fazowy układu V_2O_5-MoO_3-Ag_2O", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

157. P. Weroński, Z. Jiang, S. Rasmussen "Application of Molecular Dynamics Simulations in the Design of a Minimal Self-Replicating Molecular Machine", 27th Annual CNLS Conf. Complexity of Biological and Soft Materials, Santa Fe, 2007

158. P. Weroński, Z. Jiang, S. Rasmussen "Application of Molecular Dynamics Simulations in the Design of a Minimal Self-Replicating Molecular Machine", 4th Annual Conf. on Fundations of Nanoscience: Self-Assembled Architectures and Devices FNANO'07, Snowbird 2007

159. A. Węgrzynowicz, M. Derewiński "Wpływ warunków syntezy na właściwości fizykochemiczne cienkich filmów zeolitowych (typu MFI i BEA)", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

160. J. Węgrzyńska, G. Para, J. Chlebicki, P. Warszyński, K. A. Wilk, "Adsorption Mechanism of Multiple Ammonium Salts at the Air Solution Interface", Int. SURUZ Conf. Surfactants and Dispersed Systems in Theory and Practice, Książ 2007

161. J. Węgrzyńska, G. Para, J. Chlebicki, P. Warszyński, K. A. Wilk "Wetting Ability of Multiple Ammonium Salts", Int. SURUZ Conf. Surfactants and Dispersed Systems in Theory and Practice, Książ 2007

162. M. Witko, P. Hejduk "Theoretical Description of Ammonia Adsorption at Different Low-indices V_2O_5 Surfaces", 20th North American Catalysis Society Meeting, Houston 2007

163. W. Włodarczyk, A. Gaweł, K. Bahranowski, R. Janik, T. Machej, R. Dula, E. M. Serwicka "Montmorillonity podpierane tytanem lub cyrkonem jako nośniki katalizatorów do usuwania lotnych chlorowcopochodnych organicznych", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

164. D. Wodka, A. Struska, P. Nowak "Elektrokatalityczne właściwości cienkich warstw TiO_2 dotowanego jonami metali przejściowych, otrzymanych metodą zol-żel", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

165. D. Wodka, A. Struska, P. Nowak "Electrocatalytic Properties of Titanium Dioxide Gels Doped with Transition Metals Ions and Prepared by Sol-gel Method", COST D43 Workshop Functional Interfaces – Theory and Experiment & SURUZ Workshop Surfactants and Dispersed Systems, Kraków 2007

166. M. Zając, K. Freindl, K. Matlak, M. Ślęzak, T. Ślęzak, N. Spiridis, J. Korecki "Structural and Magnetic Properties of Ultrathin Oxide Layers Formed on Fe(001)", Workshop on Nano-Scale Materials: Growth-Dynamics-Magnetism, Grenoble 2007

167. M. Zając, K. Freindl, K. Matlak, M. Ślęzak, T. Ślęzak, N. Spiridis, J. Korecki "CEMS Studies of Ultrathin Fe Films on MgO(001)", Workshop on Nano-Scale Materials: Growth-Dynamics-Magnetism, Grenoble 2007

168. P. Zarzycki "Molecular Dynamics Study of Water Structure. Classical and Quantum Rigid Water Model", The 2007 Berkeley Mini Statistical Mechanics Meeting, Berkeley 2007

169. J. Zawała, M. Krasowska, K. Małysa "Influence of the Bubble Kinetic Energy on Rupture of Liquid Films at Liquid/gas and Liquid/solid Interfaces", COST D43 Workshop Functional Interfaces – Theory and Experiment & SURUZ Workshop Surfactants and Dispersed Systems, Kraków 2007

170. A. Zięba, A. Drelinkiewicz "Transesterification as a Method of Biodiesel Production", Integrated Course on Applied Catalysis, Kraków 2007

171. A. Zięba, T. Kasza, A. Bielański, A. Drelinkiewicz "Wytwarzanie bioestrów (Biodiesel) w procesie katalitycznej transestryfikacji olejów roślinnych", Int. Conf. on Chemistry at the Service of Society "Why Chemistry ?!", Kraków 2007

172. M. Zimowiska, M. Bazarnik, K. Bahranowski, Z. Czuła, J. Połtowicz, E. M. Serwicka "Charakterystyka teksturalna mezoporowatych sit molekularnych typu FSM-16 zawierajacych metaloorganiczne makrokompleksy", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

173. M. Zimowska, M. Bazarnik, K. Bahranowski, Z. Olejniczak, D. Su, E. M. Serwicka "Określenie natury centrów glinowych w aluminowanych sitach molekularnych typu FSM-16 metodą MAS NMR", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

174. M. Zimowska, R. Dula, J. Plona, B. Napruszewska, R. Janik, T. Machej, J. Gurgul, R. P. Socha, E. M. Serwicka "Mixed Oxide Phases Formed in the Cu-Mn-Al-O System: Nature and Role in the Catalytic Combustion of Toluene", Int. Symp. on Air and Water Pollution Abatement AWPA, Zakopane 2007

175. M. Zimowska, Z. Olejniczak , E. M. Serwicka, M. Bazarnik, K. Bahranowski "^{27}Al MAS NMR and ^{29}Si MAS NMR Study of Kanemite Precursor of FSM-16 Mesoporous Sieves", EUROCLAY Conf., Aveiro 2007

176. M. Zimowska, H. Pálková, K. Bahranowski, Z. Olejniczak, E. Serwicka "Analiza procesu powstawania porowatych heterostrukur ilastych typu PCH", 39. Ogólnopolskie Kolokwium Katalityczne, Kraków 2007

177. M. Zimowska, J. Połtowicz, R. Socha, E. M. Serwicka, M. Bazarnik, K. Bahranowski, Z. Olejniczak "Metod of Alumination as Mean of Controling the Physico-chemical and Catalytical Properties of FSM-16", 8th European Congr. on Catalysis EuropaCat-8, Turku 2007

LECTURES IN SCIENTIFIC INSTITUTIONS AND SOCIETIES

1. J. Barbasz "Struktura i morfologia powierzchni a adsorpcja CO na Au/Fe3O4(001)", Institute of Physics, Jagiellonian University, Kraków 2007

2. J. Barbasz "Mono- i wielowarstwowe struktury hierarchiczne o kontrolowanej architekturze", Institute of Physics, Jagiellonian University, Kraków 2007

3. T. Borowski "Mechanism for Cyclization Reaction by Clavaminic Acid Synthase. Insights from Modeling Studies", Faculty of Chemistry, Berlin Free University, Berlin 2007

4. T. Borowski "Electrostatic Calculations for [Ni,Fe]-Hydrogenase", Faculty of Chemistry, Berlin Free University, Berlin 2007

5. E. Brocławik "Theoretical Modeling of Metal Active Sites in Zeolites", Tohoku University, Sendai 2007

6. E. Brocławik "Electronic and Steric Factors in Enzymatic Oxidation on Oxyferryl Iron Sites: Challenges for Quantum Chemistry", Lund University, Lund 2007

7. J. Haber, M. Nattich, T. Macchj "Alkali-metal Promoted Rhodium-on-alumina Catalyst for Nitrous Oxide Decomposition", Université Pierre et Marie Curie Paris VI, Paris 2007

8. J. Haber "The Nobel Prize in Chemistry 2007", Krakow Physical Seminar, Jagiellonian University, Kraków 2007

9. J. Haber "The Nobel Prize in Chemistry 2007", Department III of the Polish Academy of Sciences, Warszawa 2007

10. P. Hejduk "Katalizator widziany oczami teoretyka", Assocuation of Chemistry Students, Maria Curie Sklodowska University, Lublin 2007

11. J. Korecki "Druga młodość (anty-)efektu Mössbauera: Fonony w skali nano"; Faculty of Physics, Warsaw University, Warszawa 2007

12. J. Korecki "Jądrowe, rezonansowe rozpraszanie promieniowania synchrotronowego, czyli druga młodosc efektu Mössbauera", Faculty of Physics and Applied Informatics, AGH University of Science nd Technology, Kraków 20007

13. J. Korecki "Rezonansowe rozpraszanie promieniowania synchrotronowego, a badania fononów", Chair of Physics, Rzeszów Technical University, Rzeszów 2007

14. A. Kowal "Pt/Rh/SnO_2 - a New Anode for Direct Ethanol Fuel Cell ?", Seoul National University, Seoul 2007

15. A. Kowal "New Catalyst for Electrochemical Oxidation of Etanol: Pt/Rh/SnO_2", IHTM Institute of Electrochemistry, Belgrade University, Belgrade 2007

16. R. Kozłowski "W sercu Mony Lizy", Conservation Seminar, National Museum, Kraków 2007 (series of 3 lectures)

17. R. Kozłowski "Pomiary mikroklimatu w obiektach zabytkowych", Conservation Seminar, National Museum, Kraków 2007

18. M. Krzan, K. Małysa "Interrelations between Development of a Dynamic Structure of Adsorption Layer and Local Velocities of Rising Bubbles", GRASP Group for Research and Analysis in Statystical Physics, Liege University, Liege 2007

19. M. Krzan, S. Cohen-Addad, R. Höhler, M. Marinic "Rheology and Stability of Particle Laden Aqueous Foams", GRASP Group for Research and Analysis in Statystical Physics, Liege University, Liege 2007

20. W. Łasocha, A. Rafalska-Łasocha "Chemical Applications of the Powder Diffraction", National Autonomous University of Mexico, Mexico City 2007

21. M. Łukomski "Sukiennice – zamek w Niepołomicach. Przeprowadzka stulecia", Conservation Seminar, National Museum, Krakówie 2007

22. A. Rafalska-Łasocha, W. Łasocha, A. Jasińska "Chemistry and Art Objects", National Autonomous University of Mexico, Mexico City 2007

23. M. Ruszel "Au Nanoparticles on Oxide Supports as Catalysts in Oxidation of CO and of Hydrocarbons", Fritz-Haber Institute MPG, Berlin 2007

24. B. Sulikowski "Properties of Zeolites and Remarks on Their Modifications", Instituto de Catálisis y Petroleoquímica, CSIC, Madrid 2007

25. M. Szaleniec "Dehydrogenaza etylobenzenowa. Beztlenowa hydroksylacja związków alkiloaromatycznych i alkiloheterocyklicznych. Teoria i eksperyment", Faculty of Medical Biochemistry Collegium Mediucum, Jagiellonian Univerrsity, Kraków 2007

26. P. Warszyński "Multilayer Polyelectrolyte Structures", Faculty of Technology, Tomas Bata University, Zlin 2007

27. P. Weroński, M. Kolasińska, J. Barbasz, Z. Adamczyk "New Approach to Modeling Multilayer Irreversible Adsorption of Charged Nanospheres", Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati 2007.

LECTURES FOR STUDENTS AND PhD STUDENTS

1. A. Bielański "Ions Condensation i Aqueous Solition: Olation and Oxalation", lecture for 2nd course students of chemistry, Jagiellonian University, 1 hour

2. T. Borowski "Quantum Chemistry of Macromolecules", classes for 3rd course students of biophysics, Jagiellonian University, 30 hours

3. E. Brocławik "Structure Spectroscopu an Interactions", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 14 hours

4. E. Brocławik "Materials Molecular Modeling", monographic lectures for cycle"new materials and catalysis at the Faculty of Chemistry, Jagiellonian University, 30 hours

5. E. Brocławik " Quantum Chemistry of Macromolecules ", lectures for students of biophysics, Jagiellonian University, 30 hours

6. E. Brocławik "Applied Quantum Chemistry", lectures for PhD students of Postdgraduate Studies at the Faculty of Chemistry, Jagiellonian University, 30 hours

7. M. Derewiński "Introduction to IR and Raman Spectroscopy", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 4 hours

8. A. Drelinkiewicz "Thermodynamics", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 32 hours

9. B. Grzybowska-Świerkosz "Fundamentals od Heterogeneous Catalysis and Main Catalytic Reactions Mechanisms", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 15 hours

10. B. Grzybowska-Świerkosz "Oxidation Reactions on Nano-oxide and Nano-metal (Au) Species Dispersed on Oxide Supports", lectures for 5th course students and PhD students, Dipartimento di Chimica Industriale e dei Materiali, Universita di Bolonia, 5 hours

11. B. Jachimska "Advanced Analytical Techniques, Dynamic Light Scattering Method (DLS), Size of Colloidal Particles Measurement", lectures for 4th course students, Faculty f Material Engineering and Ceramics, AGH University of Science and Technology, Krakow, 2 hours

12. B. Jachimska "Advanced Analytical Techniques, Laser Doppler Velocimetry, Electrphoretic Mobility of Colloidal Particles", pomiary ruchliwości elektroforetycznej cząstek koloidalnych", lectures for 4th course students, Faculty of Material Engineering and Ceramics, AGH University of Science and Technology, Krakow, 2 hours

13. B. Jachimska "Advanced Analytical Techniques, Colloidal Systems Characterization", classes for PhD students of International Postgraduate Studies at ICPC PAS, 2 hours

14. J. Korecki, didactic pensum, AGH University of Science and Technology, Krakow

15. J. Korecki, lectures for PhD students of International Postgraduate Studies at ICPC PAS

16. A. Kowal, seminar and classes of AFM and STM Techniques Using Nanoscope DI Microcsope, University of Estern Sarajevo, Departament of Technology, Zvornik, 20 hours

17. A. Kowal, seminar and classes of AFM and STM Techniques Using Nanoscope DI Microcsope, Institute of Electrochemistry ICTM, Belgrade University, Belgrade, 36 hours

18. A. Kowal, consultation of PhD Thesis of J. Lović i S. Terzić, Institute of Electrochemistry ICTM, Belgrade University, Belgrade, 2 weeks

19. A. Lubańska "Gas Chromatography – Fundamentals, Applications and Catalytic Test", lectures and classes for pupils of Chemical High School in cooperation with Department of Teaching Methodology, Faculty f Chemistry, Jagiellonian University, 18 hours

20. W. Łasocha "X-Ray Diffraction", lectures and exams for PhD students of International Postgraduate Studies at ICPC PAS, 4 hours

21. W. Łasocha "Solid State Physicochemistry and Methods of Examination" Fizykochemia ciała stałego i metody badań", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 4 hours

22. P. Nowak "Semiconductors Electrochemistry", monographic lectures for students of Faculty of Chemistry, Jagiellonian University, 15 hours

23. P. Nowak "Electrochemistry" , lectures for PhD students of International Postgraduate Studies at ICPC PAS, 4 hours

24. P. Nowak "Electrochemistry; Electrochemical Methods of Physicichemial Investigations", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 4 hours

25. E. Serwicka-Bahranowska "ESR Using for Loamy Clay Minerals Investigation" lectures at Faculty of Geology, Geophysics and Environment Protection, AGH University of Science and Technology, Kraków, 5 hours

26. B .Sulikowski "Physicochemistry of Solids", lectures and exams for 4th course students of Faculty of Chemical Enguneering ad Tehnology, Krakow Technical University, Kraków, 15 hours

27. B. Sulikowski "Physicochemistry of Solids", lectures and exams for PhD students of Faculty of Chemical Enguneering ad Tehnology, Krakow Technical University, Kraków, 15 hours

28. P. Warszyński "Physical Chemistry", lectures for PhD students of International Postgraduate Studies at ICPC PAS, 14 hours

ACENET Integrated Course of Applied Catalysis

1. E. Brocławik "Catalysts Characterization – Theoretical Modeling"

2. E. Brocławik "Kinetics and Reaction Mechanisms - Mechanistic Cycles"

3. A. Drelinkiewicz "Fundamentals of Catalytic Reactions"

4. P. Nowak "Electrocatalysis"

5. E. M. Serwicka "Catalyst Characterization"

SCIENTIFIC SEMINARS IN THE INSTITUTE

LECTURES OF INVITED GUESTS

1. M. Asztemborska (Institute of Physical Chemistry PAS, Waszawa) "Rozróżnianie enancjomerów monoterpenoidów w chromatografii gazowej"

2. P. Bahadur (Department of Chemistry, University of South Gurajat, Surat) "Block Copolymers - the Versatile Multiphase Polymeric System with Potential Applications"

3. K. Burda (Institute of Physics, Jagiellonian University, Kraków, Institute of Nuclear Physics PAS, Kraków)"Zagadka fotosyntezy"

4. N. Kruse (Université Libre de Bruxelles) "Catalysis on the Nanoscae"

5. W. Makowski (Faculty of Chemistry, Jagiellonian University, Kraków) "Zastosowanie równowagowej termodesorpcji n-alkanów jako metody badań zeolitów i materiałów mezoporowatych"

6. S. Motilla (University of Turku) "Surface Studies of Metal Chalcogenides"

7. P. Pencakowski (University of Fine Arts, Kraków) "Co przedstawia kamienny krucyfiks Wita Stwosza w Kościele Mariackim w Krakowie ?" - Easter lecture

8. S. Rodziński (University of Fine Arts, Kraków) "Tajemnica procesu twórczego. Pomiędzy wzruszeniem ia rygorem" - Christmas lecture

9. P. Ruiz (Catholic University, Louvain-la-Neuve) "New Concepts Concerning the Activation of CO_2 and Advances in Catalytic Processes Dedicated to Energetic Production"

10. K. Sadlej (Instituty of Fundamental Technical Problems PAS, Warszawa) "Opór hydrodynamiczny agregatów czastek - teoria i przykłady obliczeń numerycznych"

11. M. Staszak (Poznań University of Technology) "Symulacja dynamiki zmian powierzchni międzyfazowej metodą objętości skończonych w układzie oktan-woda wraz z weryfikacją eksperymentalną"

12. W. Taborski (GlaxoSmithKline, Poznań) "Wykorzystanie lasera do znakowania kapsułek miękkich"

LECTURES OF INSTITUTE STAFF

1. J. Barbasz "Ilościowy opis nieodwracalnej adsorpcji cząstek koloidalnych na powierzchniach heterogenicznych"

2. Burkat-Dulak, V. Pashkova, A. Węgrzynowicz M. Derewiński "Monodyspersyjne, koloidalne zawiesiny nanokryształów zeolitów i ich wykorzystanie jako prekursory w preparatyce nowych układów dla procesów katalitycznych i rozdziału"

3. Burkat-Dulak, V. Pashkova, A. Węgrzynowicz M. Derewiński "Membrany i układy o miltimodalnej strzukturze porowatej""

4. A. Drelinkiewicy "Od biomasy do biochemikalii"

5. A. Drelinkiewicz, T. Kasza, A. Zięba "Układy metal-polimer w katalizie"

6. M. Grzywa "Hybrydowe organiczno-nieorganiczne materiały warstwowe: synteza i badania strukturalne i fizykochemiczne"

7. M. Grzywa "Stałe superkwasy oraz nowe perokso związki Mo(VI), W(VI) i V(V) - synteza

8. J. Janas "Centrum Ekspertyz Zanieczyszczeń Środowiska - nowe laboratorium Instytut"

9. R. Karcz "Synteza i badania właściwosci katalitycznych kompleksów metali przejściowych w procesie utleniania węglowodorów"

10. M. Łukomski "Monitorowanie stanu powierzchni obiektów zabytkowych przy zastosowaniu metod optycznych"

11. A. Micek-Ilnicka "Kinetyka i mechanizm syntezy eteru etylo-tert-butylowego (ETBE) z etanolu i izobutenu w układzie uwodnionym"

12. Ł. Mokrzycki "Synteza i właściwości nowych katalizatorów zeolitowych do procesów transformcji węglowodorów alkiloaromatycznych i terpenowych"

13. P. Nowak "Elektrokataliza w ogniwach paliwowych"

14. A. Pacuła "Synthesis of Carbon Materials via Chemical Vapour Deposition (CVD) Using Different Templates"

15. P. Rejmak "Metale przejściowe jako centra aktywne w zeolitach i enzymach: modelowanie metodami chemii kwantowej"

16. W. Rojek "Katalityczne utlenianie sadzy samochodowej"

17. M. Ruszel, K. Samson, M. Śliwa "Badania statutowe zespołu Kataliza II"

18. B. Sulikowski, U. Filek, Ł. Mokrzycki, R. Rachwalik, E. Włoch "Synteza i właściwości nowych katalizatorów zeolitowych do procesów transformacji węglowodorów alkiloaromatycznych i terpenowych"

19. B. Świątkowska "7. Program Ramowy Unii Europejskiej"

LECTURES AT "OPEN DOORS DAY" OF THE INSTITUTE

1. Bielański, "Woda - związek bardzo pospolity"

2. J. Haber "Energia - warunek rozwoju ludzkości"

3. K. Małysa "Flotacja i tańczące pęcherzyki"

4. D. Rutkowska-Żbik "Jak teoretyk widzi katalizator ?"

5. J. Szaleniec, M. Szaleniec "Zobaczyć niewidzialne. Chmia i fizyka w medycznej diagnostyce obrazowej"

POPULARIZED SCIENTIFIC LECTURES

1. J. Barbasz "Chemia wody", Krakowskie Stowarzyszenie Akwarystów, Instytut Botaniki UJ, Kraków 2007

2. J. Barbasz "Morskie inaczej", Krakowskie Stowarzyszenie Akwarystów, Galeria Przyrody, Kraków 2007

3. A. Bielański, "Wegiel - pierwiastek o stu twarzach", 8 Festiwal Nauki, Kraków 2007

4. Drelinkiewicz "Biomasa, biodiesel, biochemikalia", 8 Festiwal Nauki, Kraków 2007

SCIENTIFIC DEGREES AND TITLES AWARDS

PROFESSORS

1. Bogdan Sulikowski
2. Wiesław Łasocha (at Faculty of Chemistry, Jagiellonian University)

DSc IN CHEMISTRY

1. R. Grabowski "Modelowanie kinetyki utleniającego odwodornienia alkanów na katalizatorach tlenkowych"
2. W. Piasecki "Opis równowag i kinetyki adsorpcji jonów prostych na granicy faz tlenek metalu/roztwór elektrolitu oparty na modelu jednostopniowej protonacji powierzchni tlenku oraz statystycznej teorii transportu międzyfazowego"

PhD IN CHEMISTRY

1. S. Jakieła "Emisja akustyczna drewna w obiektach zabytkowych pod wpływem fluktuacji klimatu" (promotor R. Kozłowski)
2. T. Kasza "Badanie właściwości fotokatalitycznych i charakterystyka fizykochemiczna nanokrystalicznych filmów TiO_2 na podłożu ceramicznym" (at Faculty of Chemical Engineering and Technology, Krakow University of Technology)
3. A. Michna "Mechanizm oddziaływania cząstek koloidalnych z powierzchniami heterogenicznymi wyznaczony przy pomocy badań adsorpcji oraz zjawisk elektrokinetycznych" (promotor Z. Adamczyk)
4. M. Nattich "Mechanizm działania katalizatora Rh w reakcji rozkładu podtlenku azotu" (promotor J. Haber)
5. K. Samson "Utleniające odwodornienie izobutanu na domieszkowanych układach tlenków chromu i wanadu na nośnikach tlenkowych" (promotor B. Grzybowska-Świerkosz)
6. M. Szaleniec "Ethylbenzene Dehydrogenase - Biocatalytic Oxidation of Aromatic and Alkylaromatic Compounds" (promotor M. Witko)
7. E. Tabor "Porównanie właściwości katalitycznych metaloporfiryn i ich μ-oxo kompleksów w procesach utleniania węglowodorów" (promotor J. Haber)
8. A. Waksmundzka-Góra "Wpływ właściwości nośników polimerowych na aktywność katalizatorów palladowych w uwodornianiu związków karbonylowych", (at Faculty of Chemistry, Jagiellonian University)

CONFERENCES AND SCIENTIFIC EVENTS ORGANIZED IN THE INSTITUTE

1. 39. Ogólnopolskie Kollokwium Katalityczne [39th Annual Polish Conference on Catalysis], Kraków March 14-16, 2007. (B. Sulikowski)

2. COST D43 Workshop Functional Interfaces – Theory and Experiment & SURUZ Workshop Surfactants and Dispersed Systems, Kraków, March 19-21, 2007 (Z. Adamczyk)

3. ACENET Integrated Course on Applied Catalysis, Kraków, March 26-30, 2007 (E. Serwicka-Bahranowska)

4. 14. Forum Zeolitowe [14th Zeolite Fotum], Kocierz, September 16-21, 2007 (M. Derewiński)

5. IDECAT Workshop "From Idea to Results - Effective Research Project Management", Kraków, June 14-15, 2007 (M. Witko)

6. Open Doors Day of the Institute, Kraków, October 16, 2007 (M. Derewiński)

7. Workshop "New Colloidal Systems for Nano and Biotechnology", Kraków, November 15-16, 2007 (B. Jachimska)