

## Department of Catalysis and Reaction Engineering

### HEAD

OLGA ŠOLCOVÁ

### DEPUTY

PETR KLUSOŇ

### RESEARCH STAFF

LIBUŠE HANKOVÁ, VLADIMÍR HEJTMÁNEK, LADISLAV HOLUB, KVĚTUŠE JIRÁTOVÁ, LUDĚK KALUŽA, JAN KLEMPA, YWETTA MALÉTEROVÁ, MARTINA MATĚJKOVÁ, LENKA MATĚJOVÁ, ROBERT PONEC, KAREL SOUKUP, HANA ŠNAJDAUFOVÁ, PAVEL TOPKA, ZDENĚK VÍT  
Part time: JANA BALABÁNOVÁ, JANA GAÁLOVÁ, DANIELA GULKOVÁ, KAREL JEŘÁBEK, JAROMÍR JIRKOVSKÝ, FRANTIŠEK KAŠTÁNEK, PETR KAŠTÁNEK, HANA KMENTOVÁ (ŽABOVÁ), JOSEF KRÝSA, PETR SCHNEIDER, KRASIMIRA SOUKUPOVÁ, MIROSLAV ZDRAŽIL

### PHD STUDENTS

PAVEL DYTRYCH, SIMONA KREJČIKOVÁ, PAVEL KRYSŤYNÍK, JANA LUDVÍKOVÁ, MAGDALENA MOROZOVÁ, LUCIE SPÁČILOVÁ

### TECHNICAL STAFF

Part time: BARBORA PAPEŽOVÁ, HELENA SOUČKOVÁ

## Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N<sub>2</sub>O
- Design of new theoretical models for structure-activity relationships
- Morphology and application properties of catalysts based on functional polymers
- Preparation of hierarchic nanomaterials
- Temperature programmed techniques in characterization of catalysts
- Texture of porous solids
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Transport processes in porous solids
- Preparation and characterization of the electrospun nanofibrous membranes and catalytic supports
- Unconventional preparation of metal oxide nanostructures by pressurized fluid extraction and supercritical drying

## Applied research

- Catalytic combustion of volatile organic compounds
- Oxidation processes for environment
- Textural characteristics of structural materials

## Research projects

### Hydrogen Oriented Underground Coal Gasification (UCG) for Europe - Environmental and Safety Aspects (HUGE2)

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2011-00002)

This project is focused on safety and environmental aspects of underground coal gasification. Underground trial will be performed in mine testing two borehole system and reactive barriers usage. The most serious environmental concerns related to UCG will be investigated that is contamination of underground aquifers and potential leakage of poisonous and explosive gases into the surrounding strata. The work will be focused on finding practical solutions of possible leakages prevention by use of reactive barriers. Complex system of environmental telemetric monitoring will be built and tested. Also technical and ecological risk assessment will be performed. [Refs. 23, 83]

### Hierarchic nanosystems for microelectronics

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with JH IPC, IMC, Institute of Microbiology of the ASCR, v. v. i., Institute of Physics of the ASCR, v. v. i., ICT, CU, UJEP, and Research Institute of Organic Syntheses Pardubice; supported by ASCR, grant No. KAN400720701)

Project developed the complex composite systems with precisely defined performance applicable in microelectronics. Prepared composite structures - various types of hierarchical nanostructures were designed, produced and functionally described, with direct implications in many types of advanced sensors; long-life humidity sensor, photoelectric gas sensor, oxalic acid sensor, etc. [Refs. 2, 11, 12, 16-18, 25, 26, 59, 64-66, 68, 69, 72, 73, 86]

### Advanced photocatalytic processes - nanotechnology for environment

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Institute of Microbiology of the ASCR, v. v. i., and UPa; supported by GACR, grant No. 104/09/0694)

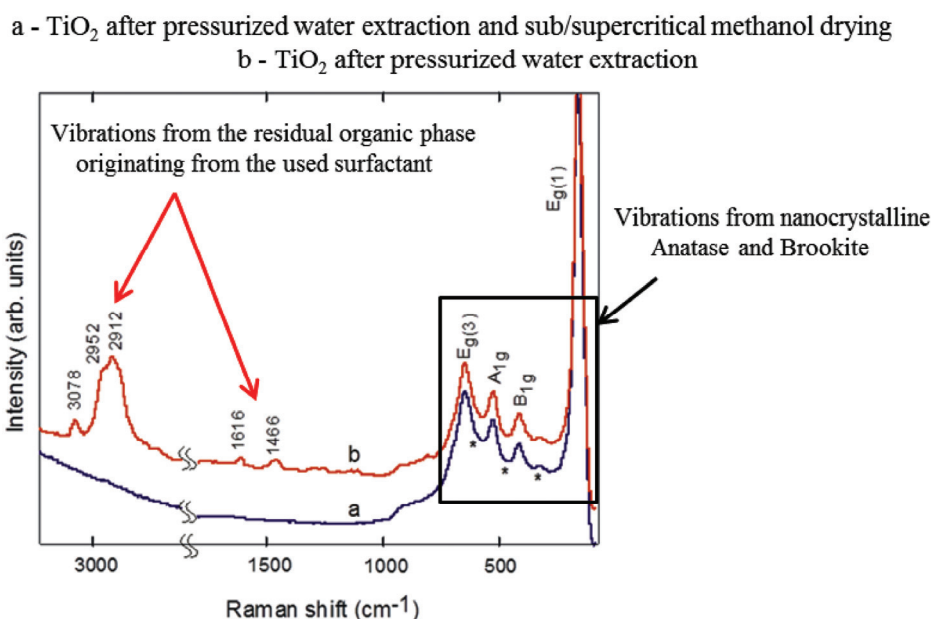
This project was focused on preparation and characterization of specially designed photoactive materials applied for decomposition of the large series of potential water contaminants ranging from phenols, chlorinated phenols, polybrominated diphenyl ethers and alcohols to herbicides, pesticides, pharmaceuticals, industrial colorants, pigments and dyes. The special focus was devoted to the reactor system; selectively prepared photoactive nanostructures together with design of effective photoreactors including mathematical modeling of involved physical and chemical processes and generalization of obtained results. [Refs. 6, 12, 17, 18, 25, 26, 58, 60, 70, 74, 75, 81, 85]

### Innovative preparation of nanocrystalline metal oxides with high-ordered mesoporous structure by extraction technique

(L. Matějová, [matejova@icpf.cas.cz](mailto:matejova@icpf.cas.cz); joint project with CU; supported by GACR, grant No. 104/09/P290)

Project deals with development and optimization of extraction technique for purification and total crystallization of prepared oxidic materials with high-ordered mesoporous structure. Developed extraction technique using fluids in supercritical and subcritical state will be generally applicable for synthesis of nanocrystalline metal oxides. The optimal experimental conditions (temperature, pressure, flow rate, etc.) as same as the suitable solvents will be defined and evaluated also with respect to future technical and economic realization of methodology. High-ordered mesoporous metal oxides (hexagonal, cubic, lamellar) TiO<sub>2</sub>, ZrO<sub>2</sub>, SiO<sub>2</sub>/TiO<sub>2</sub>, ZrO<sub>2</sub>/TiO<sub>2</sub>, CeO<sub>2</sub>, Nb<sub>2</sub>O<sub>5</sub>, Ta<sub>2</sub>O<sub>5</sub>, SnO<sub>2</sub> promising in photocatalysis and

sandwich structures in microelectronics will be synthesized by templating using amphiphilic and ionic surfactants in aqueous and alcoholic solution with metal chloride and alkoxide. [Refs. 25, 33, 65-69]



**Raman spectra of nanocrystalline TiO<sub>2</sub> prepared by extraction techniques**

### Structured catalysts with low concentration of active components for total oxidation of VOC

(K. Jirátová, [jiratova@icpf.cas.cz](mailto:jiratova@icpf.cas.cz); joint project with ICT, and IIC; supported by GACR, grant No. 106/10/1762)

Binary and ternary Cu, Co, Ni, Mn/Al mixed oxides prepared by calcination of co-precipitated LDH precursors were examined in total oxidation of ethanol. Formation of the chosen LDH precursors on an oxidized Al foil, a model of structured catalyst supports, under hydrothermal conditions was studied in detail and after their calcination, physical-chemical properties and activity of the resulting mixed oxides in ethanol oxidation was examined in detail. Catalysts containing Co-Mn-Al over TiO<sub>2</sub> support with various active metals distribution were prepared in order to study the effect of metals distribution on catalyst activity in ethanol oxidation. [Refs. 14, 15, 45, 46, 61-63]

### Abatement of N<sub>2</sub>O emissions in off-gas from nitric acid technology

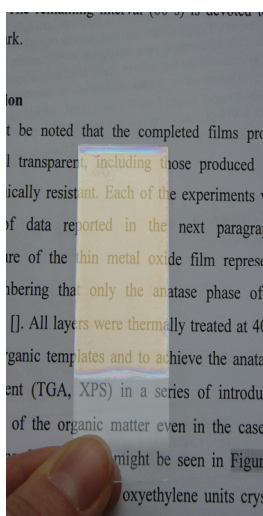
(K. Jirátová, [jiratova@icpf.cas.cz](mailto:jiratova@icpf.cas.cz); joint project with TU of Ostrava, and ICT; supported by TACR, grant No. 010220336)

The effect of promoter addition to the calcined Co-Mn-Al LDH-like compounds on the catalyst activity in decomposition of N<sub>2</sub>O was studied in detail. Potassium was found to be the best promoter of the catalyst. In addition, the effect of active metals distribution in the Co-Mn-Al/TiO<sub>2</sub> catalysts on catalytic properties was investigated. Abatement of N<sub>2</sub>O in waste by its decomposition over K-promoted Co-Mn-Al mixed oxide catalyst was simulated. [Refs. 19, 52, 53, 77]

### Advanced catalytic processes and materials

(J. Hanika, O. Šolcová, [hanika@icpf.cas.cz](mailto:hanika@icpf.cas.cz), [solcoca@icpf.cas.cz](mailto:solcoca@icpf.cas.cz); joint project with JH IPC, ICT, CU, and UPa; supported by GACR, grant No. 203/08/H032)

Development of the new selective catalytic and separation processes for preparation of specialty compounds and materials, which can give rise to a progression in the field of new chemical technologies was realized. The special focus was devoted to processes in question; stereoselective and regioselective transformations on chiral catalytic centers and processes with significant environmental impact. The project theses were coordinated in the field of catalysis, e.g., developed Rh catalysts were tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts were tested in organic synthesis (ICT, UPa, ICPF), oxidation polymerization (CU) and synthesis of chemical specialties (JH IPC); new mesoporous materials prepared at JH IPC were used in all other partner laboratories, etc. [Refs. 8, 12, 17, 18, 57, 61-63, 71-75]

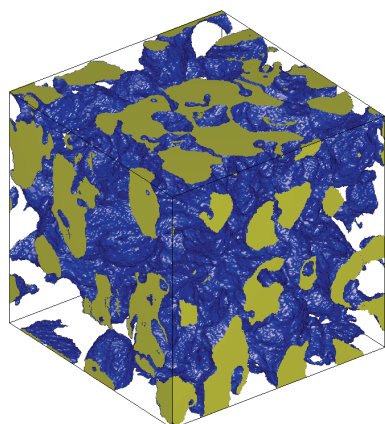


The thin transparent TiO<sub>2</sub> layer on glass

### Routes to separation performance enhancement for composite membranes based on linear polyimides

(V. Hejtmánek, [hejtmank@icpf.cas.cz](mailto:hejtmank@icpf.cas.cz); joint project with JH IPC, and ICT; supported by GACR, grant No. 203/09/1353)

The principal project goal, i.e. a development of preparation procedure for polyimide (PI) based composites with different content of microporous inclusions (silicalite-1, ZIF-8), was fulfilled. The application of a coupling species APTES enhanced mechanical stability of composites and prevented void formation at interface boundary and thus deterioration of separation factor. Prepared materials were suitable for a fundamental study of relation between macroscopic properties of the heterogeneous material on one side and microscopic descriptors of the material, self-diffusion coefficients of the gases and their occurrence probability in either phase on the other. 3D models of composite membranes microstructure were constructed using the method of stochastic reconstruction developed in the first project stage. The obtained replicas were used to simulate mass transport in the composites using a Monte Carlo algorithm. Another novel technique used in this project is the preparation procedure of polyamic acid (PAA which is the precursor of PI) based films and membranes on solid preferentially porous supports, which involves the electrophoretic deposition (EPD) of PAA solution from its emulsion in acetone. [Refs. 1, 34, 42]

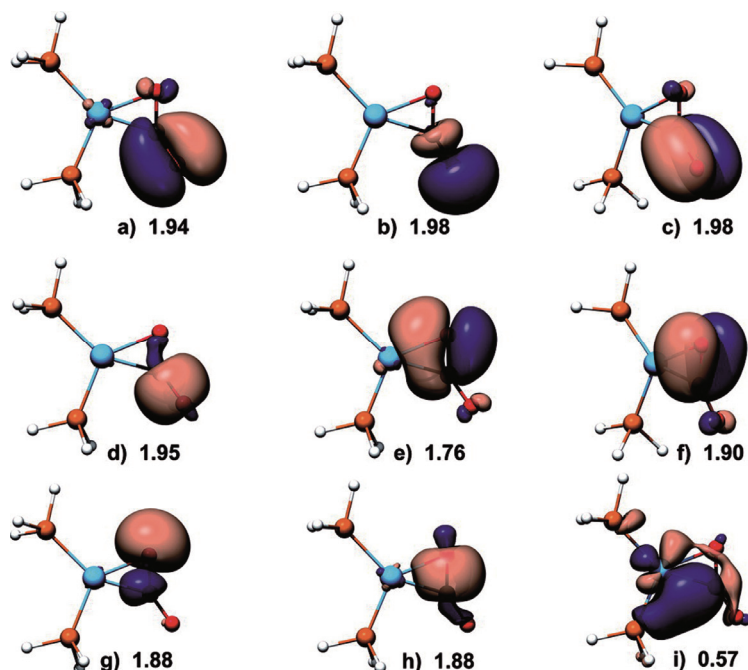


The zeolite-polyimide membrane replica ( $64 \times 64 \times 64 \mu\text{m}$ ). Polyimide phase is transparent, polyimide-silicalite interface is blue and intersections of the silicalite phase and the cut planes are yellow

### Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, [rponec@icpf.cas.cz](mailto:rponec@icpf.cas.cz); joint project with University of Pécs, Hungary, Univerzity of Girona, Spain; supported by GACR, grant No. 203/09/0118)

The project is a part of longer-term efforts at the systematic exploitation of the pair density as new source of the information about the molecular structure and nature of chemical bond. This density represents the basic theoretical quantity allowing us to describe the behaviour of electron pairs in microscopic systems. In the past several years it was proven to provide new valuable insights into the role of electron pairing in chemical bond. Especially useful in this respect were found the approaches known as the analysis of domain averaged Fermi holes and the generalized population analysis. These approaches have been applied to the interpretation of the bonding in molecules with complicated bonding pattern like metal-metal bonding, multicenter bonding, all metal aromaticity, etc. The formalism of the analysis of domain averaged Fermi holes was generalized beyond the scope of closed shell systems and the attention was also paid to the manifestation of the chemical bonding in momentum space. [Refs. 7, 21, 30, 31, 78-80]



Graphical representation of the eigenvectors of the DAFH of the  $\text{CO}_2$  fragment with the corresponding eigenvalues



### **Study of hydrodesulfurization and its inhibition by hydrogenation (denitrogenation) over catalysts containing small amounts of noble metals**

(Z. Vít, [vít@icpf.cas.cz](mailto:vít@icpf.cas.cz); joint project with Department of Chemistry, Physics and Environment, University of Udine, Italy; supported by GACR, grant No. 104/09/0751)

Alternative acidic supports and active phases based on noble metals were studied for hydrodesulfurization (HDS) of model compounds such as thiophene and benzothiophene. Mesoporous silica-aluminas modified by acid extraction were studied as supports of Pd and bimetallic Pd-Pt catalysts. The acid extraction led to higher accessible surface areas and exposed the Brønsted acid sites of supports which both improved the HDS activity of catalysts. HDS activity was also greatly influenced by the precursor of noble metal. The inhibition effects of pyridine and toluene on HDS of thiophene was studied on sulfided Rh, Ru, Mo, Rh-Mo, Ru-Mo and CoMo/alumina catalysts. Noble metal catalysts were generally less sensitive to pyridine inhibition than conventional CoMo catalysts. Their higher nitrogen tolerance was related to higher C-N bond hydrogenolysis activity. Comparative inhibition with toluene confirmed that poisoning of conventional Mo and CoMo catalysts is due to basicity of inhibitor while not to its aromatic character. [Refs. 27, 28, 38, 39, 91, 92]



**Pressure flow microreactor with fixed bed of catalyst for hydrodesulfurization**

### **Functional macroreticular polymers as catalyst carriers**

(K. Jeřábek, [kjer@icpf.cas.cz](mailto:kjer@icpf.cas.cz); joint project with Department of Chemical Sciences, University of Padova, Italy; supported by ASCR, grant No. M200720902)

In the project, polymer-based catalysts bearing either covalently bonded acidic groups and/or metal nanoparticles are investigated. Using combination of various physico-chemical methods, morphology and steric conditions in polymeric catalysts of both laboratory and commercial origin has been examined. There was developed a feasible method for modification of chemical nature of ion exchanger catalyst for applications in processes involving lipophilic reagents. [Refs. 29, 32, 40, 43, 44]

### **Post-polymerization hypercrosslinking of monolytic polymers**

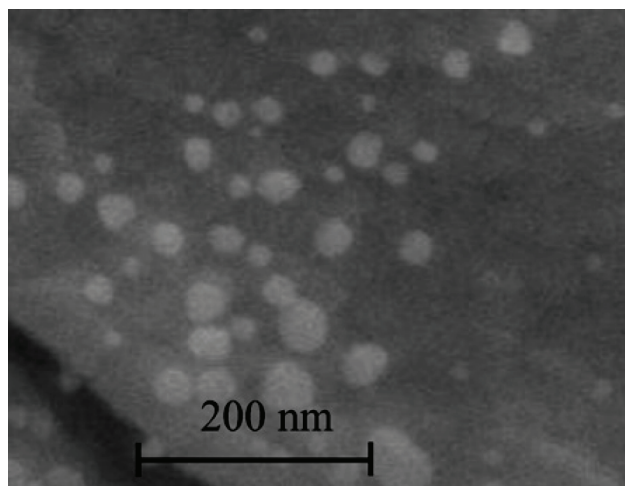
(K. Jeřábek, [kjer@icpf.cas.cz](mailto:kjer@icpf.cas.cz); joint project with University of Maribor, Slovenia, supported by MEYS, grant No. MEB091107)

Within this project are investigating possibilities of modifications of morphology of monolytic porous polymers by additional crosslinks introduced to the already polymerised monolithic material. In this manner, much smaller pores are created thus significantly enlarging the surface area while leaving the larger pores intact. [Refs. 13, 41]

### **New catalysts for VOC oxidation**

(P. Topka, [topka@icpf.cas.cz](mailto:topka@icpf.cas.cz); joint project with Department of Process and Environmental Engineering, University of Oulu, Finland, supported by ASCR, grant No. M200720901)

Novel oxidation catalysts based on noble metals supported on ceria-zirconia mixed oxides were developed, characterized and their catalytic activity in total oxidation of model volatile organic compounds was studied. In collaboration with the Finnish partner, platinum and gold catalysts with noble metal content in the range from zero to 2.5 wt. % were tested in total oxidation of dichloromethane. Their physicochemical properties (dispersion of noble metal, reducibility, acidobasic properties) were correlated with their catalytic performance and activity/selectivity vs. composition/structure relationships were proposed. [Refs. 20, 36, 37, 47]



**Gold nanoparticles on ceria-zirconia support as seen by field-emission scanning electron microscope**

### **Development of oxide catalysts for total oxidation of ethanol**

(J. Gaálová, [gaalova@icpf.cas.cz](mailto:gaalova@icpf.cas.cz); supported by GACR, grant No. 106/10/P019)

The second year of the project was focused on catalytic testing of newly developed catalysts in the oxidation of ethanol. The results of the project revealed that ceria-zirconia mixed oxides exhibited high activity and low formation of undesired reaction by-products. Novel catalysts were prepared by doping of ceria-zirconia with noble metals. It was shown that the addition of gold and platinum can dramatically affect the efficiency of the catalysts.

The effect of metal content and metal dispersion was investigated and correlated with activity and selectivity of the catalysts. Except the experiments with powder catalysts, new methods for the synthesis of monolithic catalysts were proposed and tested. [Refs. 5, 36, 47, 87]

### **Unconventional composition and preparation of sulfide hydrotreating catalysts**

(L. Kaluža, [kaluza@icpf.cas.cz](mailto:kaluza@icpf.cas.cz); supported by GACR, grant No. 106/11/0902)

The principles of the ZrO<sub>2</sub>-CeO<sub>2</sub> support synthesis and impregnation of the carries Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub>, and SiO<sub>2</sub>- Al<sub>2</sub>O<sub>3</sub> with the use of complexing agents to deposit transition metals (Co, Ni, Mo, and selected platinum metals) and with the use of organic solvent solubility precursors e.g. metals acetylacetonates were studied to prepare highly active catalysts in model hydrodesulfurization of thiophene, benzothiophene, hydrodeoxygenation of rape-seed oil and isomerization of 1-methyl-cyclohex-1-ene. The synergism in the activities and the relative C-S hydrogenolysis/ C=C hydrogenation/C=C isomerization and triglycerides hydrogenolysis / triglycerides decarboxylation selectivities were determined. The original method of slurry impregnation (solvent-assisted spreading) was successfully modified for direct synthesis of the catalysts. [Refs. 5, 28, 48-51, 92]

### **Reactive chemical barriers for decontamination of heavily polluted waters**

(P. Klusoň, [kluson@icpf.cas.cz](mailto:kluson@icpf.cas.cz); joint project with Dekonta a.s.; supported by MIT, grant No. FR-TI1/065)

The project is focused on the practical development of special oxidation processes used for decontamination of industrially polluted subsurface waters. The used methods were: photocatalytic oxidation with titanium dioxide, photocatalytic oxidation with synthetic porphyrines and oxidations with various organic peroxides and hydrogen peroxide. The project deals in a complex manner with the problem of industrial pollution with a range of organic chemicals at concentrations and the area scale that can hardly be treated in any other way. The Recheba concept represents a kind of passive approach, however, assisted with highly advanced processes for effective water decontamination. The systems were tested on a laboratory scale, in parallel they were modified and scaled-up for practical testing on three selected industrial sites. The efficiencies of the chosen methodologies were compared and the most suitable one were implemented to the final form. This system will be produced and long-term tested. [Refs. 9, 10, 24]

### **Composed molecular templates for preparation of assembled functional nanoparticles**

(P. Klusoň, [kluson@icpf.cas.cz](mailto:kluson@icpf.cas.cz); joint bilateral project with Bangor University, School of Chemistry, Wales, UK; supported by ASCR, grant No. M200720904)

To emulate at least some of the effectiveness of NATURE in making smart functional structures and systems man has had to develop many different empirical and also scientific concepts. These attempts were reflected in the steep growth of interest in nanoscience and nanotechnologies. There was much progress in the synthesis, assembly and fabrication of nanomaterials. Similar new technologies are expected to have an impact on chemistry, energy production, energy storage, electronics, machinery, aircrafts, space exploration, environment protection, etc. Independently of types of new materials (or their application), one of the most important points concerns chemical (or physical) pathways that are capable to yield them. Among the suitable methods, bottom-up approaches involving templates have dominated for the preparation of one-dimensional or multidimensional nanostructures. This pathway is particularly useful if precise replication is achieved in the nanometer precision. It corresponds to the assembly of well-defined nanobuilding blocks consisting of perfectly calibrated objects keeping their integrity in the final material. [Refs. 8, 30, 31, 35, 56]



### **Utilization of combined thermal desorption and catalytic oxidation methods for solid waste decontamination**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with Dekonta a.s.; supported by MIT, grant No. FR-TI1/059)

Project develops and verifies a new technology for decontamination of solid waste containing toxic organic substances, which is based on treatment of the waste by thermal desorption process and subsequent catalytic oxidation of desorbed organic contaminants. Research activities aimed at solution of some technical problems related to full-scale application of the developed technology will be realized together with testing under real conditions. [Ref. 5]

### **Use of PFG NMR, stochastic reconstruction and molecular simulation to estimate transport-related texture characteristics of advanced porous materials**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); joint project with CU, supported by GACR, grant No. 204/11/1206)

Searching after the functional relationship between diffusion of fluid in disordered solids (e.g. porous solids) and their microstructure is an active field of research in membrane science, catalysis, biophysics, civil engineering and other branches of research and development. During several past decades the pulsed field gradient (PFG) NMR technique has proved to be a powerful tool for measuring of self-diffusion in such systems. The focus of the project will be on investigation of transport of liquid species contained in porous materials (non-consolidated and consolidated) with monodisperse and bidisperse porous structure with excursions to adjacent supercritical regions. A rational system of transport-related structure characteristics to predict transport behavior of liquids and supercritical fluids will be searched by combined application of PFG NMR, image analysis of porous materials and molecular simulation of self-diffusion in selected two-phase systems. [Refs. 22, 42, 82, 84]

### **Removal of endocrine disruptors from waste and drinking water by photocatalytic and biological processes**

(O. Šolcová, [solcova@icpf.cas.cz](mailto:solcova@icpf.cas.cz); supported by TACR, grant No. 01020804)

The necessity to find alternative solutions for environmental protection leads to the development and use of the new technologies. Photo-catalysis using semiconductor oxides have found an increasing interest to solve the global pollution problems. Compared to the other photo-catalysts  $\text{TiO}_2$  (and/or doped  $\text{TiO}_2$ ) seems to be the most promising material not only in advanced oxidation photo-catalytic processes (AOP). It is well established that titanium oxide and related nanostructure materials in the presence of UV light (in dependence on conditions also in the presence of visible-light) can create very active species that are able to restore and preserve a clean environment by decomposing harmful organics; killing bacteria and viruses and being easily self-cleaned. Our investigation insists on the photo-catalyst immobilization in the form of a thin film trying to improve the efficiency of photocatalytic processes. [Refs. 42, 54, 55, 82, 84]

### **New heterogeneous catalysts for environmental protection**

(L. Kaluža, [kaluza@icpf.cas.cz](mailto:kaluza@icpf.cas.cz); joint bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria; supported by ASCR)

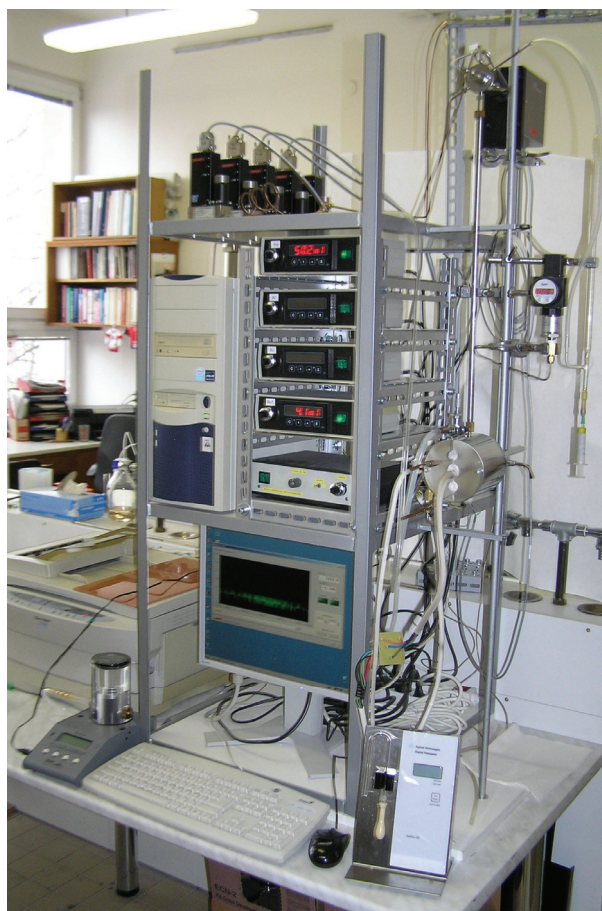
The hydrotreating  $\text{NiMo}/\gamma\text{-Al}_2\text{O}_3$  catalyst (12 wt% Mo and 1.1 wt% Ni) has been prepared by impregnation of the support with the Anderson-type heteropolyoxomolybdate  $(\text{NH}_4)_4[\text{Ni}(\text{OH})_6\text{Mo}_6\text{O}_{18}]$ . The modified catalysts have been synthesized by impregnation of the support with an aqueous solution of  $\text{H}_3\text{BO}_3$ ,  $\text{Co}(\text{NO}_3)_2$  or  $\text{Ni}(\text{NO}_3)_2$  before the deposition of heteropolyoxomolybdate. The addition of Co, Ni, or B has influenced both the phase

composition and catalytic activity of the 1-benzothiophene hydrodesulfurization reaction. Preliminary loading of Ni, Co or B increased the sulfidity of the NiMo/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts, which was confirmed by X-ray photoelectron micro-analysis. Nanoparticles of TiO<sub>2</sub>-ZrO<sub>2</sub> mixtures and tungsten-modified SBA-15 and HMS were studied for hydrotreating reactions. Acid-base properties of K-promoted (K,Ni)Mo/Al<sub>2</sub>O<sub>3</sub> catalyst and its activity in the sour water-gas shift were examined. [Refs. 3, 49, 50, 76]

### Transport characteristics of novel biocompatible materials

(K. Soukup, [soukup@icpf.cas.cz](mailto:soukup@icpf.cas.cz); supported by GACR, grant No. 106/11/P459)

The development and design of advanced bioactive and biocompatible porous materials for medical applications requires a thorough understanding of the texture and transport properties impact on their clinical efficiency. The proposed project will be focused on mass transport measurements and the transport characteristic determination of biocompatible clinical valuable materials consisted of apatite, hydroxyapatite and nanofiber membranes. Transport characteristics will be determined in liquid/solid as well as gas/solid systems by combination of inverse liquid chromatography and Graham's diffusion cell methods. Effective diffusion coefficients in liquid phase will be evaluated using a method based on the fitting of a set of experimental chromatographic profiles to the Kubín-Kučera model. Fitting of the gas diffusion data obtained from Graham's diffusion cell to the Mean Transport-Pore Model will provide transport characteristics. The obtained transport parameters will be compared with characteristics from standard textural analyses. [Refs. 81, 82, 84]



Inverse gas chromatography setup

## International co-operations

- University of Ghent, Ghent, Belgium: Theory of chemical bond, theoretical characterization of aromaticity
- Institut Scientifique de Service Public, Liege, Belgium: Transport characteristics for coal gasification
- University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity, molecular basis of structure activity relationships
- Institute of Catalysis, BAS, Sofia, Bulgaria: New heterogeneous catalysts for environmental protection
- University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
- University of Paris VI, Paris, France: Theory of chemical bond
- University of Poitiers, Poitiers, France: New catalysts for VOC elimination
- University of Strasbourg, Strasbourg, France: Determination of transport characteristics of novel materials with hierarchical pore structure
- University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
- University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
- Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes
- Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
- Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
- Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
- University of Kragujevac, Serbia: Multicenter bonding, quantitative characterization of aromaticity
- Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of Poly-HIPE materials
- University of Vigo, Vigo, Spain: Multicenter bonding, theoretical characterization of aromaticity
- Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
- University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
- University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
- UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
- University of Udine, Udine, Italy: Characterization of noble metal catalysts and desulfurization on unconventional catalysts
- Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
- Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes

## Visitors

- M. Boltz, University of Strasbourg, France
- L. Bučinský, Slovak Technical University Bratislava, Slovakia
- P. Bultinck, Ghent university, Belgium
- D. Cooper, University of Liverpool, United Kingdom

B. Corain, University of Padua, Italy  
P. Krajnc, University of Maribor, Slovenia  
P. G. Mezey, Memorial university of New Foundland, Canada  
M. Mitoraj, Jagellonian university Krakow, Poland  
S. Ojala, University of Oulu, Finland  
S. Pitkääho, University of Oulu, Finland  
A. Spojakina, Institute of catalysis, BAS, Sofia, Bulgaria  
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

## Teaching

P. Klusoň: UJEP, course "Toxicology"  
R. Ponec: CU, course "Structure and reactivity"  
O. Šolcová: ICT, postgraduate course "Texture of porous solids"

## Publications

### Original papers

- [1] Čapek P., Hejtmánek V., Kolafa J., Brabec L.: Transport Properties of Stochastically Reconstructed Porous Media with Improved Pore Connectivity. *Transp. Porous Media* 88(1), 87-106 (2011).
- [2] Černá I., Klusoň P., Bendová M., Floriš T., Pelantová H., Pekárek T.: Intensification of the Use of Ionic Liquids as Efficient Reaction Co-Solvents in Asymmetric Hydrogenations. *Chem. Eng.Process.* 50(3), 264-272 (2011).
- [3] Dimitrov L., Palcheva R., Spojakina A., Jirátová K.: Synthesis and Characterization of W-SBA-15 and W-HMS as Supports for HDS. *J. Porous Mat.* 18(4), 425-434 (2011).
- [4] Floriš T., Klusoň P., Slater M.: Stereoselective Hydrogenation of Methyl Acetoacetate over Structurally Different Chiral Ruthenium Complexes. *React. Kinet. Mech. Cat.* 102(1), 67-74 (2011).
- [5] Gaálová J., Topka P., Kaluža L., Šolcová O.: Gold versus Platinum on Ceria-Zirconia Mixed Oxides in Oxidation of Ethanol and Toluene. *Catal. Today* 175(1), 231-237 (2011).
- [6] Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dehalogenation of Polychlorinated Biphenyls (PCB) by Nucleophile Reactants at the Presence of Ionic Liquids and under Application of Microwaves. *Global NEST J.* 13(1), 59-64 (2011).
- [7] Kegl T., Ponec R., Kollar L.: Theoretical Insights into the Nature of Nickel-Carbon Dioxide Interactions in  $\text{Ni}(\text{PH}_3)_2(\eta^2\text{-CO}_2)$ . *J. Phys. Chem. A* 115(45), 12463-12473 (2011).
- [8] Klusoň P., Krýsa J., Malato S., Oller I.: Selected Contributions of the 6<sup>th</sup> European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications (SPEA 6), 13-16 June 2010, Introduction. *Catal. Today* 161(1), 2 (2011).
- [9] Klusoň P., Hejda S., Hejdová M., Krýsa J.: A Genuine Way to Mimic the Solar-Light Conditions in UV Driven Heterogeneous Photocatalytic Reactions. *Reac. Kinet. Mech. Cat.* 104(2), 273-280 (2011).
- [10] Klusoň P., Hejda S., Koudleková L., Hejdová M., Krýsa J.: Je možné objektivně srovnávat aktivitu heterogenních fotokatalytických reakcí? (Czech) Is it Possible to Compare Objectively Activities of Heterogeneous Photocatalysts in a Liquid Phase? *Chem. Listy* 105(10), 738-744 (2011).
- [11] Kment S., Hubička Z., Kmentová H., Klusoň P., Krýsa J., Gregora I., Morozová M., Čada M., Petráš D., Dytrych P., Slater M., Jastrabík L.: Photoelectrochemical Properties of Hierarchical Nanocomposite Structure: Carbon Nanofibers/TiO<sub>2</sub>/ZnO Thin Films. *Catal. Today* 161(1), 8-14 (2011).

- [12] Kočí K., Zatloukalová K., Obalová L., Krejčíková S., Lacný Z., Čapek L., Hospodková A., Šolcová O.: Wavelength Effect on Photocatalytic Reduction of CO<sub>2</sub> by Ag/TiO<sub>2</sub> Catalyst. *Chin. J. Catal.* 32(5SI), 812-815 (2011).
- [13] Kovačič S., Jeřábek K., Krajnc P.: Responsive Poly(acrylic acid) and Poly(N-isopropyl-acrylamide) Monoliths by High Internal Phase Emulsion (HIPE) Templating. *Macromol. Chem. Phys.* 212(19), 2151-2158 (2011).
- [14] Kovanda F., Jirátovej K.: Supported Layered Double Hydroxide-Related Mixed Oxides and Their Application in the Total Oxidation of Volatile Organic Compounds. *Appl. Clay Sci.* 53(2), 305-316 (2011).
- [15] Kovanda F., Jirátovej K.: Supported Mixed Oxide Catalysts for the Total Oxidation of Volatile Organic Compounds. *Catal. Today* 176(1), 110-115 (2011).
- [16] Matěj Z., Matějová L., Novotný F., Drahokoupil J., Kužel R.: Determination of Crystallite Size Distribution Histogram in Nanocrystalline Anatase Powders by XRD. *Z. Kristallogr. Proc.* 1, 87-92 (2011).
- [17] Morozová M., Klusoň P., Krýsa J., Dzik P., Veselý M., Šolcová O.: Thin TiO<sub>2</sub> Films Prepared by Inkjet Printing of the Reverse Micelles Sol-Gel Composition. *Sens. Actuator B-Chem.* 160(1), 371-378 (2011).
- [18] Morozová M., Klusoň P., Krýsa J., Gwenin Ch., Šolcová O.: Oxalic Acid Sensors Based on Sol-Gel Nanostructured TiO<sub>2</sub> Films. *J. Sol-Gel Sci. Technol.* 58(1), 175-181 (2011).
- [19] Obalová L., Jirátovej K., Karásková K., Kovanda F.: Simulation of N<sub>2</sub>O Abatement in Waste Gases by Its Decomposition over a K-Promoted Co-Mn-Al Mixed Oxide Catalyst. *Chin. J. Catal.* 32(5(SI)), 816-820 (2011).
- [20] Ojala S., Pitkäaho S., Laitinen T., Koivikko N.N., Brahmí R., Gaálová J., Matějová L., Kucherov A., Päivärinta S., Hirschmann C., Nevanperä T., Riihimäki M., Pirilä M., Keiski R.L.: Catalysis in VOC Abatement. *Top. Catal.* 54(16-18), 1224-1256 (2011).
- [21] Ponc R.: Bond Indices in Solids: Extended Analytical Model. *J. Comput. Chem.* 32(14), 3114-3121 (2011).
- [22] Salejová G., Grof Z., Šolcová O., Schneider P., Kosek J.: Strategy for Predicting Effective Transport Properties of Complex Porous Structures. *Comput. Chem. Eng.* 35(2), 200-211 (2011).
- [23] Soukup K., Rogut J., Grabowski J., Wiatowski M., Ludwik-Pardała M., Schneider P., Šolcová O.: Preparation and Microstructure Characterization of Iron Oxide Pellets for Hydrogen Storage. *Int. J. Systems Applications, Engineering & Development* 5(3), 334-341 (2011).
- [24] Šolcová O., Klusoň P., Soukup K., Krystyník P., Wimmerová L.: Texturní a transportní charakteristiky půdních vzorků v areálu bývalého chemického výrobního závodu Deza Ostrava. (Czech) Textural and Transport Characteristics of the Soil Samples from the Area of the Former Chemical Production Plant Deza Ostrava. *Waste Forum* 4(1), 42-49 (2011).
- [25] Šolcová O., Matějová L., Topka P., Musilová Z., Schneider P.: Comparison of Textural Information from Argon (87 K) and Nitrogen (77 K) Physisorption. *J. Porous Mat.* 18(5), 557-565 (2011).
- [26] Topka P., Karban J., Soukup K., Jirátovej K., Šolcová O.: Preparation of Al-SBA-15 Pellets with Low Amount of Additives: Effect of Binder Content on Texture and Mechanical Properties. Application to Friedel-Crafts Alkylation. *Chem. Eng. J.* 168(1), 433-440 (2011).
- [27] Vít Z., Kaluža L., Gulková D.: Nitrogen Tolerant Hydrodesulfurization Catalysts Based on Rh and Ru Promoted Mo/Al<sub>2</sub>O<sub>3</sub>. *Top. Catal.* 54(16-18), 1325-1330 (2011).
- [28] Vít Z., Kmentová H., Kaluža L., Gulková D., Boaro M.: Effect of Preparation of Pd and Pd-Pt Catalysts from Acid Leached Silica-Alumina on Their Activity in HDS of Thiophene and Benzothiophene. *Appl. Catal., B* 108(1-2), 152-160 (2011).



**Patents**

- [29] Jeřábek K., Hanková L., Holub L., Corain B., Zecca M., Centomo P., Bonato I.: Silně kyselý ionexový katalyzátor s afinitou k lipofilním reagentům a způsob jeho přípravy. (Czech) Strongly Acidic Ion Exchanger Catalysts Having Affinity towards Lipophilic Reagents and Method of Its Preparation. Pat. No. *PV2011-146*. Applied: 11.03.22.

**International conferences**

- [30] Baranov A.I., Kohout M., Ponec R.: Domain Averaged Fermi hole Orbitals for Extended Systems. Prague Workshop on Theoretical Chemistry, Book of Abstracts, p. 7-8, Praha, Czech Republic, 26-29 September 2011.
- [31] Barcs B., Kollár L., Ponec R., Kégl T.: Electronic Structure of Ni(0) Complexes Containing Ligands with Cumulative Double Bonds. Prague Workshop on Theoretical Chemistry, Book of Abstracts, p. 28-30, Praha, Czech Republic, 26-29 September 2011.
- [32] Centomo P., Bonato I., Hanková L., Holub L., Jeřábek K., Zecca M.: Ion Exchanger Catalyst Modification for Reactions Involving Lipophilic Reagents. XXIV Congresso Nazionale della Società Chimica Italiana, Atti del Congresso, p. 607, Lecce, Italy, 11-16 September 2011.
- [33] Čapek L., Smoláková L., Prielcel P., Kutálek P., Hájek M., Bulánek R., Kubičková I., Matějová L.: Analysis of Basic Sites at Solid-Base Catalysts. 4<sup>th</sup> International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 110, Riviera Resort, Bulgaria, 6-9 September 2011.
- [34] Čapek P., Veselý V., Kolafa J., Hejtmánek V., Brabec L.: Simulace transportu hmoty v replikách pórovitých látek pro účely odhadu jejich efektivních transportních vlastností. (Czech) Mass Transport Simulation in Replicas of Porous Material: Effective Transport Properties Estimation. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 25 (B1.2), Srní, Šumava, Czech Republic, 24-27 October 2011.
- [35] Dytrych P., Klusoň P., Floriš T., Lísal M., Slater M.: Theoretical Interpretation of Enantioselectivity Trends in (*R*)-Ru-BINAP Catalyzed Hydrogenation of Methylacetoacetate in the QAS Ionic Liquid Phase. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 35 (C1.5), Srní, Šumava, Czech Republic, 24-27 October 2011.
- [36] Gaálová J., Kaluža L., Topka P.: New Catalysts for VOC Oxidation Based on Ce-Zr Mixed Oxides. 25<sup>th</sup> National Chemistry Congress, Abstracts Book for Poster Presentations, p. 208 (OP-183), Ankara, Turkey, 27 June - 2 July 2011.
- [37] Gaálová J., Kaluža L., Topka P., Matějová L.: Total Oxidation of Ethanol and Dichloromethane over Ceria-Zirconia Mixed Oxides Doped with Platinum and Gold. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1302-1303, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [38] Gulková D., Vít Z.: Inhibitive Effect of Pyridine and Toluene on HDS of Thiophene over Mo/Al<sub>2</sub>O<sub>3</sub> Based Catalysts. 43. Symposium on Catalysis, Program Book of Abstracts, P06A, Prague, Czech Republic, 7-8 November 2011.
- [39] Gulková D., Vít Z., Kaluža L., Kmentová H., Zdražil M., Boaro M.: Activity of Pd and Mo HDS Catalysts Supported on Modified Silica-Alumina. 8<sup>th</sup> European Congress of Chemical Engineering, P 19.06, Berlin, Germany, 25-29 September 2011.
- [40] Hanková L., Holub L., Jeřábek K.: Ion Exchanger Catalyst Modification for Reactions Involving Lipophilic Reagents. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1190-1192, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [41] Hanková L., Jeřábek K.: Modeling of Swollen State Morphology of Functional Polymers. 9<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 031, Santiago de Compostella, Spain, 17-22 July 2011.

- [42] Hejtmánek V., Čapek P.: 3D Microstructure Modelling of Real Porous Steel Material from 2D Images. 7<sup>th</sup> International Conference on Porous Metals and Metallic Foams MetFoam2011, Abstracts Book, p. 269, Busan, South Korea, 18-21 September 2011.
- [43] Jeřábek K., Holub L., Hanková L., Corain B., Centomo P.: Adsorption Assisted Ion Exchanger Catalyst for Fatty Acid Esterification. 19<sup>th</sup> IUPAC International Conference on Chemical Research Applied to World Needs (CHEMRAWN XIX) 2011, Programme and Abstracts, p. 18, Kuala Lumpur, Malaysia, 27-29 September 2011.
- [44] Jeřábek K., Holub L., Hanková L., Corain B., Centomo P., Zecca M.: Adsorption Assisted Ion Exchanger Catalyst for Fatty Acid Esterification. 43<sup>th</sup> Symposium on Catalysis, Book of Abstracts, OP14, Praha, Czech Republic, 7-8 November 2011.
- [45] Jiráková K., Kovanda F.: Total Oxidation of Toluene over Calcined Layered Double Hydroxides Containing Various Transition Metals. European Clay Conference EUROCLAY 2011, Book of Abstracts, p. 345, Antalya, Turkey, 26 June - 1 July 2011.
- [46] Jiráková K., Mikulová Z., Klempa J., Kovanda F.: Modification of Calcined Ni-Mg-Mn and Co-Mn-Al LDHs with Platinum: Properties and Activity in Total Oxidation of VOC. Europacat X, PM111, Glasgow, Great Britain, 29 August - 2 September 2011.
- [47] Kaluža L., Gaálová J., Topka P., Matějová L., Gulková D.: Total Oxidation of Model Volatile Organic Compounds over Ceria-Zirconia Mixed Oxides Doped with Platinum and Gold. 8<sup>th</sup> European Congress of Chemical Engineering, P05.01, Berlin, Germany, 25-29 September 2011.
- [48] Kaluža L., Kubička D.: Hydrodeoxygenation of Rapeseed Oil over Sulfided Ni, Mo and NiMo Catalysts. 8<sup>th</sup> European Congress of Chemical Engineering, P20.01, Berlin, Germany, 25-29 September 2011.
- [49] Kaluža L., Palcheva R., Spojakina A., Jiráková K., Tyuliev G.: Hydrodesulfurization Activity of Alumina Supported Anderson Heteropolymolybdates Doped with Co, Ni and B. Europacat X, Posters, PT63, Glasgow, Great Britain, 29 August - 2 September 2011.
- [50] Kaluža L., Palcheva R., Spojakina A., Jiráková K., Tyuliev G.: Alumina Modified with Co, Ni and B as a Support of Hydrodesulfurization Catalysts Prepared from Anderson Heteropolymolybdates. 43<sup>th</sup> Symposium on Catalysis, Book of Abstracts, P12A, Prague, Czech Republic, 7-8 November 2011.
- [51] Kaluža L., Sýkora J., Karban J., Žáček P., Vít Z., Zdražil M.: Hydrodesulfurization of Model Feed Containing Olefins over Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, and ZrO<sub>2</sub> Supported Transition Metal Sulfides. 8<sup>th</sup> European Congress of Chemical Engineering, Programme, P19.01, Berlin, Germany, 25-29 September 2011.
- [52] Karásková K., Chromčáková Ž., Študentová S., Obalová L., Jiráková K.: Co-Mn-Al Mixed Oxide Supported on TiO<sub>2</sub> for N<sub>2</sub>O Decomposition. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, p. 155, Zakopane, Poland, 4-7 September 2011.
- [53] Karásková K., Kulová T., Obalová L., Jiráková K., Kovanda F.: Alkali Metals Promoted Co-Mn-Al Mixed Oxide for N<sub>2</sub>O Catalytic Decomposition. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1304-1309, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [54] Kaštanek F.: Biotechnologie pro chemický průmysl. (Czech) Biotechnology for Chemical Industry. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 99 (C4.1), Srní, Šumava, Czech Republic, 24-27 October 2011.
- [55] Kaštanek F., Sobek J., Kaštanek P., Šolcová O., Hájek M.: Dehalogenation of Polyhalogenated Compounds Dissolved in Organic Solvents with the Help of AOPs in a Two-Phase Solvent-Water System under the Influence of Ultrasound. 12<sup>th</sup> International Conference on Environmental Science and Technology CEST 2011, Proceedings, p. 114, Dodecanese, Rhodes Island, Greece, 8-10 September 2011.
- [56] Klusůň P., Hejda S.: Critical Notes on Heterogeneous Photocatalysis on TiO<sub>2</sub> Photocatalysts. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 52 (C2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

- [57] Kočí K., Krejčíková S., Lacný Z., Šolcová O., Obalová L.: Photocatalytic Decomposition of N<sub>2</sub>O on Ag-TiO<sub>2</sub>. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, pp. 159-161, Zakopane, Poland, 4-7 September 2011.
- [58] Krejčíková S., Kočí K., Obalová L., Čapek L., Šolcová O.: Optimized Doped Titania for Photocatalysis Applications. 2<sup>nd</sup> Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 54 (PP-6), Ostrava, Czech Republic, 27-29 April 2011.
- [59] Krejčíková S., Maléterová Y., Matěj Z., Šolcová O.: Preparation and Characterization of Doped Titania Layers for Polluted Water Cleaning. 9<sup>th</sup> International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 78, Dresden, Germany, 5-8 June 2011.
- [60] Krejčíková S., Maléterová Y., Šnajdaufová H., Šolcová O.: Doped Titania Photocatalysts for Poluted Water Cleaning; Preparation and Characterization. 9<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 031, Santiago de Compostela, Spain, 17-22 July 2011.
- [61] Ludvíková J., Jiráková K., Klempa J.: Titania Supported Co-Mn-Al Catalysts in Total Oxidation of Ethanol. 4<sup>th</sup> Czech-Italian-Spanish Symposium on Molecular Sieves and Catalysis, Book of Abstracts, O21, Liblice, Czech Republic, 15-18 June 2011.
- [62] Ludvíková J., Jiráková K., Kovanda F.: Mixed Oxides of Transition Metals as Catalysts for Total Ethanol Oxidation. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 231, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [63] Ludvíková J., Jiráková K., Kovanda F., Klempa J.: Úplná oxidace organických látek obsažených ve vzduchu na oxidických katalyzátorech. (Czech) Total Oxidation of Organic Compounds in Air over Oxide Catalysts. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 692-697, Kouty nad Desnou, Czech Republic, 11-13 April 2011.
- [64] Maléterová Y., Krejčíková S., Šnajdaufová H., Cajthaml T., Šolcová O.: Comparison of Various Titania Photocatalysts by the Contaminated Water Cleaning. 9<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 032, Santiago de Compostella, Spain, 17-22 July 2011.
- [65] Matějová L., Fajgar R., Matěj Z., Maléterová Y., Šolcová O.: Metal Oxide Aerogel. 2<sup>nd</sup> Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 11(OP-5), Ostrava, Czech Republic, 27-29 April 2011.
- [66] Matějová L., Matěj Z., Fajgar R., Schneider P., Šolcová O.: Highly-Porous Metal Oxide Aerogels; Preparation and Characterization. 9<sup>th</sup> International Symposium on Characterization of Porous Solids - COPS 9, Book of Abstracts, p. 181, Dresden, Germany, 5-8 June 2011.
- [67] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Water Extraction in Crystallization of Highly-Porous Titania, Titania-Zirconia and Titania-Ceria Aerogels. 12<sup>th</sup> Conference of the European Ceramic Society ECerS XII, Poster Session II, p. 72 (2132), Stockholm, Sweden, 19-23 June 2011.
- [68] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Drying in Preparation of Crystalline Metal Oxides Aerogels. 4<sup>th</sup> International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 72, Riviera Resort, Bulgaria, 6-9 September 2011.
- [69] Matějová L., Šnajdaufová H., Matějková M., Fajgar R., Matěj Z., Šolcová O.: Optimization of Pressurized Fluid Extraction for Preparation of Metal Oxide Nanostructures. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, pp. 1207-1210, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [70] Morozová M., Klusoň P., Dzik P., Veselý M., Krýsa J., Šolcová O.: Thin Sol-Gel TiO<sub>2</sub> Films Prepared by Inkjet Printing – Photoelectrochemical Properties. 4<sup>th</sup> Czech-Austrian Workshop: New Trends in Photo- and Electro- Catalysis, Hnanice, Czech Republic, 5-7 December 2011.

- [71] Morozová M., Klusoň P., Hejda S., Kment Š., Šolcová O.: Thin Functional Films of TiO<sub>2</sub> Nanoparticles. 44<sup>th</sup> Heyrovský Discussion - Nanostructures on Electrodes, Book of Abstracts, p. 56, Třešť, Czech Republic, 26-30 June 2011.
- [72] Morozová M., Klusoň P., Krýsa J., Veselý V., Dzik P., Šolcová O.: Thin TiO<sub>2</sub> Sol-gel Layers Deposited by Three Various Methods. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, pp. 1211-1213, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [73] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: The Ink-Jet Printed Nanostructured TiO<sub>2</sub> Film Electrode. 2<sup>nd</sup> Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 12 (OP-6), Ostrava, Czech Republic, 27-29 April 2011.
- [74] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: Photo-Electrochemistry on the Thin TiO<sub>2</sub> Sol-Gel Layers Deposited by Ink-Jet Printing. 12<sup>th</sup> Conference of the European Ceramic Society ECerS XII, Poster Session II, p. 72 (2133), Stockholm, Sweden, 19-23 June 2011.
- [75] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: Photo-Electrochemical Characterization of Thin TiO<sub>2</sub> Sol-Gel Layers Deposited by Dip-Coating and Injekt Printing. 9<sup>th</sup> International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 99, Dresden, Germany, 5-8 June 2011.
- [76] Nikolova D., Edreva-Kardjieva R., Spojakina A., Jiráťová K.: Potassium Influence on Acid-Base Properties of the Sour Water-Gas Shift (K,Ni)Mo/γ-Al<sub>2</sub>O<sub>3</sub> Catalysts. Europacat X, Posters, PM271, Glasgow, Great Britain, 29 August - 02 September 2011.
- [77] Obalová L., Jiráťová K., Kovanda F.: NO<sub>2</sub> Catalytic Decomposition - from Laboratory Experiment to Industry Reactor. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, p. 97, Zakopane, Poland, 04-07 September 2011.
- [78] Ponec R., Cooper D.L.: Splitting and/or Formation of Chemical Bonds. Insights from Momentum Space. 4<sup>th</sup> JCS Symposium on Theoretical Chemistry 2011, Conference Book, p. 1, Liblice, Czech Republic, 18-20 May 2011.
- [79] Ponec R., Kohout M.: Bond Indices in Solids. A Numerical Approach to Analytical Model. Prague Workshop on Theoretical Chemistry, Book of Abstracts, pp. 44-50, p. 7, Praha, Czech Republic, 26-29 September 2011.
- [80] Ponec R., Salvador P., Ramos-Córdoba E.: Bonding Quandary in Cu<sub>3</sub>S<sub>2</sub> Core. Insights from the Analysis of Domain Averaged Fermi holes and the Analysis of the Local Spin. 9<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists, Posters, PI 037, Santiago de Compostella, Spain, 17-22 July 2011.
- [81] Soukup K., Klusoň P., Šolcová O.: Electrospun Polymer Nanofibers-Gas Transport Measurements in Graham's Diffusion Cell. 8<sup>th</sup> European Congress of Chemical Engineering, Programme, P05.08, Berlin, Germany, 25-29 September 2011.
- [82] Soukup K., Petráš D., Topka P., Slobodian P., Šolcová O.: Preparation and Characterization of Electrospun Poly(p-phenylene oxide) Membranes. 10<sup>th</sup> International Conference on Catalysis in Membrane Reactors, Book of Abstracts, pp. 210-211, Saint-Petersburg, Russia, 20-24 June 2011.
- [83] Soukup K., Stanczyk K., Rogut J., Schneider P., Šolcová O.: Effect of Process Parameters on the Mass Transport Phenomena during Underground Coal Gasification. 4<sup>th</sup> International Conference GeoProc2011: Cross Boundaries Through THMC Integration, Conference Program, GP036, (6 pp. full text on CD-ROM), Perth, Australia, 6-9 July 2011.
- [84] Soukup K., Topka P., Petráš D., Šolcová O.: Transportní a katalytické vlastnosti polymerních nanovlákných vrstev připravených technikou elektrostatičkého zvlákňování. (Czech) Transport and Catalytic Properties of Polymeric Nanofibrous Layers Prepared by Electrospinning. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 53 (C2.3), Srní, Šumava, Czech Republic, 24-27 October 2011.

- [85] Šolcová O., Cajthaml T., Krejčíková S., Kaštánek F., Maléřová Y.: Application of Titania Thin Layers for Contaminated Water Cleaning. 9<sup>th</sup> International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 84, Dresden, Germany, 5-8 June 2011.
- [86] Šolcová O., Maléřová Y., Šnajdaufová H., Krejčíková S.: Thorough Characterization of Prepared TiO<sub>2</sub> - ZrO<sub>2</sub> Mixed Oxides for Photocatalytic Oxidation. 9<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 035, Santiago de Compostella, Spain, 17-22 July 2011.
- [87] Topka P., Kaluža L., Gaálová J.: Total Oxidation of Ethanol and Toluene over Platinum and Gold Supported on Ceria-Zirconia Mixed Oxide. 6<sup>th</sup> Asia Pacific Chemical Reaction Engineering Symposium, Abstract Coll., p. 127, Beijing, China, 18-21 September 2011.
- [88] Vajglová Z., Vychodilová H., Kotas P., Kaštánek F., Jiříčný V.: Degradace polybromovaných difenyl éterů. (Czech) Degradation of Polybrominated Diphenyl Ethers. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 698-704, Kouty nad Desnou, Czech Republic, 11-13 April 2011.
- [89] Vajglová Z., Vychodilová H., Tříška J., Kaštánek F., Jiříčný V.: Degradation Methods for Polybrominated Diphenyl Ethers in Liquid Wastes. 38<sup>th</sup> International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 141-145, Tatranské Matliare, Slovakia, 23-27 May 2011.
- [90] Vajglová Z., Vychodilová H., Křišťál J., Kaštánek F., Jiříčný V.: Selected Methods of Dehalogenation of Polybrominated Diphenyl Ethers. 8<sup>th</sup> European Congress of Chemical Engineering, Programme, P05.04, Berlin, Germany, 25-29 September 2011.
- [91] Vít Z., Kmentová H., Gulková D., Kaluža L.: Mesoporous Silica-Alumina Modified by Acid Extraction as Support of Pd and Pd-Pt Catalysts in HDS of Model Compounds. 43<sup>th</sup> Symposium on Catalysis, Program and Book of Abstracts, P16B, Prague, Czech Republic, 7-8 November 2011.
- [92] Vít Z., Kmentová H., Gulková D., Kaluža L.: Mesoporous Silica-Alumina Modified by Acid Extraction as Support of Pd and Pd-Pt Catalysts in HDS of Model Compounds. Europacat X, Posters, PT28, Glasgow, Great Britain, 29 August - 2 September 2011.