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HELENA SOUČKOVÁ

Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N_2O
- 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
- Unconventional preparation of supported molybdenum catalysts
- Preparation and characterization of electrospun nanofibrous membranes

Applied research

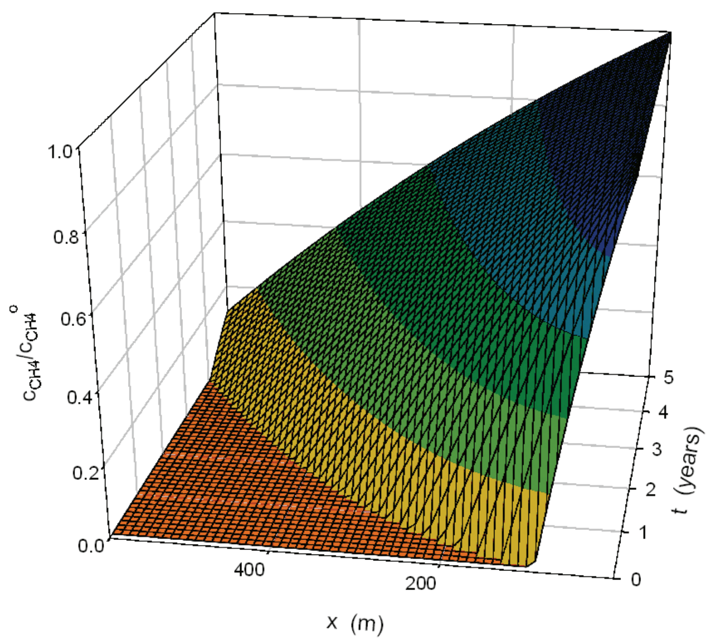
- Catalytic combustion of volatile organic compounds
- Esterification of free fatty acids in low-cost raw materials for biodiesel production
- Oxidation processes for environment
- Textural characteristics of structural materials

Research projects

Hydrogen oriented underground coal gasification for Europe

(O. Šolcová, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00006)

Project explores technology for hydrogen production through underground gasification of coal in a dynamic geo-reactor. Process is controlled through purposed dynamic changes in temperature and pressure of the reactants and products. The project addresses CBM usage and CO_2 sequestration in coal deposits. The environmental fingerprint of the technology on air, water and strata stability is evaluated. Locations of demonstration plants are chosen through computer modelling and simulation. Large scale production of hydrogen from coal is crucial for coal mining industries and will serve the needs of energy, chemistry and transportation sectors of Europe. [Refs. 27, 47, 110-112]

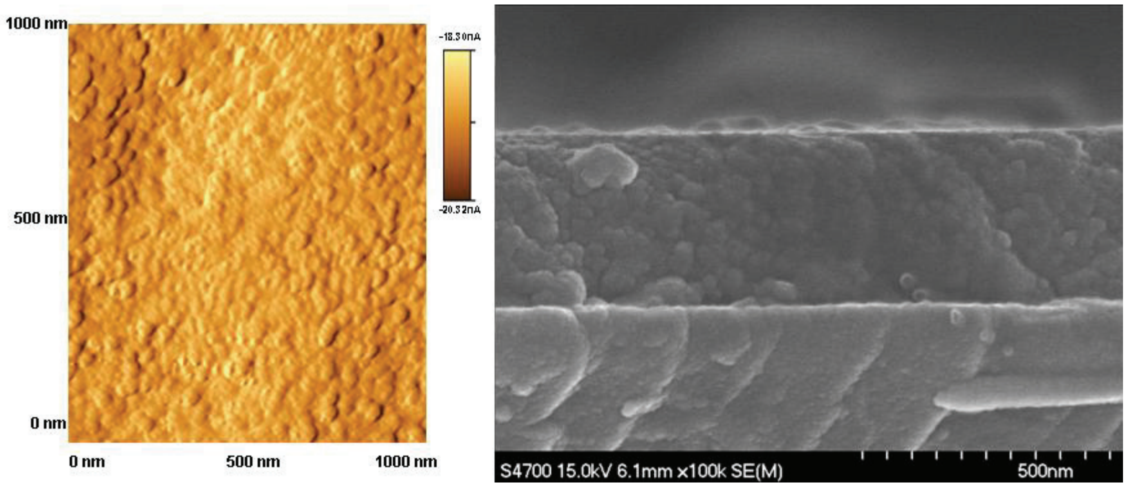


Gas transport through the porous stratum

Hierarchic nanosystems for microelectronics

(O. Šolcová, 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, project No. KAN400720701)

Project develops the complex composite systems with precisely defined performance applicable in microelectronics. The individual components are formed by small arranged particles which ensure partial function inevitable for functioning of the whole system. These composite structures should be directly applicable as elements of special sensors, photoelectric energy sources, microelectrodes for analytic instruments etc. The general aim of the project is the accumulation of sufficient amount of high-quality experimental data to be applied for design and implementation of practical nanotechnologies. Professionally, this project is focused on the study of preparation of hierarchic nanostructures, inclusive the structural and functional characterization, as well as on prediction of properties by means of mathematical modelling. [Refs. 5, 13-15, 21, 31, 37, 43, 73, 82, 95, 100]



Detail of a sensor surface

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

(O. Šolcová, joint project with Dekonta, a.s., supported by MIT, grant No. FR-TI1/059)

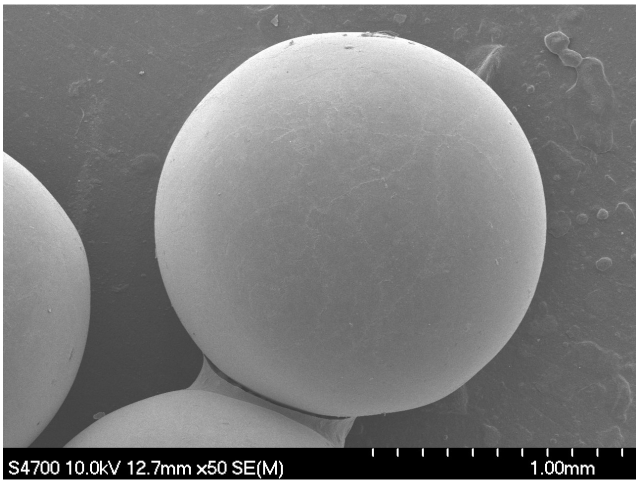
Project develops and verifies a new technology for decontamination of solid waste containing toxic organic substances, which is based on treatment of waste by the thermal desorption process and a subsequent catalytic oxidation of desorbed organic contaminants. Research activities aimed at solution of some technical problems related to full-scale application of the developed technology will be realized together with testing under real conditions. [Refs. 10, 12, 48, 50, 51, 80, 81, 115]

Pilot unit for catalytic oxidation of desorbed organic contaminants

Advanced photocatalytic processes - nanotechnology for environment

(O. Šolcova, joint project with Institute of Microbiology of the ASCR, v. v. i., and UPCE, supported by GACR, grant No. GA104/09/0694)

This project is focused on preparation and characterization of specially designed photo-active materials and their utilization for decomposition of a large series of potential water contaminants ranging from phenols, chlorinated phenols, polybrominated diphenyl ethers and alcohols to herbicides, pesticides, pharmaceuticals, industrial colourants, pigments and dyes. The special focus is devoted to design the reactor system; selectively prepared photo-active nanostructures together with design the effective photoreactors including mathematical modelling of involved physical and chemical processes and generalization of obtained results. [Refs. 3, 11, 19, 36, 89, 91, 101, 116]



Supported titania nanocrystals for water treatment

Advanced catalytic processes and materials

(J. Hanika, O. Šolcová, joint project with JH IPC, ICT, CU, and UPCE, supported by GACR, grant No. GD203/08/H032)

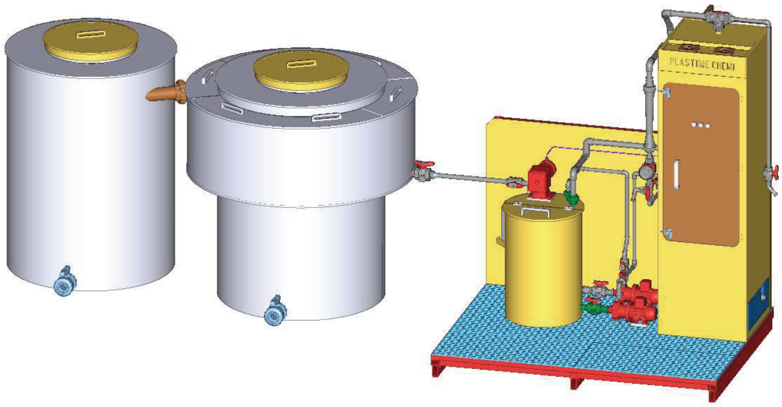
This project is aimed at development of the new selective catalytic and separation processes for preparation of special compounds and materials which can give progression in the field of the new chemical technologies. Processes in question are stereoselective and regioselective transformations on chiral catalytic centres and processes with significant environmental impact. Coordination of thesis projects is planned in the field of catalysis, e.g., developed Rh catalysts can be tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts can be tested in organic synthesis (ICT, UPCE, ICPF), oxidation polymerization (CU) and synthesis of chemical specialties (JH IPC); new mesoporous materials prepared at JH IPC will be used in all other partner laboratories, etc. [Refs. 18, 23, 38, 44, 46, 61, 62, 83-85, 90, 92, 93, 102, 117, 118]

Newly designed nanoadsorbents for photocatalysis

Reactive chemical barriers for decontamination of heavily polluted waters

(P. Klusoň, joint project with Dekonta a.s., supported by MIT, grant No. FR-TI1/065)

This project aims at the practical development of special oxidation processes used for decontamination of industrially polluted subsurface waters. The used methods are: 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 are now tested on a laboratory scale, in parallel they will be modified and scaled-up for practical testing on three selected industrial sites. The efficiencies of the chosen methodologies will be compared and the most suitable one will be implemented to the final form that will be produced and long-term tested. [Refs. 24, 30, 52, 53, 59, 68]

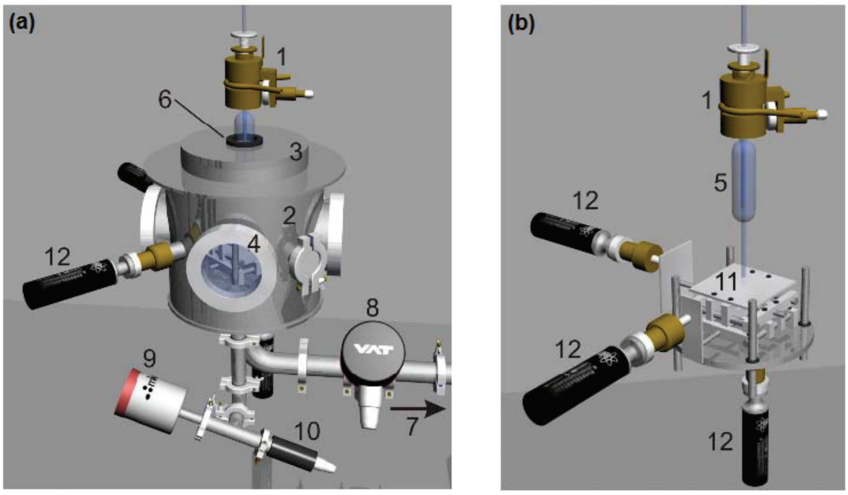


Scheme of the chemical barrier decontamination system

Composed molecular templates for preparation of assembled functional nanoparticles

(P. Klusoň, 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 later also scientific concepts. Currently such attempts are reflected in the steep growth of interest in nanoscience and nanotechnologies. Although there has already been much progress in the synthesis, assembly and fabrication of nanomaterials, their potential applications in a wider range of practical technologies are still rare. These 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. 6, 16, 17, 49, 54, 60, 63, 103]

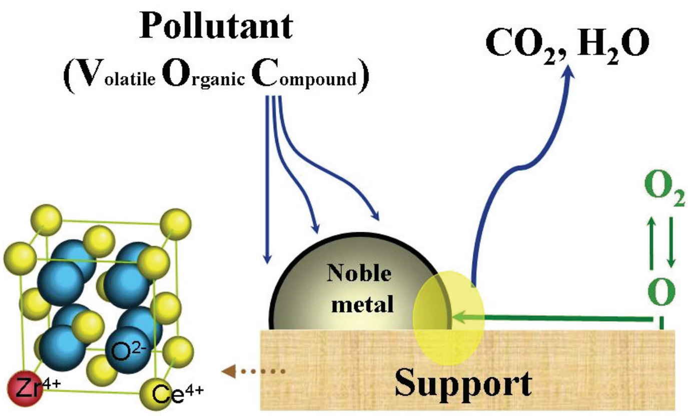


Experimental set-up: (a) surfatron plasma source, (b) inside facility of the chamber

New catalysts for VOC oxidation

(J. Gaálová, joint project with Department of Process and Environmental Engineering, University of Oulu, Finland, supported by ASCR, grant No. M200720901)

The aim of this project is development of catalyst for oxidation of the volatile organic compounds (VOCs) based on noble metals. Ceria-zirconia mixed oxides attracted special attention due to their unique property of storing and releasing oxygen and excellent thermal and mechanical resistance. Platinum catalysts supported on Ce-Zr mixed oxides that were recently developed in this project exhibited comparable performance to commercial catalysts even with lower Pt loading. On the other hand, gold supported on Ce-Zr mixed oxides proved better selectivity to CO_2 than its platinum and commercial analogues, with activity being only slightly worse. Tailored synthesis of monolithic catalysts based on these systems will be studied in near future. [Refs. 42, 65, 114]

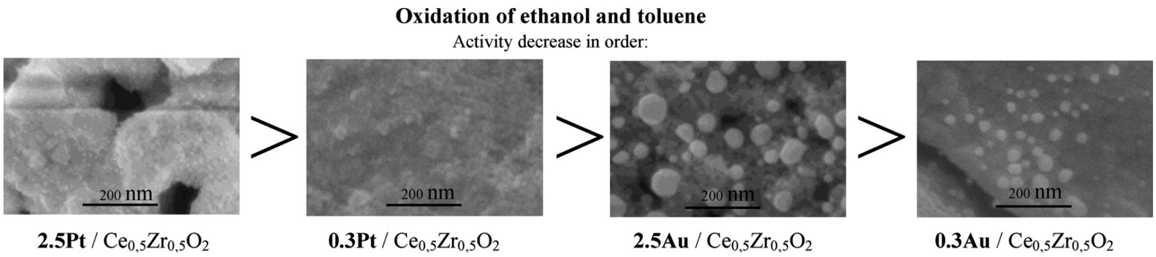


The Ce-Zr mixed oxide as support for noble metal in oxidation of VOC

Development of oxide catalysts for total oxidation of ethanol

(J. Gaálová, supported by GACR, grant No. P106/10/P019)

This project is focused on development of catalysts with higher activity and selectivity for ethanol oxidation to CO_2 than those studied previously. Importance of the project contributions is underlined by taking advantages from analogies between ethanol and other volatile organic compounds (VOC), and multiple the use of those materials. The research investigates the expansion of information about activity of mixed oxide based catalysts and effect of their promoters in VOC oxidation. Project clarifies selectivity of the catalytic materials. Predications of the new directions about their preparation and composition are formulated, which could helps to solve important environmental problem. [Refs. 34, 66, 106]

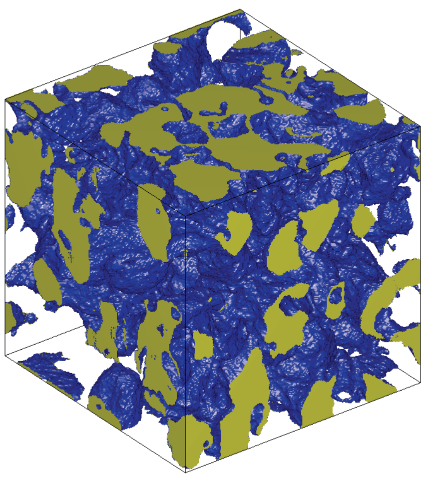


Activity of the Ce-Zr mixed oxides as supports for Pt and Au in oxidation of ethanol and toluene

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

(V. Hejtmánek, joint project with JH IPC and ICT, supported by GACR, grant No. GA203/09/1353)

Aromatic polyimides (PI) exhibit very good chemical and mechanical stability up to 250 ºC. They also exhibit a high selectivity for membrane separation of small molecules as hydrogen. The main drawback PI membranes preventing their wide application, e.g. in membrane reactors is a very low species flow. The principal goal of the project is thus, enhancement of species flow without essential deterioration of the selectivity. The approaches considered to enhance species flow through membranes are: (i) thinning of the PI layer upon introducing porous supports or armour, (ii) formation of PI layer upon radial stress, (iii) producing local stress fields by introducing inclusions, (iv) introducing porous inclusions at concentrations near to percolation threshold. To optimize two-phase membrane composition, it is intended to perform a rigorous treatment of mass transport in composite media using image analysis together with computer experiment. [Refs. 2, 57, 58, 64, 69, 70]

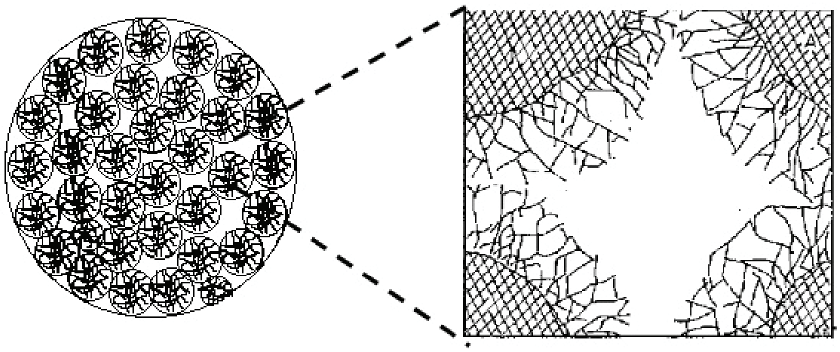


The zeolite-polyimide membrane replica (64×64×64 μm). Polyimide phase is transparent, polyimide-silicalite interface is blue and intersections of the silicalite phase and the cut planes are yellow

Functional macroreticular polymers as catalyst carriers

(K. Jeřábek, joint project with Department of Chemical Sciences, University of Padua, 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. Methods for modification of porous structure of functional polymers by additional post polymerization cross-linking were also studied. In starting stages is the investigation of modification of chemical nature of polymer catalyst carriers for applications in highly lipophilic environment. [Refs. 7, 28, 71, 72, 74, 75]

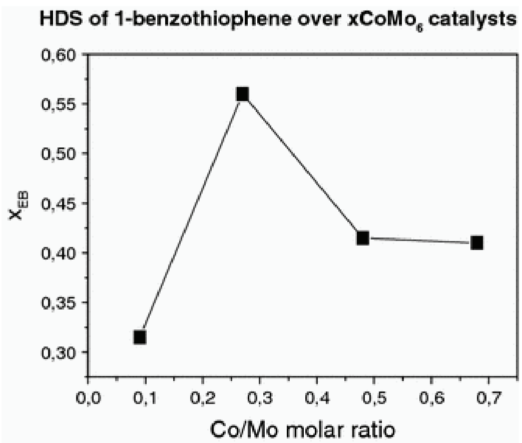


Schematic depiction of macroreticular polymer morphology

Synergistic effects in hydrodesulfurization and oxidation reactions

(K. Jirátová, bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria, supported by ASCR)

The effect of cobalt amount on hydrodesulfurization activity of Al_2O_3-supported hetero-molybdate was studied, as well as the effect of various supports (TiO_2-ZrO_2 mixtures, tungsten-modified SBA-15 and HMS). [Refs. 20, 25, 29, 33]

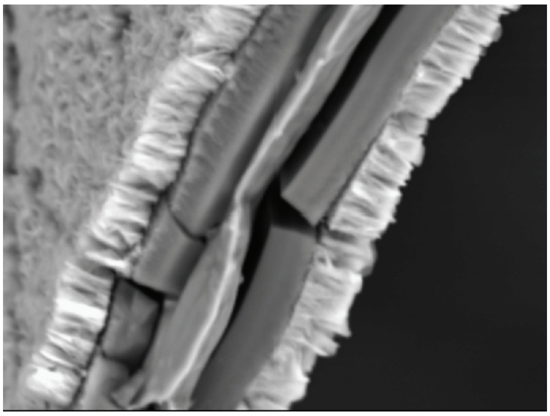


Effect of Co on HDS activity of alumina-supported heteropolymolybdate

Deposition of oxide catalysts for oxidation of VOC onto preformed support and their modification by nanoparticles of noble metals

(K. Jirátová, joint project with ICT, and IIC, supported by GACR, grant No. GA104/07/1400)

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, activity of the resulting mixed oxides in ethanol oxidation was also examined in detail. [Refs. 35, 39, 40, 76, 77, 86-88, 94, 105]

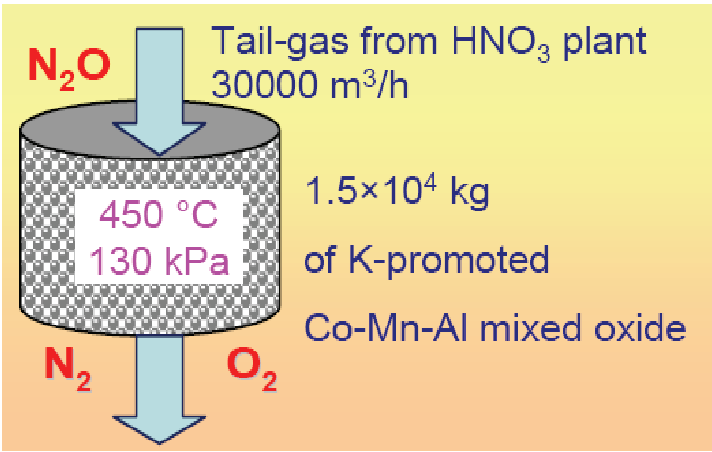


SEM of Co-(Mn)-Al catalyst precursor of LDH type grown on an oxidized Al foil

Supported oxidic catalysts containing low amount of active species as catalysts for N_2O decomposition

(K. Jirátová, joint project with TU of Ostrava, and ICT, supported by GACR, grant No. GA106/09/1664)

The effect of promoter addition to the calcined Co-Mn-Al LDH-like compounds on the catalyst activity in decomposition of N_2O was studied. Potassium was found to be the best promoter of the catalyst. Abatement of N_2O in waste by its decomposition over K-promoted Co-Mn-Al mixed oxide catalyst was simulated. [Refs. 9, 104]

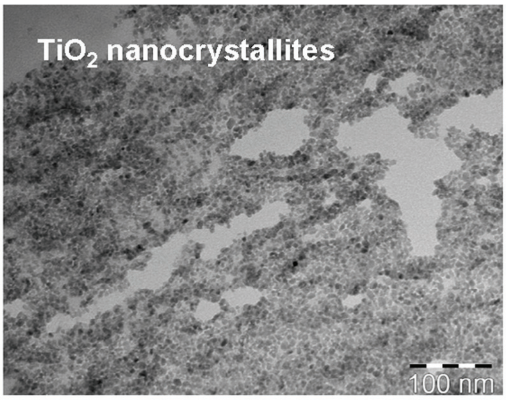


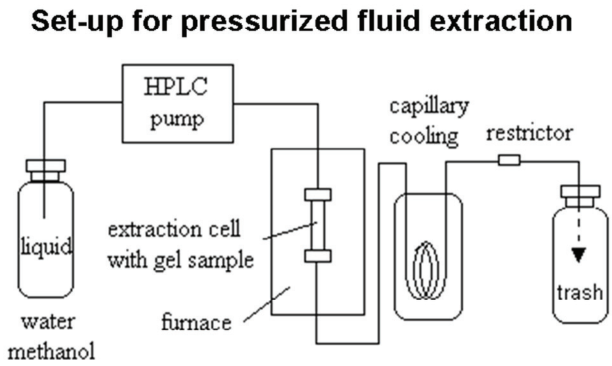
A K-promoted Co-Mn-Al mixed oxide catalyst derived from a layered double hydroxide (LDH)

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

(L. Matějová, supported by GACR, grant No. GP104/09/P290)

Project deals with development and optimization of extraction technique for purification and total crystallization prepared oxidic materials with high-ordered mesoporous structure. Developed extraction technique using fluids in supercritical and subcritical state was generally applicable for synthesis of nanocrystalline metal oxides. The optimal experimental conditions (temperature, pressure, flow rate, etc.) as same as the suitable solvents were defined and evaluated also with respect to future technical and economic realization of methodology. High-ordered mesoporous metal oxides (hexagonal, cubic, lamellar) TiO_2, ZrO_2, SiO_2/TiO_2, ZrO_2/TiO_2, CeO_2, Nb_2O_5, Ta_2O_5, SnO_2 promising in photocatalysis and sandwich structures in microelectronic were synthesized by templating using amphiphilic and ionic surfactants in aqueous and alcoholic solution with metal chloride and alkoxide. [Refs. 22, 41, 96-99, 113]



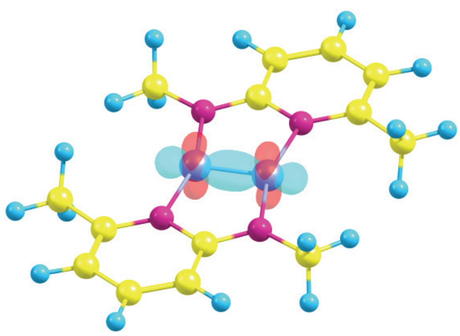


TiO_2 nanocrystallites; set-up for pressurized fluid extraction and purification

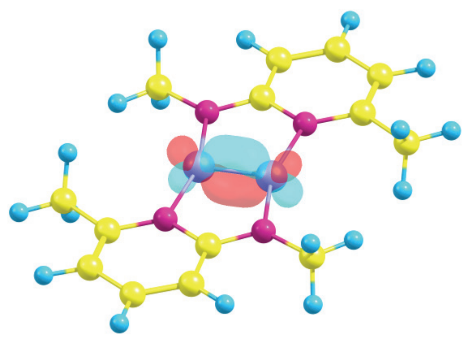
Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, supported by GACR grant No. 203/09/0118)

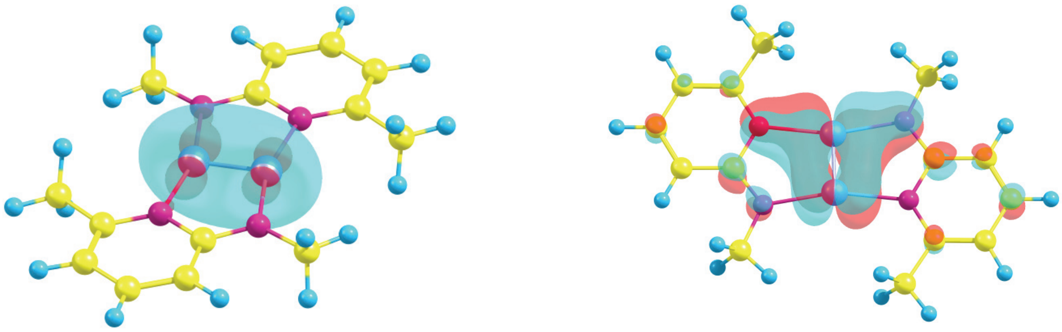
The project is a part of longer-term efforts at the systematic exploitation of the pair density as new source of the information about the molecular structure and nature of chemical bond. This density represents the basic theoretical quantity allowing us to describe the behaviour of electron pairs in 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 (DAFH) 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, multicentre 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. 1, 4, 26, 45, 55, 56, 107-109]



a) 0.982



b) 0.996



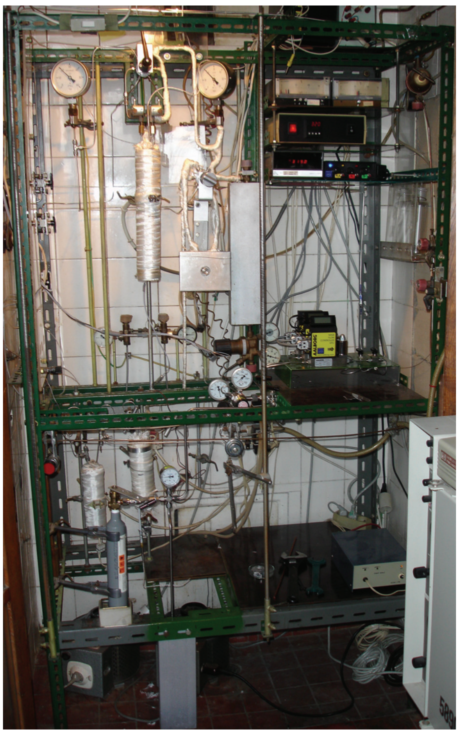
c) 0.928 d) 0.909

Results of DAFH analysis for the studied complex with multiple Cr-Cr bond. Selected eigenvectors (and associated eigenvalues) of the Fermi holes corresponding to broken valences of Cr-Cr bond for the holes averaged over the domain involving one Cr atom respectively

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

(Z. Vít, supported by GACR, grant No. 104/09/0751)

Alternative supports and active phases for hydrodesulfurization (HDS) were studied. Mesoporous silica-aluminas modified by acid extraction were studied as supports of Pt and Pd catalysts. The extraction led to higher surface areas and Brønsted acidities of supports which improved the HDS activity of Pt and Pd catalysts. Rh sulfide deposited on different alumina supports and CoMo catalysts prepared from the heteromolybdate precursors were studied in HDS of thiophene. The HDS and hydrogenation activities of different transition metal sulfides deposited on alumina, titania and zirconia were studied in reactions of benzothiophene and 1-methylcyclohexene. Inhibition effect of pyridine on HDS of thiophene was studied on Rh and Ru promoted Mo/alumina catalysts. [Refs. 8, 32, 67, 78, 79, 119, 120].



Microreactor with fixed bed of catalyst

International co-operations

Bangor University, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
Catholic University of Louvain, Louvain-la-Neuve, Belgium: Development of VOC oxidation catalysts
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
European Membrane Institute, Montpellier, France: Synthetic porphyrites
Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of Poly-HIPE materials
Institute of Catalysis, Sofia, Bulgaria: Synergistic effects in hydrodesulfurization and oxidation reactions
Institute of Computational Chemistry, University of Girona, Girona, Spain: Theory of chemical bond
Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes
Institut Scientifique de Service Public, Liege, Belgium: Transport characteristics for coal gasification
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
University of Ghent, Ghent, Belgium: Theory of chemical bond, theoretical characterization of aromaticity
University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity, molecular basis of structure activity relationships
University of Kragujevac, Serbia: Multicentre bonding, quantitative characterization of aromaticity
University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
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 Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
University of Udine, Udine, Italy: Characterization of noble metal catalysts
University of Vigo, Vigo, Spain: Multicentre bonding, theoretical characterization of aromaticity

Visits abroad

P. Krystynik: Bangor University, Bangor, Wales, United Kingdom (2 months)
L. Matějová: University of Oulu, Oulu, Finland (2 months)

Visitors

M. Boaro, University of Udine, Italy
R. Brahmi, University of Chouaib Doukkali, Morocco
L. Bučinský, Slovak Technical University Bratislava, Slovakia
B. Corain, University of Padua, Italy
O. Dudarko, Institute of Surface Chemistry NAS, Ukraine
P. Hudec, Slovak Technical University Bratislava, Slovakia
S. Ojala, University of Oulu, Finland
J. Penttinen, University of Oulu, Finland
S. Pitkäaho, University of Oulu, Finland
A. Spojakina, Institute of catalysis, Sofia, Bulgaria
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

Teaching

F. Kaštánek: ICT, Faculty of Chemical Engineering, postgraduate course "Application of chemical engineering in technologies for environment"
P. Klusoň: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
P. Klusoň, UJEP, Faculty of Environment, course "Toxicology"
R. Ponec: CU, Faculty of Science, course "Structure and reactivity"
O. Šolcová: ICT, Faculty of Chemical Engineering and Faculty of Chemical Technology, postgraduate course "Texture of porous solids"

Publications

Original papers

[1] Bultinck P., Cooper D.L., Ponec R.: The Influence of Atoms-in Molecules Methods on Shared Electron Distribution Indices and Domain Averaged Fermi Holes. (Eng) J. Phys. Chem. A 114(33), 8754-8763 (2010).

[2] Čapek P., Hejtmánek V., Kolafa J., Brabec L.: Transport Properties of Stochastically Reconstructed Porous Media with Improved Pore Connectivity. (Eng) Trans. Porous Media 88(1), 87-106 (2011).

[3] Doušková I., Kaštánek F., Maléterová Y., Kaštánek P., Doucha J., Zachleder V.: Utilization of Distillery Stillage for Energy Generation and Concurrent Production of Valuable Microalgal Biomass in the Sequence: Biogas-Cogeneration-Microalgae-Products. (Eng) Energy Conv. Manag. 51(3), 606-611 (2010).

[4] Feixas F., Ponec R., Fišer J., Roithová J., Schröder D., Price S.D.: Bonding Analysis of the $[C_2O_4]^{2+}$ Intermediate Formed in the Reaction of CO_2^{2+} with Neutral CO_2. (Eng) J. Phys. Chem. A 114(24), 6681-6688 (2010).

[5] Floriš T., Klusoň P., Muldoon M., Pelantová : Notes on the Asymmetric Hydrogenation of Methyl Acetoacetate in Neoteric Solvents. (Eng) Catal. Lett. 134(3-4), 279-287 (2010).

[6] Floriš T., Klusoň P., Slater M.: Stereoselective Hydrogenation of Methyl Acetoacetate over Structurally Different Chiral Ruthenium Complexes. (Eng) React. Kinet. Mech. Cat. 102(1), 67-74 (2011).

[7] Jeřábek K., Hanková L., Holub L.: Working-state Morphologies of Ion Exchange Catalysts and Their Influence on Reaction Kinetics. (Eng) J. Mol. Catal. A: Chem. 333(1-2), 109-113 (2010).

[8] Kaluža L., Vít Z., Zdražil M.: Support Effect in the Hydrodesulfurization of Thiophene over Rhodium Sulfide. (Eng) React. Kinet. Mech. Cat. 101(1), 63-72 (2010).

[9] Karásková K., Obalová L., Jirátová K., Kovanda F.: Effect of Promoters in Co-Mn-Al Mixed Oxide Catalyst on N_2O Decomposition. (Eng) Chem. Eng. J. 160(2), 480-487 (2010).

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