ANNUAL REVIEW 2012

BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCES

ANNUAL REVIEW 2012

http://catalysis.ru

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of Activities in Basic Research Areas
2011

BORESKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

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Boreskov Institute of Catalysis
Pr. Akademika Lavrentieva, 5
Novosibirsk, 630090
Russia

Phone: (007) 383 330 82 69
FAX: (007) 383 330 80 56
E-mail: bic@catalysis.ru
http:// catalysis.ru

Dear Colleagues,

This issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covers the year 2011 and follows the scheme which has been accepted by BIC for such kinds of reviews many years ago.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and the fSU countries, but also in many western and oriental countries. It is the world oldest and world largest specialized institution which was organized to provide any kind of R&D in the area of catalysis. Since 1960’s it remains the largest Russian chemical research institution in the Asian part of Russia, but now it appears to be one of the largest R&D chemical institutions of Russia as a whole. BIC has many deep and stable traditions in providing basic and applied research in nearly all fields of catalysis. The interests of BIC spread from the sophisticated areas of purely academic research to the real applied problems which reflect Russia entering into the market economy and thus include development of commercial catalysts and catalytic technologies.

BIC is affiliated to the Siberian Branch of the Russian Academy of Sciences. However, according to realities of new Russia, a lot deal of BIC’s activity is devoted not only to basic research, but also to numerous industrially oriented topics. The intensity and quality of the research and engineering activity at the Institute became at the new period of the Russian history much higher as before, since in the current Russian reality some academician research institutes are performing the functions of the former industrial institutions. However, according to the Russian and international data bases of citation, for several years BIC has been positioned as a leading Russian chemical institution from the point of view. This means that BIC gained in research in catalysis fundamentals, thus continuing the old traditions originated from the beginning of the Institute due to a very powerful starting impulse of its creator and first director Academician Georgii K. Boreskov, as well as the master ideas of the second director Academician Kirill I. Zamaraev. Hope, the readers will feel that themselves, when comparing the materials of this and previous issues of the Annual Review, which can be easily found at the BIC website.

The BIC has a strategic collaboration with some industrial companies, both Russian and foreign, which is nowadays, undoubtedly, the very important feature of the current scientific activity of the Boreskov Institute.

Since 1998 the Institute has been united with few other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a now informal association which was called the United Institute of Catalysis (UIC). In 2004 there were some rearrangements in the UIC structure, since the Omsk Division of the BIC has separated from BIC as a new legal entity, the Institute of Hydrocarbons Processing (IHP), while the Volgograd Scientific center with large flexible pilot facilities for fine organic synthesis has joined BIC as its Volgograd Division. Thus, now UIC consists of two large legal entities: BIC and IHP. In addition to the Volgograd pilot plant, UIC's facilities include two extra flexible and powerful semi-industrial plants capable of manufacturing the first industrial batches of various catalysts and specialty chemicals. Thus, BIC together with UIC is now one of the most powerful Russian specialized R&D organizations in the industry-oriented chemistry with unique facilities for scaling up numerous innovations for that industry. Indeed, the current management of the Institute realizes the existing problems of the large R&D structure operation and tries to take care of the maintenance of high R&D activity and productivity of BIC and UIC in both fundamental and applied areas as the goal of the highest priority.

The very important issue for BIC in the year 2011 was its entering the "Skolkovo Project" which was initiated by the top Russian authorities and is aimed at acceleration of the development of the modern style innovation climate in Russia. One of the ways on this path is the creation of a set of small spin-off enterprises to accelerate penetration of some BIC innovations into the market economy.

Hope, the current issue of the Annual Review of the Boreskov Institute of Catalysis will succeed in exhibiting many sides of the Institute potentialities in basic research on catalysis, catalysts and catalytic technologies. As to the activity of the Institute in the applied areas, which is now much more active than ever in the past, we publish special leaflets. Also, we invite the readers to visit BIC's website at **www.catalysis.ru**.

Valentin N. Parmon

BORESKOV INSTITUTE OF CATALYSIS OF THE SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCES

More than the 50-year-long history of the Institute is a glowing example of fruitful interaction between fundamental science and industry and of the profound realization that solving scientific problems should be aimed at some practical result. The accomplishments of the Institute embody its original conception, which includes studies at the atomic/molecular level and commercialization of the results. It is due to this approach that the Institute has made a significant contribution to the material and technical basis necessary for the rapid development of the Russian chemical industry and became one of the world's most prominent research centers in chemical catalysis.

The Institute was founded in the summer of 1958 as a part of Siberian Branch of the USSR Academy of Sciences. Initiator of the Institute and its permanent director up to 1984 was Academician Georgii K. Boreskov (1907-1984), an eminent scientist with international recognition, an outstanding physical chemist and chemical technologist. In 1992 the Institute of Catalysis was named after Academician G.K. Boreskov.

In 1969 the Institute of Catalysis was awarded The Red Banner of labor for the contribution to development of chemical science and for training high-skilled personnel.

In 1976 Professor Kirill I. Zamaraev has been invited by Academician G.K. Boreskov to join the Institute of Catalysis as a Deputy Director. Kirill Ilyich has come to Novosibirsk at early 1977 together with a large team of young chemical physicists, thus largely widening the studies of elementary catalytic reactions on molecular-atomic level through application of modern physical and kinetic instrumental methods of investigation.

In 1984 Professor Zamaraev became the Director of the Institute of Catalysis, and since that time he was the real leader of all research and development activity of this huge Institute. K.I. Zamaraev, the former President of the International Union of Pure and Applied Chemistry, Foreign Fellow of the Indian National Science Academy and of the Korean Academy of Science and Technology, holder of the Silver Medal of the Royal Chemical Society of Great Britain as a centenary lecture, has passed away in the prime of his brilliant scientific career on 26 June 1996.

In 1995 Professor Valentin N. Parmon, prominent specialist in the field of catalysis, chemical kinetics and photocatalysis, headed the third generation of the directorate of the Institute.

Since 1998 the Institute has been united with some other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a new R&D association: the United Institute of Catalysis headed by the director of the Boreskov Institute of Catalysis. Now the United Institute of Catalysis (UIC) affiliates the Boreskov Institute of

Catalysis with its St. Petersburg and Volgograd Departments, the Institute of Hydrocarbons Processing in Omsk and three pilot plants.

The scope of the Institute's activities is extremely wide, ranging from solving fundamental problems of catalysis to creating new catalytic technologies and organizing commercial scale production of catalysts.

The high level of the fundamental research carried out by the Institute is reflected by numerous monographs, as well as articles published in prestigious international journals and collections of works. The Institute publishes more than 300 works per year in peer-reviewed journals. According to the interdisciplinary server www.scientific.ru, the Institute has the highest total citation index among the Russian chemical institutions over the last 8 years. The average citation index of one article is above 6 and is high on the citation index list of articles from chemical instructions of the Siberian Branch of the Russian Academy of Sciences.

The Institute patents over 40 discoveries and maintains more than 30 foreign patents annually. The Institute is the avowed intellectual property protection leader among the Russian academic institutions.

The Institute is designing new generations of catalysts and technologies to meet the present-day global trends. Throughout its more than 50-year-long history, the Institute has been among the leaders in developing new technologies for the chemical and petrochemical industries, power engineering, and environmental protection.

The numerous exploratory and prospective studies of the Institute in the field of catalytic technologies include advancement of a large complex of environmental and energy-saving technologies, use of nontraditional feedstock in the production of various motor fuels and oil processing products, fine synthesis of medicines and plant protection chemicals, etc.

The Institute designed original devices for studying the properties of catalysts and has organized small-scale production of automated devices and installations for investigation and control of the physicochemical properties of various substances and materials. The novel, high-efficiency catalysts and technologies developed by the Institute satisfy the present-day requirements and are in demand in Russian markets and around the world.

The Institute is widely known abroad for its achievements and is a partner of many Russian and foreign companies.

STRUCTURE OF THE INSTITUTE

The Boreskov Institute of Catalysis unites about 1000 employees, among its 400 researchers being 1 academician, 4 Corresponding Members RAS, more than 70 Drs. Sci., more than 200 PhD's, more than 60 PhD students and about 80 graduate students.

The Institute is a unique association of specialists in various fields of science and technology that are capable of solving any catalytic problems from fundamentals to design of industrial catalysts and processes.

The Institute structure comprises 9 research departments. Supporting and service departments provide the smooth work of the Institute.

The successful research activities are based on the overall access to the latest and reliable scientific data. There is the **Information and Library Center** in the Institute, and the library is one of the best scientific libraries in Siberia.

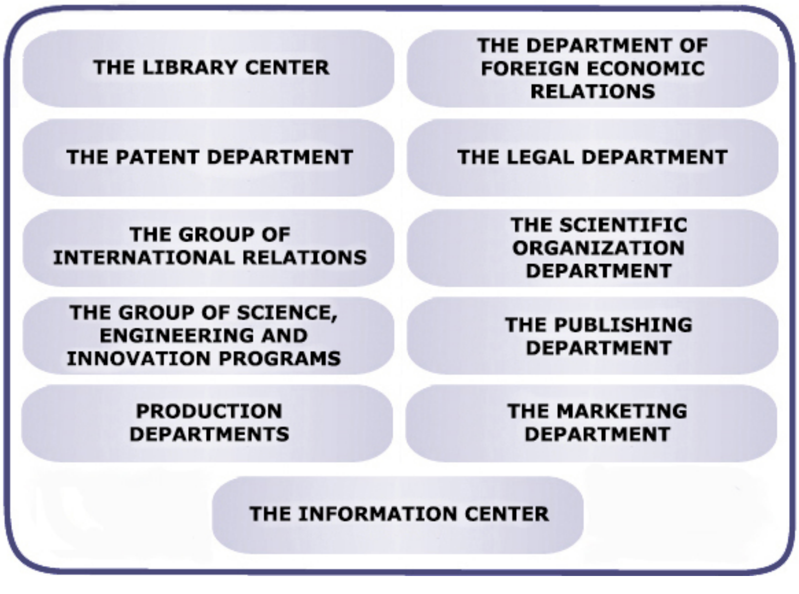
The **Scientific Organization Department** deals with scientific events such as conferences, seminars, schools, meetings, presentations of various companies and equipment producers, discussions. There is a museum where the information on catalytic science is collected.

Advertising and Exhibits Department of the Institute is active in competence, perfect service in the field of organization of exhibitions of the new inventions and successive achievements of the Institute.

The activities of the **Group of Science, Engineering and Innovation Programs** are aimed at the participation of the Institute in State priority competitive programs for creation of technologies and materials to make Russia an economically independent country.

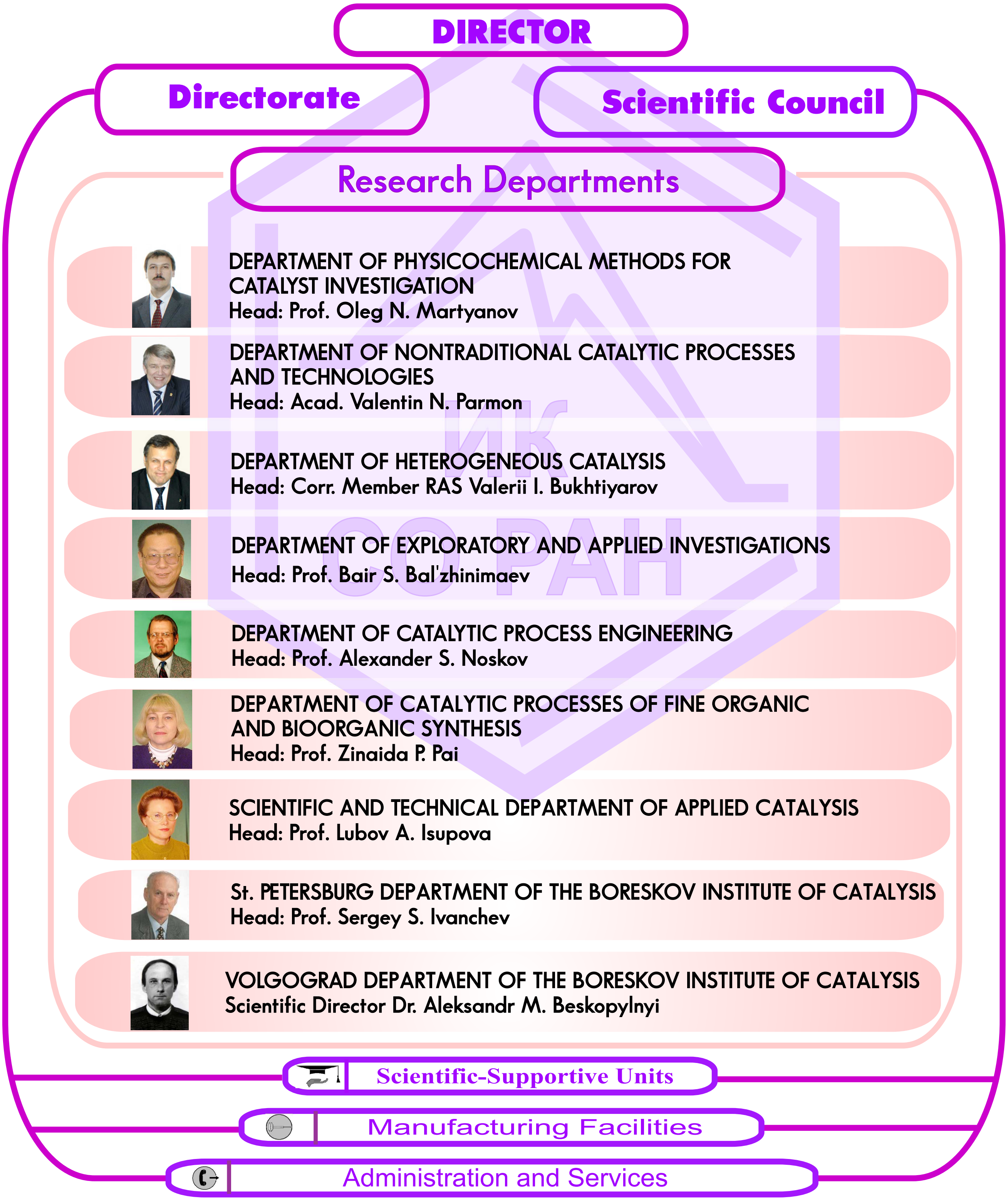
The **Publishing Department** concentrates its activities on supporting the R&D process inside the Institute, as well as on public information about the BIC's advances. Among the published items are Annual Reports, Proceedings of conferences organized by the Institute, information bulletins, manuals, etc.

Production departments provide engineering and technical support of the research activities, exploitation and modernization of the available facilities.



STRUCTURE OF THE INSTITUTE

Directorate:
A.A. Vedyagin, I.A. Kamolkin, B.S. Bal'zhinimaev, S.E. Glaznev, O.N. Martyanov
V.I. Bukhtiyarov, N.V. Mukhina, V.N. Parmon, A.S. Noskov



DIRECTOR

Directorate

Scientific Council

Research Departments

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
Head: Prof. Oleg N. Martyanov

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES AND TECHNOLOGIES
Head: Acad. Valentin N. Parmon

DEPARTMENT OF HETEROGENEOUS CATALYSIS
Head: Corr. Member RAS Valerii I. Bukhtiyarov

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS
Head: Prof. Bair S. Bal'zhinimaev

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING
Head: Prof. Alexander S. Noskov

DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS
Head: Prof. Zinaida P. Pai

SCIENTIFIC AND TECHNICAL DEPARTMENT OF APPLIED CATALYSIS
Head: Prof. Lubov A. Isupova

St. PETERSBURG DEPARTMENT OF THE BORESKOV INSTITUTE OF CATALYSIS
Head: Prof. Sergey S. Ivanchev

VOLGOGRAD DEPARTMENT OF THE BORESKOV INSTITUTE OF CATALYSIS
Scientific Director Dr. Aleksandr M. Beskopylnyi

Scientific-Supportive Units

Manufacturing Facilities

Administration and Services

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

HEAD OF THE DEPARTMENT PROF. OLEG N. MARTYANOV

Laboratory of Adsorption
Head: Prof. Oleg N. Martyanov

Laboratory of Analytical Chemistry
Head: Prof. Vladimir N. Sidelnikov

Laboratory of Investigation of the Mechanisms of Catalytic Reactions
Head: Prof. Eugenii P. Talsi

Laboratory of Catalyst Texture Studies
Head: Dr. Maxim S. Melgunov

Laboratory of Quantum Chemistry
Head: Dr. Igor L. Zilberberg

Laboratory of Spectral Methods
Head: Prof. Dimitrii I. Kochubey

Laboratory of Structural Methods
Head: Prof. Sergey V. Tsybulya

Group of Low Temperature Catalysis by Metals
Head: Prof. Vladimir V. Gorodetsky

Group of Solid-State NMR Spectroscopy
Head: Prof. Olga B. Lapina

Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion
Head: Prof. Alexander G. Stepanov

Group of Nanostructural Analysis
Head: Prof. Fedor V. Tuzikov

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES

HEAD OF THE DEPARTMENT ACADEMICIAN VALENTIN N. PARMON

Laboratory of Catalytic Methods of Solar Energy Conversion
Head: Academician Valentin N. Parmon

Laboratory of Hydride Compounds Studying
Head: Prof. Valentina I. Simagina

Laboratory of Catalytic Processes for Desulfurization
Head: Dr. Olga N. Kovalenko

Laboratory of Energy Accumulating Processes and Materials
Head: Prof. Yuriy I. Aristov

Group of Adsorption-Catalytic Processes for Fuel Cells
Head: Dr. Alexey G. Okunev

Group of Aerosol Catalysis
Head: Dr. Valerii N. Snytnikov

Group of Biocatalysis
Head: Prof. Galina A. Kovalenko

Group of Catalysts on Carbon Supports
Head: Dr. Irina L. Simakova

Group of Metal Complex Catalysis
Head: Prof. Nina I. Kuznetsova

Group of Sulfide Catalysts
Head: Prof. Anatolii N. Startsev

Group of Energy-Chemical Processes and Technologies
Head: Prof. Vladimir I. Anikeev

Group of Biodegradable Polymers
Head: Dr. Aleksandr G. Potapov

Group of Experimental Kinetics
Head: Dr. Ilya Yu. Pakharukov

Group of Vortex Processes and Apparatuses
Head: Dr. Andrey O. Kuzmin

DEPARTMENT OF HETEROGENEOUS CATALYSIS

Head of the Department Corr. Member RAS
Valerii I. Bukhtiyarov

Surface Science Laboratory
Head: Corr. Member RAS Valerii I. Bukhtiyarov

Laboratory of Catalytic Processes in Fuel Cells
Head: Prof. Vladimir A. Sobyanin

Laboratory of Heterogeneous Selective Oxidation
Head: Dr. Vladimir I. Sobolev

Laboratory of Catalysts for Deep Oxidation
Head: Prof. Vladislav A. Sadykov

Laboratory of Oxidative Catalysis over Zeolites
Head: Prof. Aleksandr S. Kharitonov

Laboratory of Catalysts Preparation
Head: Prof. Aleksandra S. Ivanova

Laboratory of Ecological Catalysis
Head: Prof. Zinfer R. Ismagilov

Laboratory of Catalytic Conversion of Carbon Oxides
Head: Dr. Tatyana P. Minyukova

Group of Supported Metal Oxide Catalysts Investigation
Head: Prof. Andrey I. Boronin

Group of Noble Metal Based Heterogeneous Catalysts

Head: Prof. Anatolii V. Romanenko

Group of Surface Compounds Synthesis

Head: Dr. Vladimir L. Kuznetsov

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING

HEAD OF THE DEPARTMENT PROF. ALEKSANDR S. NOSKOV

Laboratory of Unsteady-State Catalytic Methods for Gas Purification
Head: Prof. Aleksandr S. Noskov

Laboratory of Catalytic Hydrocarbon Conversion
Head: Prof. Gennadii V. Echevsky

Laboratory of Catalytic Polymerization
Head: Prof. Vladimir A. Zakharov

Laboratory for Catalytic Processing of Renewable Sources
Head: Dr. Vadim A. Yakovlev

Group of Kinetics of Catalytic Processes
Head: Prof. Sergei I. Reshetnikov

Group of Development and Optimization of Catalytic Processes with Catalyst Deactivation
Head: Dr. Nadezhda V. Vernikovskaya

Group of Membrane-Catalytic Processes
Head: Dr. Ilya V. Mishakov

Group of High Temperature Catalytic Processes
Head: Dr. Andrey V. Porsin

Group of Catalytic Methods for Production and Application of Syn-Gas
Head: Prof. Valerii A. Kirillov

Group of Complex Engineering Processes

Head: Dr. Victor A. Chumachenko

Group of Hydrogenation Processes

Head: Dr. Galina A. Bukhtiyarova

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS

HEAD OF THE DEPARTMENT PROF. BAIR S. BAL'ZHINIMAEV

Laboratory for Characterization and Testing of New Materials for Catalysis
Head: Prof. Bair S. Bal'zhinimaev

Laboratory of Zeolites and Acid Base Catalysis
Head: Prof. Eugenii A. Paukshtis

Group of Catalytic Conversion of Sulfur-Containing Compounds
Head: Prof. Anna V. Mashkina

DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS

HEAD OF THE DEPARTMENT PROF. ZINAIDA P. PAI

Laboratory of Liquid-Phase Catalytic Oxidation of Organic Compounds
Head: Prof. Zinaida P. Pai

Group of Catalysts and Processes Based on Heteropoly Acids
Head: Prof. Elena G. Zhizhina

Group of Heterogeneous Catalysts for Selective Liquid-Phase Oxidation
Head: Prof. Oxana A. Kholdeeva

SCIENTIFIC AND TECHNICAL DEPARTMENT OF APPLIED CATALYSIS

Head of the Department Prof. Lyubov A. Isupova

Group of Catalysts and Supports for High Temperature Processes
Head: Prof. Lyubov A. Isupova

Group of Aerogel Materials
Head: Dr. Alexander F. Danilyuk

Assurance Group
Head: Sergey A. Lopatin

Group of Catalysts Preparation
Head: Vasilii Yu. Kruglyakov

Group of Catalysts Testing
Head: Alexander S. Bobrin

Group of Pilot Plants and High Pressure
Head: Victor N. Korotkikh

Group of Preparative Synthesis
Head: Dr. Yurii I. Amosov

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Director
Prof. Sergey S. Ivanchev

Vice-Director Dr. Valery P. Tulmankov

VOLGOGRAD DEPARTMENT OF THE BORESKOV INSTITUTE OF CATALYSIS

Scientific Director
Dr. Aleksandr M. Beskopylnyi

Chief Executive Igor V. Tertishnikov

SCHOOLS OF THE BORESKOV INSTITUTE OF CATALYSIS

The successful development of the Institute has been possible only due to the existence of scientific schools headed by the Institute's leading scientists in a variety of important research areas.

Academician G.K. Boreskov

Theory of heterogeneous catalysis. The nature of the interaction between the reactants and the catalyst. The effect of the reactant–catalyst bonding energy on the catalytic activity and selectivity. The concepts of stepwise and associative mechanisms of redox catalytic reactions. Unsteady-state catalysis. Development of industrial catalysts.

Academician K.I. Zamaraev

Theory of tunneling transfer of electrons in solids. The coordination chemistry of metal complex solutions. Studies of stepwise mechanisms of homogeneous and heterogeneous catalytic reactions, active site structure at the atomic/molecular level. Search for novel areas in catalysis.

Academician V.N. Parmon

Catalysis and photocatalysis in renewable and non-traditional energetics. Photochemical and thermochemical methods of solar energy conversion. Radiation and thermal catalysis. The role of photocatalysis in the global chemistry of the terrestrial atmosphere. Abiogenic catalysis in the nature. Synthesis of nanomaterials. New types of chemical reactors.

M.G. Slin'ko, Corresponding Member of the Russian Academy of Sciences

Methods of mathematical modeling of catalytic processes and reactors based on hierarchical models. Optimization and modeling of processes in fixed and fluidized beds; liquid-phase, multiphase, and unsteady-state processes. Design of industrial reactors.

R.A. Buyanov, Corresponding Member of the Russian Academy of Sciences

Scientific basis of catalyst preparation and technology. Enhancing the reactivity of solid phases. Mechanochemistry in catalysis. Catalyst deactivation. Theoretical basis of the synthesis of carbon–mineral composites. Theory of nonbranched-chain free-radical catalytic reactions. Development of industrial catalysts.

V.A. Likholobov, Corresponding Member of the Russian Academy of Sciences

Molecular design of catalytic compositions for organic syntheses. "Tailoring" of active sites of metal complex catalysts. Synthesis of porous supports with the desired textural and surface properties.

Professor Yu.I. Yermakov

Targeted synthesis of supported catalysts with the desired composition and dispersion using immobilized organometallic compounds. Catalytic polymerization of olefins. Development of industrial catalysts.

Professor V.A. Dzis'ko

Formation of oxide catalysts of complex composition. Control of the chemical and phase compositions, acid–base surface properties, textural and strength characteristics, and thermal stability of the catalysts. Development of industrial catalysts and supports.

Professor G.M. Zhidomirov

Heterogeneous catalysis theory. Principles of the IR spectroscopy of the surface. Quantum chemical modeling of catalytic systems. Calculation of the electronic structure and properties of the acid and redox sites of zeolite, oxide, and metal catalysts.

R&D ACTIVITY AREAS

Basic research

- ♦ *Fundamentals of catalysis science, prediction of catalytic action*
- ♦ *Scientific and technological bases of catalyst preparation and synthesis of new materials including functional nanomaterials*
- ♦ *In situ studies of catalysts and mechanisms of catalytic reactions*
- ♦ *Theoretical basis of developing catalytic processes*
- ♦ *Mechanisms and kinetics of practically important catalytic reactions*
- ♦ *Mathematical modeling and optimization of parameters of reactors and catalytic processes*

Applied catalysis

- *Efficient catalysts and catalytic technologies for oil & gas processing, for production of key chemicals*
- *Catalysts and catalytic technologies for synthesis of polymers with required properties, including biodegradable polymers*
- *Catalysts and processes for fine synthesis for pharmaceutical industry*
- *Sorbents, catalysts and technologies for environmental protection*
- *Reactors and processes based on membrane catalysts. Microchannel catalytic reactors*
- *Catalysts and processes for hydrogen energetics*
- *Catalytic technologies for heat power generation*
- *Catalysis for non-traditional energetics and processing of renewable resources*
- *Methods and facilities for catalyst testing*

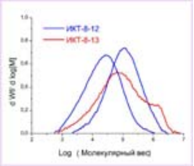
Some BIC's proprietary technologies

- **Reverse process** for gas purification
- **Zeoforming processes** for synthesis of gasoline
- **Alphox technology** for one step phenol form benzene production (in cooperation with Solutia)
- Honeycomb catalysts for oxidation of ammonia in the production of **nitric acid**
- New technology of **loading catalysts to reactors**
- **BICYCLAR** technology for production of aromatic hydrocarbons
- Direct catalytic **oxidation of H_2S** to elemental sulfur
- Treatment of mixed **radioactive organic wastes**
- Liquid-phase oxidative **treatment of industrial wastewater**
- Technology for **formaldehyde** production
- Technology for **one step formic acid** production

- Technology for **reductant atmospheres** production over honeycomb catalysts
- Catalytic technologies for production of **carbon nanofiber materials and carbon nanotubes**
- Technology for synthesis of **Nafion-type polymer materials**
- Technolohy for synthesis of **polymer hydrogel materials for soft contact lenses**
- Technologies for generation of synthesis gas from hydrocarbon fuel (natural gas, gasoline, diesel and biofuel)
- Catalytic technologies for processing of bio resources to produce biofuel

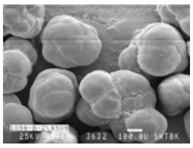
Some BIC's catalysts for industrial applications

Vanadium pentoxide catalysts for sulfuric acid production

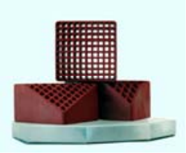


Supported catalysts ICT-8-12 and ICT-8-13 for polyethylene production

Catalyst ICT-8-20 for production of ultrahigh molecular weight polyethylene



Supported Ti-Mg catalyst IC-8-21 for polypropylene production



IC-42 series non-platinum catalysts for oxidation of ammonia in the production of nitric acid

High silica zeolite catalysts

Palladium catalyst for hydrogenation of distilled fatty acids in the production o stearine

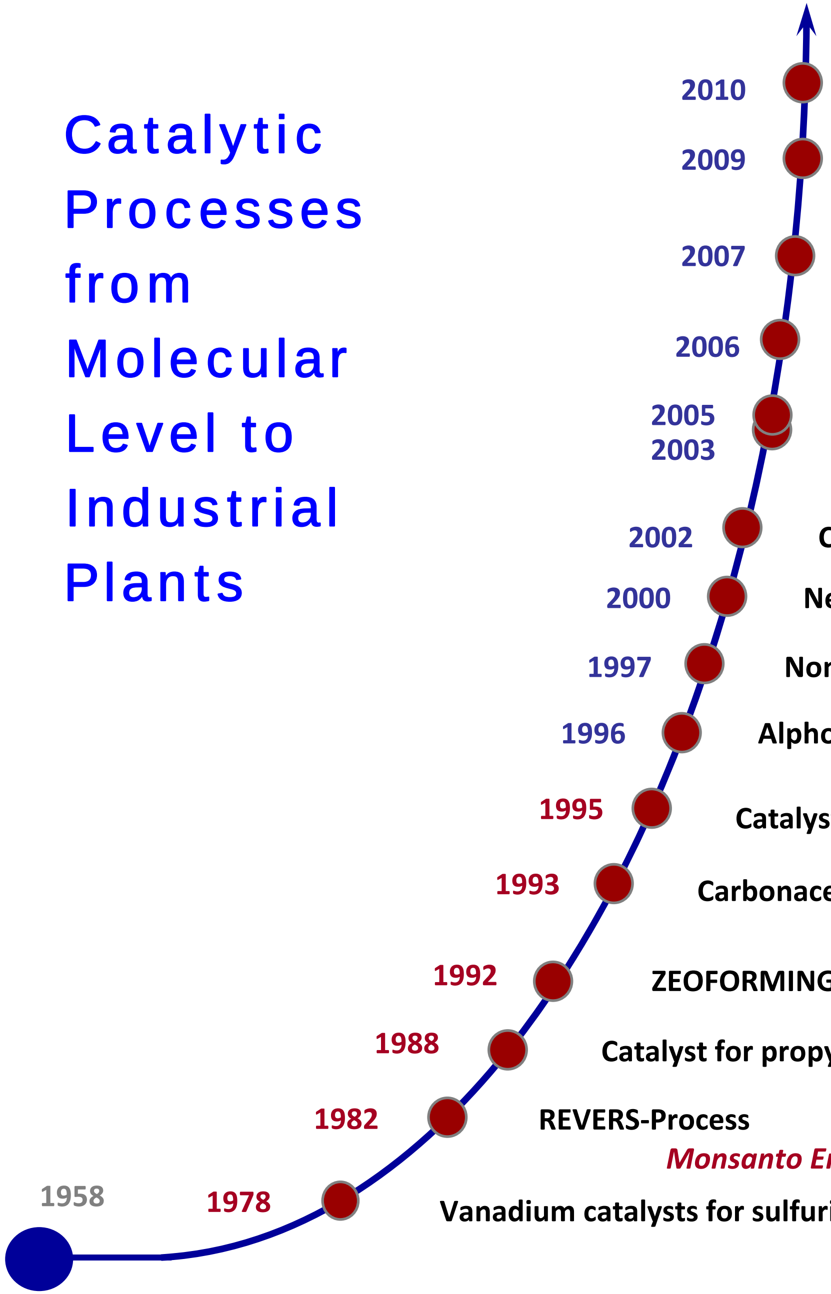
Thermostable catalyst ICT-12-40 for gas purification

Glass fiber catalysts for treatment of waste gases of the production of synthetic rubber

Photocatalytic systems for air cleaning and detoxication

CDM series dehydrogenation catalysts

Catalytic Processes from Molecular Level to Industrial Plants



2010 Catalytic heating units (CHU) for autonomous heat power generation

2009 Family of fiberglass catalysts (GFC) for treatment of industrial waste gases

2007 Catalyst for fine hydrotreatment of diesel fractions (Euro-4 and Euro-5 standards for sulfur)

2006 Catalyst for synthesis ultrahigh molecular weight polyethylene (UHMWPE)

2005
2003 New generation of LUKS series catalysts for cracking and PR and RU series catalyst for reforming

Developed in cooperation with the IHP, Omsk, Russia

2002 Composite selective water sorbents

2000 New method for loading of catalysts into industrial reactors

1997 Non-platinum catalyst for production of nitric acid

1996 Alphox technology (benzene + [N_2O] → phenol)

Developed in cooperation with Solutia, USA

1995 Catalyst for FCC (oil cracking)

1993 Carbonaceous material SIBUNIT

Since 1994 has been supplied to USA, Europe, Japan

1992 ZEOFORMING process for synthesis of gasoline

Lurgi, 1997, Germany

1988 Catalyst for propylene polymerization

DSM, 1995, the Netherlands

1982 REVERS-Process

Monsanto Enviro Chem. Systems, 1992, USA

1978 Vanadium catalysts for sulfuric acid production

1958

INSTRUMENTATION FACILITIES

The Institute engages the leading position in the world in the improvement and design of new physicochemical methods for catalyst study. The Boreskov Institute of Catalysis has specialized groups united into Department of Physicochemical Methods for Catalyst Investigation oriented at analytical and scientific studies. At the Department there are many specialists of high qualification specializing in the investigation of catalysts and nanomaterials.

Modern and, in some cases, unique physicochemical methods provide a basis for fundamental studies at the atomic-molecular level.

The types of analytical and research studies performed at the Institute and methods used for them are listed below.

Estimation of Molecular Composition of Individual Compounds and their Mixtures

- ✓ Chromatography: Gas (GC), Capillary and Multicapillary (analysis of gas and liquid phases)
- ✓ Chromato-Mass-Spectrometry (analysis of liquid and solid phases)
- ✓ Ion Chromatography
- ✓ High-temperature Gel Chromatography

Elemental Analysis of the Volume Composition of Liquids and Solids

- ✓ *Inductively Coupled Plasma Atomic-Emission Spectrometry (ICP-AES)*
- ✓ *X-Ray Fluorescent Analysis of macro and micro samples*

Solid Surface Analysis

- ✓ Photo-Electron Spectroscopy (XPS, ESCA)
- ✓ Secondary Ion Mass-Spectrometry

Phase Analysis

- ✓ X-Ray Diffraction Analysis including in-situ study
- ✓ Differential Dissolution Phase Analysis
- ✓ EXAFS Spectroscopy (for X-Ray amorphous subjects)

Morphology

- ✓ Transmission High Resolution Electron Microscopy (HRTEM)
- ✓ Scanning Electron Microscopy (SEM)
- ✓ Scanning Tunneling Electron Microscopy (STM)
- ✓ X-Ray Low Angel Scattering

Spectral methods

- ✓ Nuclear Magnetic Resonance (NMR) including *in-situ* study
- ✓ Electron Paramagnetic Resonance (EPR) including *in-situ* study
- ✓ Electron Ferromagnetic Resonance Spectroscopy (FMR) including *in-situ* study
- ✓ Ultraviolet-Visual (UV-VIS) Adsorption Spectroscopy
- ✓ Near Infrared (NIR) Spectroscopy
- ✓ Infra-Red Spectroscopy (IRS)
- ✓ Raman Spectroscopy
- ✓ Fluorescent Spectroscopy

Special Methods

- ✓ Thermal Gravimetry (TG) and Differential Thermal Analysis (DTA)
- ✓ Temperature-Programmed: Reduction (TPR), Oxidation (TPO), Desorption (TDP), Reaction (TPR)
- ✓ A Set of Calorimetric Methods
- ✓ Differential Scanning Calorimetry
- ✓ Radioisotope Methods for the study of the mechanisms and reaction kinetics
- ✓ NMR *in situ* Microtomography for Studies on Mass transfer
- ✓ Ultraspeed Chromatography Analysis
- ✓ Methods for studying polymers: melt fluidity, fractionation
- ✓ Determination of photocatalytic activity of solid samples

INTERNATIONAL COOPERATION

The scientific cooperation of the Boreskov Institute of Catalysis with the catalytic communities from various countries is effected in accordance with various forms of cooperation: conducting joint seminars on catalysis, exchanging the information and appropriate materials, exchanging research fellows, visiting scientific centers, and participating in congresses and symposia on theoretical and applied catalysis.

According to research programs, projects and grants, the fundamentals of catalysis are studied jointly with researchers from various universities, institutions, research laboratories and companies. BIC collaborates fruitfully on a commercial basis with the leading companies from more than 20 countries, sells licenses, know-how and performs research projects according to client requests.

Academician Valentin N. Parmon is the Russian representative in the European Federation of Catalytic Societies (EFCATS), Member of the International Association of the Catalysis Societies (IACS).

Visits of the specialists from the Boreskov Institute of Catalysis to foreign institutions in 2011

Austria	5	Great Britain	17	Portugal	1
Belarus	6	Greece	7	Saudi Arabia	5
Belgium	6	India	5	South Korea	1
Bulgaria	3	Italy	6	Spain	14
China	10	Japan	2	Sweden	1
Cyprus	1	Kazakhstan	1	Switzerland	1
Estonia	2	Mexico	1	Thailand	1
Finland	2	Montenegro	6	Turkey	2
France	17	Netherlands	22	Ukraine	5
Germany	33	Poland	5	USA	3
				Vietnam	2

Visits of foreign specialists to the Boreskov Institute of Catalysis in 2011

Australia	1	Japan	5	Slovakia	2
China	3	Kazakhstan	2	Spain	13
France	4	Latvia	3	United Kingdom	5
Germany	7	Mexico	2	USA	9
Iceland	1	Netherlands	1		

SCIENTIFIC COOPERATION
WITHIN THE FRAMEWORK OF CONTRACTS AND AGREEMENTS
WITH FOREIGN ORGANIZATION

FRANCE

According to the agreement between **RAS** and **CNRS** BIC collaborates with the *Institute de Recherches sur la Catalyse et l'Environnement de Lyon* (Research Institute on Catalysis and Environment), Villeurbanne, in the frame of the Russian-French European associated Laboratory on Catalysis headed by **Prof. V. Parmon** and **Dr. M. Lacroix**. The Laboratory was established by an agreement signed December 6, 2004 in Moscow by RAS and CNRS. Four areas of research were identified:

- *Catalysis and Energy: Production of Syngas and Hydrogen*
- *Catalysis and Environment: Treatment of Waste Waters*
- *Catalysis and Fine Chemistry: Pollution-Free Catalytic Processes*
- *Advanced Spectroscopic Methods: Mobility of Species in Porous Medium.*

INDIA

In the frame of RAS-DST Long Term Programme of cooperation in science and technology BIC collaborates with *National Chemical Laboratory*, Pune. Coordinators on the Program "Catalysis" are **Prof. V. Parmon** and **Prof. S. Sivaram**.

GERMANY

The cooperation in the frame of the agreement between **RAS** and **German Scientific Research Society** (GSRS) with *Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin, on the Project *"Development of in situ Methods for Study of Solid Surfaces"*. Coordinators: **Prof. V. Bukhtiyarov** (*BIC*) and **Prof. R. Schlögl** (*Fritz-Haber-Institut der MPG*)

CHINA

The cooperation in the frame of *Associated Research Laboratory* which was established by an agreement signed December 4, 2004 by the Boreskov Institute of Catalysis and Heilongjiang University, Harbin. Chief Executive officers of Laboratory are: **Prof. V. Bukhtiyarov, Prof. G. Echevsky** (*BIC*) and **Prof. Wu Wei** (*Heilongjiang University*) on the Project *"Synthesis and Modification of ZSM-12 Zeolites. Zeolite ZSM-12 in Reaction of Naphthalene Alkylation with Methanol"*.

USA

The cooperation in the frame of the bilateral agreement with the Purdue University, Indiana.

COOPERATION IN THE FRAME OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

EUROPEAN COMMUNITY SIXTH FRAMEWORK PROGRAM

I. Co-Processing of Upgraded Bio-Liquids in Standard Refinery Units

Coordinator: **Dr. Y. Solantausta**, *VTT Processes*, Espoo, Finland

Partners:

Rijksuniversiteit Groningen, The Netherlands; *Boreskov Institute of Catalysis*, Novosibirsk, Russia (Prof. V. Kirillov); *Uhde Hochdrucktechnik GmbH*, Germany; *BTG Biomass Technology Group BV*, The Netherlands; *University of Twente*, The Netherlands; *STFI-PACKFORSK AG*, Sweden; *Institute of Wood Chemistry*, Hamburg, Germany; *Slovenian Institute of Chemistry*, Slovenia; *Arkema SA*, France; *Helsinki University of Technology*, Finland; *ALMA Consulting Group SAS*, France; *INEOS Phenol, Germany*; *Metabolic Explorer*, France; *Shell Global Solutions International*, The Netherlands; *Pacific Northwest National Laboratory* (PNNL), USA; Johnson *Matthey*, UK.

EUROPEAN COMMUNITY SEVENTH FRAMEWORK PROGRAM

I. Reforming of Crude Glycerin in Supercritical Water to Produce Methanol for Re-Use in Biodiesel Plants

Coordinator: **J. Vos**, *BTG BiomassTechnology Group BV*, The Netherlands

Partners:

Acciona Servicios Urbanos, Spain; *Boreskov Institute of Catalysis,* Novosibirsk, Russia (**Prof. V. Kirillov**); *Rijksuniversiteit Groningen*, The Netherlands; *University of Maribor*, Slovenia; *UHDE High Pressure Technologies GmbH*, Germany; *SPARQLE International BV*, The Netherlands.

II. Engine and Turbine Combustion of Bioliquids for Combined Heat and Power Production

Coordinator: **J. Vos**, *BTG BiomassTechnology Group BV*, The Netherlands

Partners:

AMO ZIL, Moscow, Russia; *Aston University*, Birmingham, UK; *Boreskov Institute of Catalysis*, Novosibirsk, Russia **(Prof. V. Kirillov)**; BTG Biomass Technology Group BV, The Netherlands; *Central Scientific Automobile and Automotive Engines Institute, NAMI*, Moscow, Russia; *Encotech BV*, The Netherlands; *University of Florence*, Florence, Italy.

III. Oxidative Coupling of Methane Followed by Oligomerization to Liquids

Coordinator: **G. Marin**, *Ghent University*, Belgium

Partners:

Bayer Technology Service, Germany; *Institute de Recherches sur la Catalyse et l'Environnement de Lyon*, Villeurbanne, France; Ruhr-*Universität* Bochum, TECHEM, Bochum, Germany; *Instituto de Technologia Quimica*, Spain; *Johnson Matthey*, UK; *SINTEF*, Trondheim, Norway; *Linde Engineering*, Germany; *Cepsa R&D Center*, Spain; *Haldor Topsoe*, Denmark; *Universitetet i Oslo*, Oslo, Norway; *University of Cambridge*, UK; *ALMA Consulting Group*, France; *Boreskov Institute of Catalysis*, Novosibirsk, Russia **(V. Sadykov)**; *INEOS*, Belgium; *Institut fur Mikrotechnik Mainz Gmbh*, Germany; *Eni SpA*, Italy.

IV. Design and Manufacturing of Catalytic Membrane Reactors by Developing New Nano-Architectured Catalytic and selective Membrane Materials (DEMCAMER)

Coordinators**: Fernando Espiga Guy Marin** and/or **Inaki San Sebastian,** *Fundacion Tecnalia Research & Innovation*, Spain

Partners:

Vlaamse Instelling voor Technologisch Onderzoek N.V., *Belgium; Universita della Calabria*, Italy; *Technische Untversiteit Eindhoven*, Netherlands; *Agencia Estatal Consejo Superior de Investigaciones Cientificas*, Spain; *Fraunhofer-Gesellschaft zur Foerderung der Angewandten Forschung e.V.*, Germany; Boreskov Institute of Catalysis, Russia (**Dr. I.Z. Ismagilov**); *Institut National de l'Environnement et des Risques Ineris*, France; *Rauschert Kloster Veilsdorf GMBH*, Germany; *Ceramic Powder Technology AS*, Norway; *Hybrid Catalysis BV*, The Netherlands; *HyGear B.V.*, The Netherlands; *Abengoa Bioenergia Nuevas Tecnologias SA*, Spain; *Guascor Ingenieria S.A.*, Spain represented; *Quantis Sari*, Switzerland; Höganäs AB, Sweden; *Total Petrochemicals Research Feluy*, Belgium; *Total Petrochemicals France SA*, France.

CONFERENCE AND EXHIBITION ACTIVITIES

The advertising and information activities are universal marketing tools for establishing professional contacts. Again, this is a necessary part of the market examination to be settled in the world. Each year, achievements of the Boreskov Institute of Catalysis are demonstrated at the very prestigious exhibitions in Russia and abroad. The goal is to strengthen collaboration with the present partners and to attract attention of potential customers.

In 2011, the most important BIC's achievements in the area of applied catalysis were presented at the Exhibitions:

❖ *Exhibition "Scientific and Technological and Innovation Achievements of Russia" arranged in the frames of Year of Russia in Spain*, May 12-15, Madrid, Spain.

Diploma

❖ *Exhibition "Present Day Ceramic Materials. Properties. Technologies. Application"*, August 14-16, Novosibirsk, Russia.

❖ *XVII International Exhibition-Congress "High Technologies. Innovations. Investments" (HI-TECH 2011)*, June13-19, St. Petersburg, Russia.

Medal and Diploma of the 1st degree for "*Catalytic Heat Supply Installations*"

Medal and Diploma of the 1st degree for *"Catalytic Hot Air Generators"*

❖ *"SibPolyTech-2011"*, October 18-21, Novosibirsk, Russia.

Big Golden Medal and Diploma for "*Technology for Production of Membrane Systems of the "Nafion" Type for Fuel Cells"*

❖ *XVI International Exhibition of Chemical Industry and Science "Chemistry-2011"*, October 24-27, Moscow, Russia.

Medal and Diploma of the 1st degree for "*Technology for Production of Perfluorochemical Membrane Copolymers of "Nafion" Type for Fuel Cells"*

❖ *"RusnanotechExpo-2011" in the frames of IV Nanotechnology International Forum*, October 26-28, Moscow, Russia.

❖ *Russia-Vietnam Exhibition-Seminar "Energy Saving Technologies for Oil Chenistry and Ecology"*, November 2-4, Hanoi, Vietnam.

❖ *The Specialized Inter-Regional Exhibition "YAKUTIA: Oil. Gas. Ecology. Energo-2011"*, November 9-11, Yakutsk, Russia.

Solution of many specific problems requires joint efforts in order to promote its fastest accomplishing. International congresses, symposia, conferences, and seminars are the most productive to familiarize scientists with innovations outside their own research and to disseminate the information about the results achieved to a wider audience. One of the directions of the scientific-organizational work carried out in the Institute is aimed on conducting conferences and seminars with the participation not only of Russian scientists and researchers from fSU, but foreign participants as well.

IV SCHOOL "METROLOGY AND STANDARDIZATION IN NANOTECHNOLOGIES AND NANOINDUSTRY. FUNCTIONAL NANOMATERIALS"

April 25-29, Novosibirsk, Russia

The Organizers

- State Corporation "Russian Corporation of Nanotechnologies"
- Russian Federal Agency on Technical Regulation and Metrology (Rosstandart)
- Siberian Branch of the Russian Academy of Sciences in the person of Boreskov Institute of Catalysis and Rzhanov Institute of Semiconductor Physics.

The subject area of the school reflected International and Russian practice in the field of metrology and standardization of nanoindustry products, perspective trends of nanotechnology development for synthesis of new materials and structures, requirements to the methods of certification and testing in the field of nanoelectronics, nanophotonics and other areas of nanomaterials application.

The objective of the school includes advanced training of specialists in the fields of metrology and standardization of the R&D centers and laboratories acting in nanotechnology.

More than 200 participants form 17 regions of Russia took part in the event. 22 leading specialists in the field of metrology and standardization submitted lectures. Normative maintenance of nanotechnology infrastructure of RF, instrumentation for metrology of nanoindustry were considered in the frames of oral (about 40) and poster (about 70) presentations.

INTERNATIONAL CONFERENCE
"NANOSTRUCTURED CATALYSTS AND CATALYTIC PROCESSES FOR THE INNOVATIVE ENERGETICS AND SUSTAINABLE DEVELOPMENT"
Devoted to the Year of Spain in Russia and of Russia in Spain

June 6-10, Novosibirsk, Russia

The Organizers:

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Catalysis and Petroleochemistry, Madrid, Spain
- Russian Foundation for Basic Research.

The principal objective of the meeting was to give a broad overview of recent achievements and to discuss the latest advances in the development of catalytic technologies for energetics and sustainable chemistry, including renewable sources processing. The program was based on 27 invited presentations by leading Russian and Spanish specialists and 40 poster presentations on the following topics:

- Green Chemistry Applications
- Energy, Biofuels and Chemicals Production from the Renewable Sources
- Selective and Total Oxidation Catalysts and Processes
- Structured Catalysts for Chemical Processing and Environmental Protection
- Zeolites: Design, Synthesis and Applications.

As the event basic aim was to facilitate future cooperation between teams of both countries, seminar-discussions and round tables were organized in the frame of the presented contributions.

About 100 participants, including 13 spanish scientists, took part in the Conference.

THE VI SCIENTIFIC AND ENGINEERING CONFERENCE WITH INTERNATIONAL PARTICIPATION "SUPERCRITICAL FLUIDS: FUNDAMENTALS, TECHNOLOGIES, INNOVATIONS"

July 4-7, Listvyanka, Baikal

The Organizers:

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Moscow Lomonosov State University, Moscow, Russia
- Irkutsk Scientific Center, Irkutsk, Russia
- Baikal Museum ISC, Baikal, Russia
- Journal "Supercritical Fluids: Theory and Practice", Moscow, Russia
- ZAO "SCHAG".

Scope of the Conference

- Thermodynamics and Phase Equilibria, Transfer Phenomena, Microstructure of Homogeneous and Heterogeneous SCF Systems
- Chemical Synthesis and Reactions of SC Reactants and in SC Media
- SCF and Green Chemistry
- SCF for Energetics
- SCF for Pharmaceutics
- Synthesis, Modification and Dispersion of Natural and Synthetic Materials
- Extraction and Fractionation
- Analytical Applications of SCF
- Laboratory, Pilot and Industrial SCF Systems.

The Conference program included 5 plenary lectures, 4 invited reports, 37 oral communications, including presentations of leading commercial enterprises, 17 oral presentations of young scientists, 45 poster presentations, round tables, exhibitions of equipment and brand-name products.

Plenary lectures:

S.M. Howdle (*School of Chemistry, University of Nottingham, Nottingham, UK*) –
“Polymer Synthesis, Polymer Processing and Medical Devices: A Supercritical Approach”

O.N. Martyanov, V.N. Parmon (*Boreskov Institute of Catalysis, Novosibirsk, Russia*) –
“Physico-Chemical Aspects of Application of Supercritical Fluids in Heterogeneous Catalysis”

M. Yoshimura (*Tokyo Institute of Technology, Yokohama, Japan; National Cheng Kung University, Tainan, Taiwan*) –
“Soft Processing for Sustainable Society - Possibility of Water-Based Processing for Advanced Inorganic Materials”

M.A. Anisimov (*Institute for Physical Science & Technology and Department of Chemical & Biomolecular Engineering, University of Maryland, Maryland, USA*) –
“Liquid Water: A State Between Two Critical Points”

S.P. Gubin (*Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia*) –
“SC- Isopropanol: From Raw Materials Treatment to Nanotechnologies”.

Within the Conference, the *II All-Russian School-Conference for Young Researchers and Scientists “Supercritical Fluid Technologies for Environmental Application”* and *All-Russian Symposium “Supercritical Fluid Technologies for Pharmaceutics, Biomedical Material Science and Biotechnology”* (with international participation) were held**.**

136 participants from 8 countries (Russia, Ukraine, Kazakhstan, France, Great Britain, USA, Portugal, United Arab Emirates) took part in the Conference.

RUSSIAN CONGRESS ON CATALYSIS “RUSCATALYSIS”

October 3-7, Moscow, Russia

Main objective of the Russian Congress on Catalysis “RUSCATALYSIS” was to combine efforts of scientists and experts from industry for innovative development of chemical industry and deep processing of raw materials in Russia.

The Organizers:

- Russian Academy of Sciences
- Ministry of Education and Science of the Russian Federation
- Ministry of Industry and Trade of the Russian Federation

- Ministry of Energy of the Russian Federation
- Russian Foundation for Basic Research
- Boreskov Institute of Catalysis, Novosibirsk
- Topchiev Institute of Petrochemical Synthesis, Moscow
- Moscow Lomonosov State University, Moscow
- Zelinsky Institute of Organic Chemistry, Moscow
- Multi Gala Tours Ltd, the Official Congress service operator.

Congress Topics

Section 1. Physicochemical Fundamentals of Catalytic Processes

- Theoretical and Experimental Study of the Processes on the Catalyst Surface, in Particular, *in situ* Studies
- Mechanism of Catalytic Reactions
- Kinetics of Catalytic Processes

Section 2. Scientific Basis of Catalyst Production

- Physicochemical Basis of Catalyst Synthesis
- Scientific Basis of Technologies and Equipment for the Production of Catalysts and Supports
- Methods and Equipment for Catalyst Testing.

Section 3. Advanced Catalytic Processes

- Oil Refining
- Chemistry and Petrochemistry
- Environmental Protection
- Energy Saving and Processing of Renewable Sources.

Section 4. Industrial Catalysts and Catalytic Processes

- Catalyst Operation Under Industrial Conditions
- Catalytic Reactors: Design and Application
- Deactivation and Regeneration of Industrial Catalysts
- Catalytic Process Engineering.

Satellite symposia and round table discussions were arranged within the Congress:

- ♦ *Symposium I* “Catalytic Organic Synthesis” dedicated to the 150th anniversary of Prof. N.D. Zelinsky. Program of the Symposium comprised 5 keynote lectures and 9 oral communications
- ♦ *Symposium II* “Catalytic Processes for Low-Tonnage Chemistry”. Program of the Symposium comprised 4 keynote lectures, 7 oral communications, and 3 oral presentations of young scientists.
- ♦ *Round table discussion* “Education and Catalysis”.
- ♦ *Round table discussion* “Problems in Industrial Production of Catalysts”.
- ♦ *Round table discussion* “RFBR and State Corporation Rosnanotech”.
- ♦ *Round table discussion* “Journal “Catalysis in Industry” dedicated to the 10th anniversary of the Journal.

Scientific Program of the Congress comprised 6 invited plenary lectures, 11 invited keynote lectures, 9 invited oral communications, 126 oral communications, 26 oral presentations of young scientists and 257 poster presentations.

Plenary lectures:

I. Moiseev (*Kurnakov Institute of General and Inorganic Chemistry, Gubkin Russian State University of Oil and Gas, Moscow, Russia*) –
"Homogeneous Catalysis by Metal Complexes: Yesterday, Today and Tomorrow"

V. Parmon (*Boreskov Institute of Catalysis, Novosibirsk, Russia) –*
"Physical Chemistry and Current Problems of Heterogeneous Catalysis"

Sh. Shaikhutdinov (*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*) –
"Monolayer Catalysts: New Prospects in Terms of Surface Science"

V. Likholobov (*Institute of Hydrocarbons Processing, Omsk, Russia*) –
"Trends in Preparation of Oil Refining Catalysts"

M. Tsodikov, A. Yaroslavtsev (*Institute of Petrochemical Synthesis, Moscow, Russia*) –
"Hybrid Membrane Reactors for Selective and Fast Petrochemical Processes"

A. Noskov (*Boreskov Institute of Catalysis, Novosibirsk, Russia*) –
"Computational Hydrodynamics for Development of Catalytic Reactors".

About 450 representatives of science, industry, education and companies from 14 countries took part in the Congress.

III INTERNATIONAL CONFERENCE "BIOSPHERE ORIGIN AND EVOLUTION"

October 16-20, Rethymno, Crete, Greece

The Organizers

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Cytology and Genetics, Novosibirsk, Russia
- Paleontological Institute, Moscow , Russia

10 plenary lectures, 44 oral presentations and 70 posters were presented at the Conference on the following topics:

- Astrobiology
- Prebiotic Evolution
- The Emergence of Cells
- Living Conditions in the Early Earth. Early Biosphere
- Early Eukaryotes
- Evolution of the Geo-Biological Systems in Phanerozoic.

Plenary lectures:

M. Marov (*Vernadsky Institute of Geochemistry and Analytical Chemistry, Moscow, Russia*) –
“Earth and Planets Origin: How Do We View and Model It?”

A. Chetverin (*Institute of Protein Research, Pushchino, Moscow region, Russia*) –
“Molecular Colonies as a Pre-Cellular Form of Compartmentalization”

Yu. Zhuravlev (*Institute of Biology and Soil Science, Vladivostok, Russia*) –
“On the Complexity of Primordial Biological Objects”

R. Hoover, A. Rozanov (*NASA Marshall Space Flight Ctr., Huntsville, USA*) –
“Microfossils, Biomolecules and Biomarkers in Carbonaceous Meteorites: Implications to the Origin and Evolution of the Biosphere”

E. Galimov (*Vernadsky Institute of Geochemistry and Analytical Chemistry, Moscow, Russia*) –
“Analysis of Isotope System Data (Hf-W, Rb-Sr, J, Pu-Xe, U-Pb) as Applied to the Problem of Planet Formation. Case Study: Earth-Moon System”

A. Spirin, A. Chetverin (*Institute of Protein Research, Pushchino, Moscow region, Russia*) –
“Conveying RNA-Based Molecular Machines as a Prerequisite to the Origin and Evolution of the Ancient RNA Word”

A. Rozanov (*Borissiak Paleontological Institute, Moscow, Russia*) –
“Eukaryotes and the History of Their Appearance in the Atmosphere”

A. Kontorovich (*Trofimuk Institute of Petroleum-Gas Geology & Geophysics, Novosibirsk, Russia*) –
“Evolution of Lipid Biochemistry of Living Matter in Proterozoic and Phanerozoic”

N. Kolchanov, **D. Afonnikov**, K. Gunbin, V. Suslov (*Institute of Cytology and Genetics, Novosibirsk, Russia*) –
“Gene Networks and the Evolution of Biological Systems”

M. Fedonkin (*Geological Institute and Borissiak Paleontological Institute, Moscow, Russia*) –
“The Metal Clues of Life”.

110 scientists participated in the Conference, among them 10 from USA, Italy, India, France and Germany.

EDUCATIONAL ACTIVITIES

With that deep belief that people are a decisive factor and that the best way to educate is to teach others, many researchers of the Institute participate in the training of specialists in chemistry and, particularly, in catalysis, ensuring closest and time-tested links of the Institute with the main sources of researchers – Novosibirsk State University (NSU), Novosibirsk State Technical University (NSTU), Tomsk State University (TSU), Tomsk Polytechnical University (TPU), Kazan State University (KSU). Students studying at the following chairs realize their graduate works in the Boreskov Institute of Catalysis:

- Catalysis and Adsorption, Department of Natural Sciences, NSU
- Physical Chemistry, Department of Natural Sciences, NSU
- General Chemistry, Department of Natural Sciences, NSU
- Environmental Chemistry, Department of Natural Sciences, NSU
- Chemical and Biological Physics, Department of Physics, NSU
- Physical Methods to Study Solids, Department of Physics, NSU
- Differential Equations, Mechanico-Mathematical Department, NSU
- Environmental Engineering, Aircraft Department, NSTU
- Technological Processes and Apparatuses, Department of Mechanics and Technology, NSTU
- Physical and Colloid Chemistry, Chemical Department, TSU
- Fuel Chemical Technology and Chemical Cybernetics, Chemical-Technological Department, TPU.

About 70 scientists combine teaching and their job at the Research Institute. They present lectures, give seminars and practical classes; participate in the organization and renovation of the educational process.

Since the earliest years, the strategy of the training of students has been built up by leading scientists of BIC and combined in harmony two aspects: curricula provide the students with deep theoretical and practical knowledge in catalysis, i.e. theory of the prevision of catalytic action of substances, kinetics of catalytic reactions, scientific bases of catalyst preparation, engineering of catalytic processes, application of modern physical and mathematical methods for investigation of catalysts and catalysis; and, on the other hand, the educational process arrangement allows the scope of postgraduate activities of the students to be expanded significantly. They can work as technologists, production managers, researchers at various research organizations, teach at universities.

All these features allow students to prepare their diploma at the highest scientific level and become widely informed specialists in chemistry and catalysis. The graduates from the Chair of Adsorption and Catalysis are the principal source of recruitment of the personnel of the Institute.

BIC – NSU

The Novosibirsk State University was established as an essential part of the Siberian Branch of the Academy of Sciences; it embodies the idea of the close integration of education and science. The chief mission of the University is to train professionals for scientific institutions of the country.

From its earliest age, the University pursues *three fundamental principles*. The *first* one is that the teachers are experts engaged in the real science. The intellectual basis of the University is more than 5000 scientists of 30 research institutes of the Siberian Branch. The *second* principle is a thorough mathematical background provided to students of all the departments. And the *third* principle means that the students master theoretical disciplines during their first three years and do their practical research in academic institutes of the Siberian Branch during the last years.

The Boreskov Institute of Catalysis is a key element in the training of specialists in chemistry at NSU. Graduation works of the students are conducted at the laboratories of the Institute and are supervised by experienced researchers. Their results are usually published in scientific journals and form the basis of their future Ph.D. theses.

The *Chair of Catalysis and Adsorption* (Head Prof. V. Bukhtiyarov) is of special importance for the Institute. It is only 5 years younger than Novosibirsk State University itself. The organization of the Chair was initiated in 1964 by Academician G.K. Boreskov – the founder and first director of the Boreskov Institute of Catalysis SB RAS. The Chair is located at the Institute, which provides it with everything required for efficient training of students specializing in catalysis and technology of catalytic processes.

Courses of lectures:

- Catalysis
- Adsorption and Porous Structure
- Scientific Bases for Catalysts Preparation
- Kinetics of Heterogeneous Catalytic Reactions
- Engineering Chemistry of Catalytic Processes
- Catalysis, Environment and Sustainable Development of Civilization
- Molecular Design of Catalysts
- Modern Technique of Catalytic Experiments
- Analytical Methods
- Quantum-Chemical Methods in Catalysis
- Magnetic Resonance Spectroscopy
- Optical Spectroscopy
- X-Ray Technique
- Thermodynamics of Working Catalyst
- Physical Methods in Catalysis
- Computer Application for Catalytic Studies.

The *Chair of Physical Chemistry* (Head Prof. V. Parmon) prepares highly skilled specialists in the field of chemical kinetics and thermodynamics, application of physical methods for catalysis.

Courses of lectures:

- Physical Chemistry
- Chemical Thermodynamics
- Chemical Kinetics
- Nonequilibrium Thermodynamics
- Matter Structure
- Terminal System: Computer Modeling of Processes and Physical-Chemical Phenomena
- NMR and ESR Spectroscopy for Catalysis.

The main objective of the *Chair of General Chemistry* (Head Prof. V. Sobyanin) is teaching first year students in general and inorganic chemistry.

Courses of lectures:

- Physical Chemistry
- Inorganic Chemistry
- General and Inorganic Chemistry.

The *Chair of Physical Methods to Study Solids* (Head Prof. S. Tsybulya) prepares specialists dealing with development, design and application of physical methods for investigation of structure of solids, including functional materials of various purpose and nanosystems.

Courses of lectures:

- Crystallography
- X-Ray Diffraction
- Electron Microscopy
- XPS Spectroscopy
- Magnetic Resonance
- Thermal Analysis
- Synchrotron Radiation.

BIC – NSTU

The Novosibirsk State Technical University is one of the largest research and educational centers in Russia. The University trains and retrains qualified specialists for research and industrial complex of Siberia and the Far East. Joint training of specialists at NSTU and institutes of the Siberian Branch of RAS in the field of technology of catalytic processes is of special importance for practical application of fundamental knowledge in the field of catalysis. The basic training is conducted by the *Chair of Environmental Engineering* (Head Prof. V. Larichkin) founded at the Boreskov Institute of Catalysis.

Courses of lectures:

- Technology Bases for Environmental Protection
- Processes and Apparatuses for Environmental Protection
- Catalytic Methods for Environment Protection
- Methods and Devices for Environmental Control, Ecological Monitoring
- Mathematical Modeling of Chemical Processes and Reactors

- Organic Chemistry
- Industrial Ecology
- Technologies for Utilization of Industrial Wastes
- Oil-Gas Branch
- Analytic Chemistry and Physical-Chemical Methods of Analysis.

Chemical engineering is a science-intensive field. The engineers will be able to work successfully in the priority investment areas. The close co-operation of the *Chair of Technological Processes and Apparatuses* with research institutes of the Siberian Branch of Russian Academy of Science is the key to train high-skilled specialists.

Joint Educational Scientific Centers and Laboratories

***Educational Scientific Centers* (*ESC*)** were established according to the Government concept for the education modernization. Educational, scientific and innovational complexes give the possibility of improving professional education by providing the unity of educational, scientific and technical innovational activity at every stage of training specialists.

The Educational Scientific Center "*Catalysis*" was organized in 2008 jointly with *NSU* and *NSTU*. Executors: **Prof. Valerii I. Bukhtiyarov** (BIC), **Prof. Vladimir V. Sobyanin** (NSU), **Prof. Vladimir V. Larichkin** (NSTU).

Specialization:

- Fundamentals of Catalytic Systems Preparation and Application
- Hydrogen Energy
- Technology for Fuel and Energy Production from Organic Raw Materials
- Treatment and Utilization of Technogenic Wastes Including Catalytic Methods of Environmental Protection
- Renewable Energy Sources
- Nanotechnologies and Nanomaterials
- Energy-Saving Processes and Apparatuses
- Catalytic Reactors Modeling.

The Educational Scientific Center *"Catalytic Hydrocarbon Processing"* is organized jointly with the *Gubkin Russian State University of Oil and Gas*, Moscow, in 2009. *Executors:* ***Prof. Aleksandr S. Noskov** (BIC)* and **Prof. Vladimir M. Kapustin** (Gubkin University).

Specialization:

- Study and Development of Catalytic Processes for Oil Refining and Petrochemistry
- Design of Efficient Catalytic Reactors for Oil Refining and Petrochemistry
- Fundamentals of Nanocatalysts Synthesis for Basic Processes of Oil Refining and Petrochemistry.

The Educational Scientific Center *"Chemical Technologies and Catalysis"* was made on the basis of the *Kazan State Technological University*, Kazan, in 2008. Executors: **Prof. Aleksandr S. Noskov** (BIC) and **Prof. Kharlampii E. Kharlampidi** (KSTU).

Specialization:

- Study and Development of Catalytic Processes of Oil Refining and Petrochemistry
- Design of Efficient Catalytic Reactors for Oil Refining and Petrochemistry
- Fundamentals of Nanocatalysts Synthesis for Basic Processes of Oil Refining and Petrochemistry
- Design and Investigation of Composite Polymer Materials.

The Educational Scientific Center "*Processes and Apparatuses of Chemical Technology*" was organized jointly with *NSTU* and *Open Joint-Stock Company "Novosibirsk VNIPIET"*, Novosibirsk, in 2008. Executors: **Prof. Zinfer R. Ismagilov** (BIC), **Prof. Gennadii G. Kuvshinov** (NSTU), **Prof. Yurii V. Ostrovskii** (OJSC "Novosibirsky VNIPIET").

Specialization:

- Energy- and Resource-Saving Processes and Apparatuses of Chemical Technology
- Development of Technology and Apparatuses for Treatment and Utilization of Technogenic Wastes, Including Catalytic Methods for Environmental Protection
- Fundamentals and Technology of Catalytic Systems Design and Application
- Fundamentals and Apparatuses of Hydrometallurgical, Thermal and Catalytic Processes
- Nanotechnologies and Nanomaterials Including Composite Nanomaterials
- Hydrogen Energy
- Catalytic Reactors Modeling.

The Educational Scientific Center "*Catalytic Membranes*" was organized jointly with *NSU* and the *Budker Institute of Nuclear Physics*, Novosibirsk, in 2010. Executors: **Prof. Vladislav A. Sadykov** (BIC), **Prof. Vladimir A. Sobyanin** (NSU), **Prof. Nikolai A. Mezentsev** (BINP).

Specialization:

- Fundamentals of Controllable Synthesis of Nanocomposites and Nanocrystals as Prospect Materials for Production of a New Generation of Membranes
- Regularities of Formation of Layers with Membrane Properties from Nanocomposite and Nanocrystal Materials
- Phase, Chemical, Thermal and Structural Stability of Membranes
- Modeling of Processes in Membrane Reactors and Fuel Cells
- Development of Processes and Reactors Based on Membrane Materials
- Development of the Method for Man-Caused Wastes Purification Using Membrane Reactors.

The Educational Scientific Center "*Catalysis for Atmosphere Protection*" was organized jointly with the *Biysk Technological Institute*, a structural division of the *Polzunov Altai State*

Technical University, Barnaul, in 2010. Executors: **Prof. Aleksandr S. Noskov** (BIC), **Prof. Vladimir N. Khmelev** (BTI).

Specialization:

- Fundamentals of Preparation of Stable and Highly Active Catalysts for Waste Gases Neutralization
- Studying of the Mechanism and Kinetics of Oxidative Processes of Gases Purification
- Development of Technology for Catalytic Gases Purification in the Presence of Catalysts Poisons
- Physico-Chemical Bases for Ultrasonicon Effect on Catalytic and Topochemical Reactions
- Modeling of the Catalytic Processes for Man-Caused Waste Gases Purification
- Design of Catalytic Reactors for Gases Purification
- Study of Aero(gas)dynamic Processes in Catalytic Reactors
- Development of Scientific Bases of Technology of Sorption and Catalytic Purification of Man-Caused Waste Gases upon Ultrasound Exposure.

The Educational Scientific Center "*Functional and Structural Carbon Nanocomposites*" was organized jointly with the *Vladimir State University*, Vladimir, in 2010. Executors: **Dr. Alexey A. Vedyagin** (BIC), **Prof. Sergey M. Arakelyan** (VlSU).

Specialization:

- Fundamental and Applied Studies in the Field of Physics and Synthesis of Carbon Nanostructures for Their Further Utilization for Development of Novel Materials and Innovation Productions
- Scientific Bases for Production and Application of Catalytic Systems for Hydrocarbon Raw Materials Processing
- Development of Technology for Catalytic Hydrocarbon Pyrolysis
- Development of Technology and Catalysts for Production of Carbon Nanomaterials of Various Modification
- Potentiality of Carbon Nanostructures Application.

The Educational Scientific Center "*Natural and Synthetic Nanomaterials*" was organized jointly with the Far Eastern Federal University, Vladivostok, in 2010. Executors: **Dr. Alexey A. Vedyagin** (BIC) and **Dr. Kirill S. Golokhvast** (FESTU).

Specialization:

- Scientific Bases for Diagnostics of Toxic Properties of Synthetic and Natural Nanomaterials
- Development of a Standardized Definition of Parameters of Biosafety Upon Production and Exploitation of Nanotechnology Products
- Development of the Methods for Nanomaterials Synthesis and Isolation and Investigation of Their Physico-Chemical, Biological and Catalytic Properties
- Development of Perspective Directions of Catalytic Oil and Gas Treatment Using Nanomaterials
- Development of Method for Natural and Synthetic Nanomaterials Biotesting

- Synthesis of Carbon Nanomaterials from Hydrocarbon Raw Materials and Investigation of Their Nanotoxic Characteristics.

The Educational Scientific Center "*Physical Methods for the Investigation of Functional Materials in situ"* was organized jointly with *NSU* in 2010. Executors: **Prof. Oleg N. Martyanov** (BIC) and **Prof. Sergey V. Tsybulya** (NSU).

Specialization:

- Experimental and Theoretical Investigation of Structure and Properties of Functional Materials (Catalysts, Sorbents, Nanomaterials) Using Modern Physico-Chemical Methods
- Development of New Experimental and Computational Approach for Investigation of Functional Materials, Including *in situ*
- Experimental and Theoretical Investigation on the Atomic-Molecular Level of the Mechanisms of Catalytic Reactions, Structure and Properties of Intermediates and Active Surface Centers Using Modern Physico-Chemical Methods, Including *in situ.*

The Educational Scientific Center "*Structured and Hybrid Nanomaterials for Catalytic Processes*" was organized jointly with the *Southwest State University*, Kursk, in 2010. Executors: **Dr. Alexey A. Vedyagin** (BIC), **Prof. Aleksandr A. Kuzmenko** (SSU).

Specialization:

- Scientific Bases for Synthesis of Nanosized Particles of Metal Hybrids from Solutions
- Development of Method for Synthesis of Nanosized Platinum Group Metal and Hybrids on Their Base
- Development of Method for Synthesis of Nanosized Nickel Particles and Hybrids on Their Base
- Development of Prospect Methods for Utilization of Anodic Sludge
- Investigation of Physico-Chemical and Catalytic Properties of Nanosized Particles of Metal Hybrids.

3 Joint Laboratories were created with the purpose of integration of high education and fundamental science to increase the efficiency of joint efforts aimed at the training of high skilled specialists.

Joint **Laboratory of Catalytic Processes and Apparatuses** of the *Boreskov Institute of Catalysis* and the *Novosibirsk State Technical University,* created in 2002. Scientific Coordinators are **Prof. Aleksandr S. Noskov** (BIC) and **Prof. Gennadii G. Kuvshinov** (NSTU).

Main areas of scientific research of the Laboratory are:

- Mass and Thermo Transport Processes in Apparatuses for Chemical Engineering
- Design and Development of New Processes and Apparatuses for Energy- and Resource-Saving Chemical Technologies
- Development of the Scientific Basis for the Technology of Filament Carbon Synthesis
- Simulation of Moving Bed Apparatuses.

Joint **Laboratory of Sorption and Catalytic Processes** of the *Boreskov Institute of Catalysis* (Novosibirsk) and the *Butlerov Institute of Chemistry*, *Kazan State University*, Kazan, created in 2003. Scientific Coordinators are **Prof. Aleksandr S. Noskov** (BIC) and **Prof. Aleksandr A. Lamberov** (KSU).

Main areas of scientific research of the Laboratory are:

- Design of the Catalysts and Sorbents for Petrochemistry and Oil Refinery in Russia
- Scientific Basis of the Support Texture Formation within Industrial Synthesis and Working-Off
- Comparative Testing of Supports, Sorbents and Catalysts
- Development of New Highly Efficient Energy- and Resource-Saving Technologies for Petrochemistry and Oil Processing.

Joint **Laboratory of Engineering Chemistry** of the *Boreskov Institute of Catalysis* (Novosibirsk) and the *Volgograd State Technical University*, Volgograd, created in 2004. Scientific Coordinator is **Prof. Yurii V. Popov** (VolSTU).

Main areas of scientific research of the Laboratory are:

- Development of Novel Efficient Energy- and Resource-Saving Chemical-Technological Processes
- Design of Scientific Bases and Technology for Synthesis of Physiologically Active Substances
- Design of Scientific Bases and Technology for Heterogeneous Catalytic Processes for Chemicals Production
- Design and Study of Fuel and Oil Additives.

Dissertation Council Activities

In addition to teaching students in many Russian universities, researchers of the Institute participate in the training of young scientists of the highest qualification capable of conducting original basic and applied research in the field of catalysis. Their training has priority importance for the Institute and is related directly to its development and well being. The Institute solves these problems through the postgraduate school of SB RAS and postgraduate school of NSU. Annually 20-30 postgraduates are trained at the graduate school working at the Institute. Supervised by the researchers of the Institute, postgraduate students conduct their Ph.D. studies in chemical kinetics and catalysis, physical chemistry, chemical engineering in the BIC laboratories.

Dissertation Council D 003.012.01 was confirmed by The Order of Rosobrnadzor on May, 2010. Dissertation Council is allowed to uphold a thesis to receive an academic degree of Doctor of Science and Ph.D. on specialities: 02.00.15 “Kinetics and Catalysis” within chemical sciences and 02.00.04 “Physical Chemistry” within chemical sciences. Head of the Dissertation Council is Prof. V. Parmon.

Dissertation Council DM 003.012.02 was confirmed by The Order of Rosobrnadzor on July, 2010. Dissertation Council is allowed to uphold a thesis to receive an academic degree of Doctor of Science and Ph.D. on specialties: 02.00.15 “Kinetics and Catalysis” within chemical and technical sciences and 05.17.08 “Processes and Apparatuses for Chemical Technology” within technical sciences. Head of the Dissertation Council is Prof. Vladimir A. Sobyanin.

1 Doctor of Science and 14 Ph.D. theses have been defended in 2011.

Doctor of Science

Mariya N. Timofeeva – “*Acidity and Catalytic Properties of Homogeneous and Heterogeneous Systems Based on Heteropolyacids*”

Ph.D. Theses

Zhanna V. Veselovskaya – “*Sorption Properties of Composite Ammonia Sorbents Based on Dispersed Alkaline-Earth Metal Chlorides*”

Anton A. Gabrienko – “*Mechanisms of Activation and Transformation of Small Alkanes over Zn- and Ga-Containing Zeolites Beta According to NMR in situ*”

Marina Yu. Smirnova – “*Regularities of Formation of Sulfated Alumina and Their Activity in Reactions of Isobutane Alkylation with Butenes and n-Pentane Isomerization*”

Ruslan A. Zotov – “*Development of Catalysts Based on Alumina for Olefines Production from Alcohols*”

Tamara S. Kharlamova – “*Synthesis and Investigation of Oxygen Conducting Systems Based on Lanthanum Silicates*”

Yuliya A. Ivanova – “*Study of Kinetics and Mechanism of Selective Methane Oxidation to Syn-Gas over Pt/Ce-Zr-(La)-O Catalysts in Non-Stationary Conditions*”

Marina V. Bukhtiyarova – “*Physico-Chemical and Catalytic Properties of Catalysts Based on Aluminates of* $MAl_{12}O_{19}$ *Compositions*”

Elena M. Polyanskaya – “*Study of Catalysts Based on Nanosized Carbon Materials in Reactions of Deep Liquid Phase Oxidation of Organic Substrates with Oxygen and Hydrogen Peroxide*”

Lidiya S. Kibis – “*XPS Study of Metal and Oxidized Silver and Palladium Nanoparticles*”

Valerii S. Chernyavskii – “*MFI Zeolites in Reactions of Nitrous Oxide Decomposition and Benzene to Phenol Oxidation. Role of Iron and* α*-Centers*”

Olga V. Netskina – “*Synthesis and Study of Rhodium Containing Catalysts for Sodium Borane Hydrolysis*”

Sergei V. Budukva – “*Regeneration of Supported CoMo Catalysts for Deep Hydropurification of Diesel Fuels* ”

Elena V. Danilevich – “*Active Component of Supported Vanadium Catalysts and Kinetics of Formaldehyde Oxidation to Formic Acid*”

Irina V. Delidovich – “*Catalytic Processes for Synthesis and Oxidation of Sugars*”

There is a great demand for specialists in catalysis trained at the Boreskov Institute of Catalysis. Many of them apply their knowledge in various research centers, universities and manufacturing companies.

SCIENTIFIC SOCIAL LIFE

❖ Prize-winners of *Young Scientist Competition on Awarding Premiums Named after Outstanding Scientists of the SB RAS* became:

♦ **Dr. Sergey S. Arzumanov**, premium after Academician K.I. Zamaraev for the work "*Application of Solid State NMR for Studying Mechanism of Alkanes C1-C4 Activation and Transformation over Zn- and Ga-Containing Zeolite Catalysts*"

♦ **Dr. Ilya V. Mishakov**, premium after Academician G.K. Boreskov for the work "*Reactivity and Catalytic Properties of the Systems Based on Aerogel Magnesium Oxide*".

❖ The Ministry of Education, Science and Innovative Policy of Novosibirsk area has summed up the results of *Competitions on allocation of nominal grants, nominal premiums and grants*. Among the winners – **Pavel A. Kolinko** for his work "*Development of Photocatalytic System for Air Cleaning under Visible Light Irradiation*".

❖ *Nominal premium of the Government of Novosibirsk Area for outstanding scientific achievements in 2010 was awarded* to **Dr. Sergey V. Semikolenov** for the series of works "*Synthesis of New Type of Liquid Rubbers – Unsaturated Polyketones, for Producing Materials with Improved Characteristics*" - 1st prize in nomination "*Chemistry and Material Science*".

❖ According to Resolution of the SB RAS Presidium on the results of the *Lavrentiev Competition of SB RAS Youth Projects* three projects from Boreskov Institute of Catalysis became the winners:

♦ **E.A. Kozlova, D.V. Kozlov, P.A. Kolinko, M.N. Lyulyukin, D.S. Selishchev, D.E. Tsydenov** – "*New Composite TiO_2 Based Inorganic Materials for Solar Light Energy Utilization*"

♦ **E.N. Gribov, O.V. Netskina, I.M. Krivobokov, A.M. Ozerova, A.I. Lysikov** – "*Development of Highly Efficient Catalysts and Membrane-Electrode Assemblies for Energy Generators Based on Borohydride Hydrogen Storage*"

♦ **A.A. Lysova** (BIC, International Tomography Center) – "*Development of NMR Tomography for in situ Investigation of Catalysts and Catalytic Processe*s".

❖ Winners of the *Competition for grants of the President of Russian Federation for the state support of young Russian scientists – PhD*s *became*:

Dr. Petr M. Eletskii – "*Micro- and Mesoporous Adsorbents and Catalyst Supports from High-Ash Biomass*"

Dr. Anna A. Lysova (BIC, International Tomography Center) – "*Development and Application of NMR Tomography for in situ Studies of Heterogeneous Catalysts and Heterogeneous Catalytic Processes*"

Dr. Il'ya V. Mishakov – "*Processing of Components of Associated Gases into Carbon Nanofibres for Reinforcement of Construction Materials*"

Dr. Alexander N. Simonov – "*New Palladium Based Catalysts for High-Efficient and Ecological Power Supply*".

- On December 12-13, the annual *Competition for the best scientific research work* took place at the Boreskov Institute of Catalysis.

The first prize winner:

SILICALUMINOPHOSPHATE SAPO-31: STUDIES OF REGULAR FEATURES OF SYNTHESIS, PHYSICOCHEMICAL AND CATALYTIC PROPERTIES. DEVELOPMENT OF A CATALYST FOR *n*-ALKANE HYDROISOMERIZATION BASED THEREON

O.V. Kikhtyanin, A.V. Toktarev, A.B. Ayupov, A.E. Rubanov, M.Yu. Smirnova, G.V. Echevsky

The advanced technologies for production of low-stiffening fuel and oils are based on not removal of *n*-alkane constituents (deparaffinization) but their selective hydroisomerization. The hydroisomerization catalyst is a noble metal (hydrogenation component) containing microporous material with specific structural and acidic characteristics. The characteristics of a silicaluminophosphate with the SAPO-31 structure allow it to be considered as a promising acidic component of such a catalyst. However, the properties of this material are as yet not duly characterized because of the absence of reliable and reproducible methods for its synthesis.

The process of synthesis of SAPO-31 samples was comprehensively studied depending on the nature of initial components, as well as on the composition, preparation conditions and hydrothermal treatment of the reaction medium. The main factors determining the preparation of pure-phase SAPO-31 materials are the use of high-active aluminum sources and a high content of the structure-forming compound (template) in the reaction mixture. A reproducible method for synthesis of pure-phase silicaluminophosphates was developed for the first time.

The influence of the template type, silicon crystallinity and content in SAPO-31 on physicochcemical and catalytic properties of SAPO-31 was studied. A Russian catalyst Pt/SAPO-31 for hydroisomerization was developed and successfully tested in pilot-scale hydrotransformation of a real feedstock (diesel fraction). Metal-containing silicaluminophosphates SAPO-31 were demonstrated to be promising catalysts for hydrotransformation of vegetable oil to produce C_{15}-C_{18} fraction with a high content of isomer products.

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   Synthesis of SAPO-31 with di-*n*-Pentylamine: Influence of Chemical Composition and Crystallization Conditions,
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6. **O.V. Kikhtyanin, A.V. Toktarev, (I.D. Reznichenko), G.V. Echevsky,**
   Hydroisomerization of Diesel Fractions on Platinum-Containing Silicoaluminophosphate SAPO-31: From the Laboratory to the Pilot Scale,
   Petr. Chem., 2009, v. 49, pp. 77-82.
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   Influence of Crystallinity on the Physico-Chemical Properties of SAPO-31 and Hydroconversion of *n*-Octane over Pt Loaded Catalysts,
   Appl. Catal. A: General, 2010, v. 378, pp. 96-106.
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   Hydroconversion of Sunflower Oil on Pd/SAPO-31 Catalyst,
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   Influence of the Template on the Properties of SAPO-31 and Performance of Pd-Loaded Catalysts for *n*-Paraffin Isomerization,
   Micropor. Mesopor. Mater., 2012, v. 150, pp. 14-24.

The second prize winners:

NANOSIZE GOLD CATALYSTS: METHODS FOR SYNTHESIS AND APPLICATION FOR PRACTICALLY IMPORTANT REACTIONS

B.L. Moroz, P.A. Pyryaev, I.V. Delidovich, Yu.S. Demidova, G.N. Ilinich, V.I. Zaikovsky, D.A. Zyuzin, I.P. Prosvirin, A.V. Nartova, O.P. Taran, I.L. Simakova, E.Yu. Gerasimov, N.A. Zaitseva, E.M. Moroz, P.P. Semyannikov*, K. Kharas**

**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*

***Delphi Catalyst, Tulsa, OK, USA*

Gold was considered for long a catalytically inactive metal. In 1990's, gold dispersed to nanosize particles on various supports was discovered to reveal a very high catalytic activity and/or unusual selectivity to many reactions. The authors of the present work proposed and checked various methods for synthesis of gold nanoparticles on the surface of alumina which is one of the most abundant and technologically appropriate supports of catalytically active components. A set of methods (XRD, HRTEM, XPS etc.) were used for studying variations in the charge state and local environment of gold in preparing nanosize Au/Al_2O_3 catalysts. The epitaxial interaction of Au^o crystallites with the support that is responsible for their anomalously high stability to sintering at high temperature. When compared to commercial Pd and Pt catalysts, Au/Al_2O_3 systems are more active and thermostable in the processes of cleaning air and diesel exhaust gases from CO impurities. The developed composite Au-Pt catalysts are very stable to poisoning by CH_x impurities. It was established for the first time that gold catalyzes hydrodenitrogenation of pyridine to produce N,C-nanofibers, as well as skeletal rearrangement of α-pinene to camphene that is the key stage of the camphor production. The demonstrated high activity, selectivity and stability of Au/Al_2O_3 and $Au-Pd/Al_2O_3$ catalysts for oxidation of glucose into sodium gluconate and for hydrogenation of divinyl into butenes make these catalysts competitive to the known catalysts for these reactions.

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   Size Effects in Catalysis by Suppported Metal Nanoparticles,
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5. **B.L. Moroz, P.A. Pyryaev, V.I. Zaikovsky, V.I. Bukhtiyarov,**
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SILICA AEROGELS FOR RING IMAGING CHERENKOV DETECTORS

A.F. Danilyuk, V.L. Kirillov, A.Yu. Predein, M.D. Savelieva, A.Yu. Barnyakov*, M. Yu. Barnyakov*, V.S. Bobrovnikov*, A.R. Buzykaev*, S.A. Kononov, E.A. Kravchenko, A.P. Onuchin*

**Budker Institute of Nuclear Physics, Novosibirsk, Russia*

Ring imaging Cherenkov detectors are widely used for high energy physical experimental studies when charged particles are necessary to be identified over a wide range of pulses at a large spatial scatter of flying particles. The detector consists of a Cherenkov radiator (a layer of a transparent matter with a certain refractive index), position-sensitive photodetector and, sometimes, an optical system for light collection and focusing. When a particle flies through, photons of the Cherenkov radiation form a ring on the photodetector surface to allow the Cherenkov angle depending on the refraction index and on the particle speed to be measured, Measuring the speed and pulse of the particle makes it possible to determine the mass of the particle, i.e. to identify it.

The choice of the radiator refraction index is defined by the required pulse range where the particles are separated. In 1990's, the achieved aerogel quality allowed it to be applied for ring imaging Cherenkov detectors. Aerogel is a synthetic porous silicon dioxide; its visible light refraction index varied in the range of 1.006 to 1.20 and is chosen in the course of the synthesis.

The present work is devoted to development of methods for synthesis of packages of silica aerogels, to studies of their physical properties and efficiency of their applications as radiators of ring imaging Cherenkov detectors. Particular attention was paid to the so-called *focusing* aerogels. In 2004, a research team of the Belle collaboration (KEK, Japan) and, independently, BIC's team proposed to use packages of several aerogel layers with the refraction indices and thicknesses allowing the Cherenkov rings of different layers to overlap in plane of the photodetector. The Cherenkov radiation from different points are thus focused through the radiator thickness that makes the measurement of particle speed much more accurate in comparison to the homogeneous aerogel.

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ELECTRON STRUCTURE AND REACTIVITY OF SUPPORTED VANADIUM CATALYSTS

Molecular mechanisms of selective oxidation of formaldehyde and decomposition of formic acid

V.I. Avdeev, V.M. Tapilin, G.Ya. Popova, T.V. Andrushkevich, Yu.A. Chesalov, E.V. Danilevich, E.M. Sadovskaya, V.V. Kaichev, E.A. Ivanov

A set of physicochemical methods were used for analysis of the structure of the active component of supported vanadium catalysts V/SiO_2, V/Al_2O_3, V/ZrO_2, V/Nb_2O_5, V/TiO_2. The monomer, polymer (VO_x) and crystalline (V_2O_5) species were identified and characterized. Their catalytic properties were studied in the reactions of selective oxidation of formaldehyde $H_2C{=}O$ and decomposition of formic acid HCOOH. The V/TiO_2 catalysts with polymer VO_x species were most active and selective. Intermediates formed at the adsorption of $H_2C{=}O$ and HCOOH on the surface of the polymer samples were identified and characterized. The key species are molecular V-OCH_2, V-$OOCH_2$ and surface formate complexes V-OOCH. The data obtained were used for developing realistic models of the supported vanadium-titanium catalysts and for careful theoretical analysis of molecular mechanisms of the classical reactions of oxidation $H_2CO + O \rightarrow HCOOH$, dehydrogenation $HCOOH \rightarrow CO_2 + H_2$, dehydration $HCOOH \rightarrow CO + H_2O$, hydration-hydroxylation $H_2O + VO \rightarrow HO\text{-}V\text{-}OH$, in which the energetics and reaction pathways depend on the electron structure of the polymer VO_x species, mobility (strength) of the lattice oxygen and include processes of proton transfer, formation of Brønsted acidic VOH^+ and basic VO^- centers and the other fundamental properties of the V/TiO_2 catalysts determining their activity and selectivity to oxidation of organic compounds.

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On **August 4, 1997, Zamaraev International Charitable Scientific Foundation** was organized in the memory and honor of Professor Kirill I. Zamaraev.

The main Founders of the Foundation from the Russian side are:

- Boreskov Institute of Catalysis, Novosibirsk
- Institute of Semiconductors Physics, Novosibirsk
- Russian D.I. Mendeleev Chemical Society, Moscow
- Scientific-Industrial Company «Altay», Biysk
- «Ecogeochem Ltd.», Moscow
- Association «Russian House for International Scientific and Technological Cooperation»
- Other scientific, commercial and financial institutions.

The Foundation is supported by IUPAC and some Russian sponsors.

The Zamaraev Foundation is grateful to all sponsors for their contribution and invites Russian and foreign organizations (as well as wealthy persons) to become the honorary participants of the campaign.

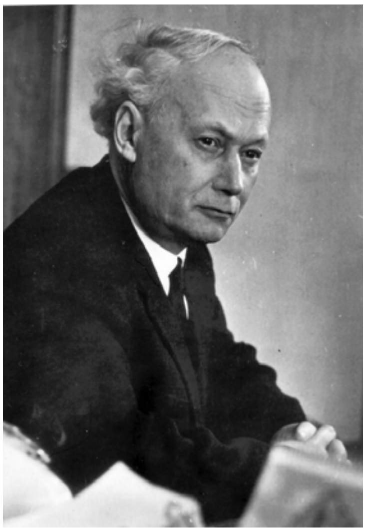
The main aim of the Foundation is to support gifted Russian scientific youth working in the field of chemical catalysis, physical methods of its research and chemical physics.

Major part of Foundation budget is spent for Zamaraev post-graduate scholarships, prizes and grants. The Foundation plans to support international cooperation of scientific youth in the field of chemical catalysis and chemical physics, i.e., their participation in international scientific conferences and seminars. In 2012 **Maxim S. Kazantsev** got the post-graduate scholarship.

❖ 17 Ph.D. students and reserach fellows of the Institute are members of the **Council of Scientific Youth.** The main principle of the Council is to represent interests of young scientists in the Institute. These are organization of competition of the youth projects, support of the young lecturers of higher educational establishments – employees of the Institute, organization of training for qualifying examinations for the Ph.D. degree, improvement of living conditions of the young scientists, and other activity areas to improve positions of young researchers in the Institute.

Memorial Rooms of Academician Georgii K. Boreskov and Academician Kirill I. Zamaraev

The **Memorial Room of Academician Georgii K. Boreskov**, the founder and first director of the Institute of Catalysis, was opened in June 1987, on the occasion of his 80th anniversary. Georgii Konstantinovich always emphasized that the foundation of the Institute was the most important cause of his life. In 1991, the Institute of Catalysis was named after Georgii K. Boreskov.



There is a small exhibition based on the documents, awards, books, Boreskov's belongings in one of the rooms of Laboratory of Oxidation, which was headed by Georgii Konstantinovich.

A series of photos dated 1930's through 1960's tell about an extremely intense and fruitful activity of G.K. Boreskov in the fields of research and science management. He headed the Laboratory of Catalysis at the Chemicoradiological Institute (Odessa) in 1932 through 1937 (the laboratory registry dated 1931 with records by Georgii Konstantinovich concerning the preparation and characterization of vanadium catalysts was kept); the Laboratory of Catalysis at the Research Institute for Fertilizers and Insecto-Fungicides (Moscow) in 1937 through 1946, the Laboratory of Technological Catalysis at the Karpov Institute of Physical Chemistry (Moscow), and in 1958 became the Director of the Institute of Catalysis (Novosibirsk).

For his contribution to the Russian science, distinguished scientific, educational, managing and social activities, his great role in establishing the Siberian Branch of the USSR Academy of Sciences, Georgii Boreskov was awarded the Badge of Honor, three Orders of Lenin, Order of the Red Banner of Labor, Golden Medal of Hammer and Sickle, he was twice USSR State Prize winner, Ukrainian SSR State Prize winner, he was awarded the title of a Hero of Socialist Labor. Among the others, these decorations are exhibited in the Museum.

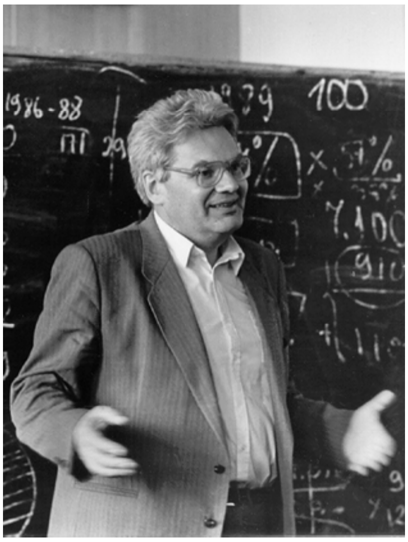
Boreskov's activity in the area of catalysis was recognized worldwide. He was a foreign member of the National Academy of Sciences of German Democratic Republic, honorary member of the New York Academy of Sciences, Doctor HONORIS CAUSA of the Wroclaw Polytechnic Institu te (Poland) and of the Poitiers University (France). Government of Bulgarian Republic awarded the Order of Kirill and Mephodium to G.K. Boreskov. Visitors can see an unusual exposition displaying the full attributes of ceremonies of awarding the HONORIS CAUSA titles to Georgii Boreskov in Wroclaw in 1976 and in Poitiers in 1981, these are black mantles and caps, an ermine scarf and leather tubules for storing the Diplomas.

Of particular interest among the exhibit is the personal book collection of Georgii Konstantinovich including more than 1000 scientific volumes and 15 sets of Russian and foreign scientific journals. There are especially memorable copies with dedicatory inscriptions by the authors and the rarities published in the end of XIX and beginning of XX century in the collection. The books capable of telling about Boreskov's educatory activity are displayed in one of the showcases, these are course descriptions and lecture summaries, books used for preparing the lectures, and the like.

There is his writing table, case, bureau and an old push-button typewriter.

Albums, arranged by the colleagues and friends in different periods of time and presented by foreign colleagues, tell about numerous scientific events, where Boreskov presented lectures, about his keenness to winter fishing and to summer "mushroom hunting", as well as about many other interesting events.

We see the same Georgii Konstantinovich in the portraits and photos, as he was – an intellectual and charming individual.



The **Memorial Room of Academician Kirill I. Zamaraev**, the Director of the Institute of Catalysis from 1984 through 1995, was opened on the 20th of May 1999, the day of 60th anniversary of K. Zamaraev. Establishment of the Memorial Room was promoted by the International Charitable Zamaraev Foundation and directly participated by Kirill Ilyich's widow, Lyudmila Aleksandrovna Zamaraeva. This small museum exposition relates to the life and activities of Academician Kirill Ilyich Zamaraev, who was a hereditary scientist.

Diplomas, awards, photo archives and belongings of Kirill Ilyich are displayed in showcases. A unique scientific book collection gathered by him is also available here.

Kirill demonstrated his brilliant potentialities in sciences as early as his school years. He finished school as the Golden Medal winner; the medal is also stored in the Museum. He continued his education in the Mendeleev Institute of Chemical Technology in Moscow, but after the third year moved to the Moscow Physical and Technological Institute (MPhTI) in order to get a strong

AN EXPERIMENTAL BENCH FOR STUDYING THE PROCESS OF SORPTIVE CATALYTIC CONVERSION OF LOW-BOILING HC

Research manager: **Dr. A. Okunev**

An experimental bench was designed and assembled for studying the process of sorptive catalytic conversion of low-boiling HC. New CO_2 absorbents, Li_2CO_3/CaO, CaO/Y_2O_3, were synthesized and studied for the first time. The original texture and its change in the cycles sorption CO_2 – regeneration were studied using a number of methods including XRD, porosimetry, elemental analysis, electron microscopy. Sorption enhanced steam methane reforming over the Li_2CO_3/CaO absorbent at 2 atm, 750°C and H_2O to CH_4 ratio of 4 using novel sorbent yielded as high as 99.8 vol. % of pure hydrogen during initial cycles.

MATHEMATICAL MODEL AND COMPUTER PROGRAM FOR CALCULATING PROCESSES IN A REACTOR FOR CATALYTIC STEAM REFORMING

Research manager: **Dr. A. Shigarov (Fig. 44)**

A mathematical model and a computer program were developed for calculating processes in a reactor for catalytic steam reforming of oil associated gas with account for non-isothermicity and internal and external diffusion limitations of the reaction rate. Experimental data on propane steam reforming over several nickel catalysts in a lab-scale flow reactor were processed using the model; parameters of the apparent 2-step kinetics were determined.

SYNTHESIS AND INVESTIGATION OF THE MODIFIED PLATINUM AND PALLADIUM BASED CATALYSTS FOR HYDROGEN AND METHANOL ELECTROOXIDATION

Research manager: **Dr. A. Simonov**

Enhancement of the specific catalytic activity of Bi-modified palladium by a factor of 3 and 20 was demonstrated for electrooxidation of H_2 on pristine and CO-blocked catalysts, respectively. Peculiarities of electrodeposition of isopolytungstates on Pt and glassycarbon electrodes were studied. It was shown that deposition of WO_x-films on Pt catalyst results in enhancement of its CO-tolerance during H_2 electrooxidation. The method for synthesis of AuPd/C catalysts was optimized. A set of AuPd/C catalysts with high loading of the active component and varied Pd:Au ratios were synthesized using different carbon supports. The promoting effect of incorporation of carbon atoms into the crystalline lattice of Pd on its electrocatalytic performance for the hydrogen electrode reactions and CO tolerance was discovered.

background in chemical physics. In the Museum, there are laboratory registries of post-graduate student Kirill Zamaraev and EPR spectra recorded by him during his post-graduate years.

The Moscow period (1956-1976) of his life and work is illustrated by the photo expositions: here is Kirill Zamaraev as a junior, then senior researcher at the Institute of Chemical Physics of the USSR Academy of Sciences; he heads a laboratory and, at the same time, he is an assistant professor in MPhTI.

Early in 1977 Kirill Ilyich was invited by Academician G.K.Boreskov; with his family and a team of young MPhTI graduates, he moved to Novosibirsk. Owing to the activity of Kirill Zamaraev and his colleagues, investigations of mechanisms of catalytic reactions at the atomic and molecular levels were considerably extended and intensified in the Institute of Catalysis.

He combined his vast research and management activity with teaching in the Novosibirsk State University.

The decade from mid-1980's to mid-1990's was the time of international recognition of his scientific achievements. The exhibition demonstrates his state awards, honorary medals of the USSR Academy of Sciences, as well as the certificate of full member of the USSR Academy of Sciences. He became a foreign member of Indian and Korean Academies of Sciences, awarded the Silver Medal by the Royal Chemical Society as an "Outstanding Lecturer of the Century", and was elected a member of Academy of Europe. In 1994 K.I. Zamaraev became a President of IUPAC, International Union of Pure and Applied Chemistry, and in 1995 was honored with the German prestigious Karpinski Award for Russian Scientists. There are diplomas and medals, as well as a number of photos of that time in the Museum.

Everyone, who knew personally Kirill Ilyich, remember his exceptional ability not to loose courage at any, even very severe, circumstances. He had a really iron character, and it was not without vain that the sport he went in for was mountaineering.

A smiling, talented, brilliant and courageous man appears before visitors to the Memorial Room.

Boreskov Institute of Catalysis SB RAS

CATALYSIS

IS THE BASIS OF HIGH-TECH CHEMISTRY

Siberian Branch of RAS –
the center of science, education
and innovations

IMPORTANT RESULTS
OF THE R&D ACTIVITY

XRD *in-situ* FOR STUDYING PHASE AND STRUCTURAL TRANSFORMATIONS OF CATALYSTS DURING THEIR PREPARATION AND ACTIVATION WITH HYDROGEN

Research manager: **Prof. L. Plyasova** (**Fig. 1**)

In-situ XRD was used for studying the phase and structural transformations of actual catalysts (Co-Al-O catalyst for the Fischer-Tropsch process; Fe-Cr-Cu-O catalysts for moderate temperature conversion of CO, a cation-substituted catalyst based on strontium hexaferrite for methane oxidation) during their preparation and activation. The studies were performed in cooperation with the Siberian Center for Synchrotron Radiation. The formation of bimetallic nanoparticles of palladium Pd-M in the course of complexes $Pd(OOCM)_4M(OH_2)$ thermoreduction was studied. The data obtained allows catalysts with controlled catalytic properties to be deliberately synthesized.

SAXS TECHNIQUE FOR STRUCTURAL AND DISPERSION ANALYSIS OF MULTICOMPONENT HETEROGENEOUS CATALYSTS

Research manager: **Prof. F. Tuzikov** (**Fig. 2**)

A new method was developed for structural and dispersion analysis of multicomponent heterogeneous catalysts to obtain direct data on the structure and dispersion of the catalyst active components. The method was tested with a series of powder heterogeneous catalysts (1%Pd-0.6%Zn)/TiO_2 and their matrix-carriers prepared by different techniques.

It was shown that algorithm for the small-angle X-ray scattering (SAXS) technique data analysis in conditions of various density contrast gives direct information on the structure and dispersity of active component of heterogeneous catalysts.

The processes of nanoparticle nucleation in the system SiO_2-P_2O_5 was studied *in situ*. The adsorption of anions of phosphoric acid on silica particles was observed during the hydrolysis of tetraethoxysilane (TEOS) in the presence of phosphoric acid and silver nitrate as a precursor of silver particles. This led to a change in the surface charge of silica to increase their coagulation that, in turn, influenced strongly the surface area and porosity of the synthesized catalyst.

IMPROVED ADSORPTION METHOD FOR STUDYING COMPONENT DISTRIBUTION THROUGH A MICROPOROUS CATALYST BULK

Research manager: **Prof. V. Gavrilov** (**Fig. 3**)

Studying the association of Cu^{2+} ions in concentrated aqueous ammonia solutions of copper nitrate shows that the ammonium concentration in the solution affects crucially the type of orbital ordering of Cu^{2+} ions in the associates. Copper ion ordering in the associates is accounted for by the presence of bridging OH groups in the axial or equatorial positions of $[Cu(NH_3)_n(H_2O)_{6-n}]^{2+}$.

SIZE EFFECT IN REACTION OF ETHYLENE EPOXIDATION OVER MODEL CATALYSTS Ag/HOPG

Research manager: **Dr. I. Prosvirin** (**Fig. 4**)

A series of model nanosized catalysts with narrow particles size distribution were prepared using HOPG as a support. Electron and catalytic properties of the Ag/HOPG catalysts with Ag particles different in size were tested for the first time in the reaction of ethylene epoxidation using *in-situ* XPS combined with PTR-MS.

ELECTRON SPIN RESONANCE SPECTRA IN SUPERCRITICAL WATER

Research manager: **Prof. O. Martyanov** (**Fig. 5**)

Electron spin resonance (ESR) spectra of VO^{2+} radical-ions in sub- and supercritical water (SCW) are observed. In subcritical conditions in the spectrum of an aqueous solution of vanadyl sulfate (with a concentration of 0.1 M and a density of 0.45 g/ml) a linear increase of the hyperfine structure (HS) lines width is observed depending on the parameter T/η (η - viscosity of the medium at temperature T). Analysis of the data allows suggesting that under isothermal conditions, the main contribution to the broadening of the HS lines makes the spin-rotational and spin-spin exchange interaction.

With increasing the temperature, the spectrum components of the hyperfine structure are broadened significantly resulting in the unresolved low-intensity line in supercritical water with $\Delta H_{pp} \sim 300$ G. The data obtained allow behavior peculiarities of the paramagnetic VO^{2+} ions in sub- and supercritical water including rotational dynamics and spin exchange between the radicals to be elucidated. The registration of the unresolved low-intensity line in supercritical conditions points to an increase in the local ion concentration in the system that can be an initial stage for the formation of vanadium-based particles in supercritical conditions.

CATALYTIC SYSTEMS BASED ON ε-Fe_2O_3 NANOPARTICLES

Research managers: **Prof. O. Martyanov, Dr. G. Bukhtiyarova** (**Fig. 6**)

Magnetostatic and magnetoresonance properties of supported ε-Fe_2O_3/SiO_2 nanoparticles with the characteristic size of ~4 nm were studied to show the existence of several magnetic subsystems irrespectively of the X-ray homogeneity. Comparative studies of the observed magnetic properties with the data of electron microscopy, XRD, ferromagnetic resonance (FMR) and Mössbauer spectroscopy made it possible to identify conditions of the formation of monophase samples and to suggest a consistent model for the magnetic ordering in the supported ε-Fe_2O_3 nanoparticles. The method of reproducible synthesis of a monodisperse system of supported magnetic ε-Fe_2O_3 nanoparticles (2-6 nm) was shown to allow catalysts containing as much as 8 wt% Fe to be developed, the catalysts being thermally stable at the temperature up to 900°C and stable to sulfiding under conditions of selective oxidation of hydrogen sulfide to provide a high selectivity of the hydrogen sulfide to sulfur conversion. *In situ* FMR was used to discover a high sensibility of magnetic properties of ε-Fe_2O_3 nanopartilces to adsorption of H_2S (FMR spectra change reversibly). The data obtained argue mainly for the formation of the nanoparticle magnetic moment owing to the surface iron ions. The system of iron-containing particles supported on silica was shown to be active to alkylation of benzene with benzyl chloride. The most active are the samples calcined at T=400°C; at a higher temperature the ε-Fe_2O_3 phase starts forming. The reaction was proved to occur on the surface of the heterogeneous catalyst. A method for its regeneration was suggested to provide the high activity on recycling.

^{13}C SOLID STATE NMR FOR STUDYING SMALL ALKANES ACTIVATION

Research manager: **Prof. A. Stepanov** (**Fig. 7**)

It is established that the activation of small alkanes (methane, ethane, propane) on gallium oxide, α-Ga_2O_3, via dissociative adsorption results in Ga-methyl (Ga-CH_3), Ga-ethyl (Ga-C_2H_5) and Ga-propyl (Ga-C_3H_7) species. These observations lead to conclude that Ga-alkyls, rather than earlier suggested alkoxy species, could be the intermediates in small alkane dehydrogenation and aromatization on gallium-modified zeolite catalysts.

In situ STUDY OF METHANOL DECOMPOSITION AND OXIDATION ON THE Pt(111) SURFACE BY XPS AND MASS SPECTROMETRIC TECHNIQUES

Research managers: **Dr. V. Kaichev, Prof. V. Bukhtiyarov** (**Fig. 8**)

Mechanisms of oxidation of hydrocarbons, methanol and CO on the surface of Pd, Pt, Rh and Ni were studied *in situ.* XPS and mass spectrometric techniques were used to study the mechanism of methanol oxidation on the Pt(111) surface at ~0.1 mbar and temperature ranging from 300 to 650 K. Two pathways of the methanol decomposition were established: complete dehydrogenation to CO and H_2 and decomposition through cleavage of the C–O bond.

STUDY OF ELECTRON STRUCTURE, THERMAL STABILITY AND REACTIVITY OF OXIDIZED METAL NANOPARTICLES Cu, Ag, Pd, DEPOSITED ON CERIUM OXIDE

Research manager: **Prof. A. Boronin** (**Fig. 9**)

Oxygen states and reactivity in oxidized metal nanoparticles (with copper, silver and palladium, deposited on cerium oxide as examples) prepared by plasma sputtering method were studied to show the interaction of the metals with surface of cerium oxide. Extending the plasma sputtering time leads to emerging of highly oxidized silver and palladium nanoparticles. The reactivity to CO is much lower than the one to oxide nanoparticles deposited on inert supports.

FORMATION OF PdO CRYSTALS OVER Pd(poly) IN O_2 ATMOSPHERE

Research manager: **Dr. A. Salanov** (**Fig. 10**)

Scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD) techniques were used to study the influence of the reaction medium of catalytic reactions of simple molecules oxidation with oxygen on chemical composition and microstructure of metal catalysts. The chemical composition and the microstructure of polycrystalline Rh, Pd and Ag foils were studied at 500-1500 K in the oxygen atmosphere. It was established that the way of the metal oxidation depends on the value of the lattice energy in the series of Rh, Pd and Ag for which the lattice structure are the same (FCC) but the lattice energy are different considerably (E = 6.10, 3.63 and 2.65 eV, respectively).

THE INTERACTION OF SO_x WITH A MODEL NSR CATALYST $Pt/(BaCO_3+CeO_2)$

Research manager: **Dr. M. Smirnov** (**Fig. 11**)

The interaction of SO_x with a model NO_x storage-reduction catalyst (NSR catalyst) $Pt/(BaCO_3+CeO_2)$ was studied using the differential charging effect in XPS. It was established that the reaction produces predominantly barium sulfate when proceeds at 150°C. Sulfation of the CeO_2 surface is observed at higher temperatures ~ 300°C and is accompanied by reduction of Ce(IV) into Ce(III), the supported platinum particles being preserved in the metal state. Reductive regeneration of the pre-sulfated at 300°C NSR catalyst in a mixture of CO and H_2O results in consecutive decomposition of Ce(III) sulfate at ≤ 500°C and then Ba sulfate at 600-700°C.

In situ XPS STUDIES OF THE REACTION OF CO + O_2 OVER Pd/CeO

Research manager: **Prof. A. Boronin** (**Fig. 12**)

Electron state and geometric structure of the active centers of disperse palladium catalysts supported on cerium-containing oxides were studied in low-temperature oxidation of carbon monoxide. *In situ* XPS studies of the reaction of CO + O_2 over Pd/CeO_2 allowed an additional CO oxidation route to be revealed, which proceeds through dissociation to form low molecular weight species of elemental carbon. The formation of active catalytic sites was studied during synthesis of the catalyst $Pd_xCe_{1-x}O_2$ to show emergence of a stable and active phase of $Pd_{2+x}Ce_{1-x}O_{2-\delta}$, containing ions of Ce^{3+} and oxygen vacancies.

BIMETAL SYSTEMS FOR METHANOL AND ETHANOL STEAM REFORMING

Research manager: **Dr. S. Badmaev**

Catalytic properties of bimetal systems for methanol and ethanol steam reforming to hydrogen-rich gas were studied. Optimal experimental conditions were determined.

THE OSCILLATORY DYNAMICS OF THE $CO+O_2$ REACTION OVER THE SUPPORTED Pd NANOPARTICLES

Research manager: **Dr. V. Elokhin**

The Monte-Carlo method was used for simulating bifurcation diagrams for the reaction $CO+O_2$ over Pt(100) and Pd(110) surfaces in the parameter space (P_i). The regions of oscillatory behavior and steady state were characterized. A variety of spatio-temporal concentration waves on the metal surfaces were revealed. The oscillatory dynamics of the $CO+O_2$ reaction over the supported Pd nanoparticles was studied with regard to the dynamically changing surface morphology of the nanoparticle surfaces.

MECHANISM OF THE STEADY-STATE REACTIONS $CO+O_2$, CO+NO, $CO+N_2O$ ON THE Pd(110)

Research manager: **Prof. V. Gorodetsky**

The mechanism of the steady-state reactions $CO+O_2$, CO+NO, $CO+N_2O$ on the Pd(110) single crystal surface were studied experimentally using TPR, TPD and molecular beam techniques. In CO oxidation, the formation of the subsurface oxygen layer is accompanied by stopping the low-temperature CO_2 formation at the 180-350 K range. In CO+NO, $CO+N_2O$ reactions, the nature of the mixed adsorption layer was established: molecular (CO_{ads}) and dissociative (O_{ads}, N_{ads}) that leads to hysteresis of the product rate formation: CO_2 and N_2.

SELF-OSCILLATIONS IN REACTION OF SELECTIVE PROPANE OXIDATION

Research manager: **A. Gladkii**

It was shown that the presence of Li (no more than 20%) in fresh Ni-catalysts leads to changes in the induction period of self-oscillations. Except this effect, Li ions influence insufficiently the region of existence of oscillations in activated catalysts.

SELF-OSCILLATIONS IN REACTION OF CO OXIDATION ON Pd/Al_2O_3(*800*)-1200 NANOPARTICLES: EXPERIMENT AND MATHEMATICAL MODELING

Research manager: **Dr. N. Chumakova** (**Fig. 13**)

Dynamics of carbon monoxide oxidation over platinum group metals were experimentally studied to describe the oscillations of the reaction rate on Pd catalyst. Based on the results obtained, a kinetic model was developed with allowance for changes in the properties of the catalyst such as, in particular, transition metal Pd^0 - oxide phase PdO. Isolated regions were identified where oscillations and isothermal self-oscillations exist. Dependencies of the oscillation period, amplitude and shape of the reaction rate auto-oscillations on the gas composition and catalyst temperature were determined.

MECHANISM OF PHOTOSTIMULATED FORMATION OF RADICAL ANIONS O^- ON THE SURFACE OF OXIDES

Research manager: **Prof. A. Volodin** (**Fig. 14**)

Procedures were developed for generation and detection of anion radicals O_2^- which appear upon decomposition of H_2O_2 and are stabilized on the surface of Zr- and Ti-containing oxide and hydroxide catalysts. An anomally high reactivity of these anions in respect of organic molecules was discovered. Particularities of the stabilization of oxygen anion radicals on the hydrated and dehydrated surfaces of oxide catalysts were studied. Quantum chemical calculations of the structure and properties of various anion radical O^- species stabilized on the partly hydroxilated surface of MgO were performed.

DFT ANALYSIS OF FORMIC ACID DECOMPOSITION PATHWAYS $HCOOH \rightarrow CO + H_2O$ ON THE SURFACE OF V_2O_5/TiO_2

Research manager: **Dr. V. Avdeev** (**Fig. 15**)

Molecular and dissociative modes of formic acid adsorption on the V_2O_5/TiO_2 model surface, possible intermediates, and transition states along of the dehydrogenation ($HCOOH \rightarrow CO_2+H_2$) and dehydration ($HCOOH \rightarrow CO+H_2O$) pathways were studied by the periodic density functional theory.

MODIFIED SOLUTIONS OF non-KEGGIN TYPE Mo-V-P HPA - HYDROLYTICALLY STABLE AND TECHNOLOGICALLY ADAPTABLE CATALYSTS FOR OXIDATION OF ORGANIC SUBSTRATES

Research manager: **Prof. E. Zhizhina** (**Fig. 16**)

Modified solutions of Mo-V-P HPA were synthesized by the methods developed earlier and studied by ^{51}V and ^{31}P NMR. In a dilute (<0.1 M) solution of $H_{11}P_4Mo_{18}V_7O_{87}$ (HPA-7), a peak of phosphoric acid is visible clearly. In the concentrated solutions ($\geq$ 0.2 M) it is strongly broadened. Perhaps such a bound state is the complex phosphate, VO_2^+, or outer-sphere complexes containing H_3PO_4, VO_2^+ and HP-anions. These features provide high thermal stability of modified HPA solutions.

BIFUNCTIONAL CATALYSTS BASED ON PEROXO POLYOXOMETALLATES

Research managers: **Prof. D. Kochubey, Prof. Z. Pai** (**Fig. 17**)

EXAFS, SAXS, IR and Raman spectroscopies were used for establishing the existence and structures of main polyoxo- and peroxopolyoxo complexes of tungsten formed through interaction of phosphorus tungsten heteropoly acid with hydrogen peroxide in aqueous solutions. The interaction was shown to reduce the nuclearity of the complexes compared to their precursor - $H_3PW_{12}O_{40}$, tetranuclear peroxopolyoxo complexes of general composition $\{PO_4[WO(O_2)_2]_4\}^{3-}$ being predominantly formed.

STUDY OF PEROXOCOMPLEX $[Me_3(n\text{-}C_8H_{17})_3N]_2\{HPO_4[WO(O_2)_2]_2\}$ (MTO) STRUCTURE IN ORGANIC SOLVENTS USING SAXS TECHNIQUE

Research manager: **Prof. F. Tuzikov** (**Fig. 18**)

SAXS technique was used for studying in detail complex $[Me(n\text{-}C_8H_{17})_3N]_2\{HPO_4[WO(O_2)_2]_2\}$ in 18 solvents. In most of the solvents, the complex is detected as individual molecules of 14.5±1.2 Å in size. The molecule structure is described in termed of the core-shell model with a dense nucleus (W-containing anion) and a loose shell.

SYNTHESIS OF ORGANIC COMPOUNDS USING IONIC LIQUIDS AS REACTION MEDIA

Research manager: **Dr. N. Adonin** (**Fig. 19, 20**)

The reactions of the carbon-halogen bond activation under the action of *in situ* generated zero-valent nickel complexes were investigated in ionic liquids as reaction media.

SYNTHESIS OF DIACETONE ALCOHOL AND TRIETHANOLAMINE IN MICROCHANNEL REACTOR

Research manager: **Prof. L. Makarshin** (**Fig. 21, 22**)

Diacetone alcohol and triethanolamine were synthesized for the first time using a microchannel reactor. The results obtained demonstrated a high efficiency of the microchannel reaction against the traditional systems, the maximal productivity corresponded to the equilibrium concentration of diacetone alcohol and reached 5 mol %.

It was established that the optimal residence time of the reagents for triethanolamine synthesis is 2.5-3 min, the ethylene oxide to ammonia ratio being 1 to 1.3.

VORTEX EMULSIFIER FOR PHASE MIXING IN CATALYTIC MULTIPHASE PROCESSES

Research manager: **Dr. A. Kuzmin** (**Fig. 23**)

A lab-scale vortex emulsifier was assembled and tested for phase mixing in catalytic multiphase processes on the liquid/liquid boundary with participation of gas component. Hydrodynamic studies were carried out to suggest a theoretical model for describing basic parameters of the vortex emulsifier.

POLYMERIZATION AND COPOLYMERIZATION OF ETHYLENE AND α-OLEFINS OVER NEW BINUCLEAR AND FUNCTIONALIZED POSTMETALLOCENE CATALYSTS

Research manager: **Prof. S. Ivanchev** (**Fig. 24**)

Nine tridentate salicylaldiimine ligands of various structures and corresponding titanium halide complexes based thereon were for the first time synthesized. A set of analytic and physicochemical methods including NMR-DOSY spectrometry and Maldi-TOF mass-spectrometry were used to prove the binuclear structure of the binuclear titanium halide complexes.

Twelve *bis*salicylaldiimine ligands of different structures also were synthesized, which were functionalized with oxy-allyl groups in phenyl bound with imine nitrogen, the corresponding complexes based thereon being prepared.

Kinetic studies of ethylene polymerization were carried out using binuclear titanium halide catalysts. The resulting catalytic systems were shown, depending on the ligand environment and the nature of bridge bonds between imines of the binuclear complexes, to feature a high thermal stability combined with the high catalytic activity. The relevant quantum chemical calculations supported the results of the kinetic studies.

Co-polymerization of ethylene and hexene-1 was studied using two of the binuclear complexes. The results obtained did not confirm the expected possibility of a selective increase in the proportion of hexene-1 involved in the co-polymer as was reported by Salata and Marks who studied copolymerization of ethylene and hexene-1 in catalytic systems based on binuclear complexes of different structure. It is our opinion that the bridge bonds between imines in systems under study make special hindrances for insertion of α-olefins (hexene-1) into the co-polymer to neutralize an increase in the proportion of hexene-1 inserted into the co-polymer.

Specific features of catalytic activity to polymerization were studied with the catalysts prepared on the basis of the synthesized titanium halide complexes which were functionalized with oxy-allyl groups of bissalicylaldiimine precursors. It was shown that the regime of the catalyst self-immobilization can be controlled in the course of polymerization depending on the position of the oxy-allyl group and on the length of the bridge (–CH_2) between the oxy-group and double bond.

ALTERNATIVE MECHANISMS OF OXIDATIVE METHANE ACTIVATION

Research manager: **Dr. E. Starokon** (Fig. 25)

It is generally accepted that oxidative activation of methane (and other hydrocarbons) proceeds through dissociative interaction with active oxygen of the catalyst. However, it is not clear which fragment of dissociating molecule (H or CH_3) is bound to the active oxygen. The prevailing opinion tending to the hydrogen abstraction is only a hypothesis having no direct experimental evidence.

For clarification of this question the convenient model is the reaction of methane with α-oxygen which is anion-radical species deposited on the FeZSM-5 surface. Reaction of CH_4 with preloaded O_α in the concentration up to 100 μmol/g, is instantly proceeds even at – 30°C.

In this work the reaction of methane with O_α was studied at its slow deposition from N_2O to the surface of FeZSM-5 at 25°C. In this case, an only fragment of methane can bind to α-oxygen. IR spectroscopic identification of the resulting surface products gave for the first time reliable experimental evidence of the widely accepted hypothesis about methane activation by the hydrogen abstraction mechanism to form $(OH)_\alpha$ groups.

MECHANISM OF OXIDATION OF BUTADIENE-1,3 ON Pd-Te/C CATALYSTS

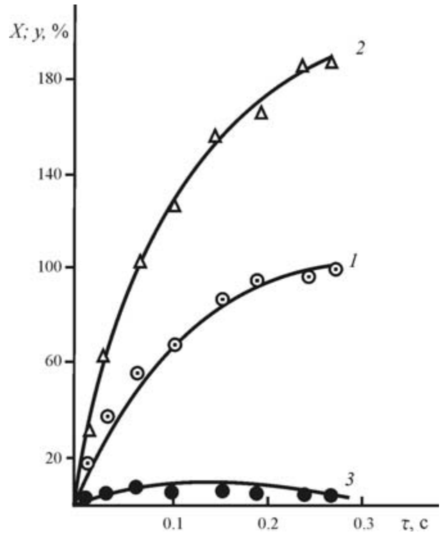
Research manager: **Prof. N. Kuznetsova** (Fig. 26)

1,4-Oxygenates, in particularly 1,4-butenediol and its ethers, are valuable reagents for polymerization and chemical synthesis. It was established that methyl alcohol is another, apart from acetic acid, solvent suitable for oxidation of butadiene-1,3 to 1,4-oxygenates in the presence of Pd-Te/C catalyst. The absence of acrolein among the oxidation products indicated strongly the non-radical mechanism provided by stabilization of the intermediate and products with methoxyl group. Variations in the catalyst (Te loading) and additives (H_2O, H_2SO_4) allowed the conditions to be identified for preferable formation of 1,4-derivatives. Oxidation of butadiene-1,3 on Pd-Te/C catalyst in the presence of H_2SO_4 gave 85% yield of GC detected products at 33% selectivity to 1,4-dimethoxybutene-2 and 50% total selectivity to 1,4-oxygenates. Under similar conditions and increased butadiene loading, the selectivity to 1,4-dimethoxybutene-2 reached 60% at 30% conversion of butadiene to the GC detected products.

CATALYTIC SYNTHESIS OF DIMETHYL SULFIDE BASED ON DIMETHYL DISULFIDE

Research manager: **Prof. A. Mashkina**

The reaction of dimethyl disulfide with methanol was studied at P = 1 atm and T = 350°C in the presence of catalysts bearing acidic and basic centers. The main sulfur-containing products are dimethyl sulfide and methanethiol. In the formation of dimethyl sulfide, the most active catalysts are those which bear simultaneously moderate-strong basic sites and strong proton and aproton centers on their surface. These are, in particular, H-zeolites and transition metal oxides supported on γ-Al_2O_3.



Dependence of dimethyl disulfide conversion upon its reaction with methanol (1) and dimethyl sulfide (2) and methanethiol (3) yields on contact time. Catalyst Cr/ γ-Al_2O_3.

HYDROXYLATION OF AROMATIC COMPOUNDS WITH NITROGEN SUBOXIDE

Research manager: **Dr. D. Ivanov** (Fig. 27)

Gas phase oxidation of phenol by nitrous oxide for preparation of (DHB) is of significant interest. However, due to experimental difficulties caused by the high boiling points of DHB

(240-285°C), this reaction has not been as yet studied in detail. In the present work, the reaction was studied for the first time using a catalytic setup specially designed for operation with high-boiling compounds.

FeZSM-5 zeolites were shown to be efficient catalysts for the title reaction. An unusual isomeric distribution of DHB depending on the reaction conditions was found. Formation of resorcinol, in addition to hydroquinone and catechol, is a particular feature of the reaction. Although the fraction of resorcinol averaged over 12 h time-on-stream is not high (6-9 mol %), in the initial period of reaction it may comprise over 70% of the total amount of DHB.

A comparison with the current liquid-phase processes of phenol oxidation by H_2O_2 showed that the oxidation by N_2O may open a new promising way for alternative production of DHB in the gas phase.

NITROUS OXIDE FUNCTIONALIZATION OF POLYMER NANOMATERIALS

Research manager: **Dr. K. Dubkov** (**Fig. 28**)

Tire rubber granules were treated with nitrous oxide (N_2O) at 180–230°C and 20–50 atm to obtain products of the rubber regeneration with different conversions of C=C bonds and destruction levels. It was shown that the sol-gel fraction comprised in the regenerated rubber contains mainly isoprene and butadiene oligomers with carbonyl (predominantly ketone) groups. The gel fraction involves a part of the polymer component of the initial vulcanizate and all of its carbon filler. The results obtained allowed the mechanisms of rubber-N_2O interaction and of the rubber destruction to be established. The reaction goes through selective interaction between N_2O and C=C bonds of the vulcanized materials (isoprene and butadiene rubbers) to form carbonyl, preferably ketone, C=O groups in polymer chains. Cleavage of a part of C=C bonds leads to the controlled destruction of polymer chains of vulcanized rubber and, consequently, to destruction of the vulcanization network to form a plastic regeneration product. Sulfide cross-bonds are formed during the rubber vulcanization but not destroyed during the reaction. The presence of polar carbonyl groups in the regeneration products obtained with N_2O makes the products applicable as adhesion modifiers in coating compositions, they make the rubber-wire binding much stringer (by a factor of 1.5) in the composition.

RELATION BETWEEN CATALYTIC PROPERTIES OF Mo-V-Te-Nb OXIDES AND THEIR ACTIVITY IN REACTION OF ISOTOPIC EXCHANGE WITH DIOXYGEN

Research manager: **Dr. E. Sadovskaya** (**Fig. 29**)

The differences in catalytic behavior of the multiphase Mo-V-Te-Nb oxide catalysts are accounted for by the different oxygen states in the constituent phases. A relatively high rate of isotopic exchange with dioxygen is characteristic of oxygen comprised in the layered phase Me_5O_{14} and hexagonal phase M2. This oxygen also is active to complete oxidation of propane and propylene, while oxygen of the orthorhombic phase M1 features the minimal rate of isotopic exchange but is active to partial oxidation.

MECHANISM OF H/D EXCHANGE OVER Pt/SZA CATALYST AND Pt/Al_2O_3+ SZA MECHANICAL MIXTURE

Research manager: **Prof. V. Goncharov** (Fig. 30)

The importance of hydrogen spillover processes in typical acid-catalyzed reactions was established. The hydrogen transfer processes have a significant impact on the side conversion of carbenium ion intermediates on the surface to decrease the fraction of molecules transformed into condensation products (coke), but the conversion of the initial reagents also decreases. The conversion decreasing can be caused by the suppression of the carbenium ions formation on Lewis acid sites due to the competition for the site between the hydrogen and paraffin molecules due to minor difference between dissociation energies of H-H and C-H bonds.

SYNTHESIS AND CHARACTERIZATION OF FIBERGLASS CATALYSTS

Research manager: **Prof. B. Bal'zhinimaev** (Fig. 31)

Three types of leached fiber glass silicate materials modified with Zr, Al and rare earth metals (REM) (Zr-Si, Al-Si and REM-Si) were nitridated with ammonia at high temperatures. According to DRIFTS and H/D exchange data, dehydroxylation of silanol groups as well as hydrolysis of NH_x species takes place along with their nitridation. *In situ* DRIFTS study showed that the limiting steps are slow chemical reactions, but not diffusion of NH_3 or H_2O molecules in the glass bulk. The concept of strained siloxane bridges formed due to dehydroxylation of two adjacent silanol groups was used for explanation of the reaction kinetics.

A series of Cs- and Pt-containing fiberglass samples were prepared via ion exchange. Only bimetal Pt-Cs FG systems revealed high performance in isobutene dimerization with conversion up to 20% and extremely high selectivity (99%), whereas the monometallic ones showed poor performance. XPS studies revealed electron transfer from Pt to Cs takes place in the glass bulk to cause the formation of Pt-Cs clusters (Cs^0 surrounded with a number of $Pt^{\delta+}$ species) which are active to isobutene dimerization. The reaction pathway was suggested with Pt-H hydride-like species, formed on Pt-Cs clusters as the key active sites.

MECHANISMS OF METHANE ACTIVATION UPON OXYCHLORINATION OVER RUTHENIUM-CONTAINING CATALYSTS

Research manager: **Prof. E. Paukshtis** (Fig. 32)

A new effective catalyst was developed for methyl and ethyl chloride production by oxychlorination of the corresponding paraffins; the catalyst is based on ruthenium oxychloride $K_4Ru_2OCl_{10}$ supported on titania. The catalysts of this type allow monochlorinated paraffins to be prepared at the selectivity not lower than 85-90% and conversion of 15-20%.

The composition of the active sites of the catalysts and the interaction of these sites with methane and ethane were studied. It was shown that, in contrast to the known catalysts based on copper chloride, the production of mono-chloride derivatives is mediated by the formation of surface methoxyl groups with participation of the bridging Ru-O-Ru oxygen.

The mechanism of paraffins oxychlorination over ruthenium oxychloride was proposed including the participation of bridging oxygen of electrophylic nature.

MECHANISM OF SELECTIVE OXIDATION OF 2-METHYL-1-NAPHTHOL WITH MOLECULAR OXYGEN

Research manager: **Dr. I. Ivanchikova** (Fig. 33)

Kinetic, spectroscopic, mass-spectrometric, isotope, and theoretical methods were used to study the mechanism of selective oxidation of 2-methyl-1-naphthol to 2-methyl-1,4-naphthoquinone (menadione, vitamin K_3) with molecular oxygen. The data obtained lead to conclude about the mechanism of selective formation of menadione at high pressure (3 atm O_2) via thermal intersystem crossing that involves the spin inversion in the rate-limiting step and the formation of zwitter-ion. At atmospheric pressure, there occurs the routine non-selective autooxidation by the classical chain radical mechanism.

NEW HETEROGENEOUS CATALYSTS MIL-101 FOR LIQUID-PHASE PROCESSES

Research manager: **Dr. O. Zalomaeva**(Fig. 34)

The mesoporous iron and chromium terephthalate-based metal-organic framework Fe- and Cr-MIL-101 catalyze the selective oxidation of cyclohexane with *tert*-butyl hydroperoxide and allylic oxidation of cyclohexene with molecular oxygen as well as carboxylation of epoxides with CO_2 to produce cyclic carbonates. All the reactions proceed efficiently in the absence of any solvent under mild reaction conditions.

NEW CATALYTIC SYSTEMS FOR ASYMMETRIC EPOXIDATION OF OLEFINS WITH HYDROGEN PEROXIDE

Research managers: **Prof. K. Brylyakov, Dr. O. Lyakin** (Fig. 35)

Non-heme catalyst systems Fe(*S,S*)-PDP/oxidant/carboxylic acid and Mn(*S,S*)-PDP/oxidant/carboxylic acid (oxidant = H_2O_2 or peroxycarboxylic acid) were tested in enantioselective epoxidation of olefins. It was found that these systems can epoxidize prochiral olefins with hydrogen peroxide and peroxycarboxylic acids with moderate to high enantioselectivities (up to 86% *ee* for iron and up to 93% *ee* for manganese), the Mn counterpart demonstrating higher turnover numbers (1000 vs. 100 TON). The systems Fe(*S,S*)-PDP/H_2O_2/carboxylic acid and Mn(*S,S*)-PDP/H_2O_2/carboxylic acid demonstrate very similar reactivity patterns, indicating similar oxygen-transferring active species.

STUDY OF CuZn-OXIDE CATALYST ACTIVATION

Research manager: **Prof. A. Khassin** (**Fig. 36**)

The studies of reductive activation of CuZn-oxide catalyst using INS, IRS *in situ* (FTIR/MS) and TG-DSC/MS showed that the reduction by hydrogen with Cu^0 formation occurs through the reversible interaction with hydrogen, accompanying with protons absorption in the form of OH^--groups ($\nu=3250$ cm^{-1} and $\delta=1430$ cm^{-1}) according to the reaction: $Cu^{2+} + 2O^{2-} + H_2 \leftrightarrow Cu^0 + 2OH^-$. At 200°C, CuZn oxide accumulates up to 6H/Cu as a hydride, hydroxyl and formate-groups to release CO_2. Isothermal study of the reduction allows estimating the kinetic and thermodynamic parameters: standard enthalpy and entropy as $\Delta_r H^\circ \approx - 110 \pm 10$ kJ/(mol$_{H2}$), $\Delta_r S^\circ \approx -140 \pm 20$ J/(mol$_{H2}$·K) and activation energy as 100 kJ/mol. H.

IMPROVEMENT OF THE PROCESS FOR SYNTHESIS OF MONOMETHYLANILINE

Research managers: **Prof. T. Yurieva, Prof. A. Khassin, Prof. A. Noskov** (**Fig. 37**)

The reason for fast deactivation of the industrial catalyst was established; this is the covering of the catalyst surface by the products of aniline interaction with side products of methanol activation. A catalyst based on Cu-containing compounds and process conditions were developed to avoid the formation of side products of methanol activation. The proposed process provides long service cycle of the catalyst and reduction of the methanol consumption. The technology for the catalyst production is adopted at the Angarsk Plant of Catalysts and Organic Synthesis (APC&OS) . The produced pilot catalyst batch (1.5 t) is tested, the expected catalyst lifetime is ca. 1 year.

A REGENERABLE SULFUR SORBENT FOR FUEL GASES

Research manager: **Dr. N. Dobrynkin**(**Fig. 38**)

Laboratory samples of carbon-supported nanosystems differing by active component ratios for selective desulfurization of gas hydrocarbons were synthesized. The sample composition and preparation conditions were optimized. The samples were tested using adsorption-catalytic and kinetic methods.

TECHNOLOGY FOR ON-SITE UTILIZATION OF OIL ASSOCIATED GASES

Research managers: **Prof. V. Kirillov, Dr. N. Kuzin, Prof. V. Sobyanin** (**Fig. 39**)

A technology for on-site utilization of oil associated gases was developed. The technology is based on low-temperature catalytic conversion of the associated wet gas into methane and synthesis gas. The relevant field-tests at the steady operation of power plants demonstrated the conversion as high as 98 % and 25 % increase in the quantity of generated electric power at meeting the EURO-4 standards.

POWER PLANT BASED ON A HT PEM FC

Research manager: **Dr. V. Belyaev** (**Fig. 40**)

A power plant prototype was manufactured based on a HT PEM FC stack and fuel processor for methanol steam reforming to hydrogen rich gas mixture. The power plant is capable of generating 220V AC and can be used for supplying various electric appliances including the household facilities of capacity up to 300 W.

BIMETAL Au-Cu CATALYSTS FOR SELECTIVE CO OXIDATION

Research manager: **Dr. P. Snytnikov** (**Fig. 41**)

The structure and properties of bimetal gold-copper catalysts supported on ceria were studied. The formation of the highly dispersed bimetal Au-Cu nanoparticles on the support surface was confirmed. A higher activity and selectivity of the 5 wt% Au_2Cu_3/CeO_2 catalyst against its monometal analogues was demonstrated.

NEW CATALYSTS FOR NO_x SCR

Research manager: **Dr. Yu. Amosov**

New catalysts were developed and the existing catalysts optimized for efficient removal of NO_x from exhaust gases of diesel engine based power plants. Catalytic methods were suggested for NO_x reduction in the gas released by lean fuel combustion in diesel and gas-piston engines of vehicles and autonomous power plants.

COBALT BORIDE CATALYSTS FOR $NaBH_4$ AND NH_3BH_3 HYDROLYSIS

Research manager: **Prof. V. Simagina** (**Fig. 42**)

Catalytic activity of cobalt boride catalysts with their active phase formed in the reaction media of $NaBH_4$ and NH_3BH_3 hydrolysis *(in situ)* were found to depend on the nature of hydride compounds, dispersion, and oxidation degree of the active particles. The use of cobalt boride catalysts in alkali-free system is more promising for the further investigations.

FUEL PROCESSOR BASED ON MICROCHANNEL REACTORS

Research manager: **Prof. L. Makarshin** (**Fig. 43**)

An integrated microchannel fuel processor built-up by six microchannel reactors, four microchannel heat exchangers/mixers and two vaporizers was developed and manufactured. The fuel processor enables production of hydrogen-rich gas with low CO content (20 ppm) and has specific power of 550 W/dm^3.

NANODISPERSE Pd-Au ALLOYS ON SIBUNIT AS NEW CO-TOLERANT CATALYSTS FOR ANODES OF FUEL CELLS

Research managers: **P. Pyryaev, Dr. B. Moroz, Dr. A. Simonov** (**Fig. 45**)

A method was developed for preparation of *alloyed* PdAu/C (C is the synthetic carbon support Sibunit) catalysts for membrane electrode units of high-temperature cells fueled by hydrogen with CO impurities. The method is based on separate supporting of the noble metals. The highest activity is characteristic of the particles with a kind of *homophilic* structure, which bear on their surface ensembles of 2-3 palladium atoms surrounded by gold atoms. In particular, the palladium-gold catalysts are preferable at a considerable increase in the CO proportion in hydrogen and at a reduced cell operation temperature.

DEVELOPMENT OF METHODS FOR SYNTHESIS OF MEMBRANE ELECTRODE ASSEMBLIES INCLUDING NEW ELECTROCATALYSTS

Research manager: **Dr. E. Gribov** (**Fig. 46**)

A set of AuPd/C and PdPtRu/C anode catalysts were tested using hydrogen-oxygen and methanol fuel cell prototypes, respectively. Specific catalytic activity of the developed AuPd/C catalysts for oxidation of pure H_2 and H_2 contaminated with CO (130 and 1100 ppm) is at least not worse than the activity of the commercial Pt-based catalytic systems. The anode PdPtRu/C catalysts are not inferior to the commercial PtRu/C catalyst in terms of the activity for methanol electrooxidation. The technique of membrane-electrode assembly (MEA) preparation using a new 20-60 wt% Pt/Sibunit-1562 as cathode electrocatalysts with high Pt dispersion and different support were shown to play an important role in the performance of Pt/C cathode catalysts in fuel cells. The specific activity of the Pt/Sibunit catalysts in the oxygen electroreduction reaction in solid polymer electrolyte fuel cell is correlated with the size of the active component, the optimal particle size of Pt being ca. 3 nm. The activity of the Pt/Sibunit catalysts was found to be superior to that of the commercial 20% Pt/Vulcan XC-72 catalyst. Additives of carbon black in the cathode layer can effectively influence its transport properties.

PHOTOCATALYSTS AND PHOTOCATALYTIC PROCESSES IN CATALYSIS

Research manager: **Prof. A. Vorontsov** (**Fig. 47-51**)

- Photocatalysts $Cd_{1-x}Zn_xS$ for hydrogen production from aqueous sulfide, ethanol and glycerol solutions were developed and studied, their highest activity being observed at x=0.7 and quantum efficiency nearly 13%. The photocatalysts loaded with Pt demonstrated a high potential for H_2 generation from glycerol solutions. It was discovered that basic pH is necessary for the reaction (Fig. 47).
- The TiO_2/SiO_2 and TiO_2/C photocatalysts were prepared and studied in air purification from organic compounds. It was shown for the first time that UO_2, when supported on TiO_2, is capable of oxidizing acetone vapor under visible light (Fig. 48-49).

- The needles – metal net corona discharge geometry was successfully developed for plasmocatalytic air treatment (Fig. 49).
- A method was developed for synthesis of polystyrene template spheres with finely tuned monodispersed particles. Inorganic materials alumina, ZSM-5, SiO_2, ZrO_2 with macroporous structure and high porosity were prepared (Fig. 50).
- Propane and ethane pyrolysis was studied under infrared laser beam in the presence of propylene and ethylene to form propylene, ethylene and methane. C_6, C_{11} and C_{16} liquid hydrocarbons were subjected to pyrolysis over metal-containing catalysts to form carbon nanostructures under microwave heating that allows obtaining a higher selectivity as compared to the conventional thermal heating (Fig. 51).

MCA SYNTHESIS OF CARBIDE MATERIALS

Research manager: **V. Goidin** (**Fig. 52, 53**)

Disperse modified tungsten monocarbide (WC) materials were synthesized by mechanochemical activation (MCA) of a mixture of tungsten metal and carbon. The activities of WC and Pt-based catalysts to hydrogen electrochemical oxidation were comparable when the electrode was poisoned with carbon monoxide.

A method was developed for accelerated preparation of cellulose triacetate (TAC) using mechanochemical activation.

SYNTHESIS OF COMPLEX OXIDES USING MECHANOCHEMICAL AND MICROWAVE PRETREATMENTS OF THE PRECURSORS

Research managers: **Prof. L. Isupova, Dr. I. Yakovleva** (**Fig. 54**)

A possibility of improving the yield of $La(Co,Fe)O_3$ perovskite at synthesis under microwave (MW) radiation of the precursors was studied by adding carbon (to increase the radiation absorption) and citric acid (to increase the solution viscosity). Monophase perovskites $LaMeO_3$ (Me=Fe, Co) with high specific surface area and catalytic activity to methane oxidation and N_2O decomposition were prepared after calcinations of MW treated precursors.

SYNTHESIS OF SINGLE OXIDES USING MC AND MW PRETREATMENT OF CRYSTALLINE HYDROXIDES

Research manager: **Prof. O. Krivoruchko** (**Fig. 55**)

The MW treatment of coarse gibbsite crystals was shown to result in the formation of an X-ray amorphous product with four coordinated Al^{+3} cations and nearly zero energy-gap width (as compared with 6.1 eV for gibbsite) after MW treatment of gibbsite. IR spectroscopic studies of adsorbed CO molecules revealed a.b. at 2187 and 2215 cm^{-1} that indicate the occurrence of two type Lewis sites (weak and moderate, respectively) on the surface of the amorphous product of MW treatment of gibbsite. A considerable narrowing of the band gap E_g from ca. 1.6 eV in gibbsite to close to zero in the amorphous phase was discovered for the first time. The observed effect is of importance both to catalysis and to synthesis of various semiconductor devices.

Zn-MOF BASED CATALYSTS FOR SELECTIVE OXIDATION

Research manager: **Prof. K. Brylyakov** (**Fig. 56**)

Catalytic properties of a series of isoreticular metal-organic frameworks based on Zn complexes were studied; these frameworks catalyze the oxidation of thioesters to sulfoxides with hydrogen peroxide at a high chemo- and size-selectivity.

NEW HETEROGENEOUS CATALYSTS MIL-101 FOR LIQUID-PHASE PROCESSES

Research manager: **Prof. O. Kholdeeva** (**Fig. 57**)

The mesoporous iron and chromium terephthalate-based organometal framework Fe- and Cr-MIL-101 catalyze selective oxidation of cyclohexane with *tert*-butyl hydroperoxide and allylic oxidation of cyclohexene with molecular oxygen as well as carboxylation of epoxides with CO_2 to produce cyclic carbonates. All the reactions proceed efficiently in the absence of any solvent under mild reaction conditions.

A principal scheme of a heat accumulator based on the adsorption equilibrium in the system POM@MIL-101(Cr) – H_2O was proposed.

OPTIMIZATION OF MEDICAL EFFECT OF SOFT CONTACT LENSES

Research manager: **Prof. S. Ivanchev**

The influence of the structure and composition of drug mixtures and of the structure (ionic nature) of therapeutic soft contact lenses on the rate of feed and release of drug components was established. The discovered phenomena allow the therapeutic effect to be optimized.

NEW MODIFICATIONS OF SUPPORTED CATALYSTS FOR GAS-PHASE SYNTHESIS OF POLYETHYLENE

Research manager: **Prof. V. Zakharov** (**Fig. 58**)

New modifications of supported catalysts were developed for production of various polyolefins, in particular, high-molecular co-polymers of ethylene with α-olefins, polypropylene with broadened molecular weight distribution (MWD), and polyethylene with bimodal MWD, synthesized by gas-phase method by one-reactor scheme.

SUPPORTING NANOSTRUCTURED ACTIVE LAYER $VO_x{\cdot}MgO$ ON POROUS MINERAL SUPPORTS

Research manager: **Dr. I. Mishakov** (**Fig. 59**)

A method was developed for supporting $VO_x{\cdot}MgO$ aerogel cover on alumina and silica based substrates. It was shown that supporting of the prepared gel rather than supporting of alcoxides followed by hydrolysis allows a larger surface area to be obtained. An extra advantage of the proposed procedure is that a constant V/Mg ratio is preserved in the sample. The synthesized samples are vanadium amorphous, CSR of MgO and γ-Al_2O_3 phases being ca. 5 nm. The activity of the immobilized aerogel samples was studied in oxidative dehydrogenation of propane. Comparable yields of propylene were observed with the supported aerogel catalysts $VO_x{\cdot}MgO/\gamma$-Al_2O_3 and $VO_x{\cdot}MgO$ catalysts prepared earlier.

NANOCRYSTAL BINARY SYSTEMS CoO_x/MgO FOR CO OXIDATION

Research manager: **Dr. I. Mishakov** (**Fig. 60**)

An aerogel procedure was developed for synthesis of nanocrystal binary systems $CoO_x{\cdot}MgO$ to produce samples with CSR no more than 8 nm and specific surface area ca. 100 m^2/g. From microscopic data, the primary particles (plates) were ca. 10–20 nm in size and 5–6 nm in thickness, and the secondary structure was long species (2–5 μm width and 5–30 μm length) built-up by fine rounded plates. XRD data show that the samples consist of a solid solution of CoO in MgO with Co_3O_4 particles incorporated epitaxially. The synthesized catalysts are very active to oxidation of CO, their stability (from cycle to cycle) being comparable to that of the traditional platinum catalysts. An increase in the activity after sample heating is accounted for by crystallization of the $MgCo_2O_4$ phase in the solid solution structure.

CATALYSTS FOR GAS-PHASE NITRATION OF AROMATIC COMPOUNDS

Research manager: **Dr. I. Mishakov**

Catalytic properties of sulfofluoropolymers (Nafion, SFP), sulfated carbon materials (SCM) and supported sulfofluoropolymers (Nafion/C, Nafion/SCM) were characterized in the reaction of gas-phase nitration of aromatic compounds. There was observed a high yield of the target product but the non-supported catalysts were less stable than the prototypes. A series of supported samples were prepared by precipitation of Nafion from isopropanol-water solution onto SCM or carbon supports. These catalysts were shown to be highly active and selective to gas-phase nitration of aromatic compounds.

NANOCOMPOSITE CATALYSTS FOR CARBON DIOXIDE CONVERSION OF METHANE

Research manager: **Prof. V. Sadykov** (**Fig. 61**)

Carbon dioxide conversion of methane over the catalysts, which are clusters of Pt, Pd and their Ni alloys anchored onto the surface of perovskite- and fluorite-like oxides with highly mobile and reactive oxygen, was studied using a number of Non-Stationary Methods (pulse techniques, kinetic methods including isotopic relaxations), *in situ* IRS, microcalorimetry. The data obtained argue for the bifunctional mechanism of the reaction. Independent stages of activation of methane (limiting) and CO_2 occur on the metal and oxide sites, respectively, while the fast surface/subsurface diffusion of oxygen (bridge species) provide conjugation of these stages including the interaction of activated CH_x fragments with oxygen atoms at the metal-oxide boundary.

DEVELOPMENT OF A PROMISING CATALYST Pd/C FOR HYDROGENATION OF SUNFLOWER OIL

Research manager: **Prof. A. Romanenko** (**Fig. 62-63**)

Regularities of the formation of Pt/Graphite catalysts prepared via redox-deposition of the metal under successive actions of $Na_2S_2O_4$ and HCOOH on the suspension of graphite in H_2PtCl_6 solution, as well as kinetic peculiarities of catalyzed hydrogenation NO to hydroxylamine in aqueous sulfuric acid were studied. A set of general factors determined the selectivity of the reaction was revealed. Optimization of some parameters of the catalyst preparation/regeneration allowed the following parameters of the industrial process of hydroxylamine production (AZOT Co.) to be achieved: substitution for approximately half a total mass of the catalyst in reactors resulted in an increase in hydroxylamine sulfate yield from 112.3 g/l to 120.5 g/l and a decrease in the yields of by-products from 13 g/l to 10 g/l (ammonium sulfate) and from 12 vol.% up to 7-8 vol% (nitrogen suboxide in off-gases).

Research managers: **Prof. A. Romanenko, Dr. V. Chumachenko** (**Fig. 64**)

The data obtained by kinetic studies of hydrogenation of sunflower oil over a Pd-catalyst were used to develop the kinetic model of the reaction, to determine activation energies and rate constants of hydrogenation and isomerization of double bonds of fatty acids. The suggested kinetic model provides a good agreement of the relevant experimental and calculated data. The method of computational hydrodynamics was used for studying the relation between the flowing mode of disperse particle and characteristics of mass transfer between the solid and liquid phases. Filtration of mixtures of hydrogenated fats and support samples of different fraction compositions (50–200 µm) was experimentally studied using a model installation with commercial textile filters in order to identify the optimal process conditions.

SYNTHESIS OF TiO_2-NANOPARTICLES FOR SUPPLYING THERAPEUTIC COMPONENTS INTO CELLS

Research manager: **Dr. E. Matus** (**Fig. 65**)

Methods for synthesis of TiO_2 nanoparticles with required structural-dispersion properties for supplying therapeutic components into cells were developed, a possibility was demonstrated for TiO_2-nanoparticles and their conjugates with oligonucleotides to penetrate into cells by way of endocytosis without any special transfection procedures, which damage cells membrane.

SYNTHESIS OF NANOSIZED MIXED COBALT AND CERIUM OXIDES ON THE SURFACE OF γ-ALUMINA

Research manager: **Dr. G. Volkova** (**Fig. 66**)

A method was developed for deliberate synthesis of nanosized mixed cobalt and cerium oxides (≤5 nm) on the surface of γ-alumina. The method is to be used for synthesis of nanosized mixed transition metal oxide (CoO, NiO and etc.) and cerium oxide on the surface of γ-alumina that allow the obtained regularities of the mixed nanooxides formation to be applied for synthesis of other catalytic systems with unique catalytic properties.

FORMATION OF NANOSIZED 1D-3D PARTICLES OF Cu, Pt AND Pd IN THE CHANNELS OF HIGH SILICA ZEOLITES AND OXIDE MESOPOROUS MATERIALS

Research manager: **Dr. S. Yashnik** (**Fig. 67**)

Dependences of the formation of nanosized particles of Cu, Pt and Pd in the channels of high silica zeolites and oxide mesoporous materials on the chemical composition and structure of aluminosilica frame, conditions of the introduction of metal cations, temperature and atmosphere used in treatment were revealed, as well as the dependences of catalytic properties and resistance to deactivation in the reaction medium (in the presence of oxygen, water vapor and sulfur organic compounds).

GENESIS OF STRUCTURE AND COMPOSITION OF Mo-Me NANOPARTICLES IN ZEOLITE MATRIX H-ZSM-5

Research manager: **Dr. E. Matus** (**Fig. 68**)

The genesis of structure and composition of metal-containing nanoparticles (Mo-Me, Me = Fe, Co, Ni), stabilized in zeolite matrix H-ZSM-5, was investigated depending on synthesis conditions (thermal treatment in O_2, Ar, CH_4) and molar ratio Me/Mo (0.04-1.0) by a complex of physical-chemical methods (XRD, EPR, ESDR, TEM, EDX, XPS). It was established that the ratio of the carbide to oxide Mo forms in Mo-Co/ZSM-5 after treatment in CH_4 at 720°C increases from ~0.2 to ~0.5 with an increase of Co/Mo from 0.08-0.4 to 0.8.

METAL NANOPARTICLES IN THE STRUCTURE OF MICRO- AND MESOPOROUS CARBON NANOMATERIALS

Research manager: **Dr. M. Kerzhentsev** (**Fig. 69**)

Dependences of the size and state of Pt and Co nanoparticles in the structure of micro- and mesoporous carbon nanomaterials on the synthesis conditions and the nature of the carbon materials were studied using XRD, XPS, TEM and adsorption methods.

SYNTHESIS OF MESOPOROUS COATING ON THE INNER SURFACE OF THE QUARTZ CAPILLARY

Research manager: **Dr. L. Okhlopkova** (**Fig. 70**)

To study the effect of preparation conditions on the properties of catalytic coating, a method for synthesis of SiO_2, $PtSn/TiO_2/SiO_2$ and $PdZn/TiO_2/SiO_2$ mesoporous coating on the inner surface of the quartz capillary was developed. Optimal parameters of the synthesis of $PtSn/TiO_2/SiO_2$ and $PdZn/TiO_2/SiO_2$ coatings on the inner surface of the capillary microreactor with controlled size and composition of metal nanoparticles and porous structure of the support were determined.

NANOSIZE Pd- AND Pt-Pd CATALYSTS OVER ALUMINA SUPPORTS

Research managers: **Prof. Z. Ismagilov, N. Shikina** (**Fig. 71**)

Correlation between the state of Pt-Pd active sites stabilized in an alumina matrix in the form of nanosize oxide and intermetal particles and behavior of Pt-Pd-CeO_2-Al_2O_3 catalysts in methane oxidation was established. It was shown that the high activity and stability of the catalysts in the methane oxidation are reached at the ratio of phases of PdO and Pt-Pd-alloy equal 0.33-1.0.

FORMATION OF MESOPOROUS SILICATE SHELL AROUND LSX ZEOLITE MICROSEEDS

Research manager: **Dr. M. Melgunov** (**Fig. 72**)

The formation of particles with the “core-shell” morphology, where LSX zeolite microseeds were used as cores and silicate mesoporous mesophase layer as a shell, was studied. The possibility of formation of mesoporous shell with thickness of 50-150 nm was shown. The textural characteristics (specific surface area and pore volume) of particles with the morphology of “nonporous core - mesoporous shell” decreased by less than 15% on storing for a year.

DESIGN OF CERAMOMETAL DEHYDROGENATION CATALYST

Research manager: **Prof. S. Tikhov** (**Fig. 73**)

Pilot testing of the ceramometal honeycomb catalysts in the fluidized bed regime was achieved in cooperation with “Sibcermet” Ltd. A high efficiency of solid fuel combustion (97.8-98.5) with low emission of pollutants (430-480 ppm CO, 340-370 ppm NO_x) close to the conventional ceramic catalyst (IC-12-70) was demonstrated, no attrition of the catalytic units being observed after 100 hours of testing.

CATALYST FOR *n*-ALKANE HYDROISOMERIZATION BASED ON SILICOALUMINOPHOSPHATE *SAPO-31*

Research manager: **Prof. G. Echevsky** (**Fig. 74**)

Specific features of synthesis of SAPO-31 were studied depending on the nature of initial components, as well as on the composition of the reaction mixture, conditions of its preparation and hydrothermal treatment. The main factors that determine feasibility of preparing phase-pure SAPO-31 materials were shown to be the use of highly active sources of aluminium and a high content of a structure-forming compound (template) in the reaction mixture. A reproducible procedure for synthesis of phase-pure silicoaluminophosphates SAPO-31 was developed for the first time. The influence of the template type, silicon crystallinity and content on physicochemical and catalytic properties of SAPO-31 was studied. A hydroisomerization catalyst Pt/SAPO-31 was developed and tested successfully at the pilot scale in hydrotransformation of a real feedstock (diesel fraction). Metal-containing silicoaluminophosphates SAPO-31 were shown to be promising catalysts for hydrotransformation of plant oil to produce C_{15}–C_{18} fraction with a high content of isomer products.

APPLICATION OF CFD MODELING FOR DEVELOPMENT OF THE THEORY OF STRUCTURED HIGH-TEMPERATURE CATALYTIC SYSTEMS

Research manager: **Dr. O. Klenov** (**Fig. 75**)

Results of CFD modeling of time-depended transitional processes show that the performance of an exothermic catalytic reaction (CO oxidation is considered as a model reaction) in the catalytic monolith with porous walls and square section channels is characterized by temperature nonuniformity inside the monolith with difference between the maximum and minimum temperatures ΔT_{cat} more than 200^o for the investigated regime at $0.6 \leq \tau \leq 4.0$ s.

ACTIVITY OF SULFIDE NiMo AND NiW CATALYSTS OVER ZEOLITE-CONTAINING SUPPORTS IN REACTION OF TETRALIN TRANSFORMATION

Research manager: **Dr. G. Bukhtiyarova** (**Fig. 76**)

The peculiarities of sulfidizing with dimethyldisulfide of NiMo and NiW catalysts prepared using zeolite-containing supports (10-30% zeolite) was investigated using gas chromatography (GC) with a thermal conductivity detector and GC with an atomic-emission detector for analysis of gas and the liquid phases, respectively. The optimum temperature and duration of interaction of organic solvent spiked with dimethyldisulfide (DMDS) with catalyst was defined for the formation of highly disperse NiMoS or NiWS phase. It was shown that sulfide nanoparticles are located on the alumina surface rather than zeolite, the NiMoS phase are in the form of monolayer particles, the NiWS particles contain 2 or 3 layers. The selectivity of tetralin transformation depends mainly on the zeolite content in the support rather than on sulfide chemical composition.

PREPARATION OF OPTIMAL SUPPORTS FOR HYDROTREATING CATALYSTS

Research manager: **Dr. O. Klimov** (**Fig. 77**)

The requirements for commercial aluminium hydroxide powders were formulated; the procedure was developed for preparation of the supports with textural and strength characteristics and grain composition optimal for hydrotreating catalysts of various oil fractions. The preparation method provides the structure preservation of Co-Mo bimetal complex compounds in the target catalyst.

COMMON FEATURES OF THE OXIDATION OF ALDOSUGARS OVER MONOMETAL CATALYSTS

Research manager: **Dr. O. Taran** (**Fig. 78**)

Systematic studies of selective catalytic oxidation of glucose, lactose and sorbose over monometal catalysts containing noble metals resulted in revealing common features of the oxidation of aldosugars (glucose and lactose). The catalytic activity increases in the series of Ru<Pt<Pd<Au.

STABILITY AND DEACTIVATION OF GOLD CATALYSTS IN α-PINENE TO CAMPHENE ISOMERIZATION

Research manager: **Dr. I. Simakova** (**Fig. 79**)

Stability and deactivation of gold catalysts in α-pinene to camphene isomerization was studied. The effect of temperature and initial concentration of α-pinene on the initial activity and stability of the Au catalyst was identified. The deactivation function was defined.

METAL COMPLEX CATALYSTS FOR HOMOGENEOUS AND PHASE-TRANSFER ASYMMETRIC REACTIONS

Research manager: **Prof. Z. Pai** (**Fig. 80**)

Metal complex catalysts based on V(IV), Rh(I) and Ru(II) with N,O-derivatives of diterpenes as chiral inductors were synthesized. Configuration of asymmetric centers of the obtained organic catalysts and ligands was studied using ^{1}H and ^{13}C NMR spectroscopy and X-ray structure analysis. The prepared catalysts will be used in homogeneous and phase-transfer asymmetric reactions.

STUDIES ON GLYCEROL COFERMENTATION WITH GLUCOSE

Research manager: **Dr. K. Sorokina** (**Fig. 81**)

Studies on glycerol cofermentation with glucose by Klebsiella pneumoniae W18 showed a 13 % increase in the 1,3-propanediol yield. It was shown that gene expression is related to cell anaerobiosis, when activated by transcriptional factors arcA and OxyR.

KINETIC PECULIARITIES OF HYDROGENOLYSIS OF BUTYL LACTATE

Research managers: **Dr. M. Simonov, Dr. I. Simakova** (**Fig. 82**)

Kinetic peculiarities of hydrogenolysis of butyl lactate over a copper-containing catalyst at atmospheric pressure were studied including the influence of temperature, residence time and concentration on lactate conversion and selectivity to propylene glycol and hydroxyacetone. Apparent activation energies, preexponential factors and reaction orders were determined.

CATALYTIC SYNTHESIS OF BIODEGRADABLE POLYMERS

Research manager: **Dr. A. Potapov** (**Fig. 83**)

Catalytic polycondensation of 2-hydroxypropionic (L-lactic) acid and combined polycondensation of L-lactic acid with aliphatic dicarboxylic acids and diols was studied including the influence of conditions of polycondensation on polymers properties.

CATALYST AND ADSORBENTS FOR DIRECT OXIDATION OF HYDROGEN SULFIDE

Research manager: **Dr. S. Khairulin** (**Fig. 84**)

The composition of a catalyst for direct oxidation of hydrogen sulfide to achieve the sulfur yield ≥ 90 % in the temperature range 230-300°C, as well as the compositions of multifunctional adsorbents providing sulfur capacity more than 20 % both for H_2S and SO_2 were developed.

DEVELOPMENT OF CATALYST FOR LOW-TEMPERATURE SULFUR DIOXIDE REDUCTION

Research manager: **Dr. S. Khairulin** (**Fig. 85**)

The catalysts based on mixed oxides of iron and manganese for low-temperature sulfur dioxide reduction by synthesis gas were developed and characterized. It was demonstrated that pretreatment of initial samples with hydrogen sulfide (sufidation) improves substantially their catalytic performance in the target reaction.

CATALYST FOR THE EFFICIENT PROTECTIVE BED IN A CLAUS REACTOR

Research manager: **Dr. G. Bukhtiyarova** (**Fig. 86**)

The chemical composition of promoters was developed for the efficient protective bed in a Claus reactor with a high catalytic activity to oxygen conversion, Claus reaction and COS hydrolysis.

DEVELOPMENT OF THE PROCESS OF FINE PURIFICATION OF GASES FROM SULFUR DIOXIDE TO GIVE ELEMENTAL SULFUR

Research manager: **Dr. O. Kovalenko** (**Fig. 87**)

Thermal decomposition of $(NH_4)_2SO_4$ solution in the presence of CO to form NH_3 and SO_2 was studied. Conditions were determined to ensure complete conversion of NH_4HSO_4 and close to stoichiometric yield of ammonia (T=300–400°C, molar ratio of $CO/(NH_4)_2SO_4 \geq 1$, the contact time – $\geq$ 240 min). It was shown that the thermal decomposition of concentrated $(NH_4)_2SO_4$ solutions can be used as the stage of regeneration of absorption solution in the process of fine purification of gases from sulfur dioxide while maintaining NH_3, which can be reused in the process of absorption of sulfur oxides.

CATALYTIC PROPERTIES AND STRUCTURE OF V_2O_5, WO_3/Ce-TiO_2, V_2O_5, WO_3/Y-TiO_2 CATALYSTS IN THE deNOx REACTION WITH AMMONIA

Research manager: **Prof. G. Zenkovets** (**Fig. 88**)

XRD and TEM techniques were used for structural studies of catalysts V_2O_5,WO_3/(Ce-TiO_2) and V_2O_5,WO_3/(Y-TiO_2) of optimal composition with high activity and stability in the deNOx reaction with ammonia (NO conversion ≥ 95-97% at 500°C). The both catalysts were shown to have a nanocrystalline structure consisting of non-coherently conjoined anatase crystals of 15-20 nm in size with interblock boundaries containing stabilized ions of Ce (Y), V and W. The state of these ions was determined by XPS and NMR. The catalyst structures were preserved for long operation in the deNOx reaction mixture.

The study of phase composition and microstructure of multipromoted catalysts for ammonia oxidation to dinitrogen showed that the active catalysts were solid solution of Ce ions in ZrO_2 of tetragonal modification with high disperse Mn oxide particles stabilized on its surface mixed with ZSM-5 zeolite containing lengthy clusters of Cu^{2+} ions stabilized on its outer surface.

TECHNOLOGICAL APPROACH FOR OXIDATION OF SO_2 IN THE REVERSE-FLOW REGIME

Research manager: **Prof. A. Zagoruiko** (**Fig. 89**)

A new technological approach was proposed for oxidation of SO_2 in the reverse-flow regime in the media of non-ferrous smelter waste gases containing significant amount of CO (up to 2% vol.). The new process is based on application of an additional beds of Pt catalyst on the fibrous Zr-Si support. According to the mathematical simulation data, mounting of these beds between beds of V catalyst and heat regenerative material makes it possible to reduce noticeably maximum temperatures in the reactor and thus to improve the SO_2 conversion and the process operation stability under significant oscillation of CO content in the waste gases. The recommendations for practical application of technology were prepared for the Mednogorsk Copper-Sulfur Combine.

STUDY OF NOVEL HIGH EFFICIENT CATALYSTS BASED ON URANIUM-CONTAINING COMPOUNDS

Research manager: **V. Kuznetsov** (**Fig. 90-91**)

The influence of preparation conditions of alumina supported mixed catalysts containing oxides of uranium and a transition metal on their physico-chemical and catalytic properties was studied. Physicochemical properties of the initial catalysts and the catalysts after reactions of chlorobenzene oxidation and methane steam reforming were characterized.

REGENERATION OF CARBON-BASED CATALYSTS-ADSORBENTS BY HYDRODECHLORINATION

Research manager: **Prof. V. Simagina** (**Fig. 92**)

The conditions of adsorptive-catalytic cycle for *o*-dichlorobenzene removal from aqueous media were optimized. It was shown that the catalyst 1%Pd/MeKS is the most effective for the process. The catalyst can be totally regenerated by liquid-phase hydrodechlorination for an hour.

DELIBERATE SYNTHESIS OF NANOSTRUCTURED CATALYSTS BASED ON MOLYBDENUM SULFIDE

Research manager: **Dr. S. Yashnik** (**Fig. 93**)

Approaches were developed for formation of Mo(W)-Ni powders providing necessary textural characteristics to catalyst-extrudates without changes in the composition and nanostructure of Mo(W)-Ni oxides and without changes of in sulfide form Mo(W)-Ni in size.

STUDYING OF OXIDATIVE DESULFURIZATION OF HYDROCARBON FUELS

Research manager: **V. Kuznetsov** (**Fig. 94**)

A laboratory setup for studying oxidative desulfurization of hydrocarbon fuels was designed, constructed and put into operation. Catalyst samples were tested in the ODS of a model mixture of octane and thiophene or dimethyldisulfide (DMDS). Adsorption and interaction of thiophene with the surface of oxide catalysts was studied by FTIR.

STABILITY OF BIMETAL Pt-Pd-CATALYSTS BASED ON MnO_x, $MnLaAl_{11}O_{19}$ IN REACTION OF METHANE OXIDATION

Research manager: **Dr. S. Yashnik** (**Fig. 95**)

High-stable catalysts containing Mn oxide or Mn hexaaluminate and Pt-Pd-nanoparticles were developed for a combustion chamber of gas turbines. Peculiarities of formation of nanostructures of oxide and metal active sites as a function of the nature of active component precursors, Pt and Pd content, Pt/Pd atomic ratio, crystal modification of alumina support and calcinations condition were studied. The optimal Pt/Pd atomic ratio providing high activity and stability of the catalysts in methane oxidation reaction was determined.

SYNTHESIS OF PEROVSKITE CATALYSTS WITH MODIFIED CELLULOSE USED AS A STRUCTURE-FORMING AGENT

Research manager: **Prof. V. Simagina** (**Fig. 96**)

A method for synthesis of perovskite catalysts was developed with modified cellulose used as a structure-forming agent that prevent aggregation and sintering of the perovskite particles. An increase in dispersion of perovskites leads to a significant increase in the combustion rate of model high-energy compounds. The factors that influence the rate of gas generation during thermolysis of ammonia borane based compositions were revealed.

SIMULATING THE CATALYTIC PROCESS OF GAS GENERATION FROM SOLID FUEL MATERIALS

Research manager: **Dr. V. Khanaev** (**Fig. 97**)

In simulating the catalytic process of gas generation from solid fuel materials, the influence of different geometry of catalytic monoliths on the gas generation rate was studied for the first time, as well as dynamics of monolith-fuel system for different geometry of catalyst.

MATHEMATICAL SIMULATION OF COMBUSTION PROCESSES IN THE CATALYST FIXED-BED

Research manager: **Prof. A. Gerasev** (**Fig. 98**)

The mathematical simulation of catalytic, filtrational and autowave processes in the catalyst fixed-bed during propane oxidation was performed.

SYNTHESIS OF NANODISPERSED Pd-CONTAINING CATALYST STABLE TO DEACTIVATION

Research manager: **Dr. I. Simakova** (**Fig. 99-100**)

A series of bicomponent catalysts containing nanosize Pd-B and Pd-N particles of metal glasses on the surface of mesoporous carbon support were prepared. Their stability in the two-step hydrodebenzylation process was tested. A possibility of non-destructive regeneration of the catalyst, as well as service time of synthesized samples was studied. The data obtained give the basis for the development of scientific approaches to the synthesis of the active bicomponent catalyst with low content of Pd for hydrodebenzylation of 2,4,6,8,10,12-hexaasabenzyl-2,4,6,8,10,12-hexaazaizowurtzitan.

Ba-CONTAINING CATALYSTS IN REACTION OF TRANSESTERIFICATION OF RAPESEED OIL

Research manager: **Dr. P. Eletskii** (**Fig. 101**)

Ba-containing catalysts were studied during transesterification of rapeseed oil in a flow fixed bed reactor during 50-60 h at 200 (228)ºC, 20 (30) atm and liquid flow rate 0.8–2 h^{-1}. The

$Ba_{0.04}La_{1.96}O_3$ catalyst kept its activity to transesterification at a very high level during 50 h but then decreased sharply. The $BaAl_{12}O_{19}$ catalyst was less active but more stable. XRD and XPS techniques were used to demonstrate that the observed decrease of the catalysts in activity is caused by a change in the phase or surface composition.

DEOXYGENATION OF LIQUID PRODUCTS OF BIOMASS PYROLYSIS

Research manager: **Dr. S. Zavarukhin** (**Fig. 102**)

In the field of hydrocarbon production from biomass pyrolysis products, the studies were focused on the influence of the nature of the active component and support on the catalyst activity and stability and the selectivity to the target products; on the kinetics and mechanism of deoxygenation of liquid products of biomass pyrolysis in the presence of the most promising catalysts.

DEVELOPING OF SYSTEM FOR SCREENING AND ISOLATION OF PROSPECTIVE MICROALGAE STRAINS

Research manager: **Dr. K. Sorokina** (**Fig. 103**)

A system for screening and isolation of prospective microalgae strains was developed and new strains of Nannochloris bacillaris, Botryococcus sudeticus, Chlorella sorokiniana identified by 18s rRNA gene sequencing. Culturing conditions were optimized for Botryococcus braunii UTEX 2441 in a photobioreactor and microalgae biomass (179 g as dry weight) was produced. The optimal catalyst for hydrocracking of lipid fraction and microalgae lipid fraction derivatives at this stage was chosen, tested in the reaction with model compounds and a microalgae oil as a feedstocks. The influence of hydrocracking conditions on the yield of hydrocarbon was studied.

THERMAL OXIDATIVE PROCESSING OF MUNICIPAL SLUDGE, HYDROLYSIS AND PULP AND PAPER INDUSTRY

Research manager: **Dr. A. Simonov** (**Fig. 104**)

In the field of combustion, pyrolysis and gasification of carbon-containing raw materials, thermal oxidative processing of municipal sludge, hydrolysis and pulp and paper industry was studied in fluidized bed of a deep oxidation catalyst. Main specific features of the process were established in order to provide stable burning at a low quantity of toxic wastes including dioxins.

THERMODYNAMIC AND KINETIC REGULARITIES OF OXIDATION PROCESSES OF ALCOHOLS OVER BIFUNCTIONAL CATALYSTS

Research manager: **Dr. A. Beskopylnyi** (**Fig. 105**)

Thermodynamic and kinetic regularities of oxidation processes were studied with an example of synthesis of benzoic acid from benzyl alcohol using bifunctional catalysts of interphase oxidation and hydrogen peroxide as the oxidant. The influence of ultrasound on oxidation of various organic substrates in two-phase systems also was studied.

A technology for synthesis of 2,3-difluoro-6-nitrophenol and 2-acetonyloxy-3,4-difluoro nitrobenzene – the key intermediates in the synthesis of antibiotic levofloxacin – was developed. The technology is six stage synthesis with intermediate isolation and purification of raw materials to the purity of no less than 95-98%

An engineering basis was developed for the semicommercial production of these compounds with reference to modular units “Ufa-1”, “Ufa-2”. A semicommercial sample of 2-acetonyloxy-3,4-difluoro nitrobenzene (35 kg) to be used for synthesis of pilot samples of levofloxacin was studied.

KINETIC FEATURES OF TRIMETHYLPHENOL TO TRIMETHYLBENZOQUINONE OXIDATION

Research manager: **Prof. E. Zhizhina** (**Fig. 106**)

Kinetic features of oxidation of 2,3,6-trimethylphenol (TMF) to 2,3,5-trimethyl-1,4-benzoquinone (TMQ) were studied in two-phase systems in the presence of modified solutions of Mo-V-P HPA. The reaction mechanism was proposed.

NANODIAGNOSTICS OF HIGHLY DISPERSED MATERIALS

Research managers: **Prof. E. Moroz, Dr. D. Zyuzin**

Wide and small angle X-ray diffraction (XRD) techniques were used for studying ultrafine grained nanostructured materials.

Complex structural investigations were carried out for a large number of oxide, metal-oxide and sulfide-oxide catalysts.

Research managers: **Prof. E. Moroz, Dr. S. Cherepanova, Dr. V. Pakharukova**

New versions of software packages were developed for creation of 3D models of nanostructures and for calculation of their XRD patterns. A principally new model of the nanodomain structure of the $SrFe_{0.95}Mo_{0.05}O_{2.5+\delta}$ solid solution was suggested. The model can be used for understanding the appearance of superstructural reflections due to the formation of 90^o twins, which have vacancy ordering typical of brownmillerite but pseudocubic lattice of perovskite.

Research manager: **Prof. O. Lapina**

A new experimental technique was implemented for acquisition of correct stationary solid state NMR spectra for quadrupolar nuclei with half integer spins QCPMG (Quadrupolar Carr-Parsel-Mebius-Gill). To develop the scale of ^{29}Si NMR chemical shifts for zirconium-silicate systems, ^{29}Si NMR parameters were obtained for a huge number of individual Na-Zr-Si-O compounds of the known structures with a set of Na-Zr-Si-O minerals. GIPAW method was applied to periodic calculation of NMR parameters for individual vanadium compounds V_2O_5 and NH_4VO_3.

STRUCTURE RESEARCH WITH SYNCHROTORON RADIATION

Research manager: **Prof. D. Kochubey (Fig. 107)**

Alkoxides complexes solutions in aliphatic alcohols were discovered to have similar structures. The hierarchical model of the structures was described. The ligand displacement was detected when solvent molecules were more compact compared to the complex' ligands.

Monoslab HNb_3O_8/MgO catalysts were synthesized. Difference in the structures of bulk and monolayer HNb_3O_8 was shown. A possibility of detecting structural changes after exfoliation and after aniline adsorption were demostrated.

Research manager: **Dr. A. Shmakov**

The temperature of phase transition Ni-enriched Ni-Cu alloy in the course of the growth of N-containing carbon nanofilaments (N-CNF) was established. It was shown that the growth of N-CNF includes stages of carbon and nitrogen dissolution in the catalyst particle but not the formation of the metal carbide phase. A new phase of $NiCu_xC_yN_z$ with the lattice constant comparable to that of copper metal is formed under these conditions at 440-460°C.

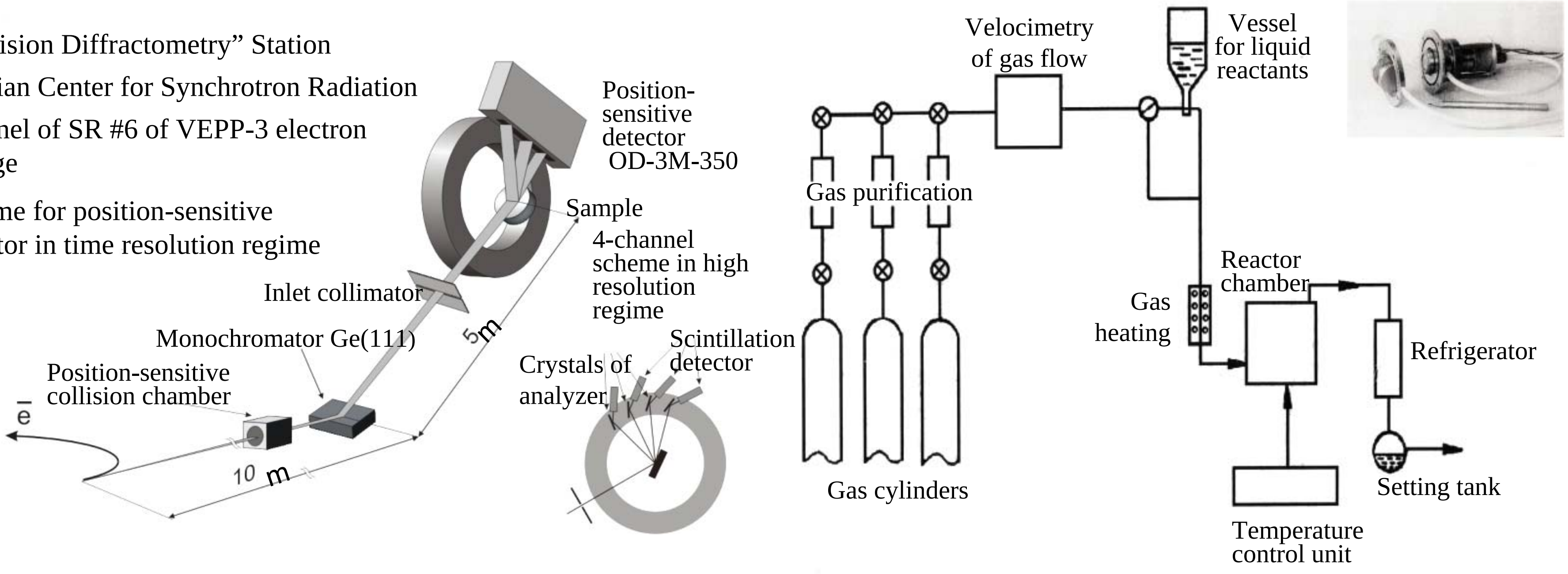
XRD *in-situ* FOR STUDYING PHASE AND STRUCTURAL TRANSFORMATIONS OF CATALYSTS DURING THEIR PREPARATION AND ACTIVATION WITH HYDROGEN

"Precision Diffractometry" Station

Siberian Center for Synchrotron Radiation

Channel of SR #6 of VEPP-3 electron storage

Scheme for position-sensitive detector in time resolution regime

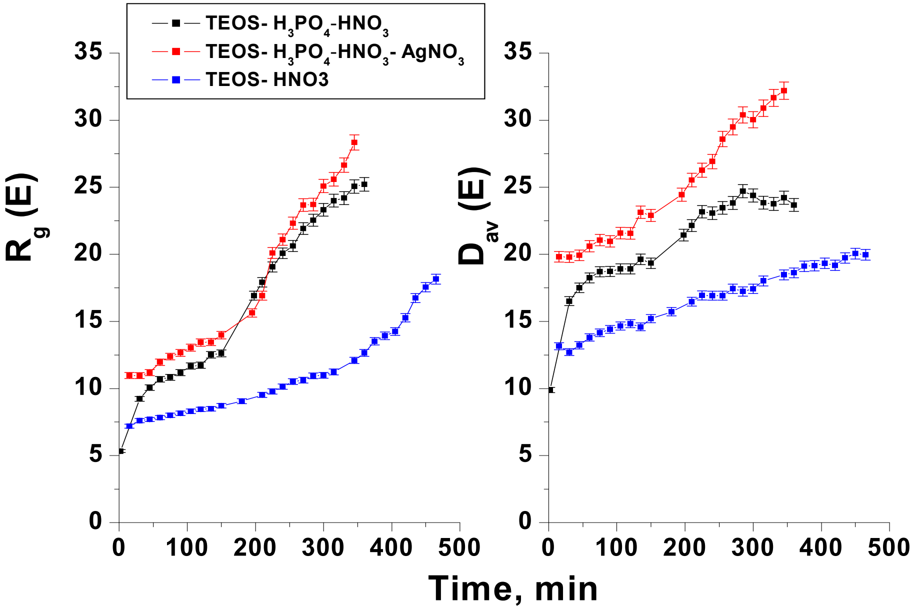


- **Specific features of structural transformations in Co-containing Fischer-Tropsch catalysts were studied at their interaction with hydrogen;**
- **Reduction of nanodisperse CuO particles was studied under the isothermal conditions;**
- **The structure of FeCrCuO catalysts under close to the reaction of CO conversion conditions was studied as dependent on the Cr/Fe ratio;**
- **The process of the formation of bimetal palladium nanoparticles with transition metals was studied**

Fig. 1

SAXS TECHNIQUE FOR STRUCTURAL AND DISPERSION ANALYSIS OF MULTICOMPONENT HETEROGENEOUS CATALYSTS

In-situ SAXS study of the metal nanoparticle nucleation in the system SiO_2-P_2O_5



Dependencies of average value of radius of gyration (R_g) and particle diameter (D_{av}) on time for 3 mixtures

Method for synthesis of the promoted silver catalyst: hydrolysis of tetraethoxysilane (TEOS) in ethyl alcohol in the presence of phosphoric and nitric acid and silver nitrate as the precursor of the silver particles

Questions and problems:

- Lack of data on the processes that occur in the system before the gel drying
- Lack of data on the structure and texture of the gel under hydrolysis
- The absence of highly sensitive and informative methods for *in situ* studying the process of TEOS hydrolysis
- The role of phosphoric acid

***In situ* SAXS**

•Formation of particles in the size range from 1 to 3 nm at $T=20^{o}C$ and 12 nm in size at $T=50^{o}C$

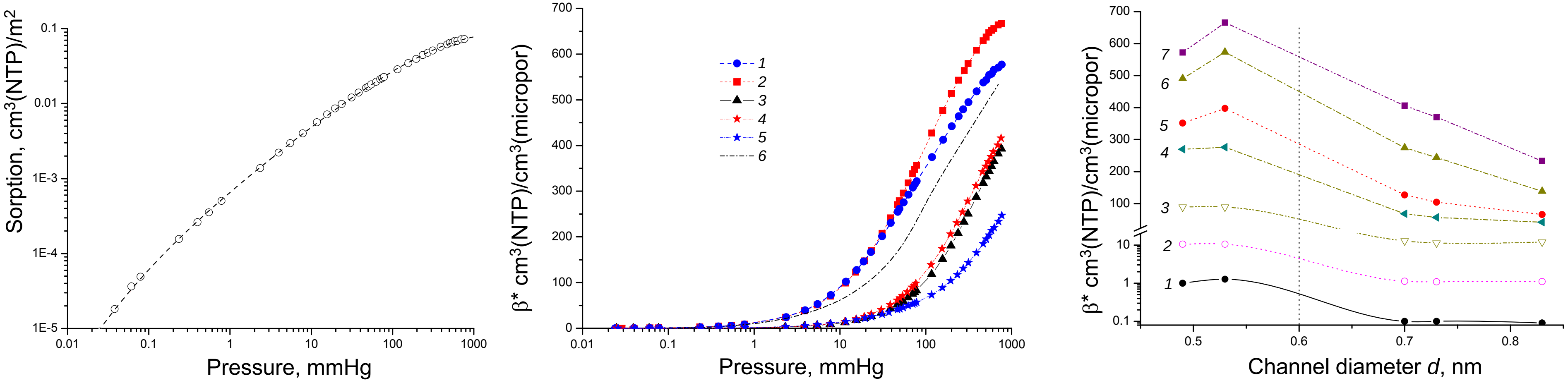
•Sorption of phosphoric acid anions on the SiO_2 surface led to a change in the surface charge of silica to increase their coagulation

Fig. 2

IMPROVED ADSORPTION METHOD FOR STUDYING COMPONENT DISTRIBUTION THROUGH A MICROPOROUS CATALYST BULK

The adsorption method for studying component distribution through a microporous catalyst bulk was improved, which includes experimental studies of two sorbates at identical temperatures when one of them is vapor and another gas

Adsorption of N_2 and H_2 at 77 K



✓ Absolute quantities of H_2 adsorption, α(P), were established for mesoporous aluminophosphates

✓ Effective density of adsorbed H_2 in the micropore bulk, β(P, d) was determined

✓ H_2 adsorption isobars were calculated

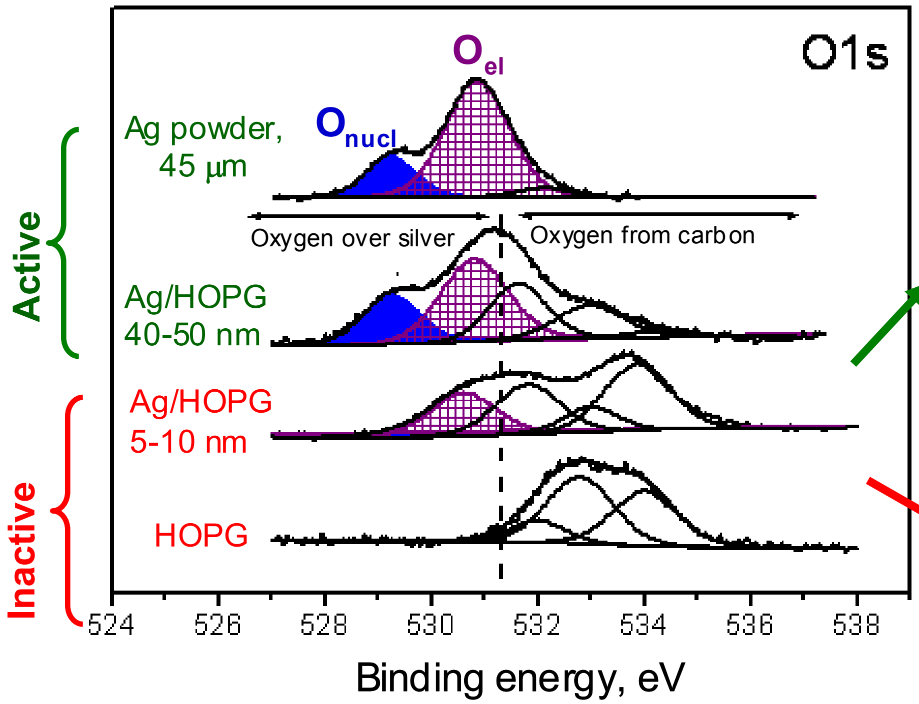
Fig. 3

SIZE EFFECT IN REACTION OF ETHYLENE EPOXIDATION OVER MODEL CATALYSTS Ag/HOPG

***In-situ* XPS:**

(source of synchrotron radiation BESSY II (Berlin))

$C_2H_4/O_2 = 2/1$, P = 0.5 mbar



PTR-MS:

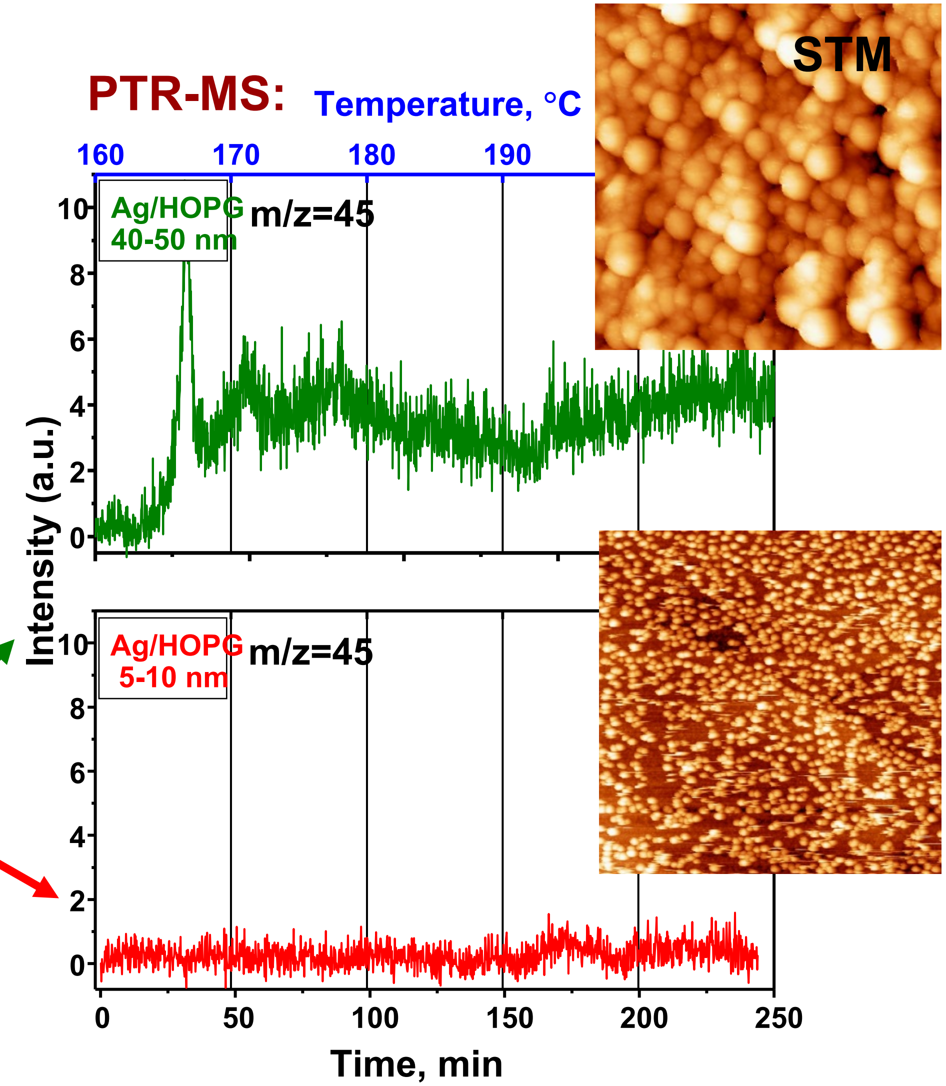
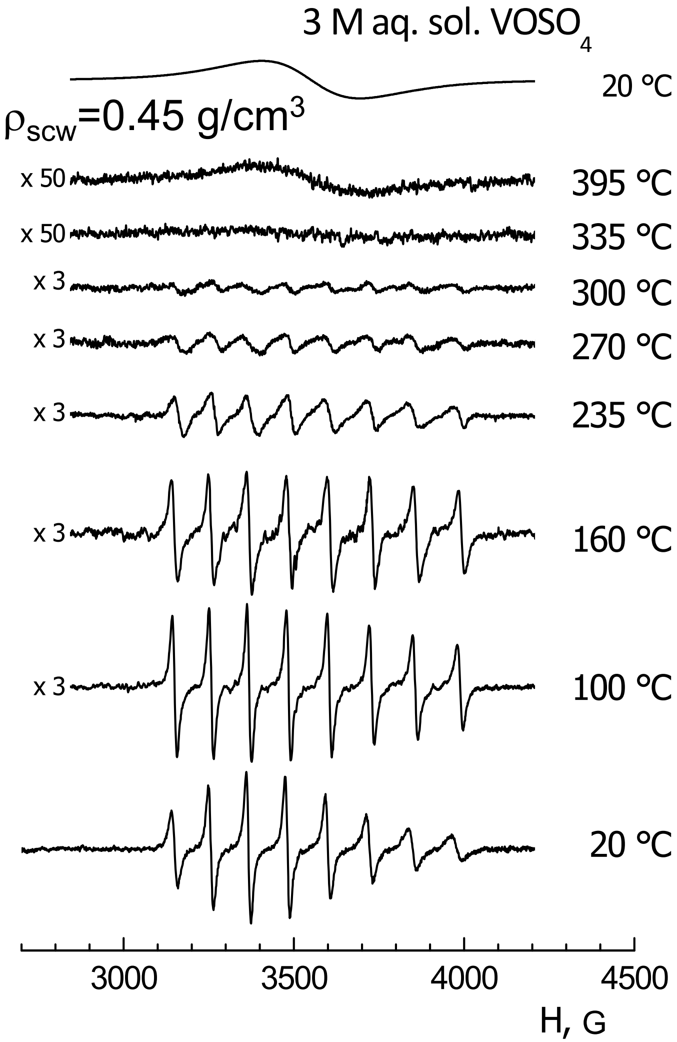
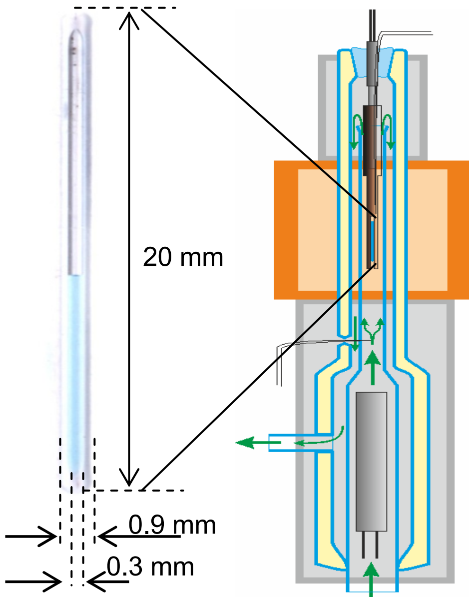


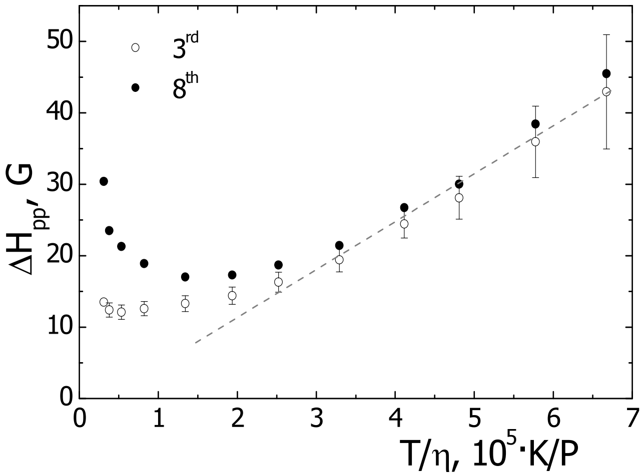
Fig. 4

ELECTRON SPIN RESONANCE SPECTRA IN SUPERCRITICAL WATER

(T_c=647 K (374°C); P_c=220 atm)







Sources of peak broadening:

1. Spin-rotary interaction
2. Spin exchange

ΔH~T/η:

Additional source of broadening**?**

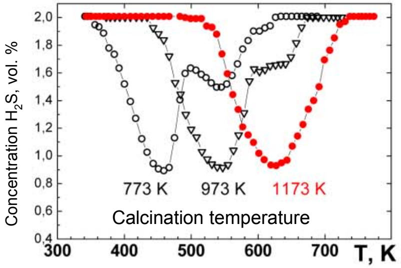
Increase in exchange interaction due to an increase in the local vanadyl ions concentration – initial stage for oxide particles formation in SCW

Fig. 5

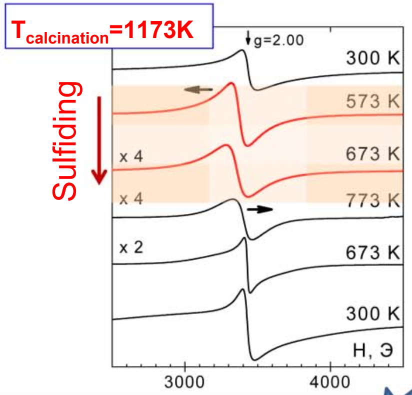
CATALYTIC SYSTEMS BASED ON ε-Fe_2O_3 NANOPARTICLES

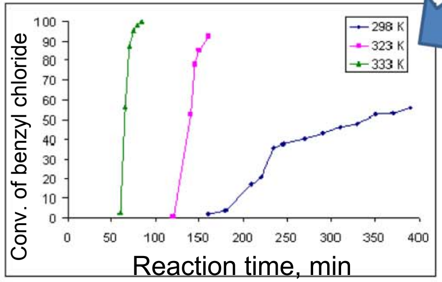
ε-Fe_2O_3

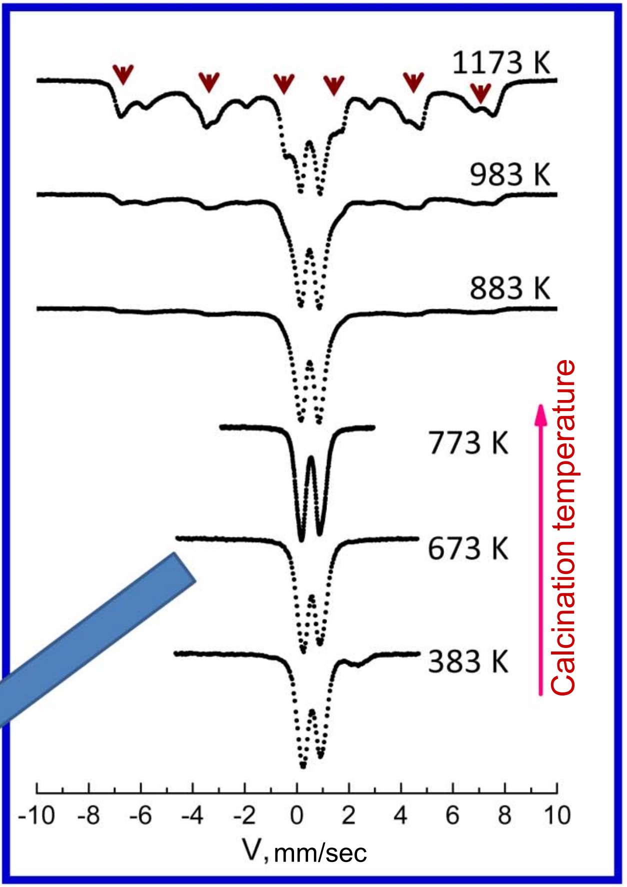
Thermostability (**up to 1200 K**) and resistance to sulfiding (**up to 500 K**)



Magnetic anisotropy and **FMR spectra change upon sulfiding *in situ***

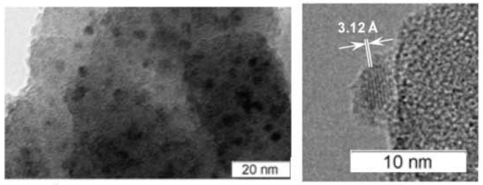


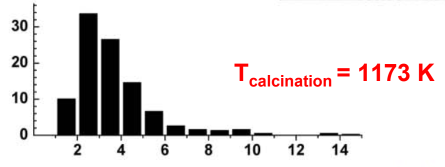


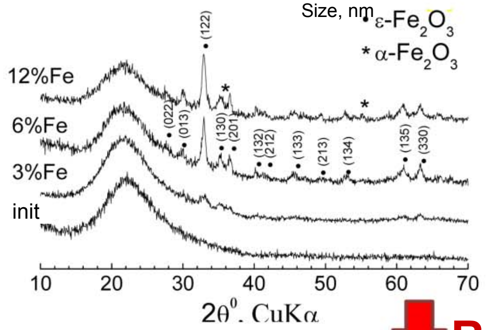


The most active are the samples calcined at $T_{calcination}$=673 K; at a higher temperature the ε-Fe_2O_3 phase starts forming

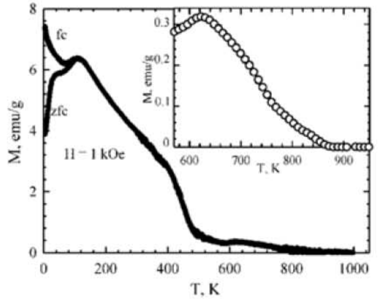
X-ray homogeneity of **ε-Fe_2O_3/SiO_2** containing as much as 8 wt % Fe







But!

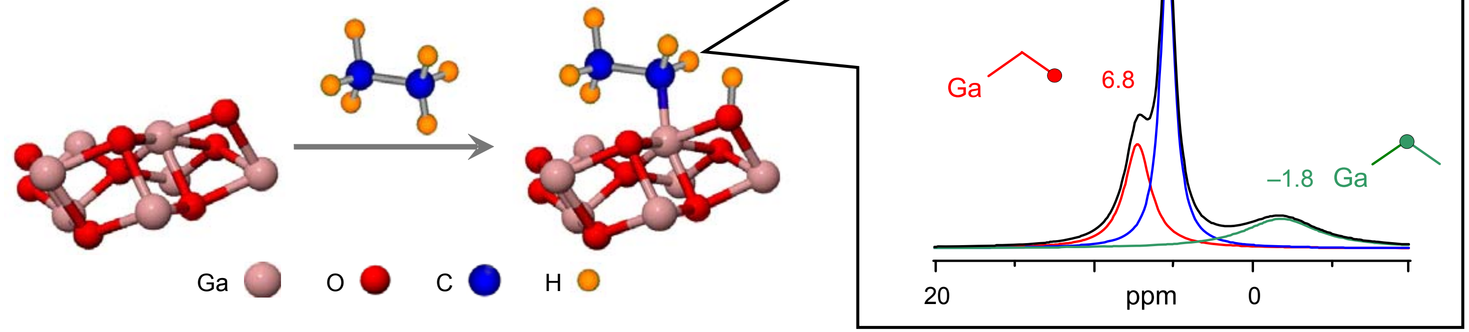


Existence of several magnetic subsystems in ε-Fe_2O_3/SiO_2 containing as much as 8 wt % Fe

Fig. 6

^{13}C SOLID STATE NMR FOR STUDYING SMALL ALKANES ACTIVATION

Ga-alkyls are probable intermediates in small alkane aromatization on gallium-modified zeolite catalysts



Joint aromatization of methane and propane over zeolite Mo/H-BEA

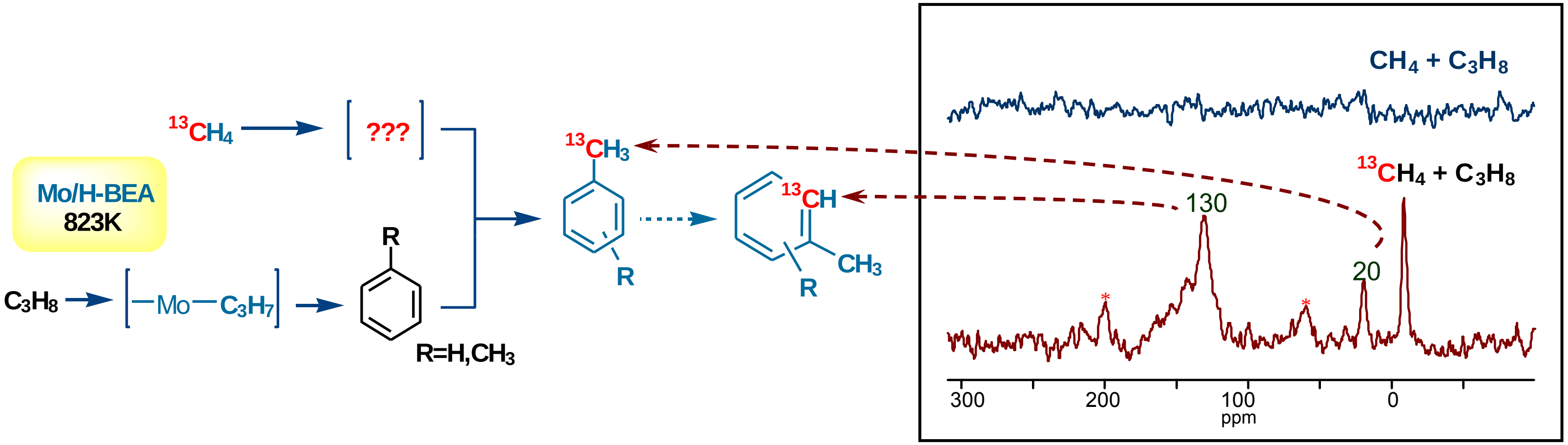
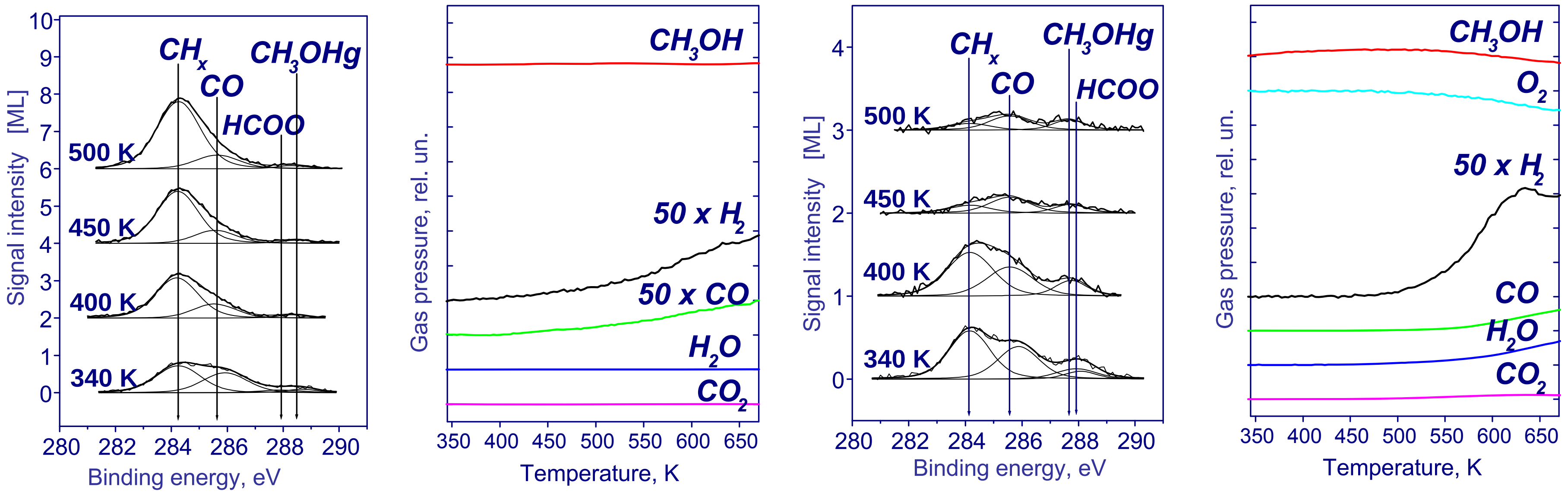


Fig. 7

In situ STUDY OF METHANOL DECOMPOSITION AND OXIDATION ON THE Pt(111) SURFACE BY XPS AND MASS SPECTROMETRIC TECHNIQUES



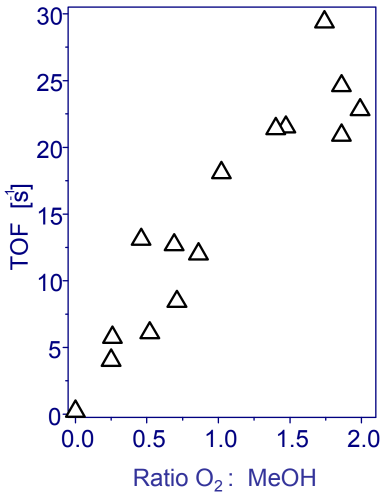
0.01 mbar CH_3OH

$CH_3OH \rightarrow CH_3O + H$

$CH_3O \rightarrow CO + 3H$

$CH_3O \rightarrow CH_3 + O$

$CH_3 \rightarrow C + 3H$



O_2 + 0.01 mbar CH_3OH

$CH_3O \rightarrow CH_2O + H$

$CH_2O + O \rightarrow HCOO + H$

$HCOO \rightarrow CO_2 + H$

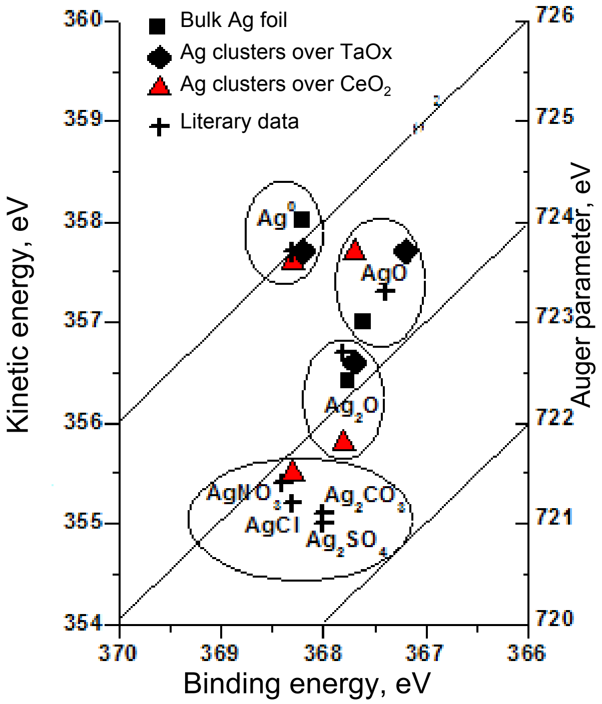
$CO + O \rightarrow CO_2$

Fig. 8

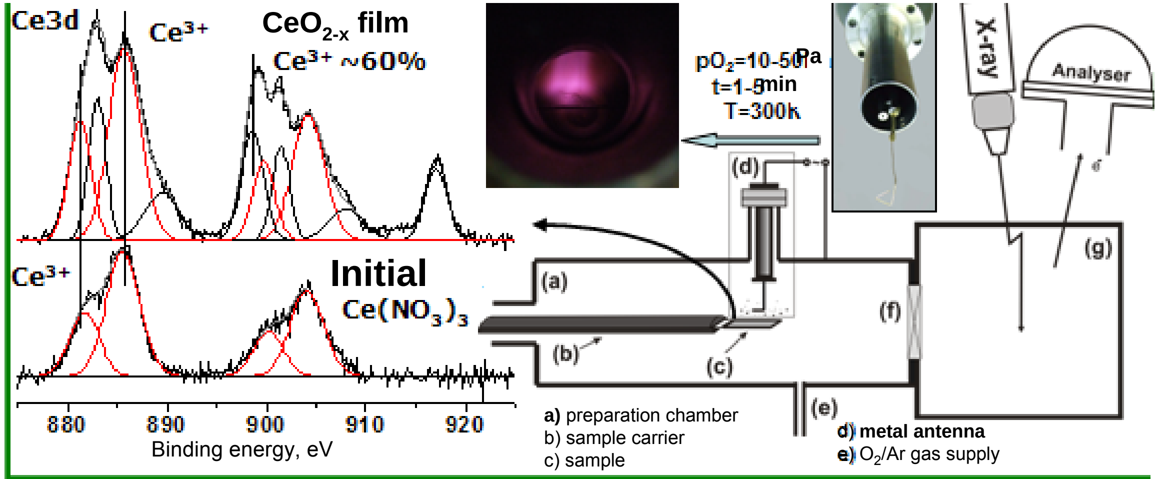
STUDY OF THE ELECTRON STRUCTURE, THERMAL STABILITY AND REACTIVITY OF OXIDIZED METAL NANOPARTICLES Cu, Ag, Pd, DEPOSITED ON CERIUM OXIDE

Silver nanoparticles

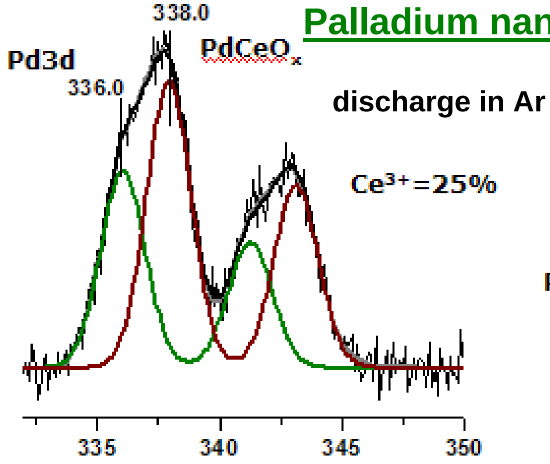
Two-dimensional Wagner map

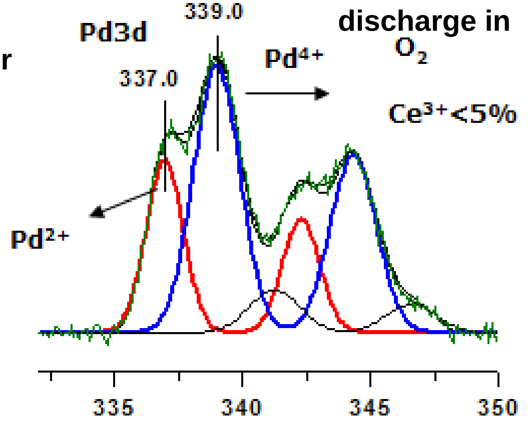


Deposition of silver particles in oxygen leads to the formation of $Ag_xCe_{1-x}O_{2-d}$ compound. Extending the plasma sputtering time leads to the formation of Ag_2O, AgO (Ag_3O_4). Reactivity of oxidized nanoparticles deposited on CeO_2 is much lower.



Palladium nanoparticles





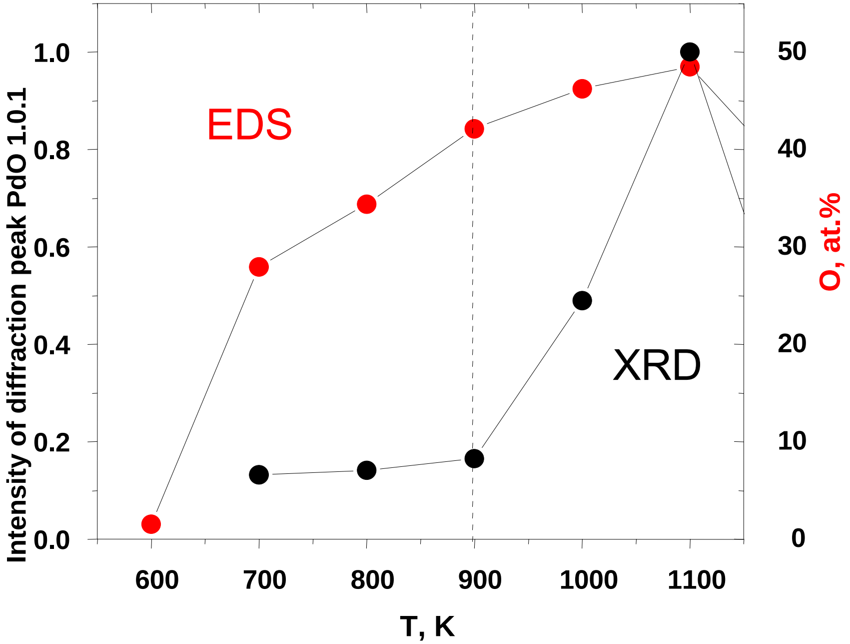
Deposition of palladium particles on CeO_2 in Ar atmosphere leads to the formation of palladium states different from the oxide structure PdO or PdO_2. Similar bond energy values of Pd3d are observed in real high active catalysts Pd/CeO_2

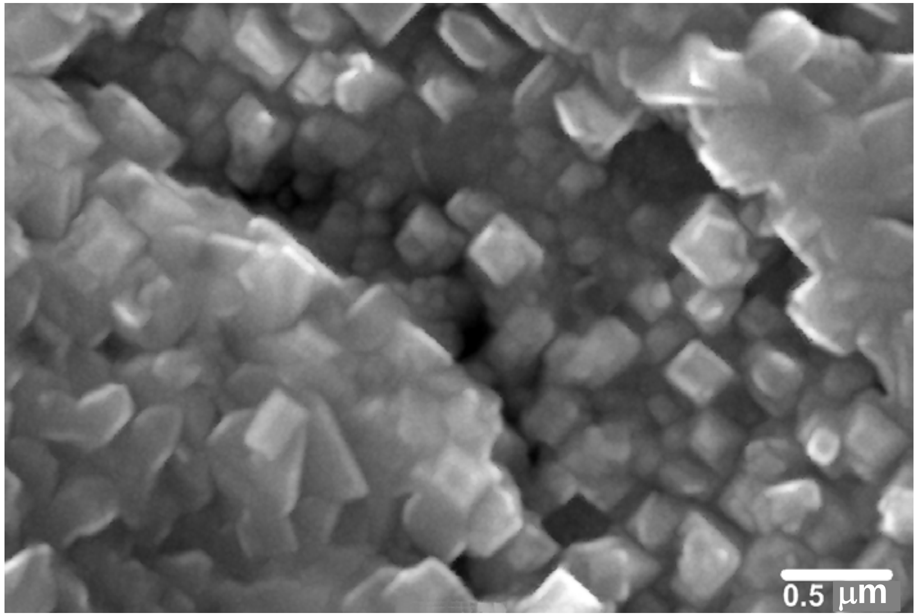
Fig. 9

FORMATION OF PdO CRYSTALS OVER Pd(poly) IN O_2 ATMOSPHERE

As the temperature rises to 1100 K, the quantity of oxygen absorbed by Pd(poly) increases up to ca. 50 % (EDS) and the diffraction peak of PdO becomes more intense (XRD)

At T = 1100 K a continuous layer of PdO crystals (250–500 nm) is formed



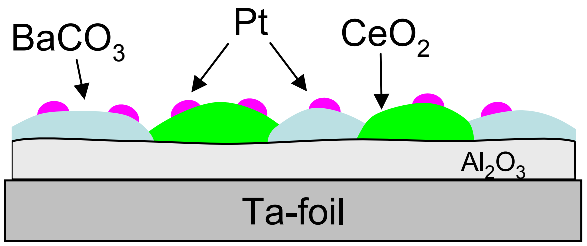


EDS – data of energy-dispersive X-ray spectroscopy
XRD – results of X-ray diffraction technique

SEM imaging of Pd(poly) surface

Fig. 10

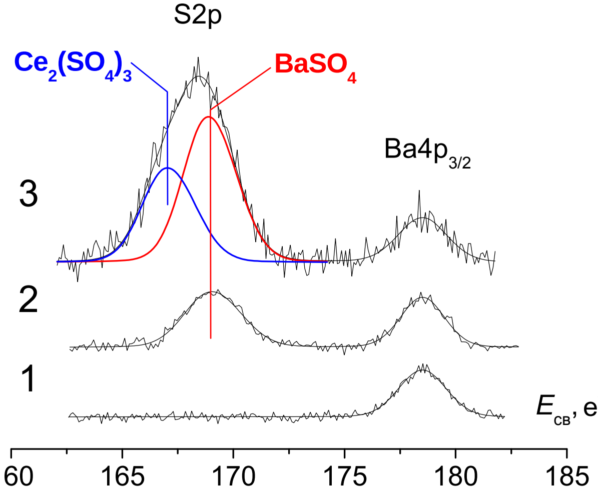
THE INTERACTION OF SO_x WITH A MODEL NSR CATALYST $Pt/(BaCO_3+CeO_2)$

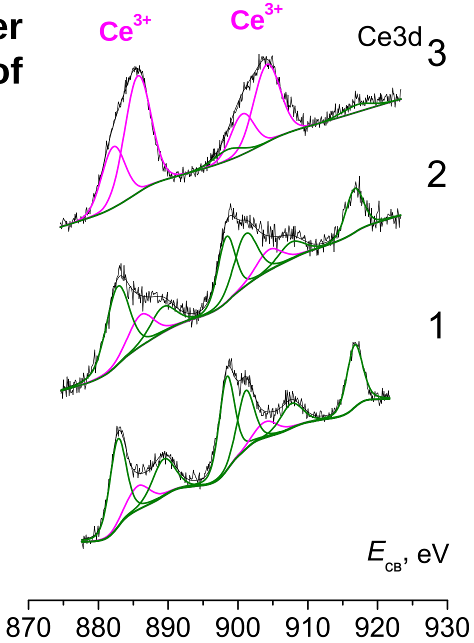


A model NSR catalyst $Pt/(BaCO_3+CeO_2)$ during neutralization of car exhaust gases was treated with a mixture of SO_x - 260 Pa SO_2 + 2600 Pa O_2 + 525 Pa H_2O

Aim: **Elucidation of the nature of surface compounds, that form upon the catalyst poisoning with sulfur oxides under oxidative conditions**

Method: **XPS is a method highly sensitive to the chemical state of sulfur; it allows surface compounds of similar chemical nature ($BaSO_4$ and $Ce_2(SO_4)_3$) to be identified under conditions of differential charging of a multicomponent sample**





1 - Initial catalyst 2 - SO_x, 150°C 3 - SO_x, 300°C

Fig. 11

Conclusion:

a) **Successive formation of Ba and Ce sulfates is observed with increasing temperature**

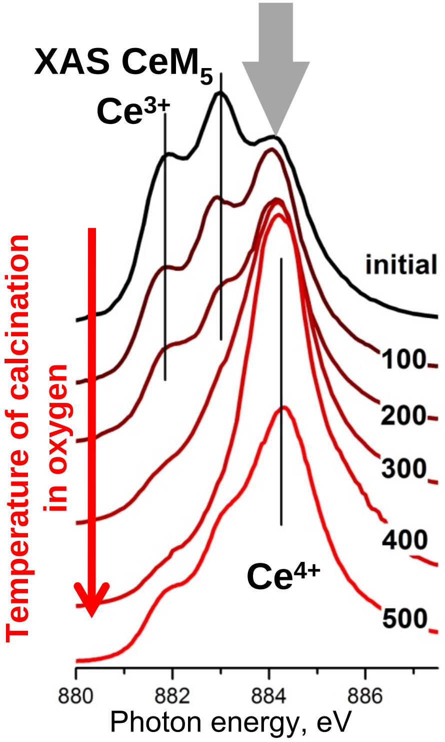
b) **Sulfation of CeO_2 is accompanied by reduction of Ce(IV) to Ce(III)**

c) **Supported Pt particles preserve their initial metal state**

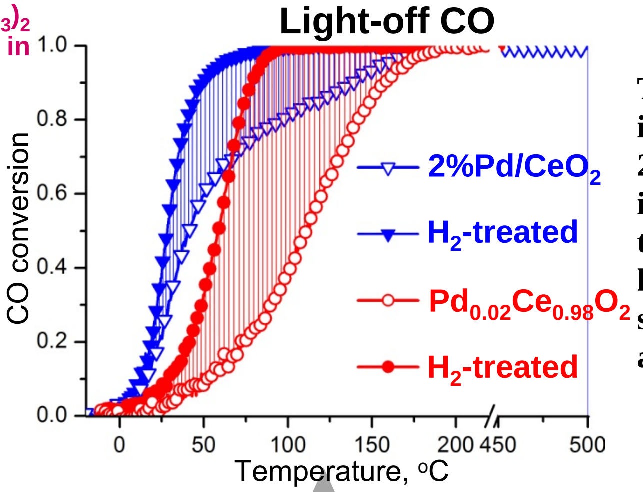
d) **On regeneration of the sulfated catalyst by heating in a mixture of 2100 Pa CO + 525 Pa H_2O, successive decomposition of surface sulfates Ce_2SO_4 is observed at below 500°C and $BaSO_4$ at the temperature range between 600 and 700°C**

In situ XPS STUDIES OF THE REACTION OF CO + O_2 OVER Pd/CeO

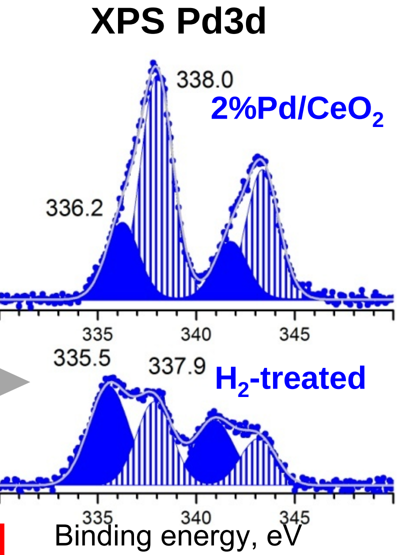
Solution of $Ce(NO_3)_3$ and $Pd(NO_3)_2$ mixture is dried and calcined in oxygen



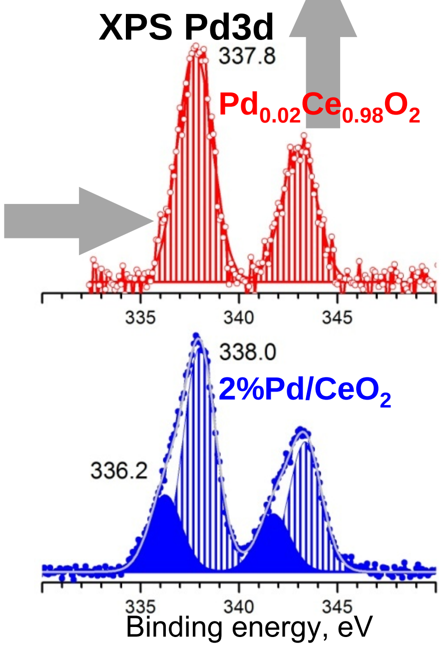
Ce^{3+} ions are completely oxidized at 400°C but elevation of the calcination temperature up to 500°C leads again to emergence of Ce^{3+} ions



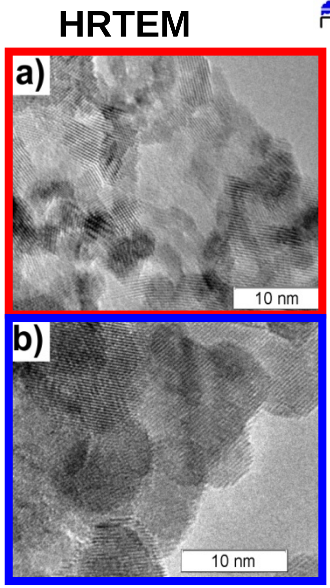
The catalyst $Pd_{0.02}Ce_{0.98}O_2$ is less active than 2%Pd/CeO_2 at identical ignition temperatures; their treatment with hydrogen results in a sharp increase in the activity of both catalysts



The treatment with hydrogen leads to the formation of reduced palladium clusters but the solid solution $Pd_xCe_{1-x}O_2$ is partly preserved



The main palladium state in the obtained catalyst is identical to that in the 2%Pd/CeO_2 catalyst prepared by impregnation; it is $Pd_xCe_{1-x}O_2$ solid solution

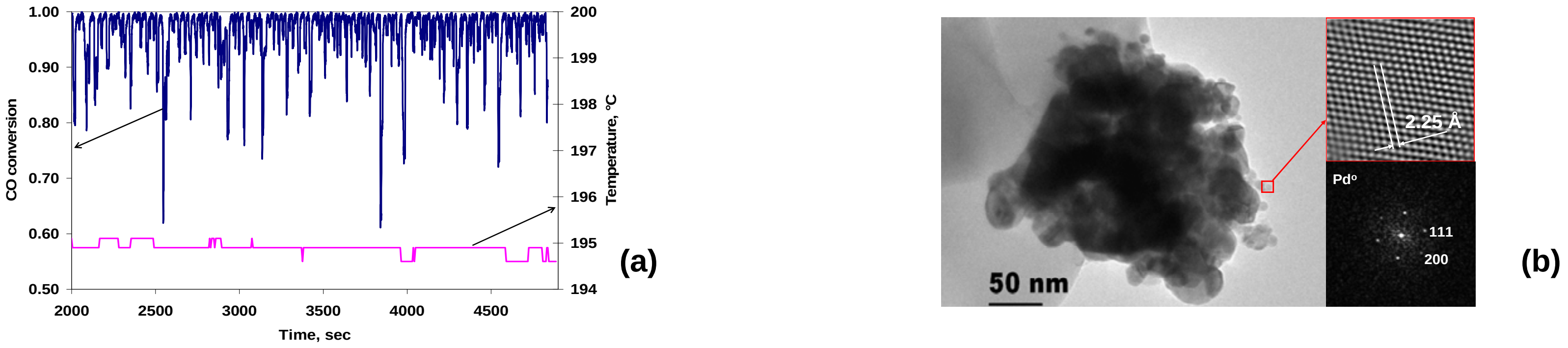


HRTEM studies do not reveal any palladium particles in the structure of both catalysts. The morphology is observed as CeO_2 nanoparticles

A method was developed for *in situ* synthesis of the $Pd_xCe_{1-x}O_2$ phase in the chamber of a spectrometer. The presence of Ce^{3+} ions is demonstrated to be necessary for the phase stabilization. It is established that this phase is responsible for the reaction ignition. Palladium clusters bear responsibility for the fast achieving the maximal conversion. The prepared model nanodisperse catalyst is close by all its parameters to the catalysts synthesized by traditional way of impregnation

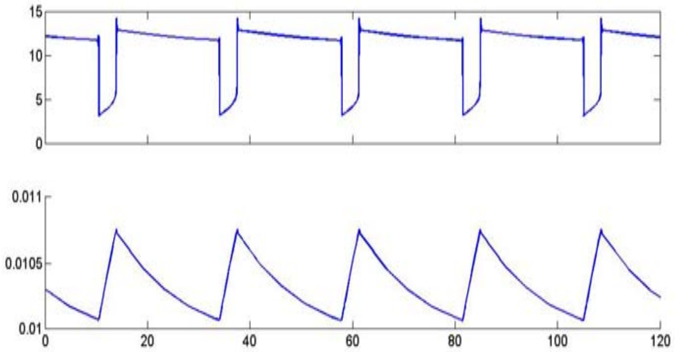
Fig. 12

SELF-OSCILLATIONS IN REACTION OF CO OXIDATION ON Pd/Al_2O_3(*800*)-1200 NANOPARTICLES: EXPERIMENT AND MATHEMATICAL MODELING



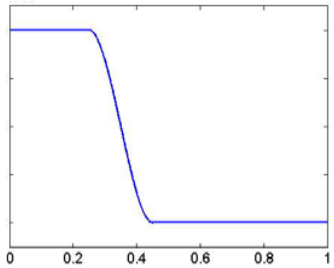
(a) **(b)**

Time dependence of CO conversion over Pd/Al_2O_3*(800)*-1200 at 195°C (a), TEM image of a Pd nanoparticle after long self-oscillations (the particle surface was cleaved into numerous finer Pd and PdO particles) (b)



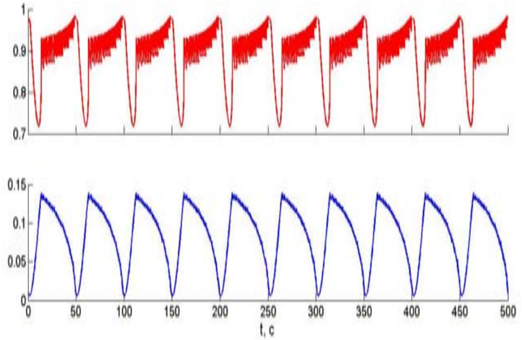
Redox model: Relaxation self-oscillations of reaction rate and part of metal surface

+



Non-linear dependence of the rate constants on concentration of adsorbed O

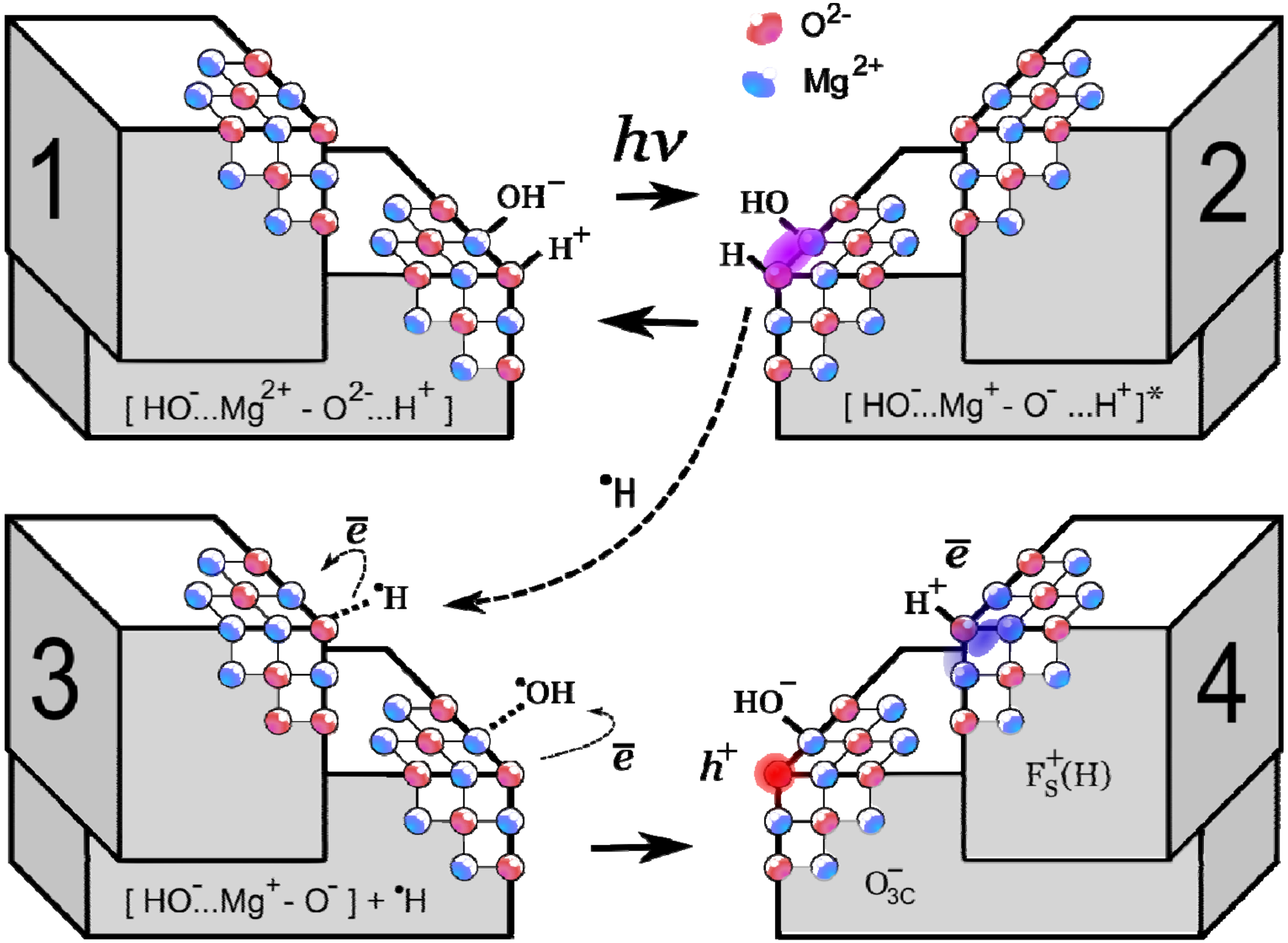
⇒



Multipeak oscillations of CO conversion and part of metal surface

Fig. 13

MECHANISM OF PHOTOSTIMULATED FORMATION OF RADICAL ANIONS O$^-$ ON THE SURFACE OF OXIDES



Photodecomposition of chemisorbed water to H$^\bullet$ and OH$^\bullet$ radicals is the key factor in the process of anion radicals O$^-$ generation. Process *does not need* the space separation of charges!

Fig. 14

DFT ANALYSIS OF FORMIC ACID DECOMPOSITION PATHWAYS $HCOOH \rightarrow CO + H_2O$ ON THE SURFACE OF V_2O_5/TiO_2

Rate determining step of dehydration reaction: **$HCOOH \rightarrow CO + H_2O$**

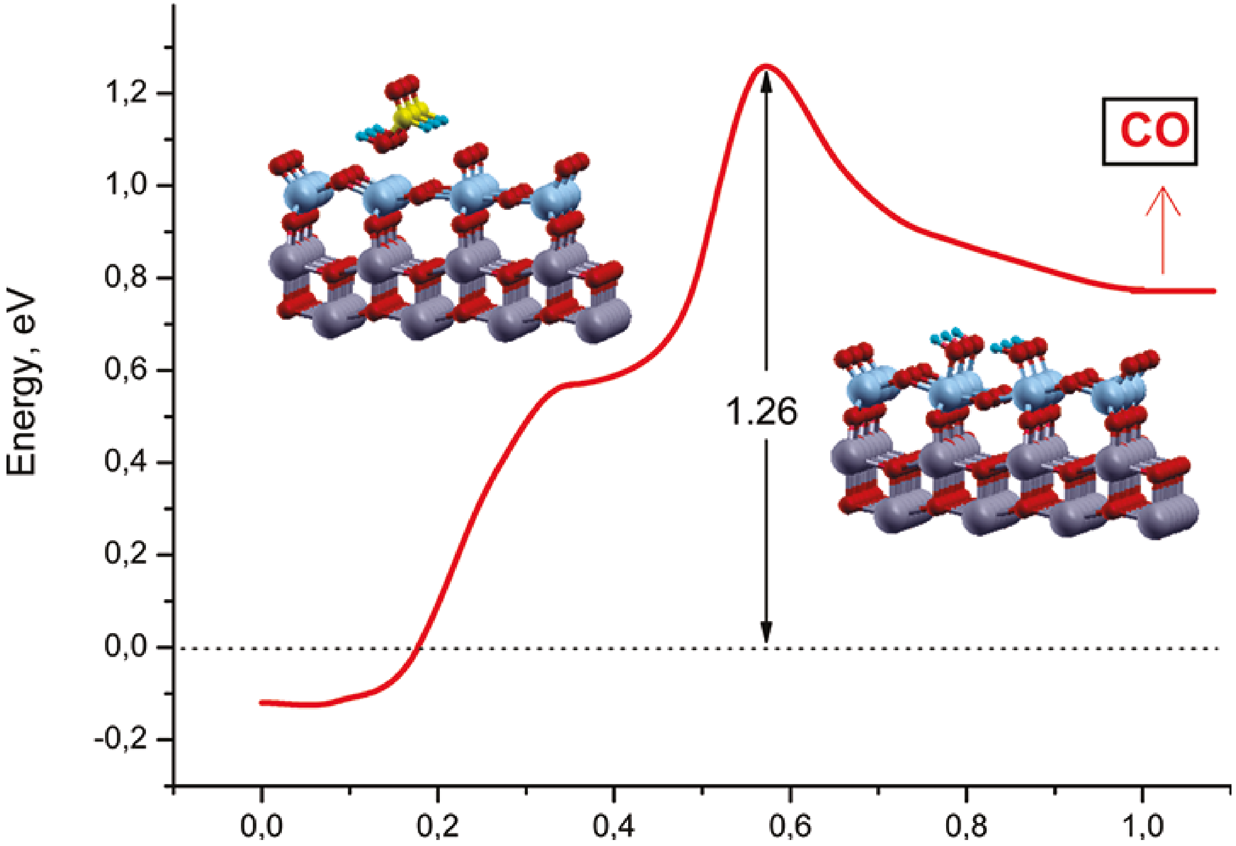
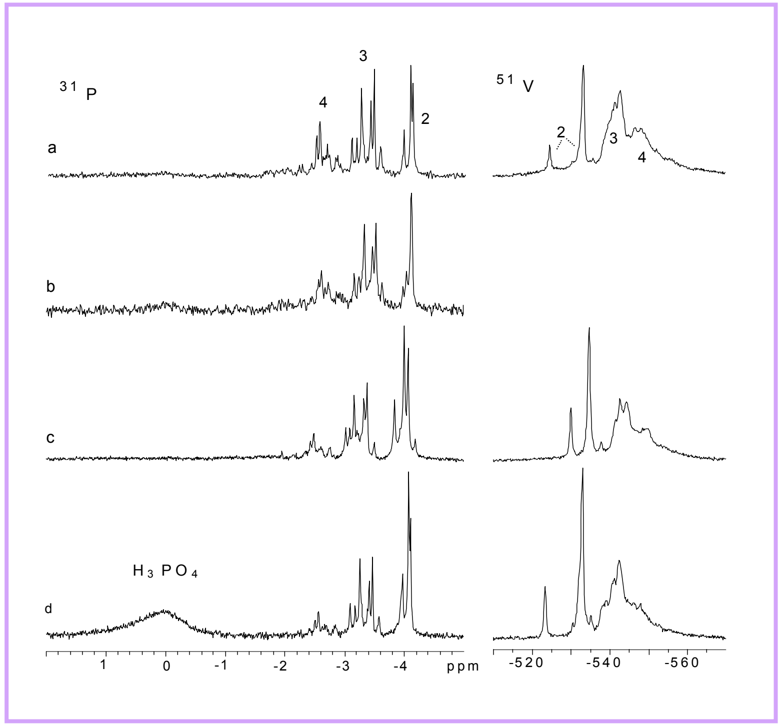


Fig. 15

MODIFIED SOLUTIONS OF non-KEGGIN TYPE Mo-V-P HPA – HYDROLYTICALLY STABLE AND TECHNOLOGICALLY ADAPTABLE CATALYSTS FOR OXIDATION OF ORGANIC SUBSTRATES



NMR ^{31}P and ^{51}V spectra of solutions $Na_{1,2}H_{5,8}PMo_8V_4O_{40}$ (0,1 M (a) and 0,02 M (в))

and $Na_{1,2}H_{15,8}P_3Mo_{16}V_{10}O_{89}$ (0,1 M (c) and 0,01 M (d))

$$H_aP_zMo_yV_{x'}O_b$$

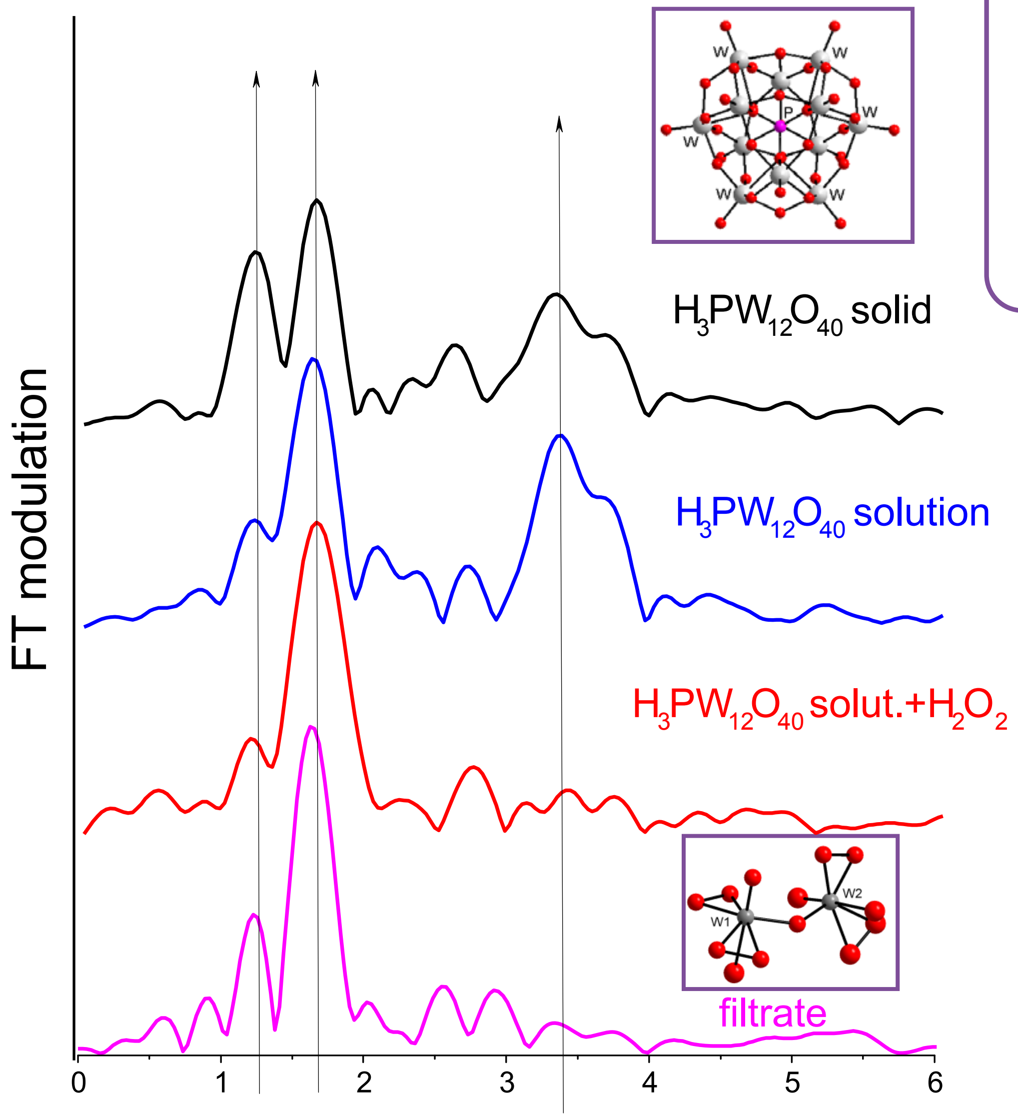
$$1 \le z \le 3;\ 8 \le y \le 18;\ 1 \le x' \le 12;$$

$$a = 2b - 6y - 5(x' + z);\ 40 \le b \le 89$$

- Methods for synthesis of two modified 0.25 M solutions (**$H_{11}P_4Mo_{18}V_7O_{87}$** (**HPA-7**) and **$H_{17}P_3Mo_{16}V_{10}O_{89}$** (**HPA-10**)) were optimized
- The synthetic procedure was made **2.5 times** shorter
- The introduced vanadium is increased in quantity to **1.75–2.5 M**
- The thermal stability is improved (**up to 170 °C**)

Fig. 16

BIFUNCTIONAL CATALYSTS BASED ON PEROXO POLYOXOMETALLATES



Structural changes in the course of complexes preparation:

- the nuclearity of the complexes is reduced
- symmetry of tungsten surrounding is changed

A new series of peroxo polyoxometallate catalysts of $Q_3\{PO_4[MO(O_2)_2]_4\}$ composition, where M = Mo and W, was synthesized

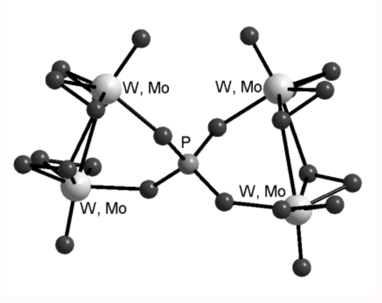
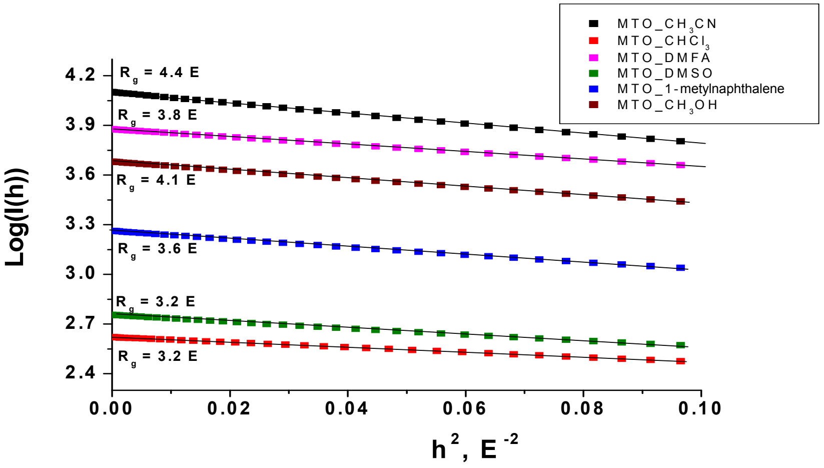
Q^+	$\{PO_4[WO(O_2)_2]_4\}^{3-}$
$[Me_4N]^+$	
$[Et_4N]^+$	
$[Bn_3MeN]^+$	
$[Me_4N]^+$	
$[Et_4N]^+$	
$[Et_2Bn_2N]^+$	

Fig. 17

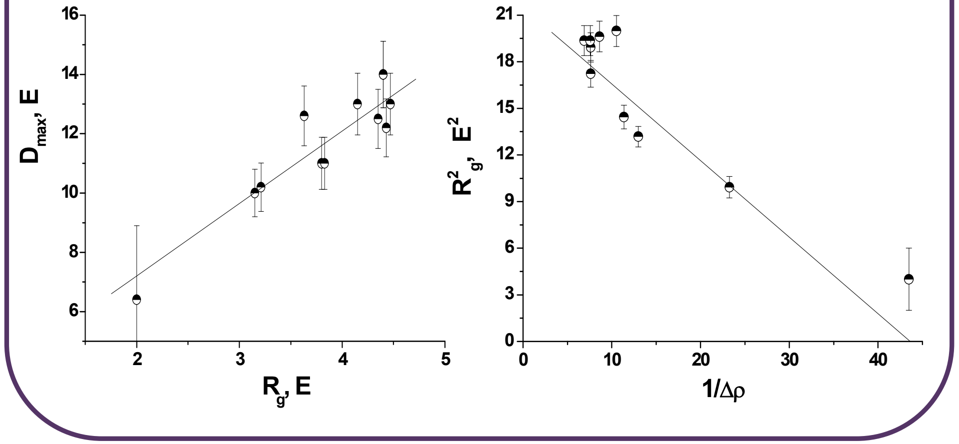
STUDY OF PEROXOCOMPLEX $[Me_3(n\text{-}C_8H_{17})_3N]_2\{HPO_4[WO(O_2)_2]_2\}$ (MTO) STRUCTURE IN ORGANIC SOLVENTS USING SAXS TECHNIQUE

SAXS data in Guinier coordinates for monodispersed particles



In 15 solvents complex exists in the form of individual molecules

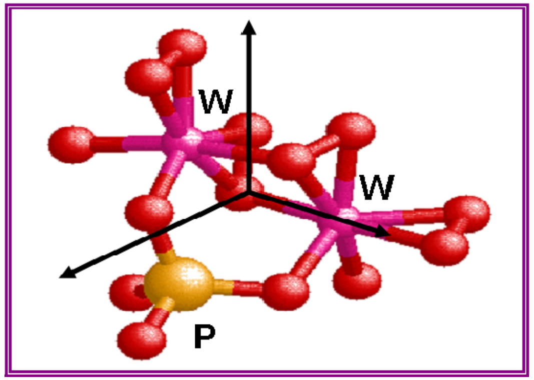
Dependencies Dmax(Rg) for MTO molecules (left) and Rg on value of relative contrast (right)



Ratio Dmax /Rg for particles of various shape

Models	Sphere	Disc	Rachis	Complex
D_{max}/R_g	2.6	2.8	3.5	3.1 ± 0.2

Anion $\{HPO_4[WO(O_2)_2]_2\}^{2-}$ structure according to X-ray



Conclusion: Structure of the complex possesses features of oblate and oblong heterogeneous nanoparticle

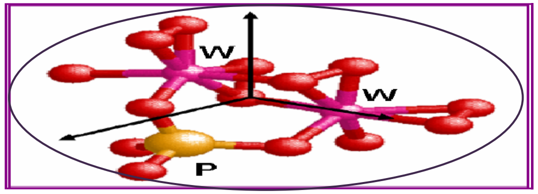
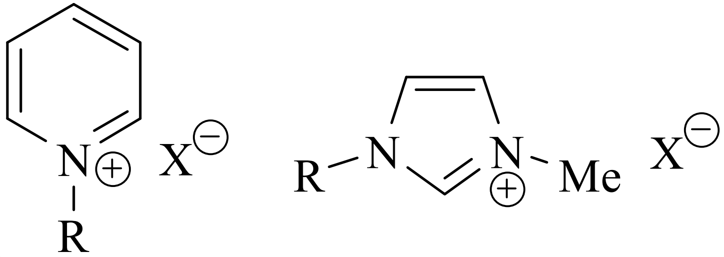


Fig. 18

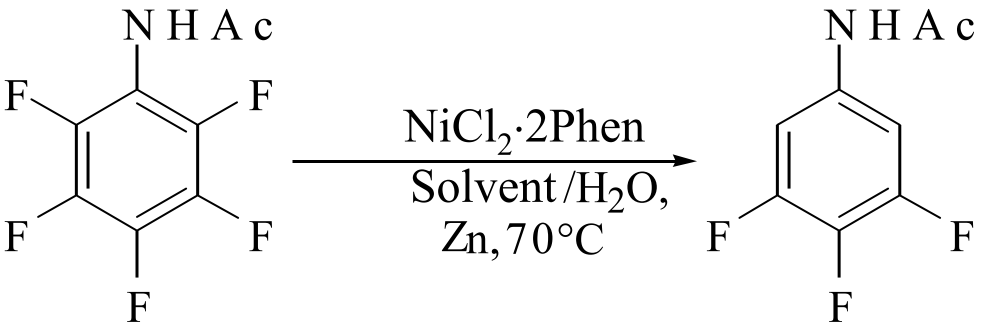
SYNTHESIS OF ORGANIC COMPOUNDS USING IONIC LIQUIDS AS REACTION MEDIA

Synthesis and characterization of ionic liquids with physico-chemical methods



R = H, Et, Bu, Hex, $C_{10}H_{21}$, $C_{12}H_{25}$, $C_{16}H_{33}$
X = Br, Cl, $Al_{n+1}Cl_{3n+3}$ (n = 0-3), $[(C_6F_5)_nBF_{4-n}]$

Ionic liquids as reaction media for C-F bond activation



Reaction time:
***N*-Methylpyrrolidone – 6 h**
BMIMBr – 2 h

BMIMBr:

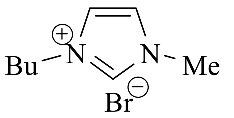
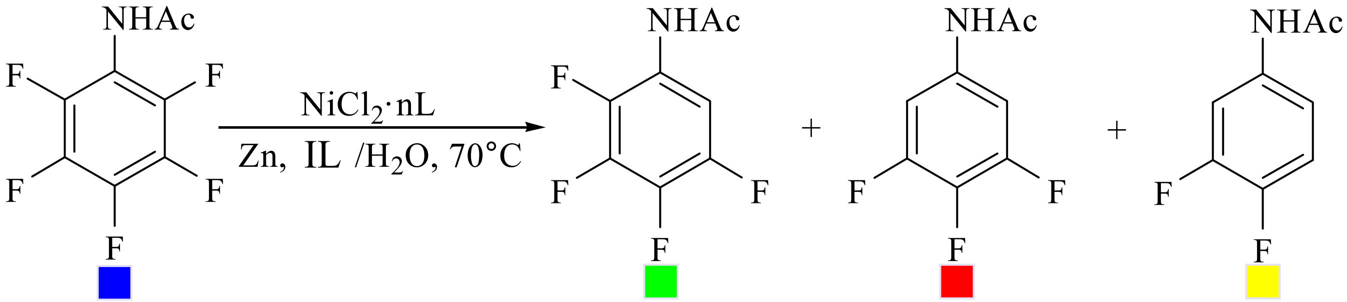


Fig. 19

SYNTHESIS OF ORGANIC COMPOUNDS USING IONIC LIQUIDS AS REACTION MEDIA

Study of the effect of ionic liquid nature on the rate and selectivity for hydrodefluorination reaction



BMIMBr: High activity of NiCl$_2$·2Phen and NiCl$_2$·3Bpy

BMIMCl: High activity of all NiCl$_2$·nBpy complexes

BMIMOAc: Low activity of all nickel complexes

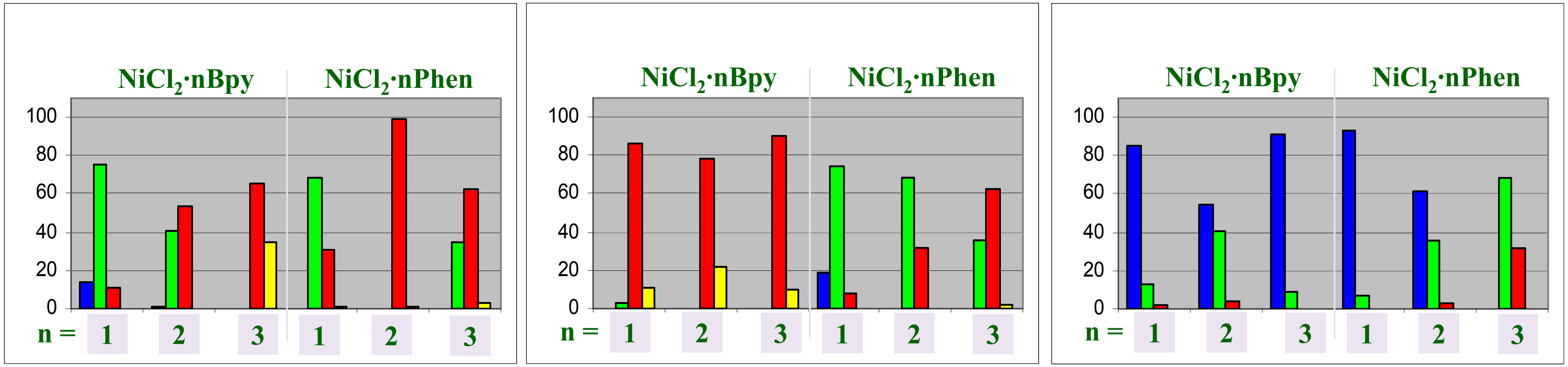
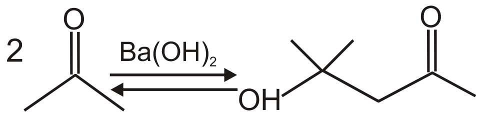
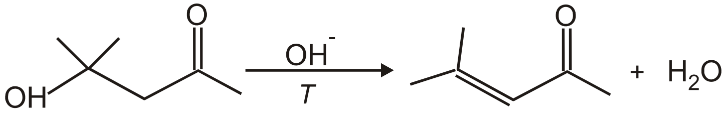


Fig. 20

DIACETONE ALCOHOL SYNTHESIS IN MICROCHANNEL REACTOR

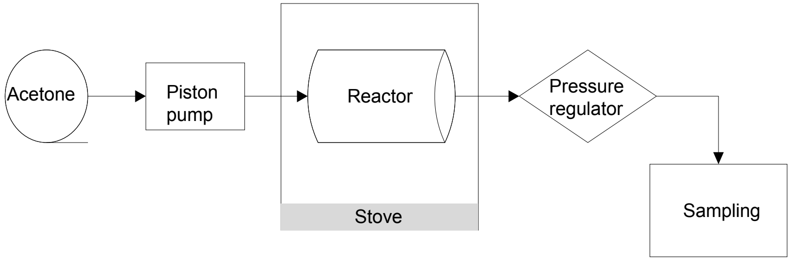


Reaction of diacetone alcohol (DAA) formation



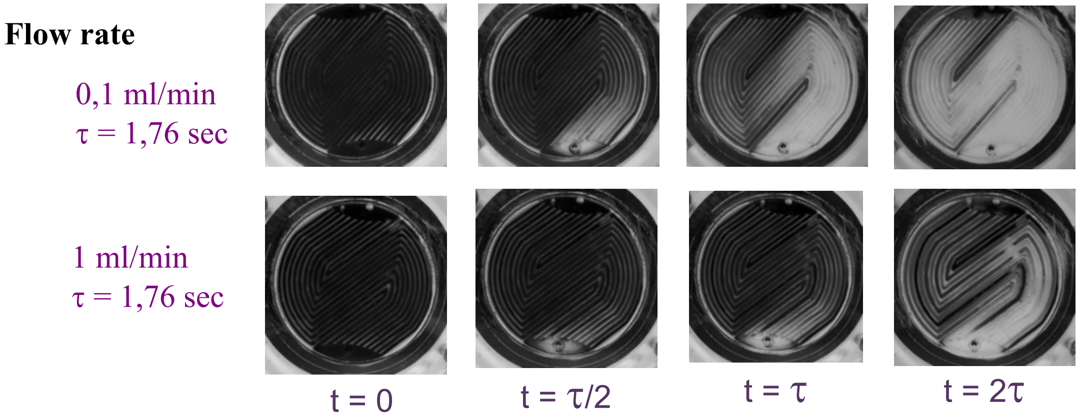
Side reaction of mesityl oxide formation (4-methyl-3-penten-2-on) (MO)

Scheme of experimental setup with working pressure 20 – 25 atm



№	T, ^{0}C	Rate of acetone supply, ml/min	Pressure, atm	Time sampling, min	Products concentration, mol. %	
					MO	DAA
1	86,5-91,2	0,5	15	80	0,54	0,37
2	95,3-94,3	0,5	20	90	0,51	1,06
3	96	1	25	60	0,82	2,24

Visualization of reagents stream over microchannel plated



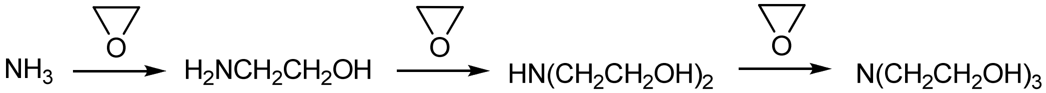
The better distribution of stream through the channels is observed at low flow rates

Optimum conditions:

✓Temperature = 20-45°C
✓Volumetric flow rate of acetone = 10-20 h^{-1}

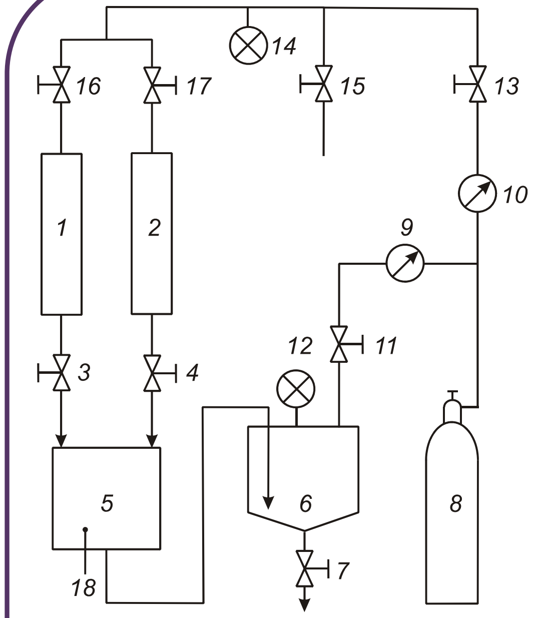
Fig. 21

TRIETHANOLAMINE SYNTHESIS IN MICROCHANNEL REACTOR



$NH_3 \longrightarrow H_2NCH_2CH_2OH \longrightarrow HN(CH_2CH_2OH)_2 \longrightarrow N(CH_2CH_2OH)_3$

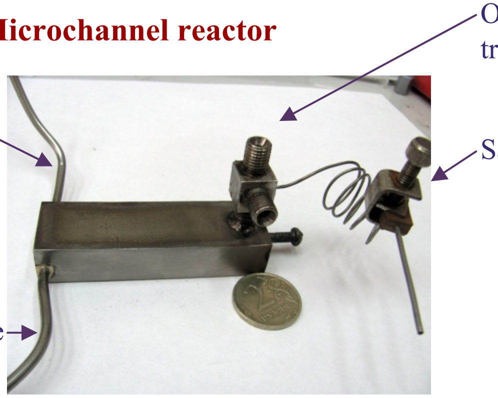
Ethylene oxide ammonolysis

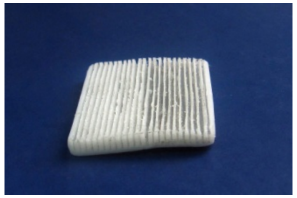


Scheme of laboratory setup for triethanolamine production

1. Vessel with ammonia
2. Vessel with ethylene oxide
3-4. Taps for ammonia and ethylene oxide flow control
5. Microreactor
6. Vessel for products
7,11,13,15-17. Stopcocks
8. Argon cylinder
9-10. Reducers
12,14. Manometers
18. Thermopair

Microchannel reactor





Microchannel plate from teflon 4

Contact time, min	Composition of resulting mixture, wt. %				OE conversion, %
	MEA	DEA	TEA	OEA	
2,4	-	-	84	15,6	56
3	-	19,5	65	14,5	69
4,3	1,4	1,5	55	37	84
7,9	14,1	12,4	14,0	59	100
10	10,4	10,2	3,1	76	100
11,5	4,2	6,3	1,6	80	100

MEA - monoethanolamine
DEA - diethanolamine
OE – ethylene oxide
TEA - triethanolamine
OEA – oxyethanol oxide

Fig. 22

VORTEX EMULSIFIER FOR PHASE MIXING IN CATALYTIC MULTIPHASE PROCESSES

Design of vortex emulsifier for phase mixing in catalytic multiphase processes on the liquid/liquid boundary with participation of gas component

- ✓ Vortex emulsifier is developed in which contact between liquids is realized in vortex layer, formed by liquid swirling via distributor with possible adding of dispersed gas

- ✓ Obtained data are evidence of high efficiency of liquid and gas mixing

Dispersed layer
(water – dispersed air)

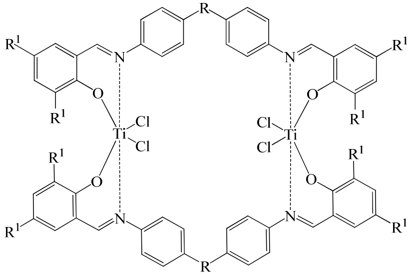
Formation of emulsion layer
(water - pentanol with dye Rhodamine G extraction)

Photo of emulsion layer
water + 5 vol. % of stained hexane

Fig. 23

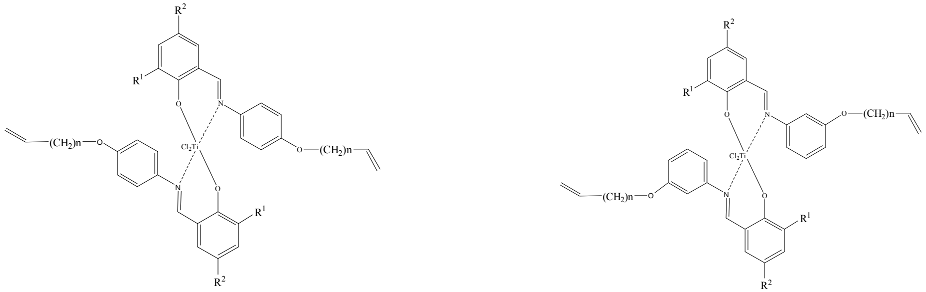
POLYMERIZATION AND COPOLYMERIZATION OF ETHYLENE AND α-OLEFINS OVER NEW BINUCLEAR AND FUNCTIONALIZED POSTMETALLOCENE CATALYSTS

1. **A set of analytic and physicochemical methods including NMR-DOSY spectrometry and Maldi-TOF mass-spectrometry were used to prove the binuclear structure of the binuclear titanium halide complexes. The resulting catalytic systems were shown, depending on the ligand environment and the nature of bridge bonds between imines of the binuclear complexes, to feature a high thermal stability combined with the high catalytic activity and MW of obtained polyethylene.**



Structure of binuclear complexes

R= $-CH_2-$, -O-; $-(p\text{-}C_6H_4)-$; $-O-(p\text{-}C_6H_4)-O-$;
$=-O-(p\text{-}C_6H_4)-C(CH_3)_2-(p\text{-}C_6H_4)-O-$
R^1= t-Bu; CMe_2Ph



Structure of bis(phenoxyimine) functionalized complexes

$R^1= CMe_2Ph$, R^2=H;
$R^1= CMe_2Ph$, R^2=Me;
$R^1= R^2= CMe_2Ph$;
n=1

$R^1= R^2= CMe_2Ph$;
n=3

Co-polymerization of ethylene and hexene-1 was studied using two of the binuclear complexes. The results obtained did not confirm the expected increase in the rate of copolymerization, and possibility of hexene-1 insertion into copolymer is not more than 1.5 % mol, the bridge bonds between imines make special hindrances for insertion of α-olefins. Similar binuclear systems reported by Marks, studied at temperatures ≤ 40°C, possess very low activity in comparison with our systems

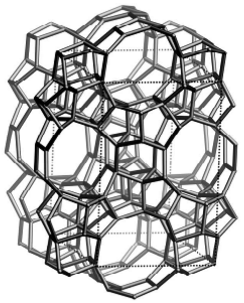
2. Specific features of catalytic activity to polymerization were studied with the catalysts prepared on the basis of the synthesized titanium halide complexes which were functionalized with oxy-allyl groups of bissalicylaldiimine precursors. It was shown that the regime of the catalyst self-immobilization can be controlled in the course of polymerization depending on the position of the oxy-allyl group and on the length of the bridge ($–CH_2$) between the oxy-group and double bond

Fig. 24

ALTERNATIVE MECHANISMS OF OXIDATIVE METHANE ACTIVATION

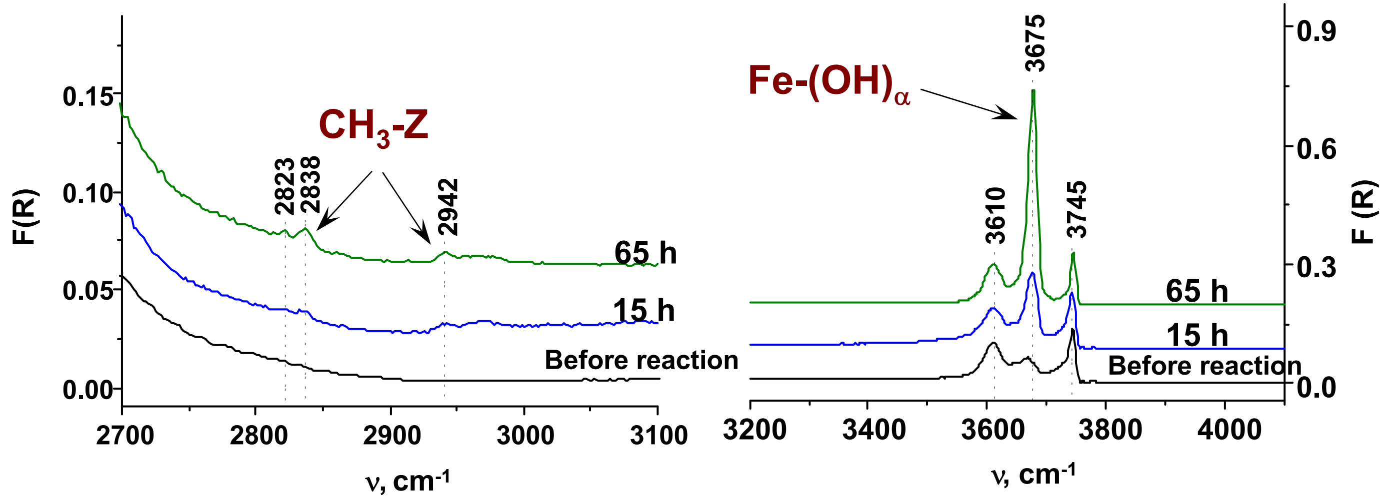
Mechanism (1): $CH_4 + Fe\text{-}(O^{\bullet -})_\alpha \rightarrow Fe\text{-}(HO)_\alpha + CH_3^{\bullet}$

Mechanism (2): $CH_4 + Fe\text{-}(O^{\bullet -})_\alpha \rightarrow Fe\text{-}(CH_3O)_\alpha + H^{\bullet}$



FeZSM-5

C_α = 100 μmol/g



Reaction $CH_4 + O_\alpha$ at 25°C results only in the formation of hydroxide groups $Fe\text{-}(OH)_\alpha$ and methyl radicals $^{\bullet}CH_3$. There are no methoxyl groups $Fe\text{-}(OCH_3)_\alpha$

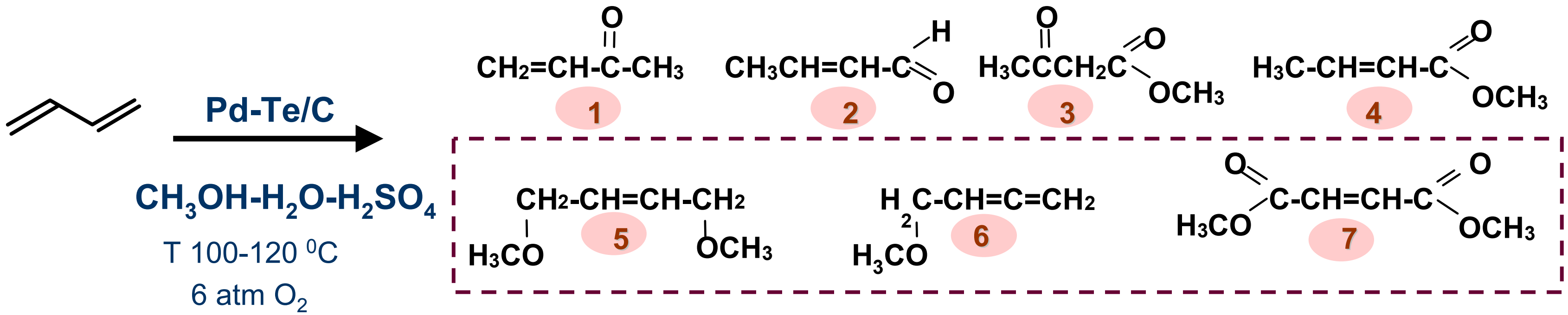
- **Conclusion: Oxidative activation of methane proceeds by mechanism (1) with hydrogen atom detachment and generation of surface OH-groups**

Fig. 25

MECHANISM OF OXIDATION OF BUTADIENE-1,3 ON Pd-Te/C CATALYSTS

Wide spectrum of products of butadiene-1,3 oxidation may be obtained upon variation of catalyst and reaction conditions.

The most valuable products are 1,4-butenediol and its derivatives (5-7)



Pd-Te/C

$CH_3OH\text{-}H_2O\text{-}H_2SO_4$

T 100-120 ^{0}C

6 atm O_2

$CH_2{=}CH\text{-}C({=}O)\text{-}CH_3$ **1**

$CH_3CH{=}CH\text{-}C({=}O)H$ **2**

$H_3CC({=}O)CH_2C({=}O)OCH_3$ **3**

$H_3C\text{-}CH{=}CH\text{-}C({=}O)OCH_3$ **4**

$H_3CO\text{-}CH_2\text{-}CH{=}CH\text{-}CH_2\text{-}OCH_3$ **5**

$H_3CO\text{-}H_2C\text{-}CH{=}C{=}CH_2$ **6**

$H_3CO\text{-}C({=}O)\text{-}CH{=}CH\text{-}C({=}O)\text{-}OCH_3$ **7**

1,4-butenediol derivatives - methyl ethers of 1,4-butenediol, allenic alcohol and maleic acid – are obtained by oxidation of butadiene-1,3 over Pd-Te/C catalyst in methanol at the selectivity 50-90%. Selectivity to 1,4-dimethoxybutene reaches 60%

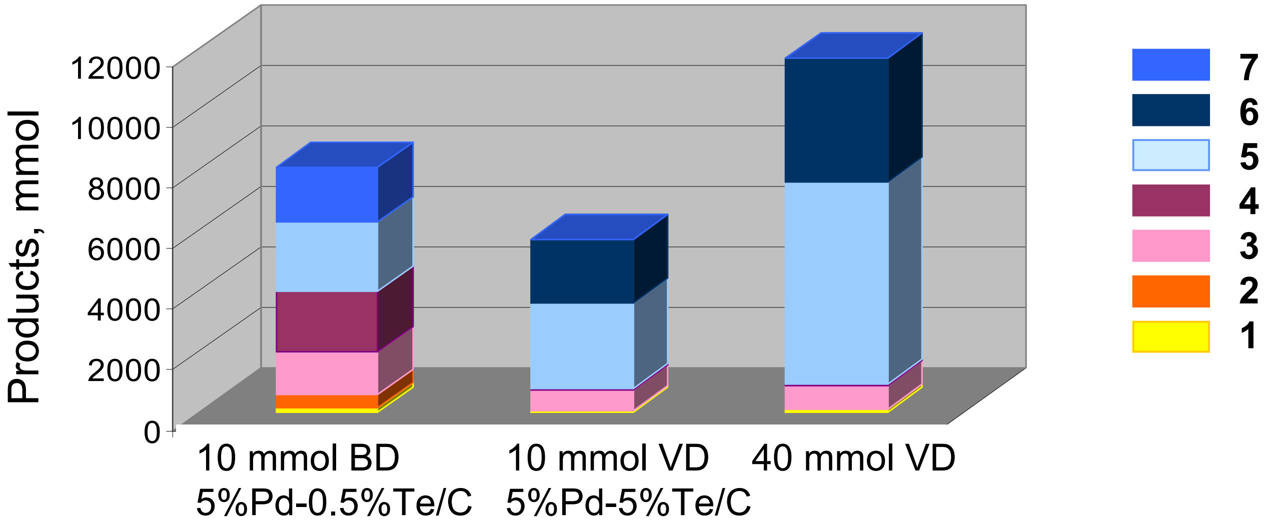
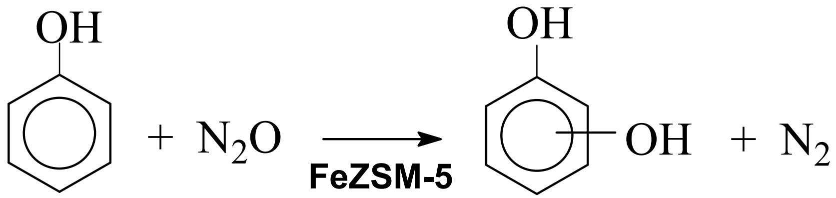


Fig. 26

HYDROXYLATION OF AROMATIC COMPOUNDS WITH NITROGEN SUBOXIDE

Reaction of phenol oxidation by nitrous oxide over FeZSM-5 zeolites was studied for the first time using a catalytic setup specially designed for operation with high-boiling compounds:



Hydroquinone	**48%**
Pyrocatechin	**38%**
Resorcinol	**6%**
Quinone	**8%**

A comparison with the current liquid-phase processes of phenol oxidation by H_2O_2 showed that the oxidation by N_2O may open a new promising way for alternative production of dihydroxybenzenes (DHB) in the gas phase

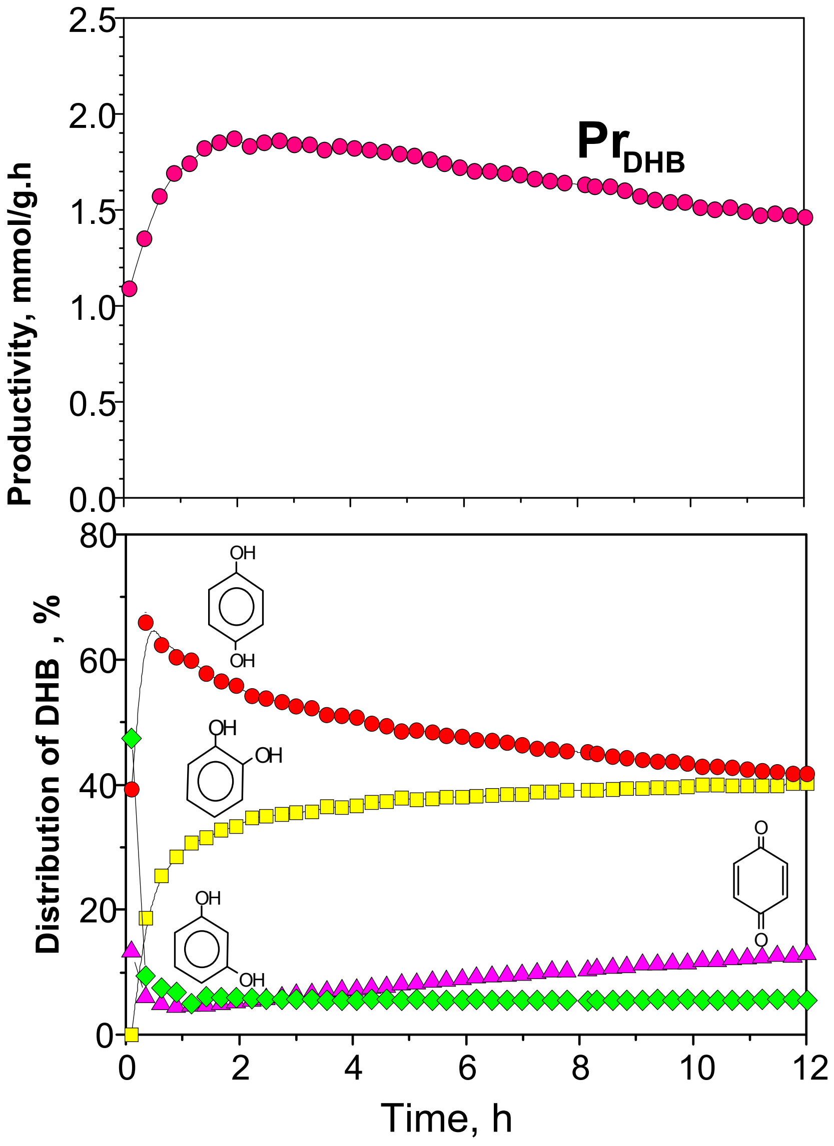
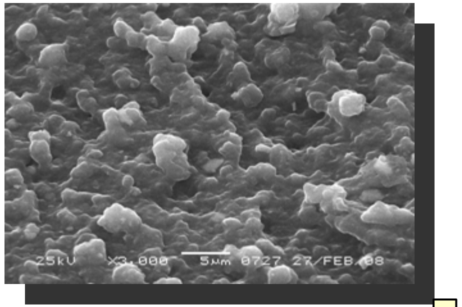


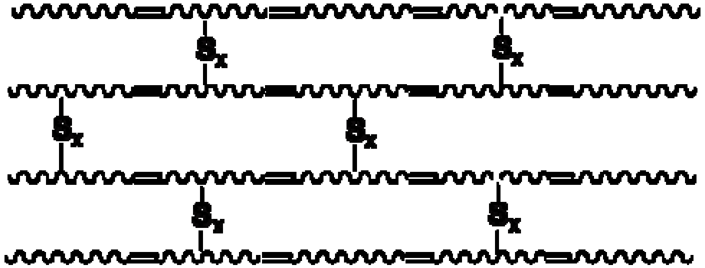
Fig. 27

NITROUS OXIDE FUNCTIONALIZATION OF POLYMER NANOMATERIALS

The reaction goes through selective interaction between N_2O and C=C bonds of the vulcanized materials to form carbonyl, preferably ketone, C=O groups in polymer chains

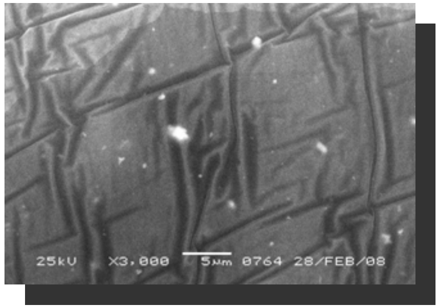
Initial rubber

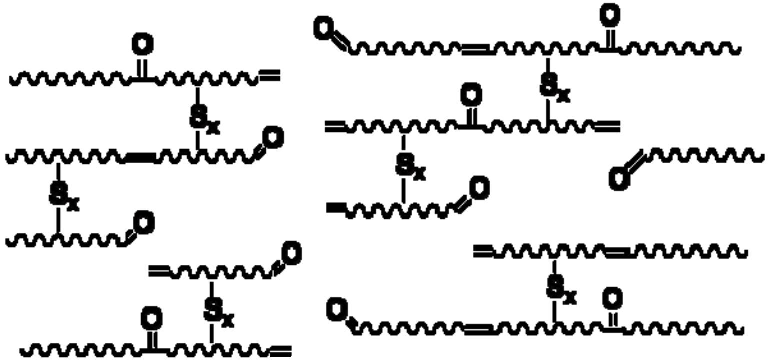




N_2O

T = 180÷230°C
P = 20÷40 atm





Regenerated rubber

Advantages:

- ***Controlled destruction of polymer chains and vulcanization network of the rubber***
- ***Formation of a plastic product***
- ***Stronger adhesion to reinforcing wire***

Fig. 28

RELATION BETWEEN CATALYTIC PROPERTIES OF Mo-V-Te-Nb OXIDES AND THEIR ACTIVITY TO ISOTOPIC EXCHANGE WITH DIOXYGEN

Chemical and phase composition of oxides, their catalytic properties

Sample	**Chem. composition**	**Phase composition**
M1	$Mo_1V_{0.31}Te_{0.14}Nb_{0.13}$	90% M1
M2	$Mo_1V_{0.31}Te_{0.19}$	97% M2
Me_5O_{14}	$Mo_1V_{0.31}Nb_{0.37}$	100% Me_5O_{14}

The activity in reaction of propane and propylene oxidation changes in the series:

M1 >> Me_5O_{14} > M2

The selectivity to the products of partial oxidation changes in the series:

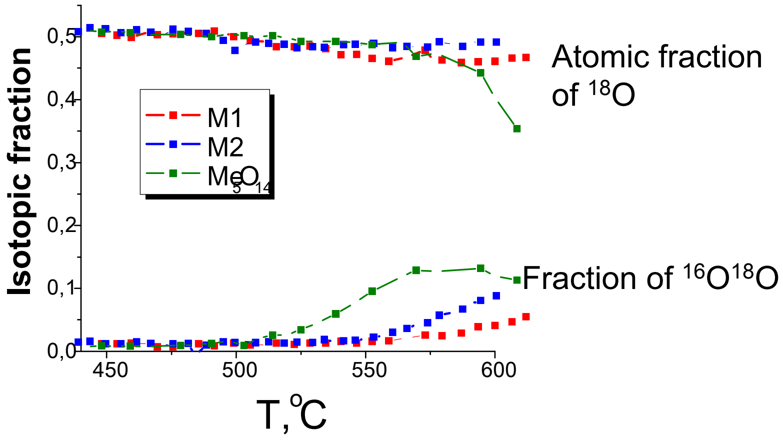
M1 > > M2 > Me_5O_{14}

The selectivity to the products of complete oxidation changes in the series:

Me_5O_{14} > M2 >M1

Thermally programmed isotopic exchange

A change in the isotopic oxygen outlet composition (inlet $0.5^{16}O_2 + 0.5^{18}O_2$)

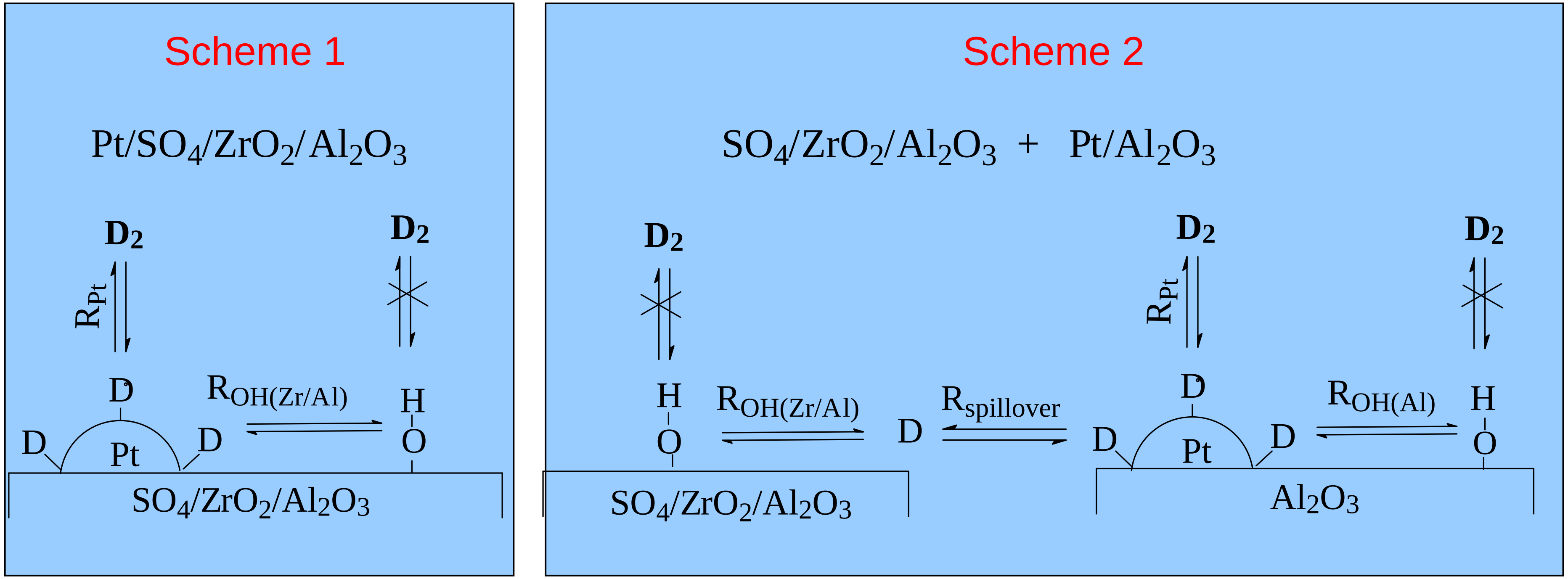


The activity to isotopic oxygen exchange changes in the series:

Me_5O_{14} > M2 > M1

Fig. 29

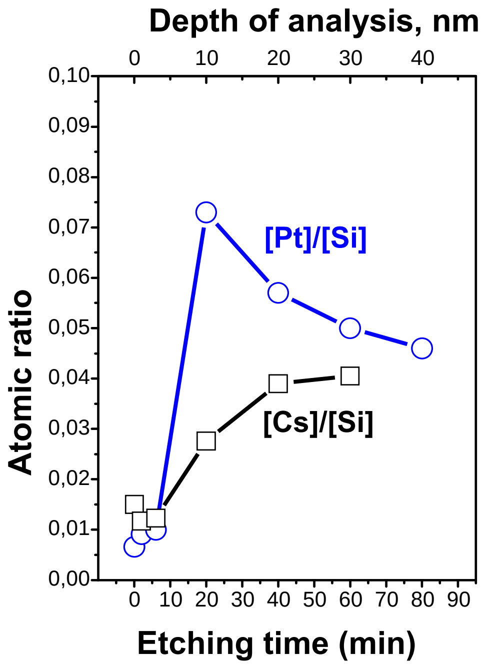
MECHANISM OF H/D EXCHANGE OVER Pt/SZA CATALYST AND Pt/Al_2O_3 + SZA MECHANICAL MIXTURE

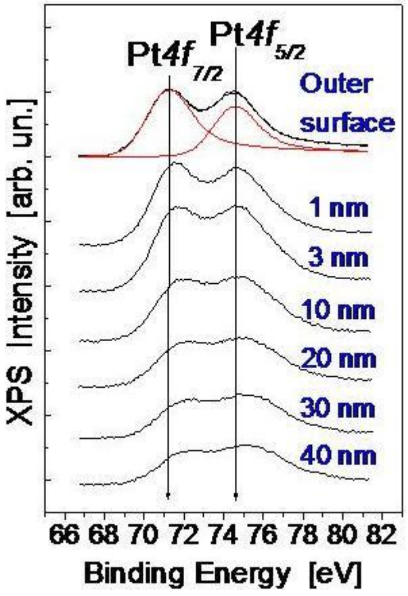


Hydrogen spillover process plays the key role for deutero-hydrogen exchange over acid catalysts

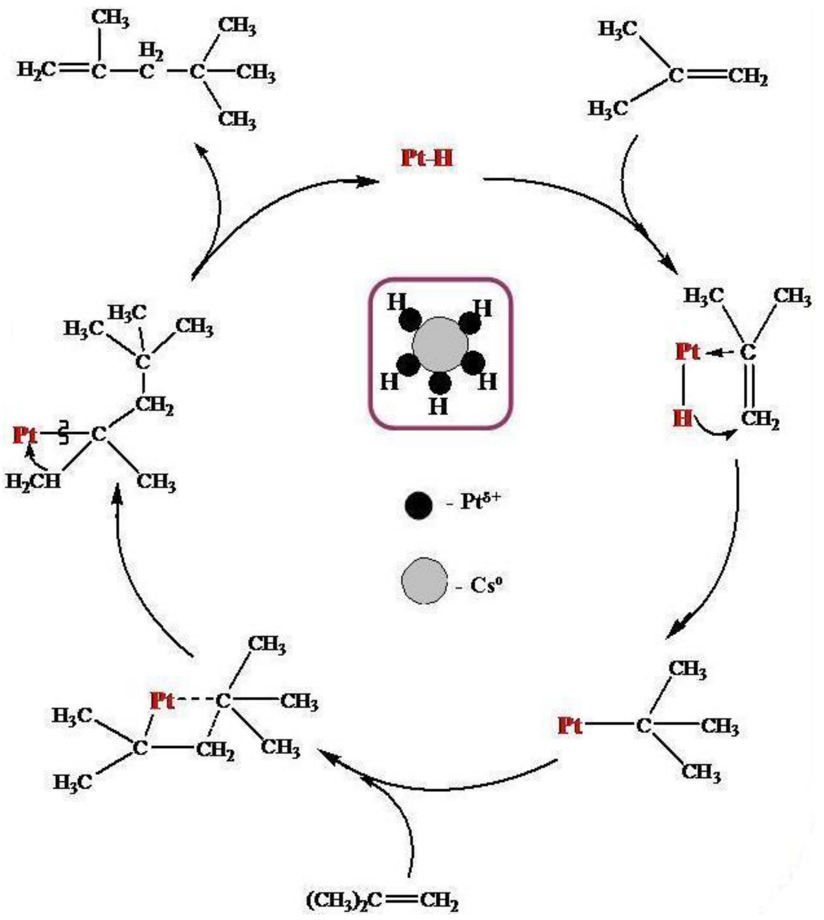
Fig. 30

SYNTHESIS AND CHARACTERIZATION OF FIBERGLASS CATALYSTS





Putative mechanism of the reaction of isobutene dimerization



- Upon the catalyst preparation, the intercalation of Cs and Pt particles into the volume of glass fibre at a depth 30-40 nm is observed

- XPS studies revealed electron transfer from Pt to Cs in the glass bulk

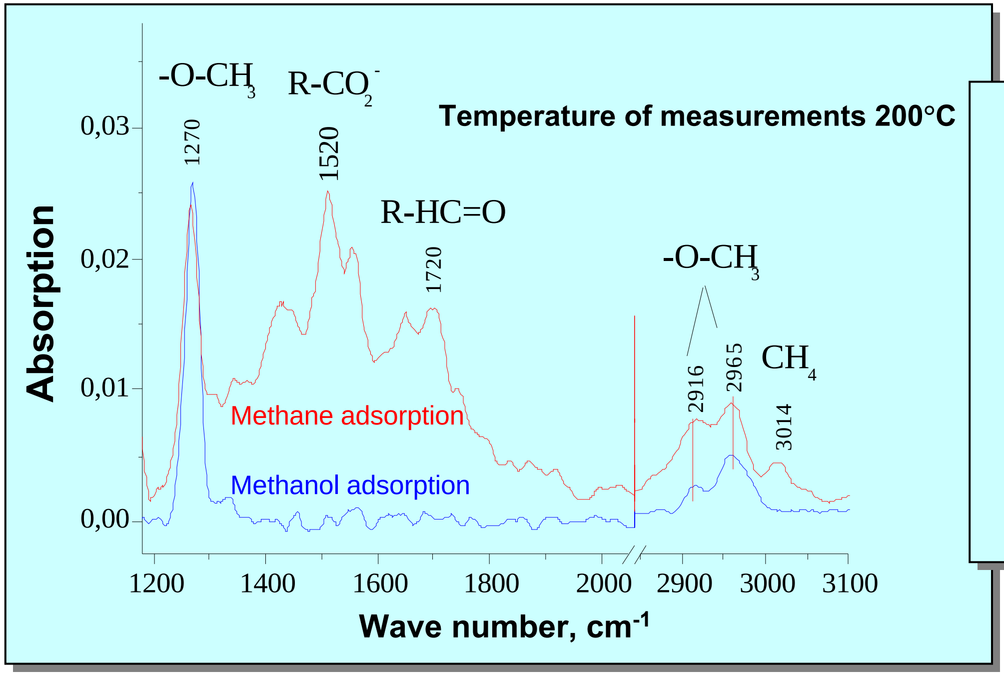
Formation of Pt-Cs particles provides isobutene dimerization with conversion up to 20% and extremely high selectivity to 2,4,4-trimethylpentene >99%

Fig. 31

MECHANISMS OF METHANE ACTIVATION UPON OXYCHLORINATION OVER RUTHENIUM-CONTAINING CATALYSTS

$$CH_4 + HCl + 1/2O_2 \longrightarrow CH_3Cl + H_2O$$

Selectivity to methyl chloride 85-90%



Structure of active center

Cl_n-Ru-O_2-Ru-Cl_n

n=3-4

(XPS data)

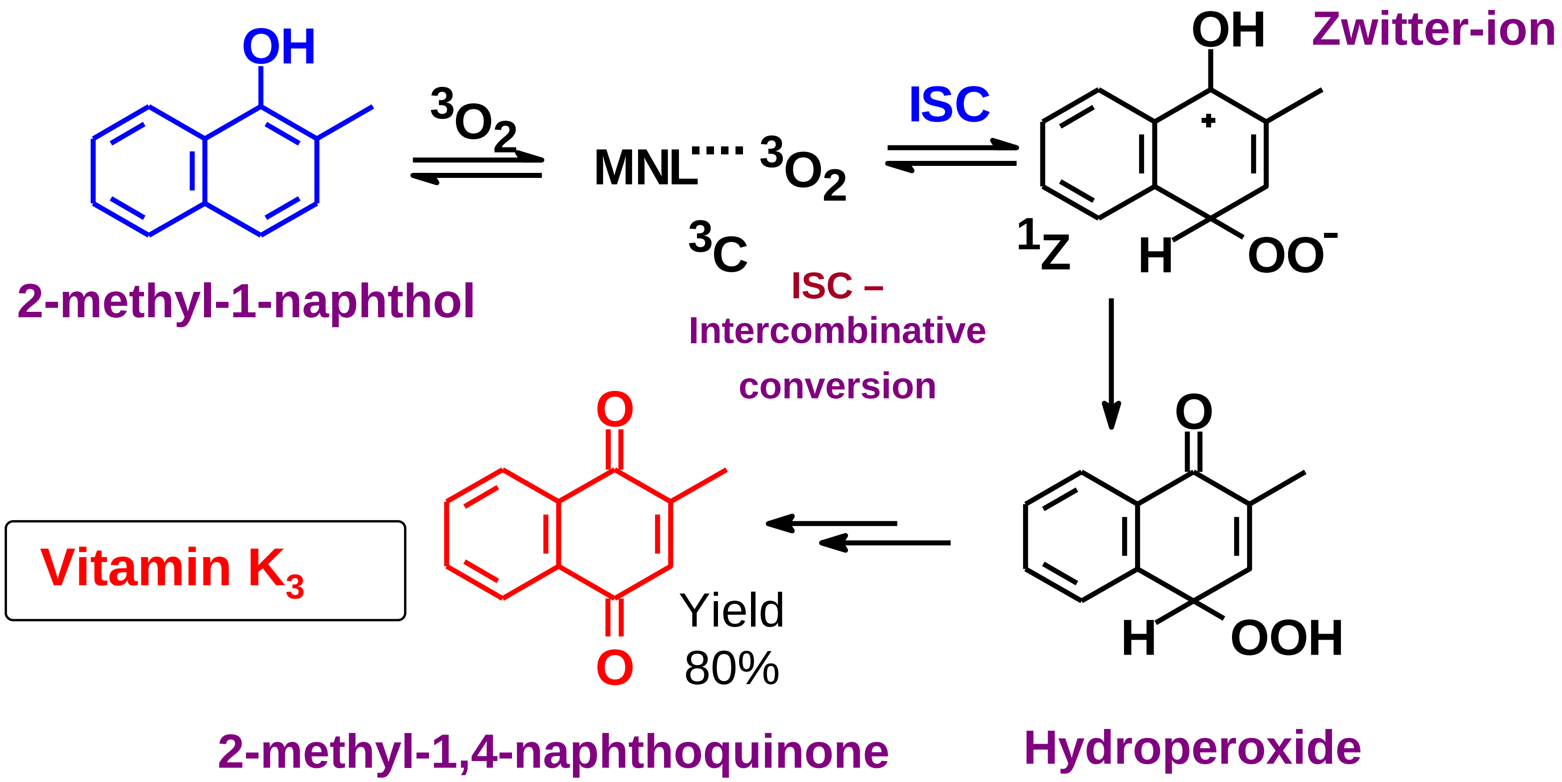
***In-situ* Fourier transform infrared spectroscopy reveals that the first stage of reaction is fromation of methoxy groups on the surface (band at 1270 cm^{-1})**

The following reaction mechanism is proposed:

1. $CH_4 + Ru\text{-}O_2\text{-}Ru \rightarrow Ru\text{-}OCH_3(OH)\text{-}Ru$
2. $Ru\text{-}OCH_3(OH)\text{-}Ru + HCl \rightarrow Ru\text{-}(OH)_2Ru + CH_3Cl$

Fig. 32

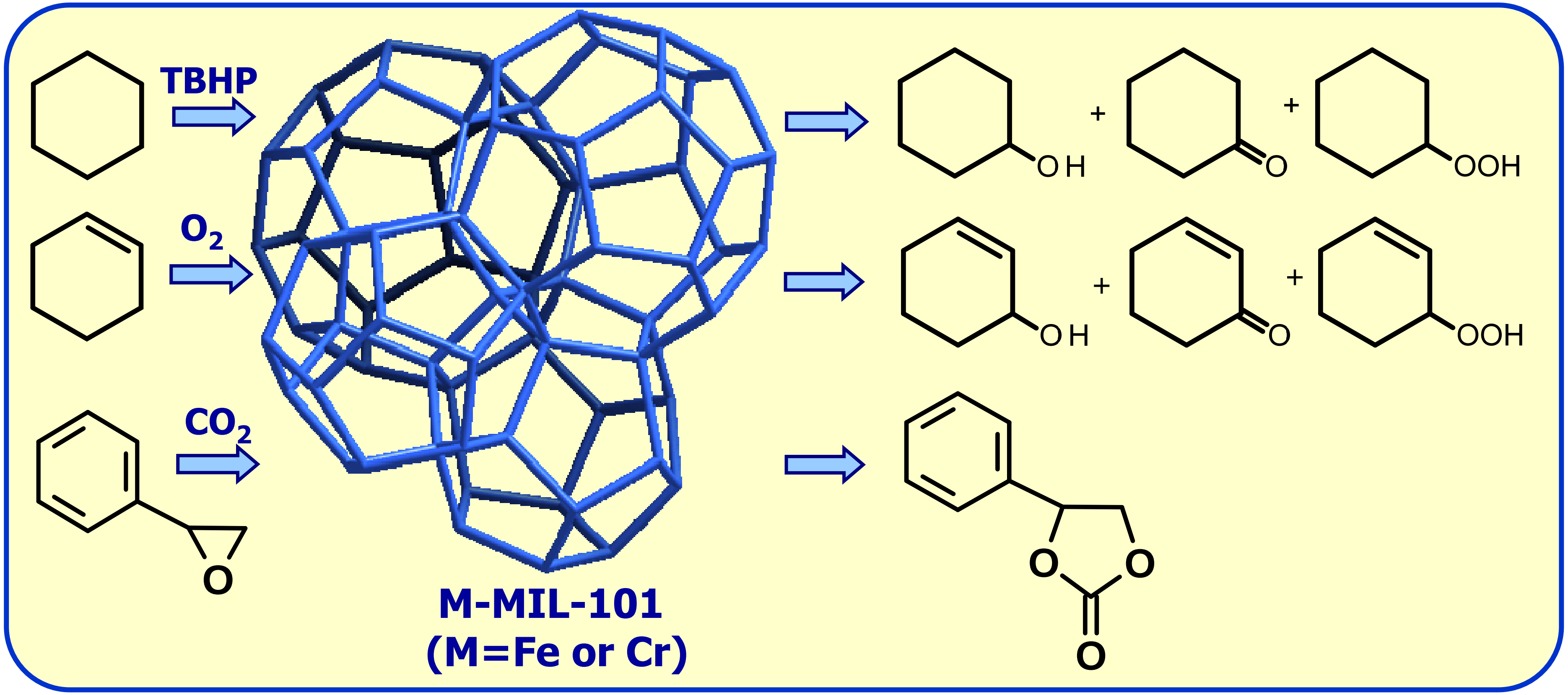
MECHANISM OF SELECTIVE OXIDATION OF 2-METHYL-1-NAPHTHOL WITH MOLECULAR OXYGEN



Oxidation of 2-methyl-1-naphthol to vitamin K_3 with molecular oxygen (3 atm) proceeds via thermal intersystem crossing that involves the spin inversion in the rate-limiting step and the formation of zwitter-ion intermediate

Fig. 33

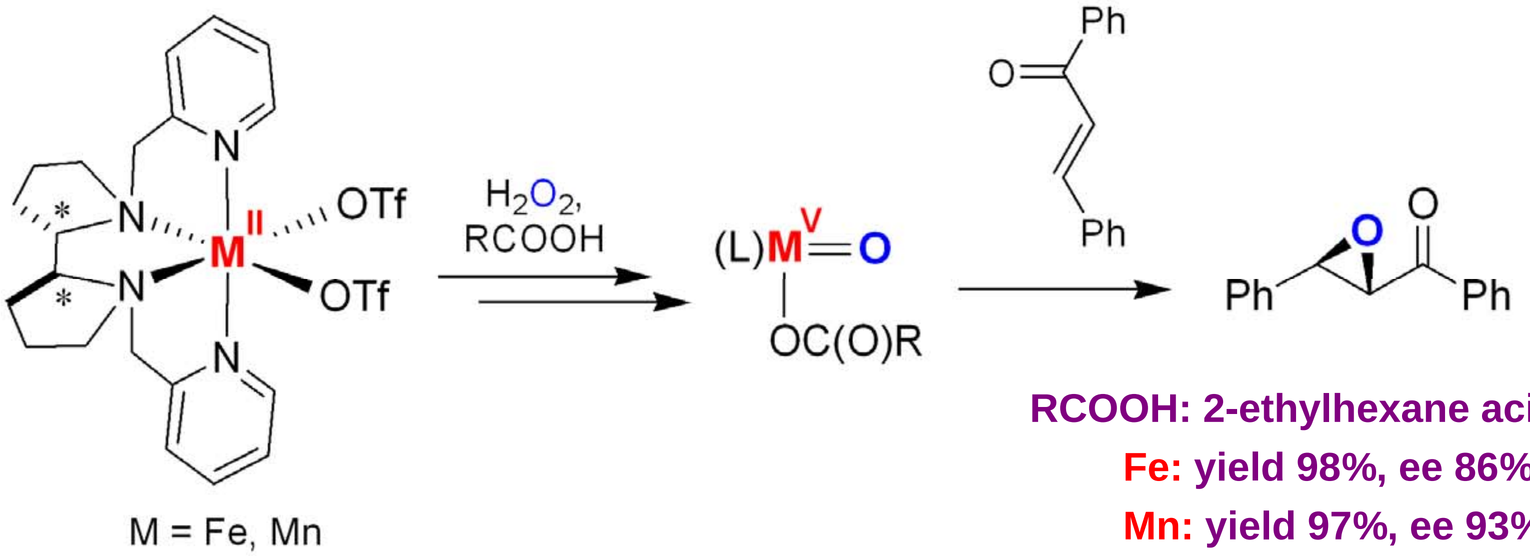
NEW HETEROGENEOUS CATALYSTS MIL-101
FOR LIQUID-PHASE PROCESSES



The mesoporous coordination polymers MIL-101 catalyze the selective oxidation of cyclohexane to cyclohexene as well as carboxylation of styrene in the absence of organic solvent

Fig. 34

NEW CATALYTIC SYSTEMS FOR ASYMMETRIC EPOXIDATION OF OLEFINS WITH HYDROGEN PEROXIDE



RCOOH: 2-ethylhexane acid

Fe: yield 98%, ee 86%

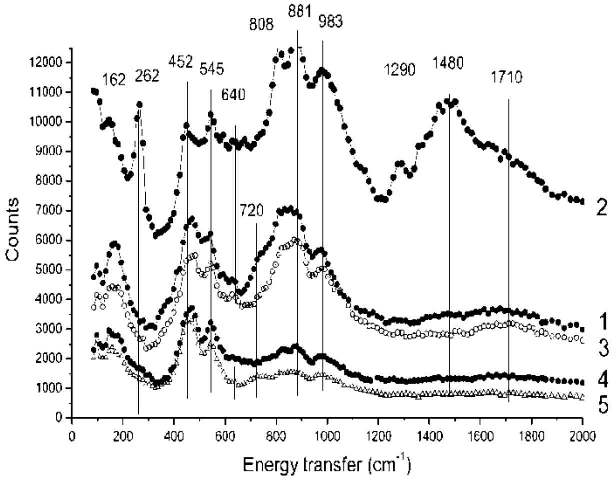
Mn: yield 97%, ee 93%

Chiral non-heme aminopyridine manganese complexes catalyze the enantioselective epoxidation of olefins with peracetic acid or hydrogen peroxide

Fig. 35

STUDY OF CuZn-OXIDE CATALYST ACTIVATION

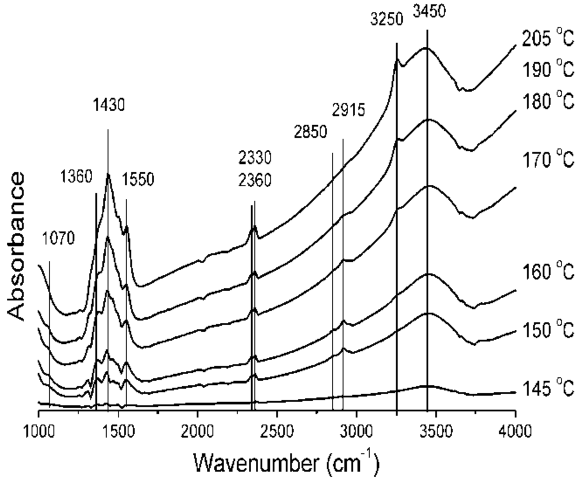
Fig. 1. Experimental INS spectra at 30-40 K



$Cu_{0.08}Zn_{0.92}O$ was treated:

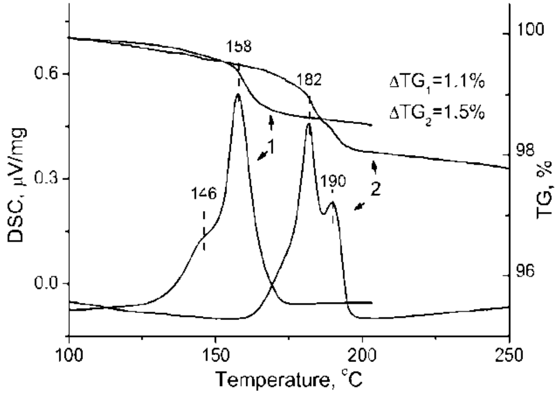
1 –in Ar at 350°C and sealed under Ar;
2 –in Ar at 350°C, in H_2 at 200 °C and sealed under H_2;
3 – in Ar at 350°C, in H_2 at 200°C, in 0.5-1 % O_2;
in Ar at 250°C, sealed under Ar;
4 – in Ar at 350°C, in H_2 at 480 °C and sealed under H_2;
5 – in Ar at 480°C and sealed under Ar

Fig. 2. Differential *in-situ* FTIR spectra of Cu-Zn oxide catalyst at hydrogen pressure 5 torr and gradual heating from 145 to 205 °C



Spectrum of the sample at 145°C in vacuum was used as background

Fig. 3. Thermal curve of reduction of the sample $Cu_{0.08}Zn_{0.92}O$ in hydrogen



Thermal curve of reduction of the sample calcined at 350 °C in inert gas

(1) without exposition on air;
(2) exposed on air during a few days. Heating rate 10 K/min

The studies of reductive activation of CuZn-oxide catalyst using INS (Fig. 1), FTIR/MS (fig. 2), and TG-DSC/MS (Fig. 3) showed that the reduction by hydrogen to form Cu^0 occurs through the reversible interaction with hydrogen, accompanied by proton absorption in the form of OH--groups (ν=3250 cm^{-1} and δ=1430 cm^{-1}) according to the reaction: $Cu^{2+} + 2O_2^- + H_2 \leftrightarrow Cu^0 + 2OH^-$

IMPROVEMENT OF THE PROCESS FOR SYNTHESIS OF MONOMETHYLANILINE

MMA – gasoline dope for increasing octane rating

Problem

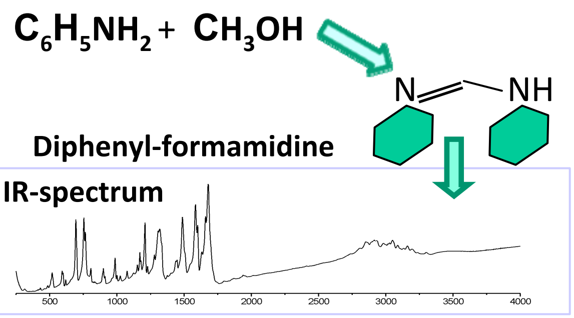
Fast catalyst KA-99 deactivation.
Lifetime - ~ 4 months

The reason for deactivation **-** covering of the catalyst surface by the products of aniline interaction with side products of methanol activation

Problem solving **–** developing a catalyst based on Cu-containing compounds and process conditions to avoid the formation of side products of methanol activation

Studies

The mechanism of side products formation was elucidated:


$C_6H_5NH_2 + CH_3OH$

Diphenyl-formamidine

IR-spectrum

Catalyst ICA-33-3:

- Highly selective for MMA,

Provides

- Grows capacity by 30%
- Methanol saving by 10%
- Prolongs service cycle by 4 times

Results

The technology for the catalyst ICA-33-3 production is adopted at the APC&OS

The produced pilot catalyst batch (1.5 t) is tested, the expected catalyst lifetime is ca. 1 year

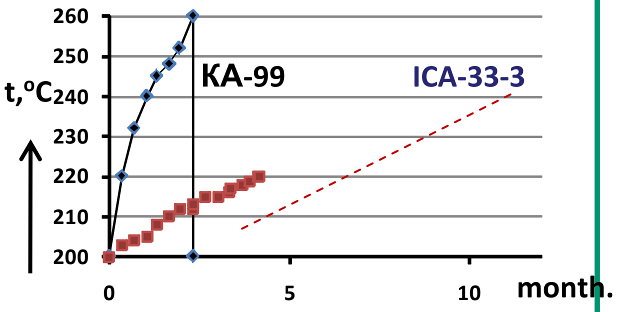
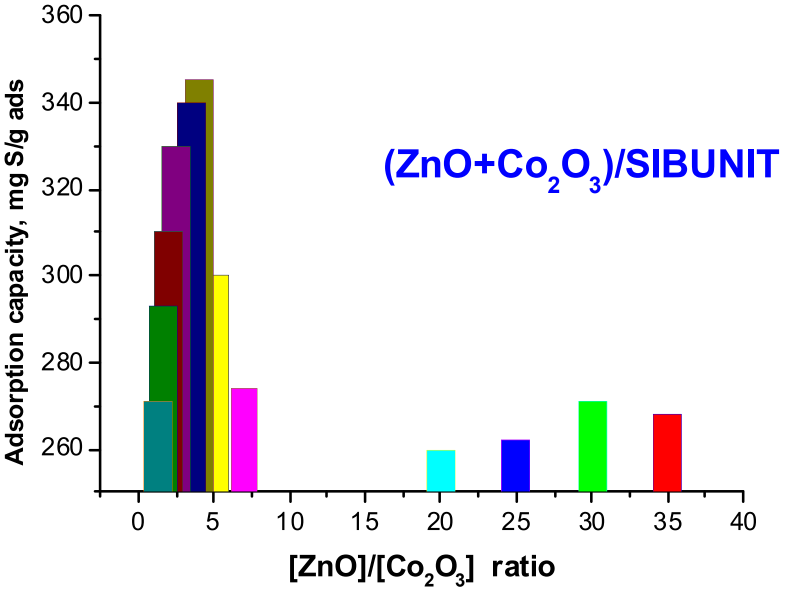


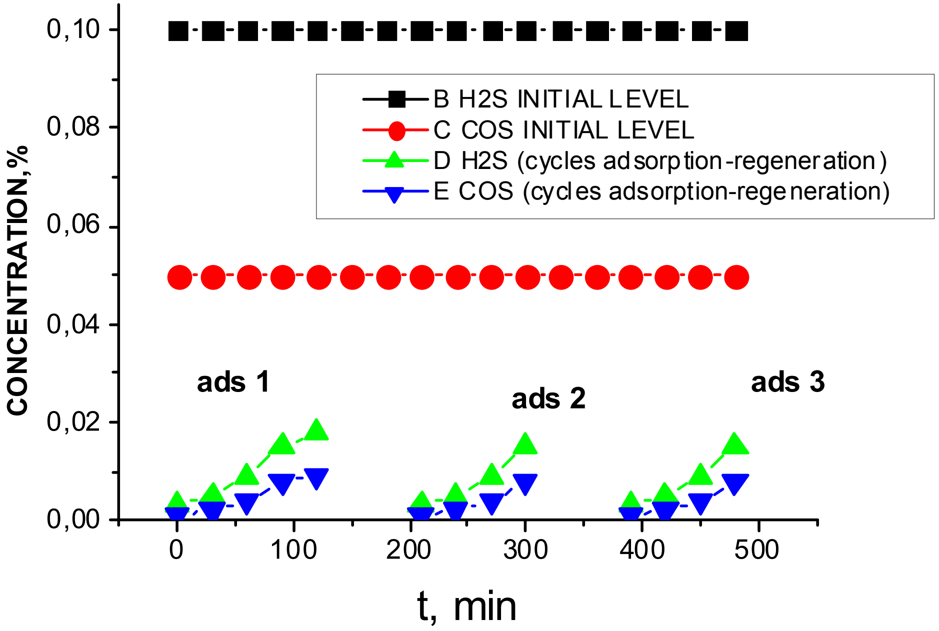
Fig. 37

A REGENERABLE SULFUR SORBENT FOR FUEL GASES

ADSORPTION CAPACITY



ZnO+Co$_2$O$_3$/SIBUNIT



0.1 % H_2S + 0.05% COS, other – N_2
adsorption - 25°C, regeneration- 220°C

Fig. 38

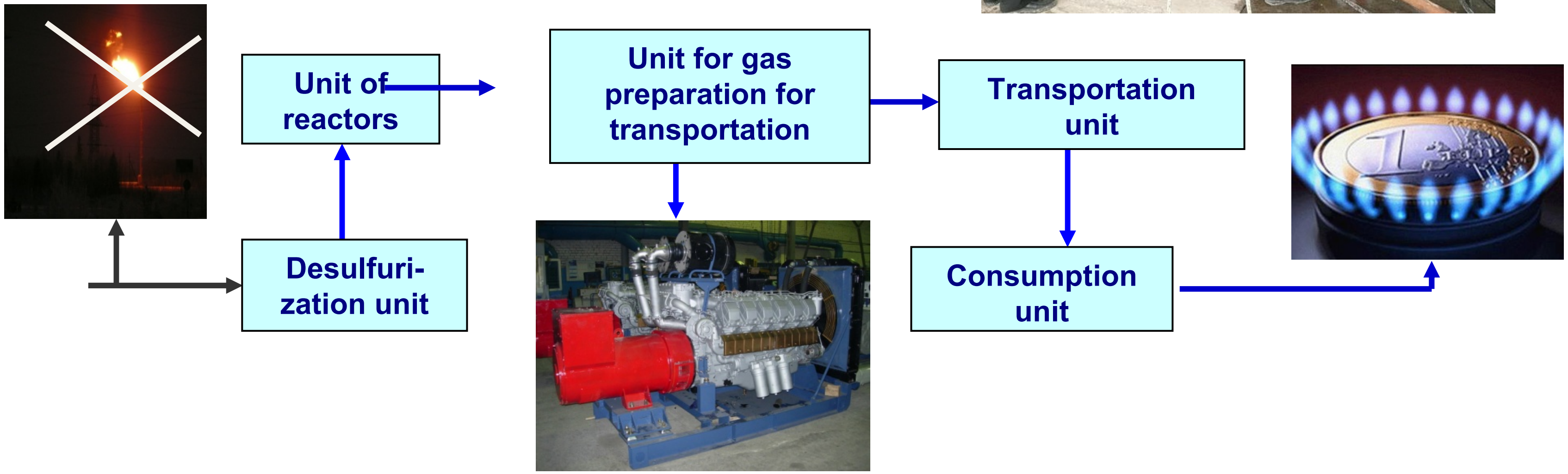
TECHNOLOGY FOR ON-SITE UTILIZATION OF OIL ASSOCIATED GASES

The technology is based on low-temperature catalytic conversion of fatty components of AWG into methane and synthesis gas at petroleum production places

Results of field-tests:

- conversion as high as 98 %
- steady operation of power plants
- 25 % increase in the quantity of generated electric power at meeting the EURO-4 standards

Field-tests in Khanty-Mansi Autonomous Okrug - Yugra



Unit of reactors

Desulfuri-zation unit

Unit for gas preparation for transportation

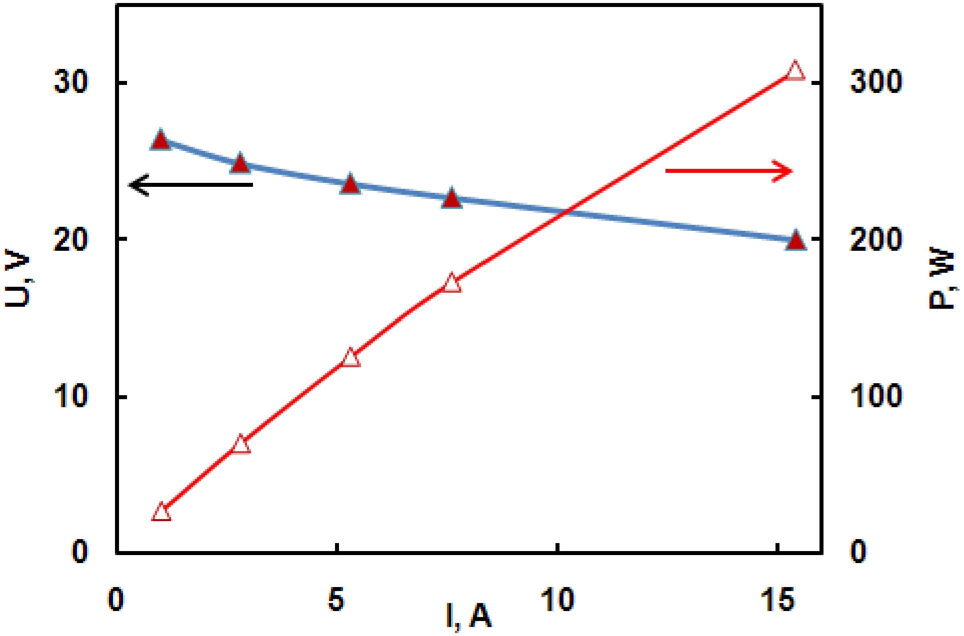
Transportation unit

Consumption unit

Fig. 39

POWER PLANT BASED ON A HT PEM FC

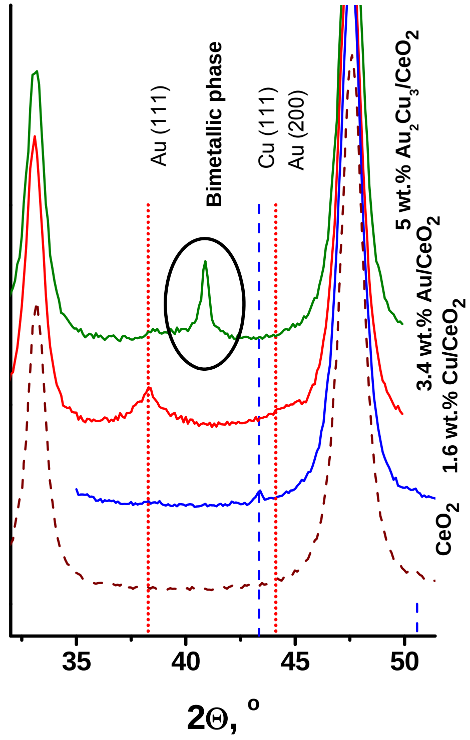
Primary fuel	- methanol, DME
Working temperature	- 170°C
Alternating voltage	- 220 V
Capacity	- 300 W

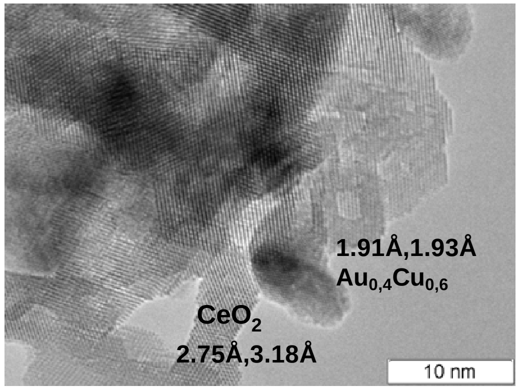


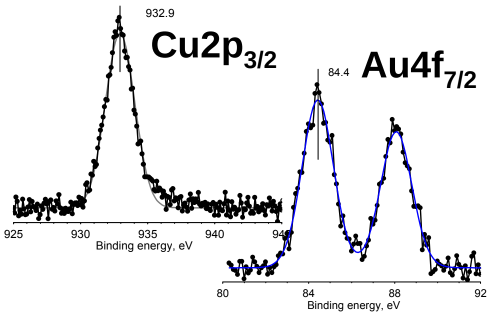
Dependencies of battery voltage and capacity on current

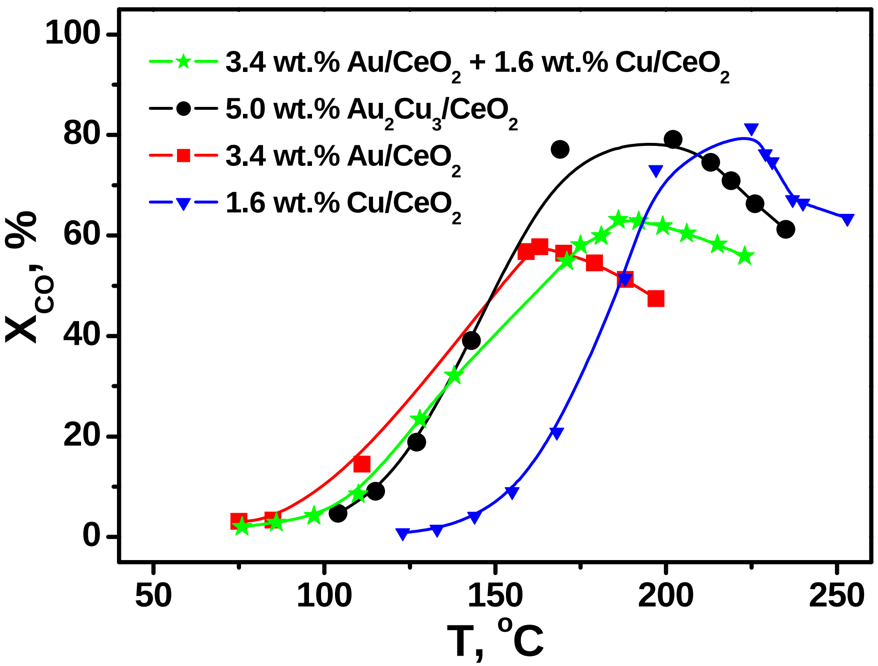
Fig. 40

BIMETAL Au-Cu CATALYSTS FOR SELECTIVE CO OXIDATION









Composition of mixture (vol.%): 1 CO, 0.6 O_2, 10 H_2O, 20 CO_2, 65 H_2 and He - balance; P = 1.4 atm; WHSV=270000 $cm^3g^{-1}h^{-1}$

According to X-Ray, TEM and XPS, the use of $[Au(En)_2]_2[Cu(Ox)_2]_3$ salt as a precursor results in the formation of highly dispersed bimetal Au-Cu nanoparticles on the support surface

Au_2Cu_3/CeO_2 catalyst possesses higher activity and selectivity as compared with monometal analogues

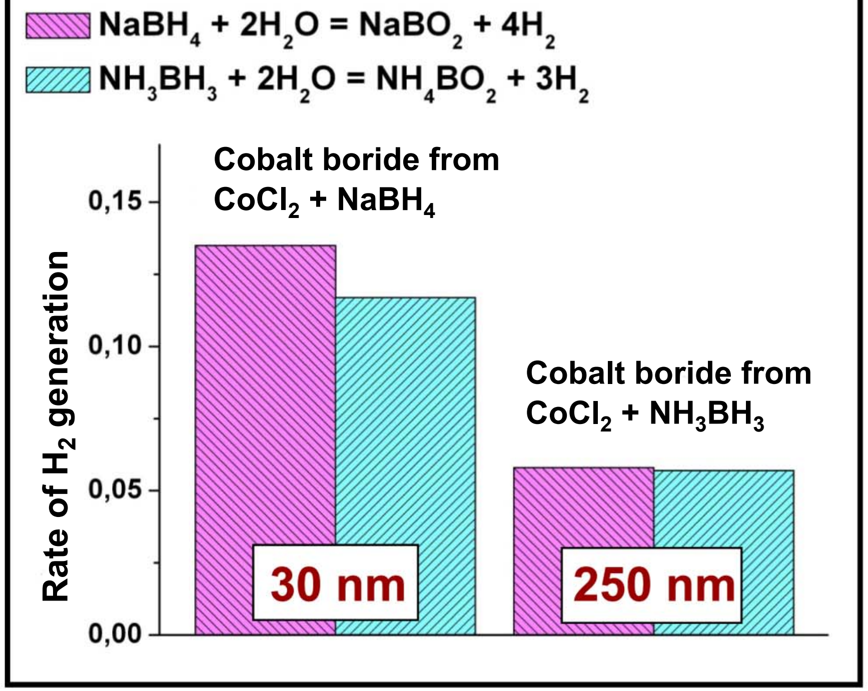
Fig. 41

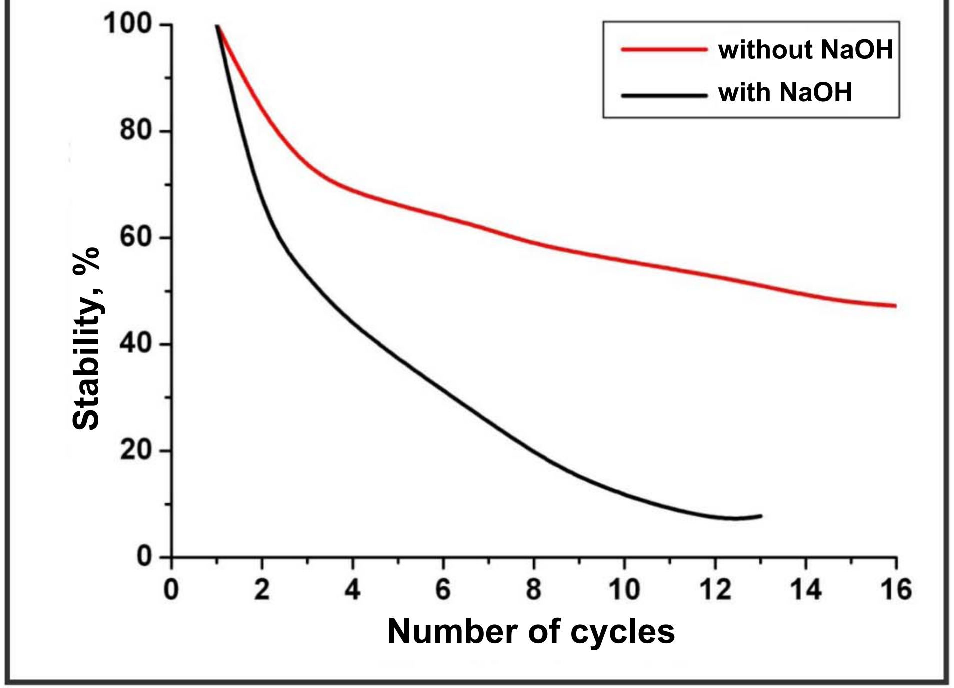
COBALT BORIDE CATALYSTS FOR $NaBH_4$ AND NH_3BH_3 HYDROLYSIS

$$NaBH_4 + 2H_2O \xrightarrow{Co_xB} NaBO_2 + 4H_2\uparrow$$

$$NH_3BH_3 + 2H_2O \xrightarrow{Co_xB} NH_4BO_2 + 3H_2\uparrow$$

$$\begin{matrix} CoCl_2 \\ Co_3O_4 \end{matrix} \xrightarrow[NH_3BH_3]{NaBH_4} Co_xB$$

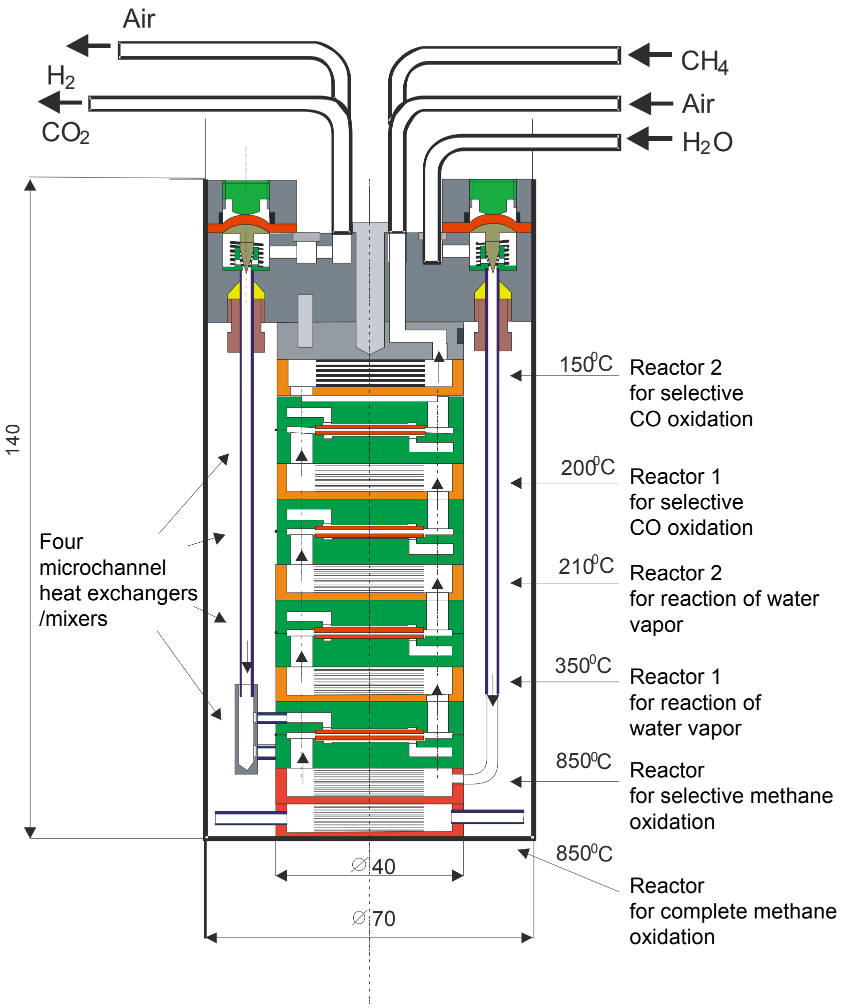


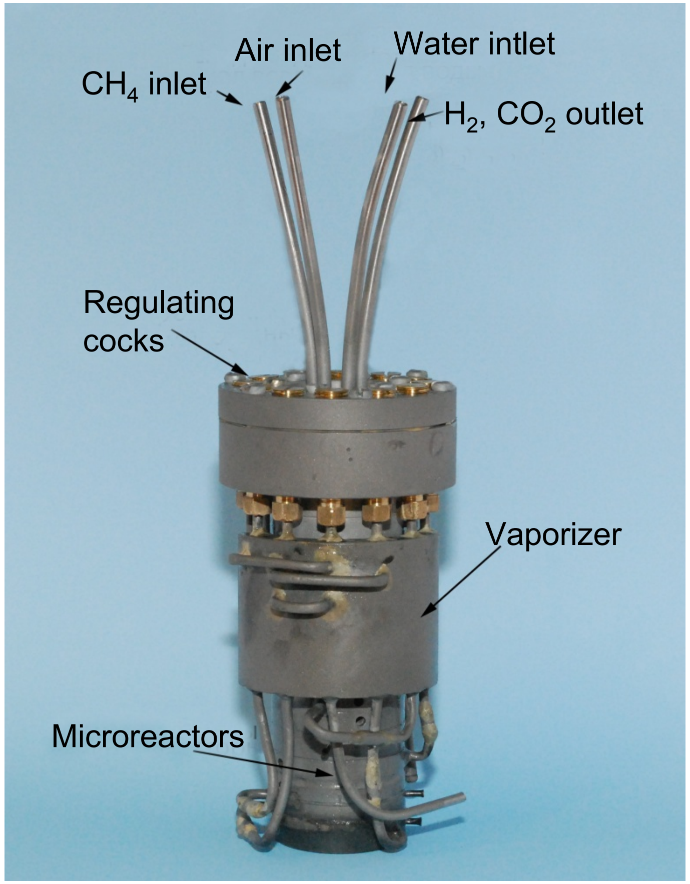


- Composition of hydride reaction media (**$NaBH_4$, NH_3BH_3**) affects the formation of catalyst active phase ***in situ***
- A negative effect of NaOH addition on the stability of **Co_xB catalysts**, formed *in situ* in **$NaBH_4$ media**, is revealed

Fig. 42

FUEL PROCESSOR BASED ON MICROCHANNEL REACTORS



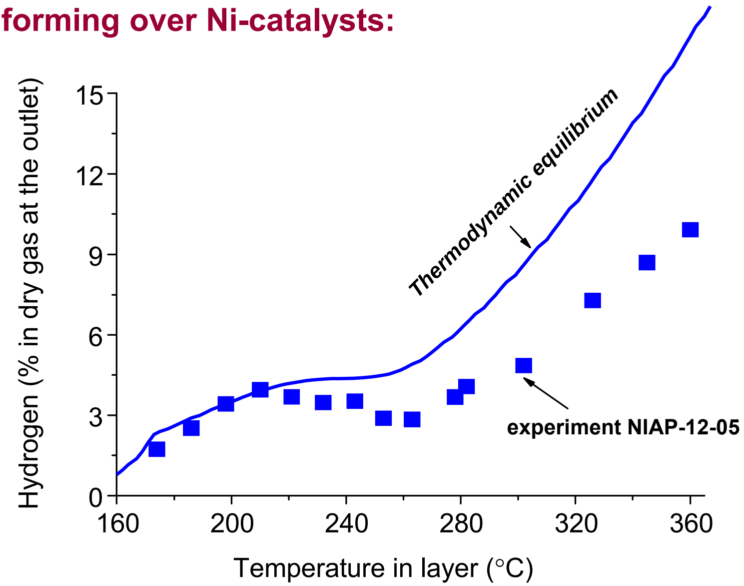


Heat capacity – 300 W

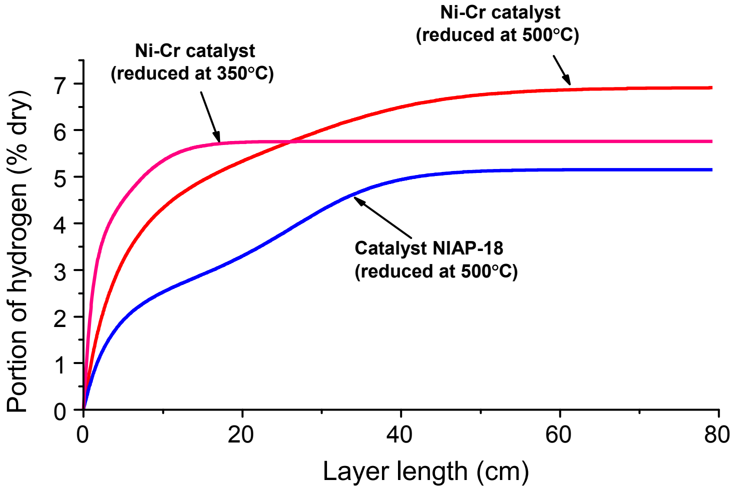
Fig. 43

MATHEMATICAL MODEL AND COMPUTER PROGRAM FOR CALCULATING PROCESSES IN A REACTOR FOR CATALYTIC STEAM REFORMING

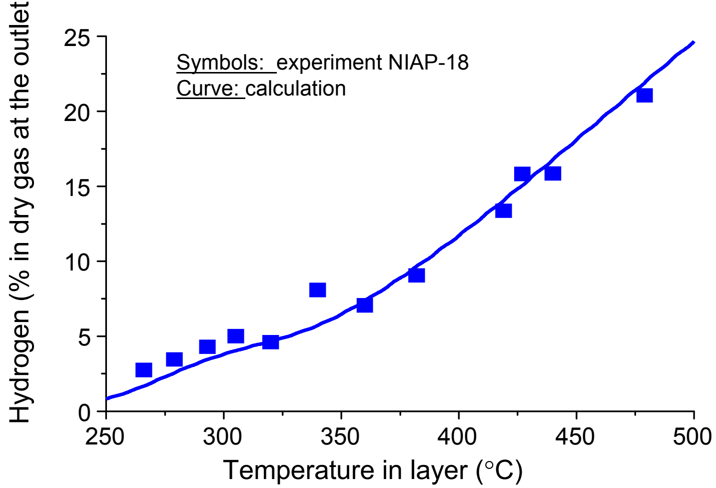
Example of thermodynamically non-equilibrium propane reforming over Ni-catalysts:



Calculating of adiabatic APG reformer:



Comparison of experimental and design data for steam propane reorming:



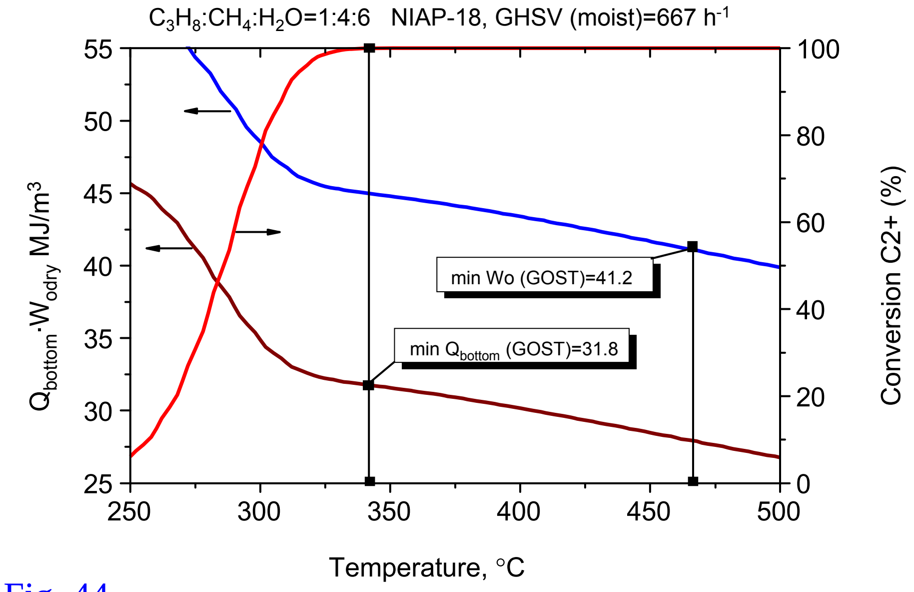
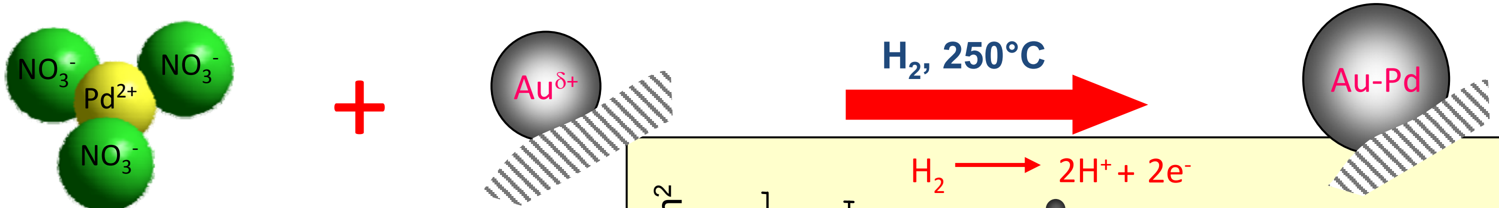
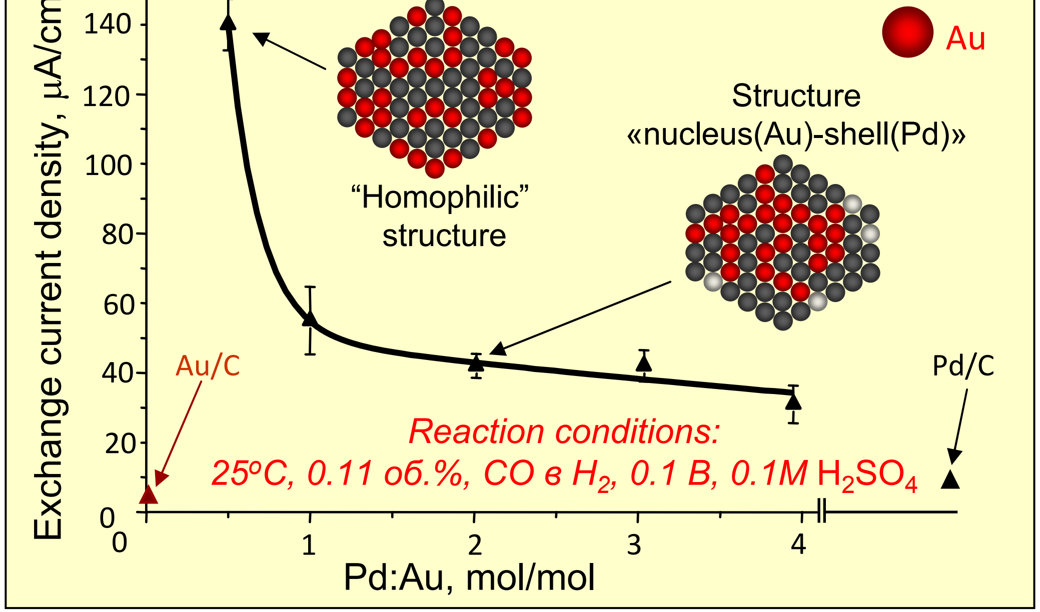


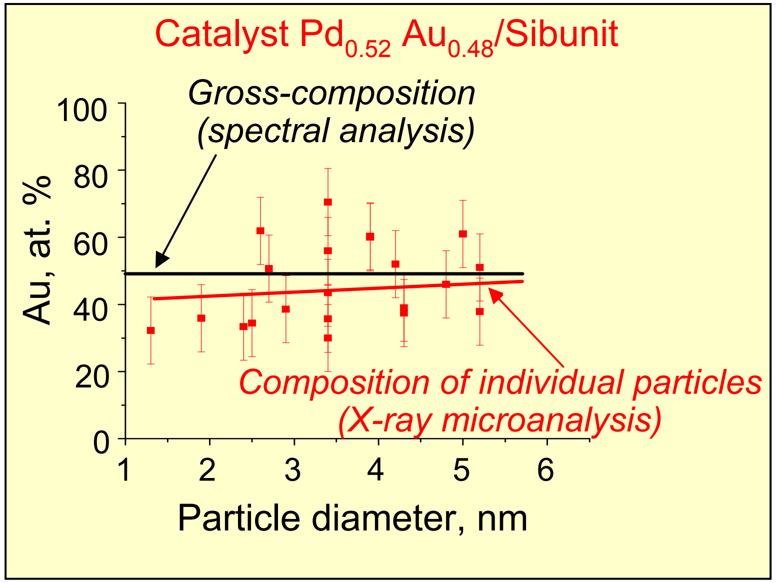
Fig. 44

NANODISPERSE Pd-Au ALLOYS ON SIBUNIT AS NEW CO-TOLERANT CATALYSTS FOR ANODES OF FUEL CELLS



The developed synthesis method allows obtaining carbon-supported catalysts that contain up to 20 wt % of metal (Pd/Au = 0.5÷3.9 *mol/mol*) in the form of alloyed Pd_xAu_{1-x} particles with the size not more than 6 nm and chemical composition close to the desired





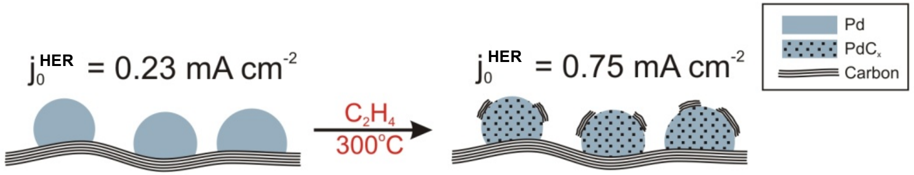
Alloyed catalysts PdAu/Sibunit are prospective for application in fuel cells fueled by hydrogen with CO impurities. A very high activity of these catalysts to anodic H_2 oxidation is accounted for by reduction of the adsorption energy of H and CO on Pd atoms due to the electron effect of Au atoms

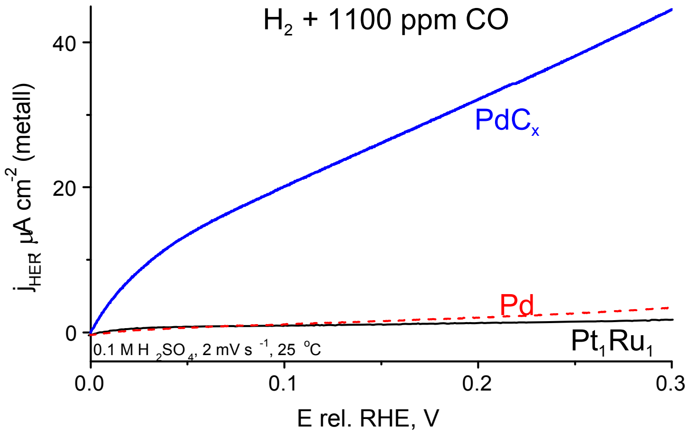
Fig. 45

DEVELOPMENT OF METHODS FOR SYNTHESIS OF MEMBRANE ELECTRODE ASSEMBLIES INCLUDING NEW ELECTROCATALYSTS

Electrochemical study of promising electrocatalysts

The promoting effect of carbon incorporated into palladium crystal lattice on the catalytic activity of metal in the hydrogen electrode reaction and on stability to contamination with CO is shown for the first time

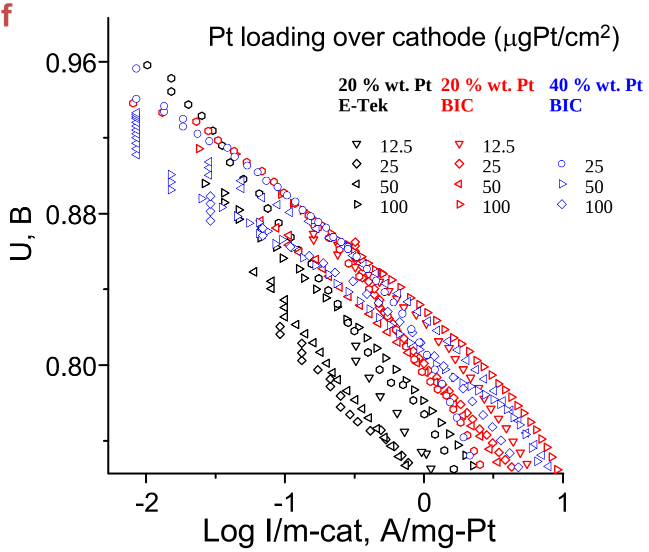


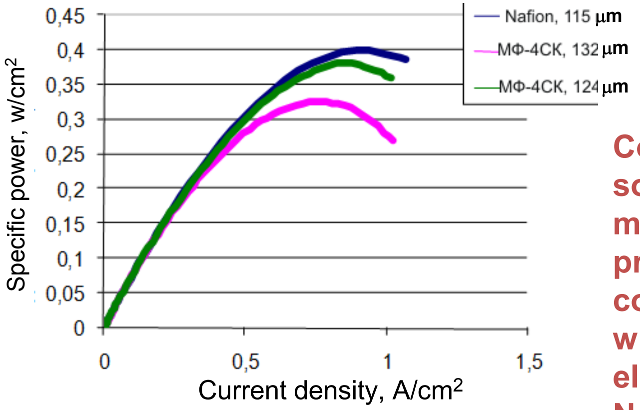


Curves of electrooxidation of hydrogen with CO admixture (1200 ppm), measured by method of rotating disk electrode for catalysts Pd/C, PdC_x/C and Pt_1Ru_1/C

Studying the efficiency of components in the solid polymer fuel cell

Catalytic activity of Sibunit supported catalysts is found to be some times superior to that of the commercial BASF catalyst in the region of working currents. Catalyst are efficient even at ultralow loadings <50 mkg/cm²





Conductivity of solid polymer membranes, prepared in BIC, compare well with the electrolyte Nafion ®

Fig. 46

PHOTOCATALYTIC HYDROGEN PRODUCTION FROM WATER

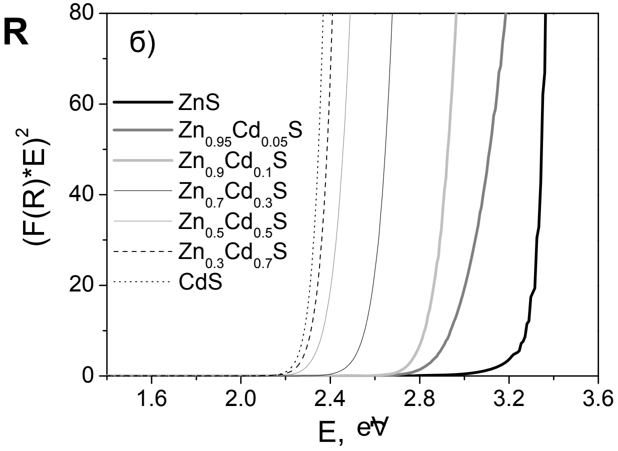
Synthesis, characterization and activity of photocatalysts $Cd_{1-x}Zn_xS$

$CdCl_2 + 2NaOH = Cd(OH)_2 + 2NaCl,$ (I)

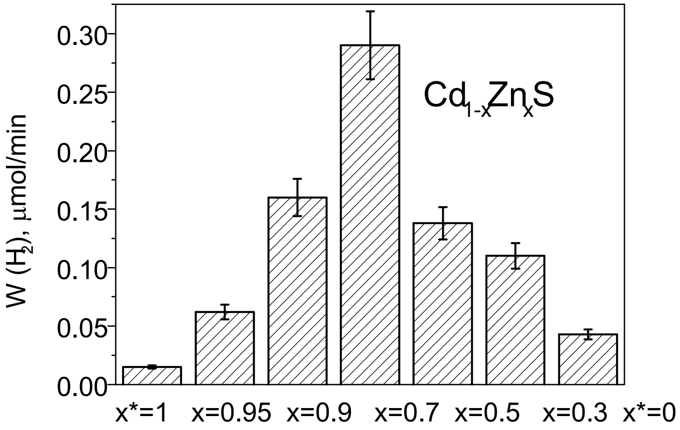
$ZnCl_2 + 2NaOH = Zn(OH)_2 + 2NaCl,$ (II)

$(1-x)Cd(OH)_2 + xZn(OH)_2 + Na_2S = Cd_{1-x}Zn_xS + 2NaOH$ (II)

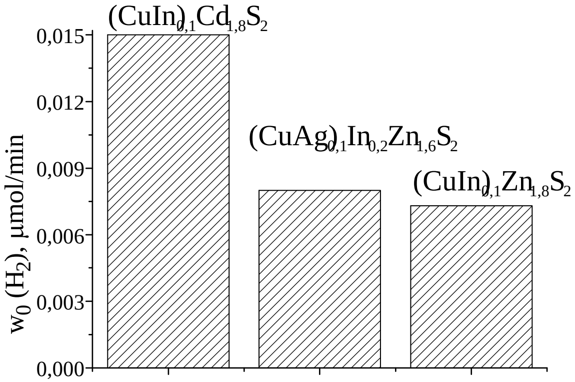
ESDR



Initial rates of photocatalytic hydrogen production from aqueous Na_2S/Na_2SO_3 solutions



Synthesis, characterization and activity of photocatalysts of complex composition



Dependence of initial rate of photocatalytic hydrogen production on initial concentration of NaOH under visible light over $Cd_{0.2}Zn_{0.8}S$

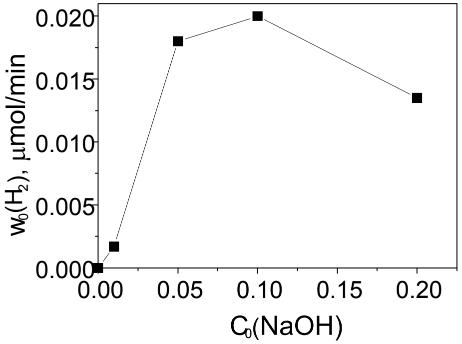
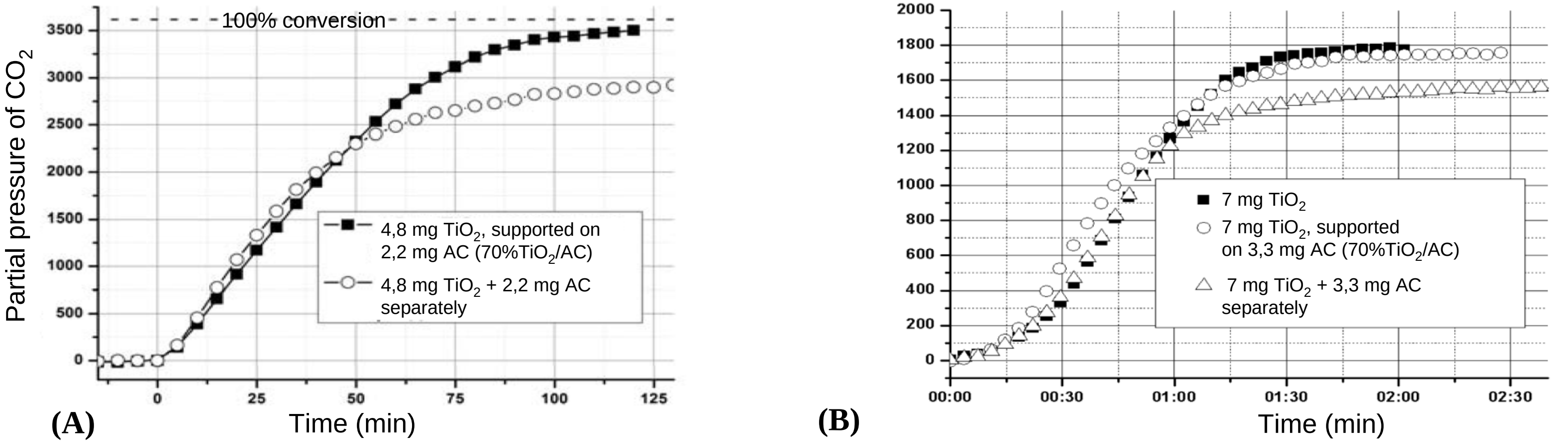


Fig. 47

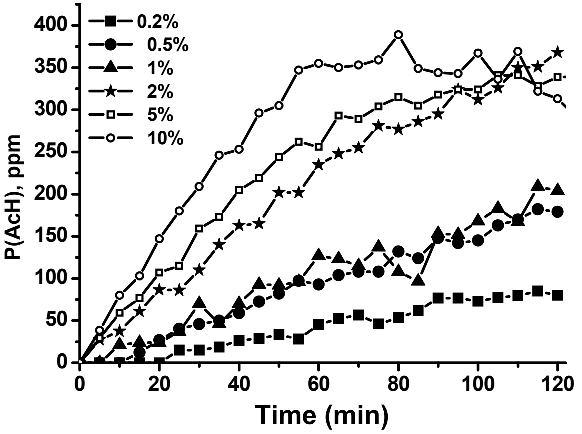
PHOTOCATALYTIC OXIDATION

Synthesis of nanostructured oxidative photocatalysts $TiO_2/SiO_2/C$ of mixed type with extended adsorption constant of oxidizable substrate

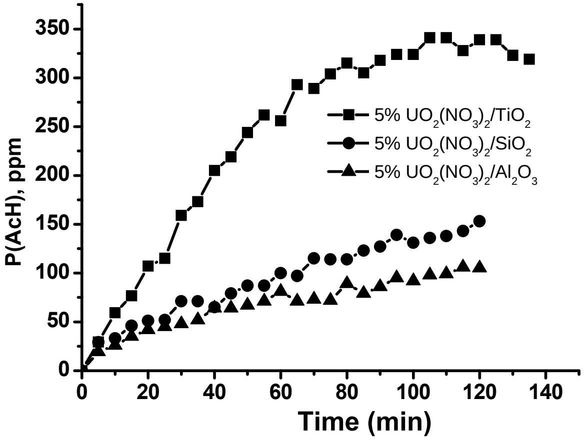


Comparison of kinetics of CO_2 conservation in the course of photocatalytic oxidation of cyclohexane (A) and ethanol (B) vapors oxidation in static reactors over 70%-TiO_2/AC sample and separate use of TiO_2 and AC

Synthesis and investigation of oxidative photocatalysts based on UO_2 and cadmium sulfide with extended spectral characteristics



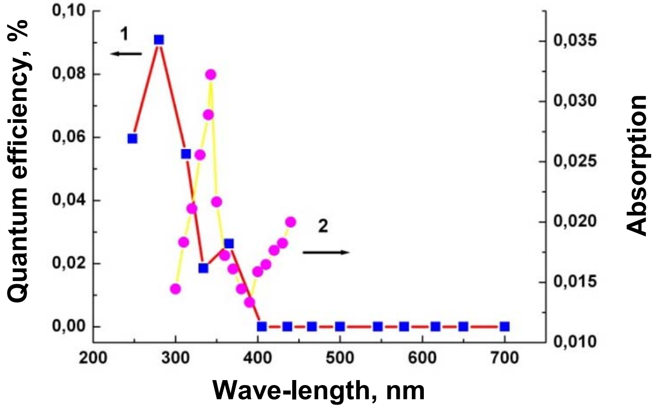
Kinetic curves of acetaldehyde production from ethanol over catalysts $UO_2(NO_3)_2/TiO_2$ in static reactor under visible light



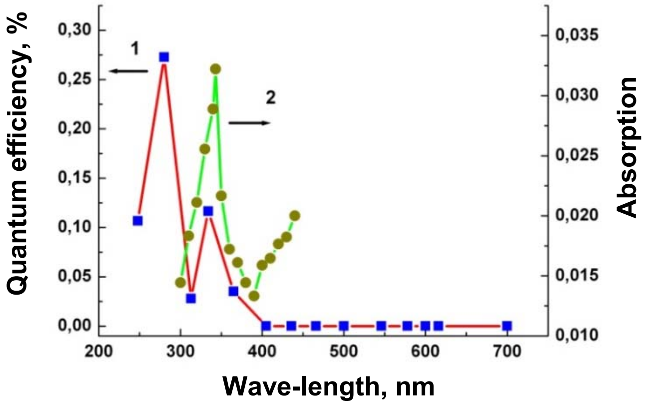
Kinetic curves of acetaldehyde production from ethanol over catalysts $UO_2(NO_3)_2/TiO_2$ (■), $UO_2(NO_3)_2/SiO_2$ (●) and $UO_2(NO_3)_2/Al_2O_3$ (▲) in static reactor under visible light

Fig. 48

Photostimulated reactions on the surface of natural materials



Quantum efficiency and spectral dependence of quantum efficiency of carbon dioxide photodesorption from $Mg(OH)_2$



Quantum efficiency and spectral dependence of quantum efficiency of carbon dioxide photodesorption after dark Freon 22 adsorption

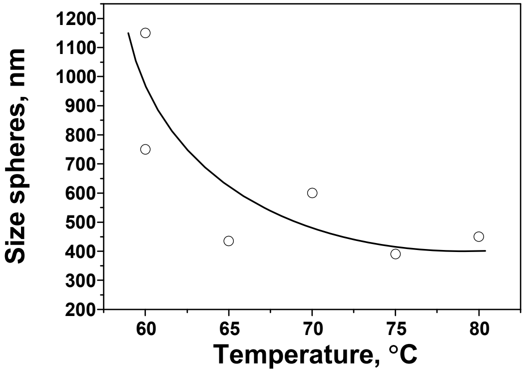
PLASMOCATALYTIC AIR TREATMENT

Acetone oxidation in corona discharge over two types of photocatalysts

Photocatalyst/exposure		Characteristic rate of acetone concentration decrease, ppm/min	Characteristic rate of CO_2 generation, ppm/min	Characteristic rate of CO generation, ppm/min
Pt/TiO_2	u/v	0.032	0.08	0
	u/v + discharge	0.204	0.3	0.11
	discharge	0.176	0.23	0.16
TiO_2 Hombifine	u/v	0.027	0.12	0.02
	u/v + discharge	0.163	0.42	0.08
	discharge	0.157	0.26	0.11

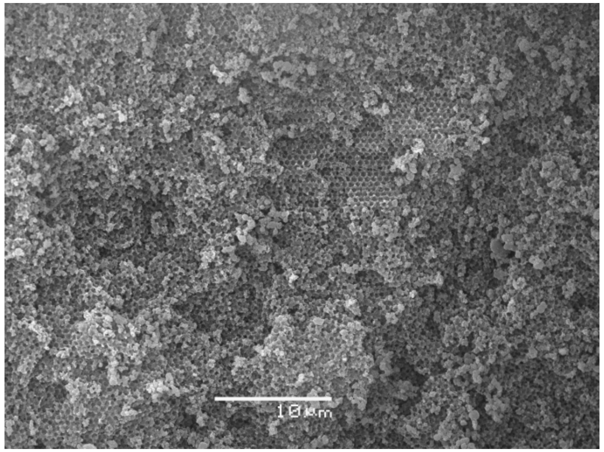
Fig. 49

SYNTHESIS OF ZEOLITE CATALYSTS AND PHOTOCATALYSTS WITH 3D MACROPOROUS STRUCTURE AND STUDY OF PHYSICO-CHEMICAL PROPERTIES



Dependence of polystyrene template spheres size on the temperature of emulsion styrene polymerization

SEM of amorphous SiO_2 samples, synthesized in the presence PS template



Textural properties of synthesized macroporous samples according to data of low temperature nitrogen adsorption

Sample	Macroporosity	Composition	Specific surface area by BET method, m^2/g	Total pore volume, cm^3/g	Outside surface, m^2/g	Part of micropores in volume extent, %
A	SiO_2	no	2.37	0.007	4.00	0
B	ZSM-5	no	416.7	0.224	26.8	80
C	ZSM-5	yes	214.7	0.436	190.5	0.1
D	FeZSM-5	yes	436.2	0.683	441.9	0
E	ZiO_2	yes	16.68	0.060	18.4	0
F	Al_2O_3	yes	131.6	0.306	136.1	0
G	$A1_2O_3$	yes	143.6	0.426	153.3	0
H	$A1_2CO_3$	no	138.5	0.361	152.1	0

Fig. 50

PROPANE AND ETHANE PYROLYSIS UNDER INFRARED LASER BEAM

Radicals generation

$C_2H_6 \rightarrow 2\ CH_3\bullet$

$C_2H_4 \rightarrow \bullet C_2H_4\bullet$

$\bullet C_2H_4\bullet + C_2H_6 \rightarrow C_3H_7\bullet + CH_3\bullet$

Chain propagation

$CH_3\bullet + C_2H_6 \rightarrow C_2H_5\bullet + CH_4$

$C_2H_5\bullet \rightarrow C_2H_4 + H\bullet$

$C_2H_6 + H\bullet \rightarrow H_2 + C_2H_5\bullet$

$C_3H_7\bullet \rightarrow CH_3\bullet + C_2H_4$

Death of radicals

$2\ C_2H_5\bullet \rightarrow C_2H_4 + C_2H_6$

Quantum-chemical calculations of reaction of ethylene biradical. Gaussian 09

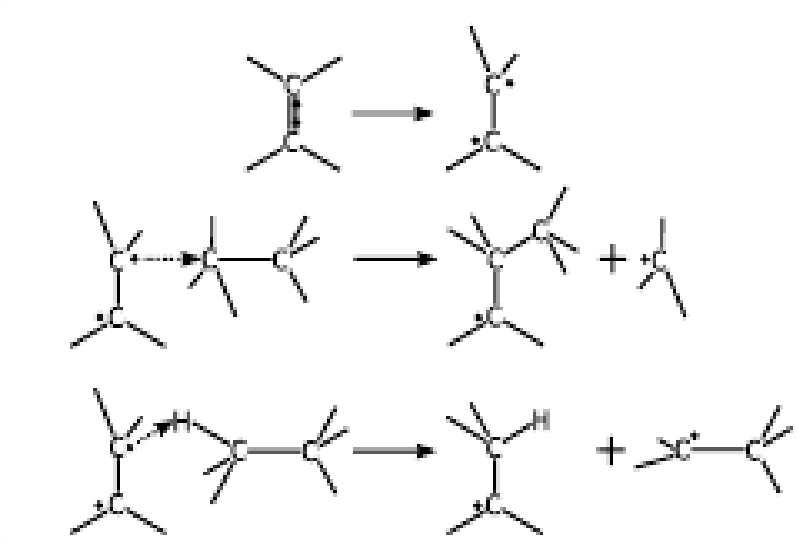
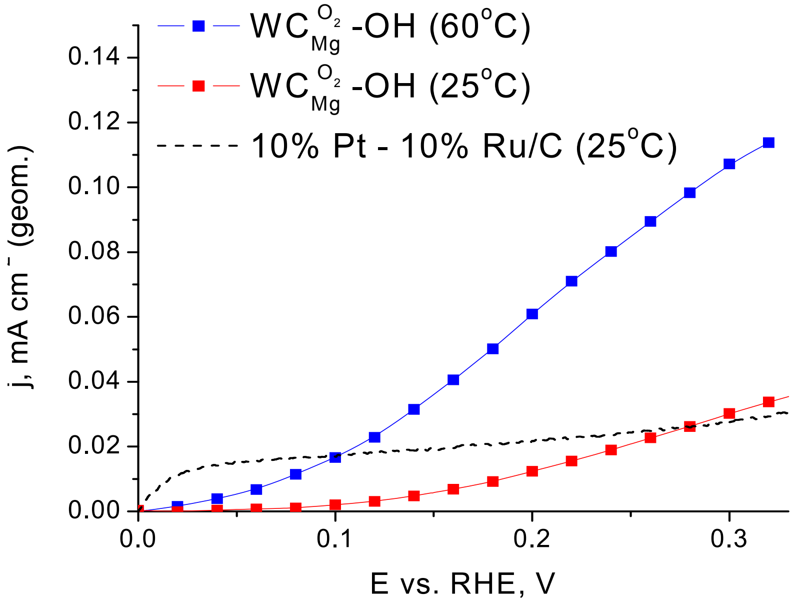


Fig. 51

MCA SYNTHESIS OF CARBIDE MATERIALS

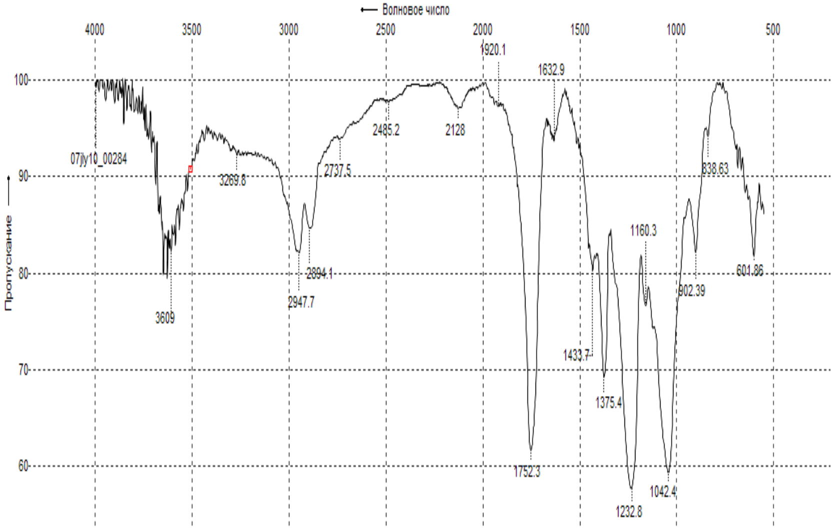


Potentiostatic oxidation of H_2 over modified samples WC_{Mg} (at 25°C) and $WC_{Mg}O^{2-}OH$ at 25 and 60°C in H_2-saturated 0.1M H_2SO_4. Potentiodynamic H_2 oxidation (dash curve) over the catalyst 20%Pt1Ru1/C, poisoned with CO at 25°C at 5 mV/s intervals

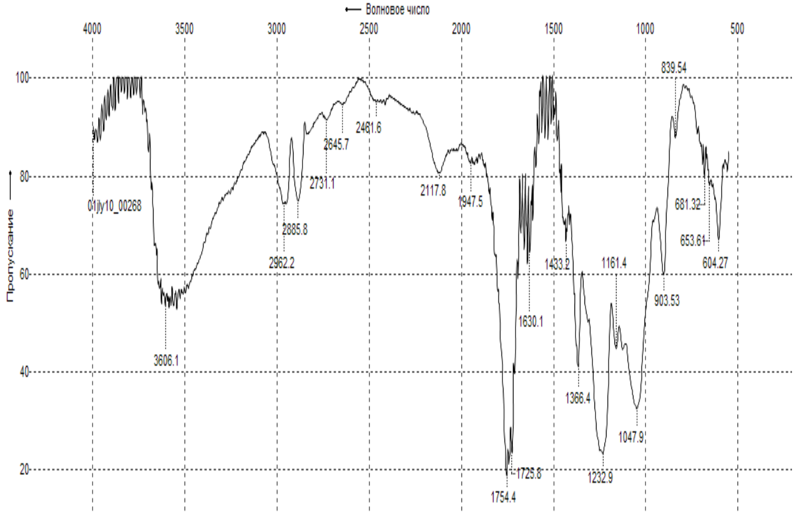
A method was developed for modification of nanodisperse tungsten monocarbide WC obtained using mechanochemical activation. The catalytic activities of WC and Pt-containing (after CO inhibition) catalyst to electrochemical hydrogen oxidation at 25°C are shown to be comparable

Fig. 52

MCA SYNTHESIS OF CARBIDE MATERIALS



IR spectra (KBr) of standard sample of TAC

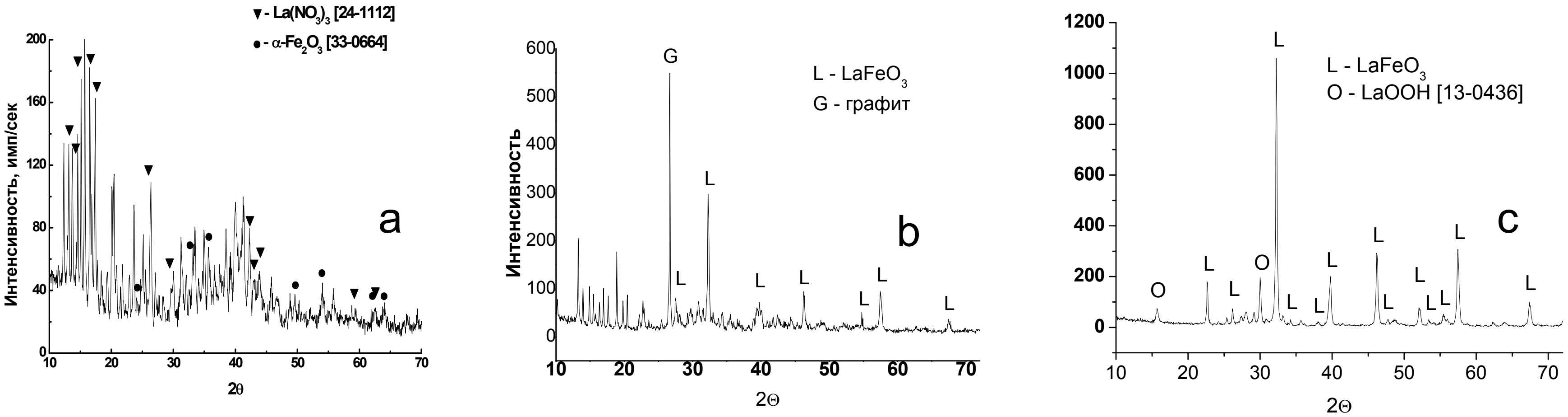


IR spectra (KBr) of TAC sample obtained using mechanochemical activation

A method was developed for accelerated preparation of cellulose triacetate using mechanochemical activation

Fig. 53

SYNTHESIS OF COMPLEX OXIDES USING MECHANOCHEMICAL AND MICROWAVE PRETREATMENTS OF THE PRECURSORS

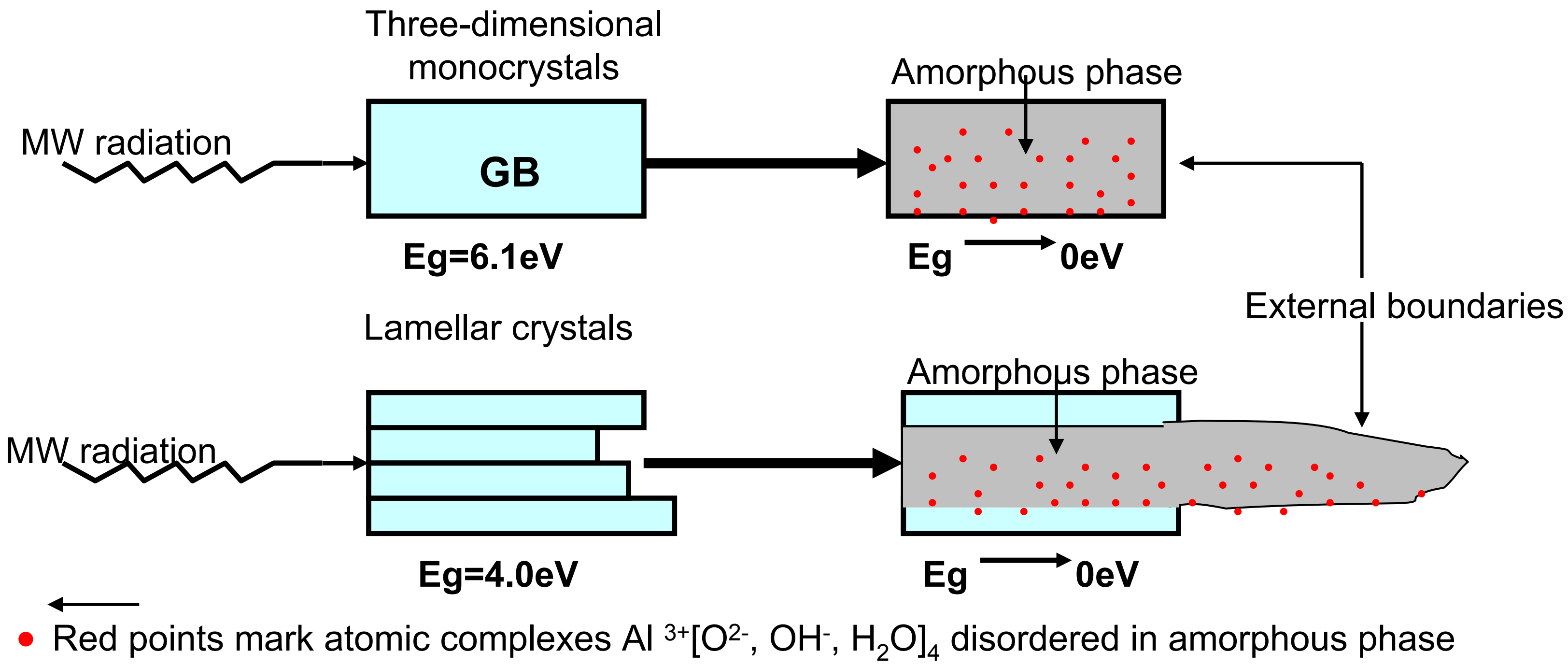


The influence of graphite (b) introduction followed by calcination at 600°C (c) on the lanthanum ferrite synthesis using MW treatment of crystal hydrates of initial salts (a)

A possibility of improving the yield of La(Co,Fe)O_3 perovskite at synthesis under microwave (MW) radiation of the precursors by adding carbon (to increase the radiation absorption) and citric acid (to increase the solution viscosity) was revealed. Monophase perovskites $LaMeO_3$ (Me=Fe, Co) with a large specific surface area (>10 m^2/g) and catalytic activity to methane oxidation and N_2O decomposition were prepared after calcinations of MW treated precursors

Fig. 54

SYNTHESIS OF SINGLE OXIDES USING MC AND MW PRETREATMENT OF CRYSTALLINE HYDROXIDES



● Red points mark atomic complexes Al $^{3+}[O^{2-}, OH^{-}, H_2O]_4$ disordered in amorphous phase

The MW treatment of coarse gibbsite crystals was shown to result in the formation of an X-ray amorphous product with four coordinated Al^{+3} cations (NMR), and characterized (ESDR) by nearly zero energy-gap width (Eg)

Fig. 55

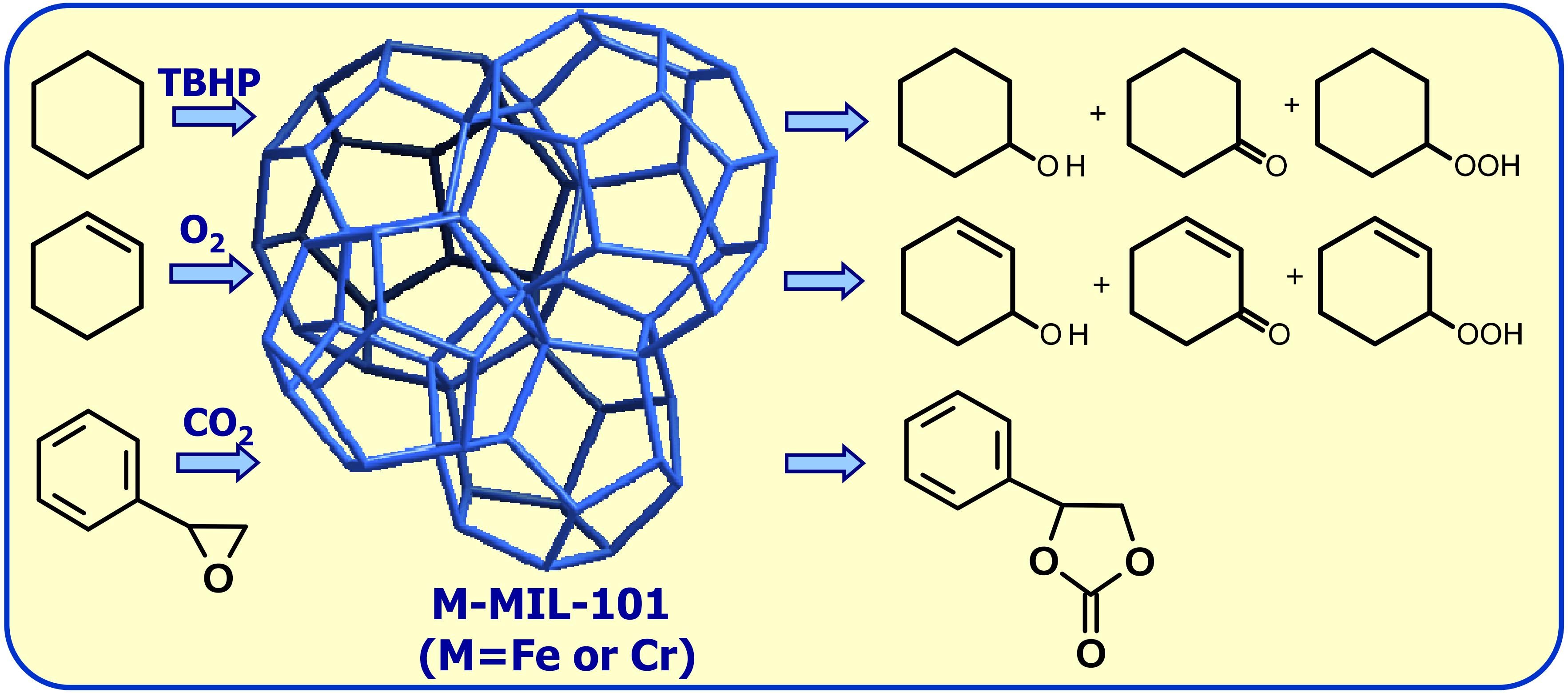
Zn-MOF BASED CATALYSTS FOR SELECTIVE OXIDATION

№	**MOF**	**Pore size, Å**	**Thioester**	**$[S]/[Zn]/[H_2O_2]$**	**Solvent**	**Conversion, %**	**Selectivity, %**
1	$[Zn_2(bdc)(S\text{-lac})]$	5 × 5	PhSMe	3:1:9	CH_3CN	92	100
2	$[Zn_2(bdc)(S\text{-lac})]$	5 × 5	PhSMe	10:1:15	CH_3CN	94	98
3	$[Zn_2(bdc)(S\text{-lac})]$	5 × 5	$PhSCH_2Ph$	1:1:4	CH_2Cl_2	3	100
4	$[Zn_2(ndc)(R\text{-man})]$	6 × 10	2-naphSMe	12.5:1:25	CH_3CN	78	99
5	$[Zn_2(ndc)(R\text{-man})]$	6 × 10	$PhSCH_2Ph$	12.5:1:25	CH_3CN	70	99
6	$[Zn_2(bpdc)(R\text{-man})]$	4 × 14	2-naphSMe	12.5:1:25	CH_3CN	57	98
7	$[Zn_2(bpdc)(R\text{-man})]$	4 × 14	$PhSCH_2Ph$	12.5:1:25	CH_3CN	78	98

Isoreticular coordinated frameworks based on Zn complexes catalyze the oxidation of thioesters to sulfoxides with hydrogen peroxide at a high chemo- and size-selectivity

Fig. 56

NEW HETEROGENEOUS CATALYSTS MIL-101 FOR LIQUID-PHASE PROCESSES



The mesoporous coordinated frameworks MIL-101 catalyze selective oxidation of cyclohexene and cyclohexane, as well as carboxylation of epoxides in the absence of organic solvent

Fig. 57

NEW MODIFICATIONS OF SUPPORTED CATALYSTS FOR GAS-PHASE SYNTHESIS OF POLYETHYLENE

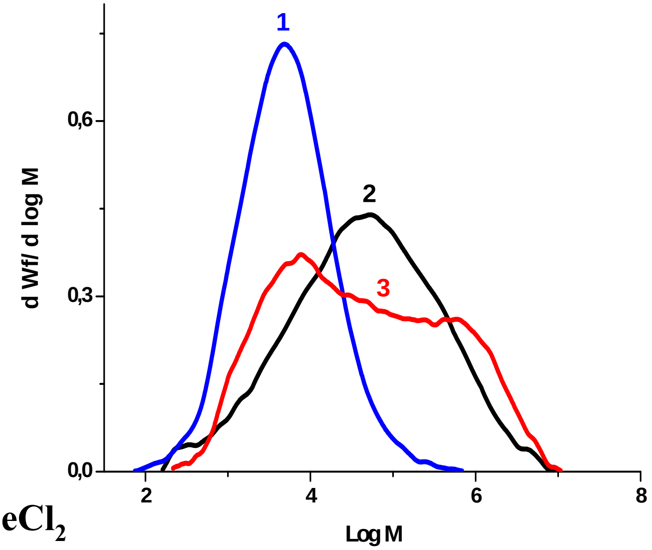
New modifications of supported catalysts were developed for production of various polyolefins, in particular, high-molecular co-polymers of ethylene with α-olefins, polypropylene with broadened molecular weight distribution (MWD), and polyethylene with bimodal MWD, synthesized by gas-phase method by one-reactor scheme

Curves of polymer MWD

1 - SiO_2/ 2,6-Cl_2LFeCl_2

2 - SiO_2/CrO_x

3 - SiO_2/CrO_x/ 2,6-Cl_2LFeCl_2

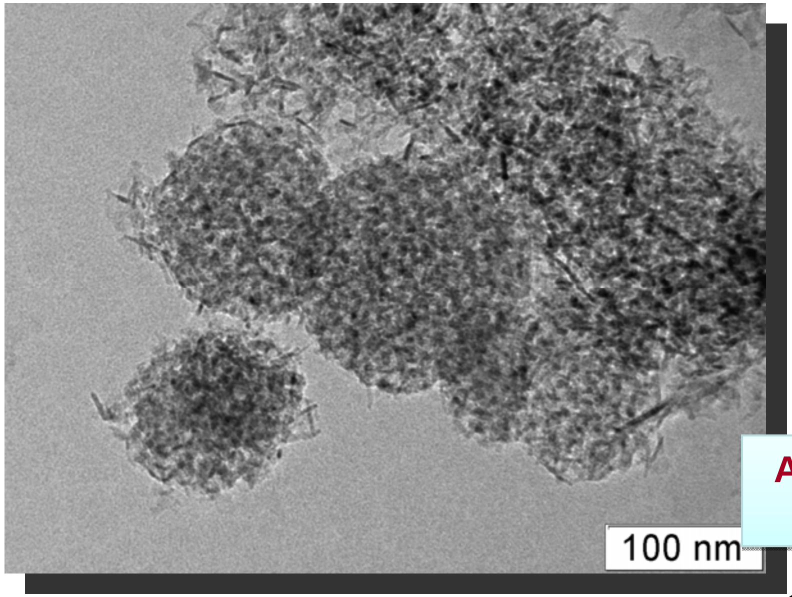


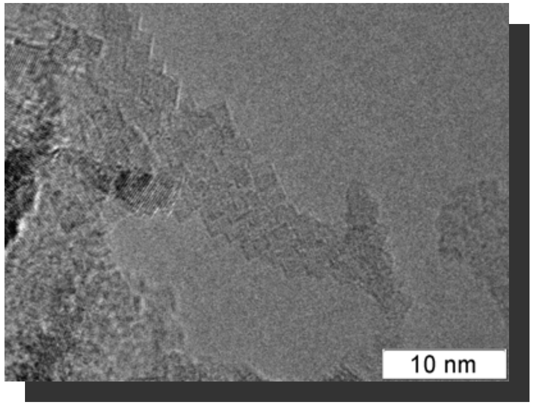
Commercial chromium oxide catalysts (monomodal MWD, high molecular weight, curve (2) was modified by introducing bis(imino)pyridyl complex of Fe(II) (a catalyst for synthesis of low molecular weight PE, curve (1)

The resulting bicomponent catalyst Cr/Fe/SiO_2 produces PE with a bimodal molecular weight distribution, curve (3)

Fig. 58

SUPPORTING NANOSTRUCTURED ACTIVE LAYER VO_x· MgO ON POROUS MINERAL SUPPORTS



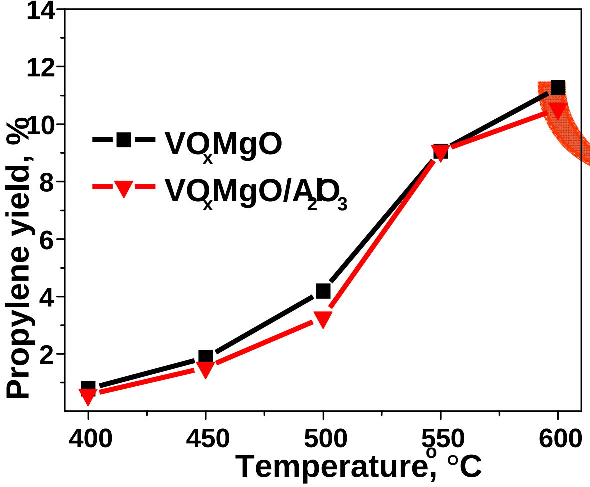


Samples :

- ❑ γ-Al_2O_3
- ❑ La_2O_3-Al_2O_3
- ❑ SiO_2

A method was developed for supporting of VO_xMgO aerogel cover on the surface of microspheric Al_2O_3 particles

The pattern of vanadium distribution and catalytic activity of immobilized aerogel samples in reaction of ODP do not change



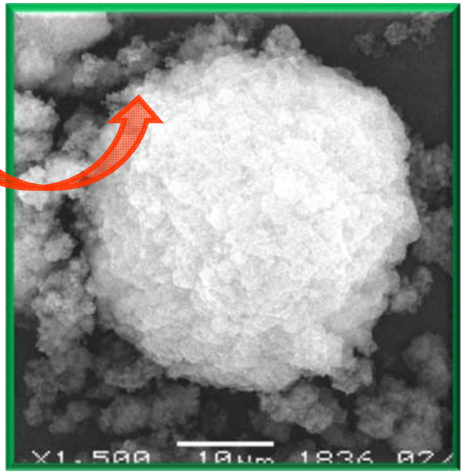
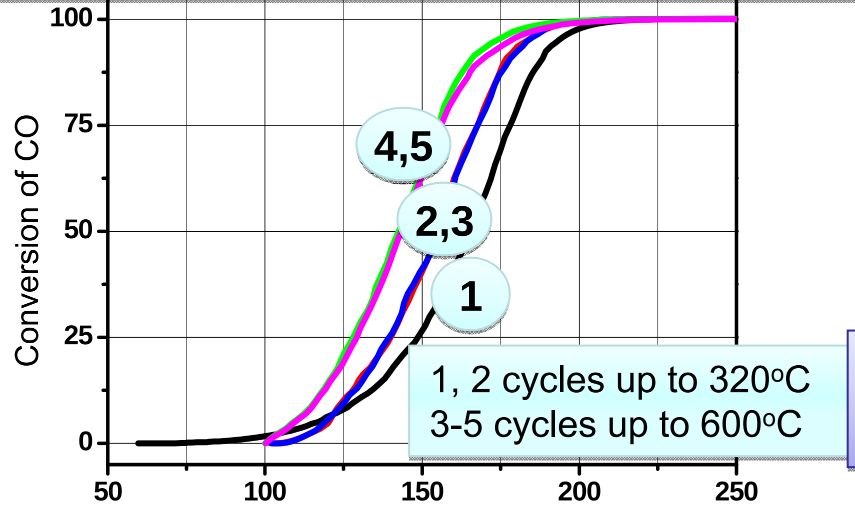


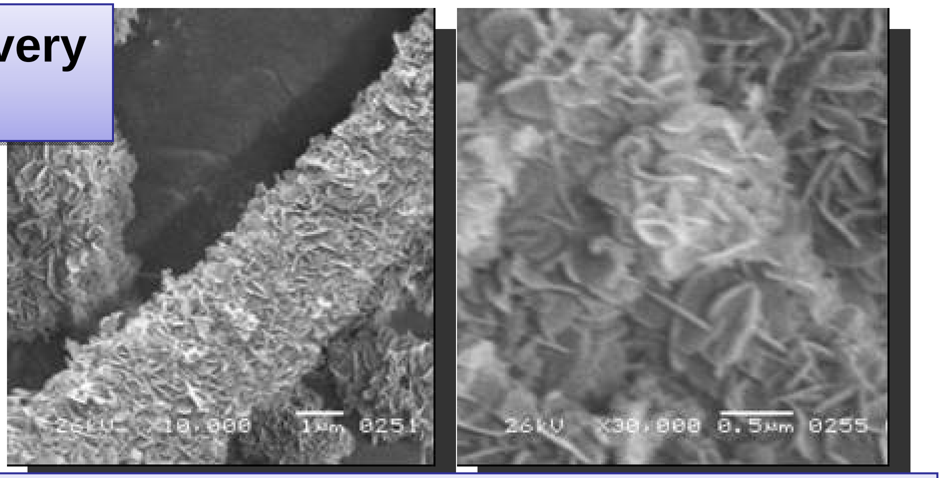
Fig. 59

NANOCRYSTAL BINARY SYSTEMS CoO_x/MgO FOR CO OXIDATION

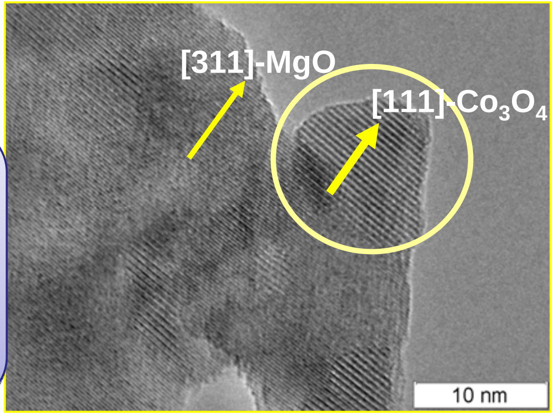
Aerogel samples CoO_x/MgO catalysts are very active to oxidation of CO



1, 2 cycles up to 320°C
3-5 cycles up to 600°C



Unique secondary structure – vertically oriented «scales»



The samples consist of a solid solution of CoO in MgO with Co_3O_4 particles incorporated epitaxially

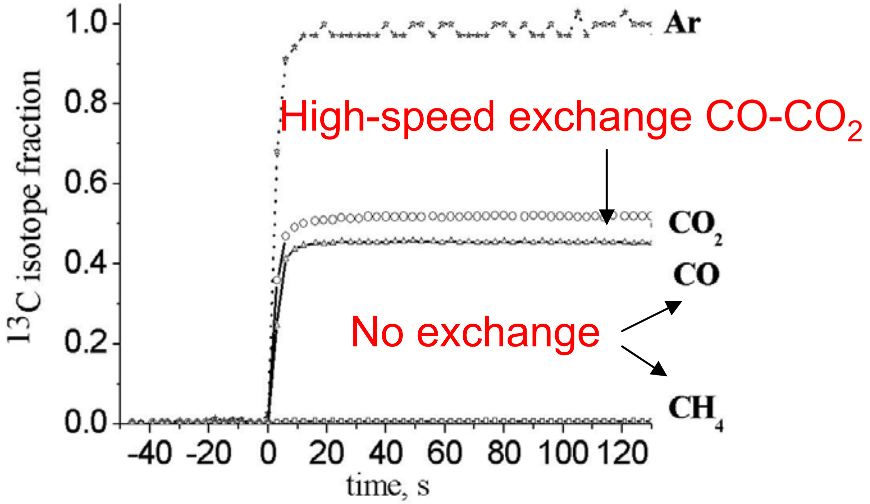
An increase in the activity after sample heating is accounted for by crystallization of the $MgCo_2O_4$ phase in the solid solution structure

Fig. 60

MECHANISM OF CARBON DIOXIDE CONVERSION OF METHANE

The mechanism of carbon dioxide conversion of methane over Me/CeZrLnO (Me=Pt, Ni+Pt, Ni+Ru) was studied by non-stationary kinetic methods

SSITKA ^{13}C: CH_4+CO_2 +He→CH_4+$^{13}CO_2$+He+Ar


High-speed exchange CO-CO_2

No exchange

Typical isotopic relaxations upon flows switching CH_4+CO_2 +He→CH_4+$^{13}CO_2$+He+Ar

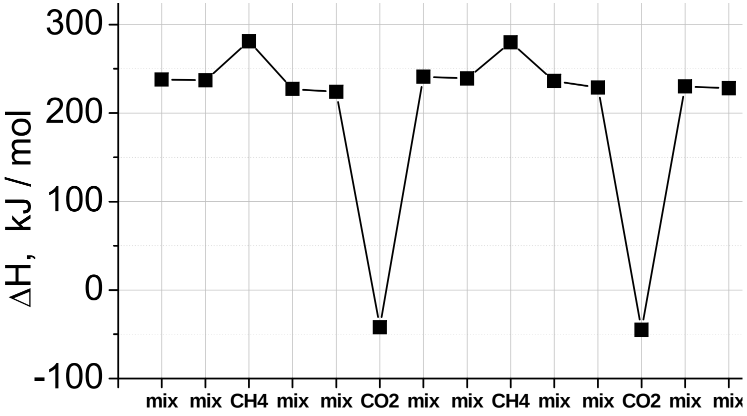
^{13}C does not convert to CH_4⇒ independent stages of activation of CH_4 и CO_2

1) [ZO] +CH_4 → [Z] + CO + 2H_2 - limit
2) [Z] + CO_2 ↔ [ZO] + CO- fast reversible

$W_2/W_1 > 10$

Thermal effects of methane pulses over stationary catalyst

Reversibility of effects

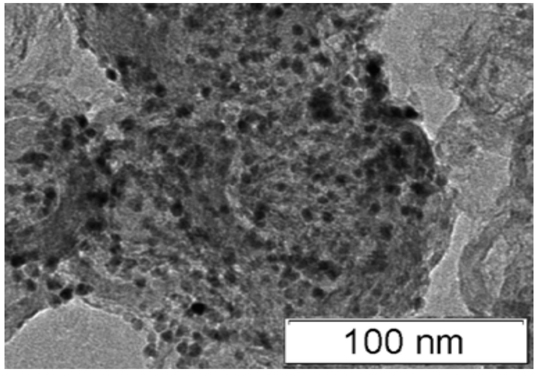


Reactive oxygen species M_2O with adsorption heat ~600 kJ/mol migrate rapidly through the oxide surface to the metal and selectively oxidize CH_4 to CO and H_2

Fig. 61

DEVELOPMENT OF A PROMISING CATALYST Pd/C
FOR HYDROGENATION OF SUNFLOWER OIL

SEM picture; 1% Pd/C



Comparison of the activity of Pd/C catalyst with the commercial Ni-containing analogues in hydrogenation of sunflower oil (SO)
(5 atm, 1200 revo, T=180°C)

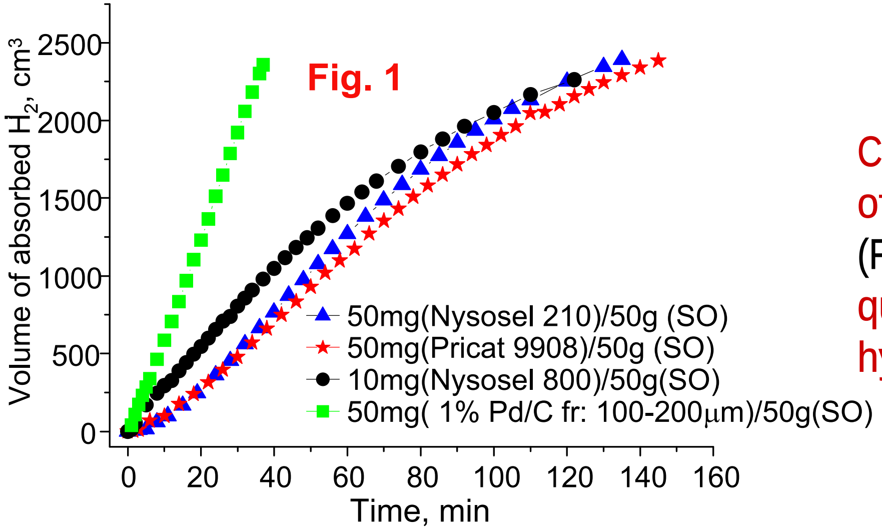


Fig. 1

Study of stability of Pd/C catalyst

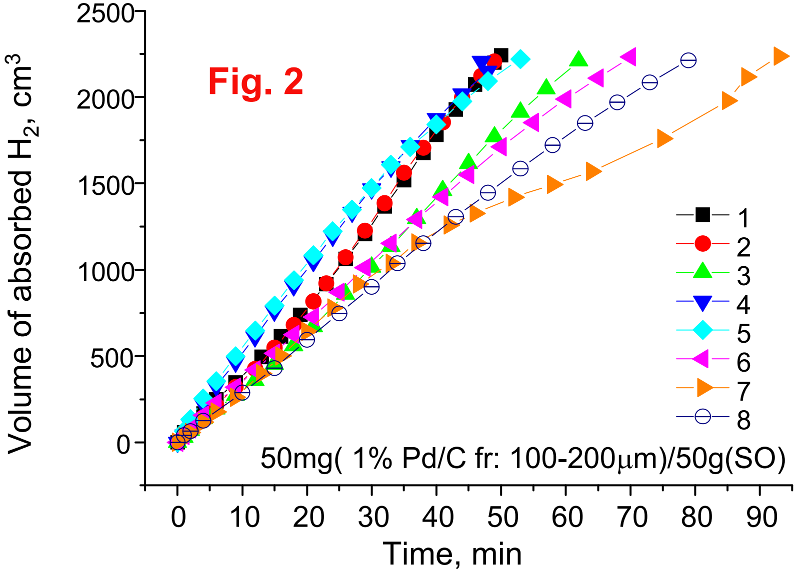


Fig. 2

Catalyst Pd/C is more active to partial hydrogenation of sunflower oil than the commercial Ni analogues (Fig. 1) and reveals high stability without change of quality of obtained product during some cycles of hydrogenation (Fig. 2)

Fig. 62

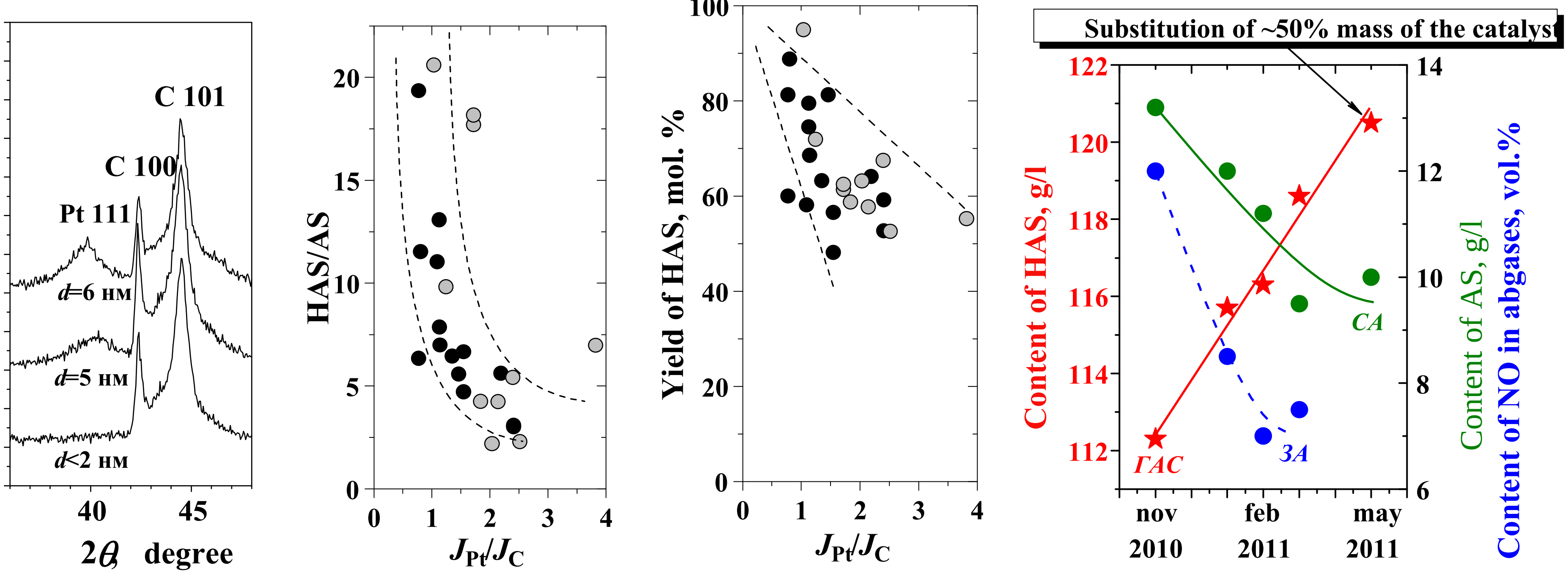
DEVELOPMENT OF IMPROVED PROCESS OF CATALYST Pt/C REGENERATION ON KOAO "AZOT

Catalyst:

$$H_2PtCl_6 + C \xrightarrow[NaOAc]{Na_2S_2O_4} Na_2PtCl_4 + C \xrightarrow[80^oC]{HCO_2H} Pt/C$$

Process:

$$NO + H_2 \xrightarrow[H_2SO_4]{Pt/C,\ 40°C} \underset{HAS}{(NH_3OH)_2SO_4} + \underset{AS}{(NH_4)_2SO_4} + \underset{NO}{N_2O}$$



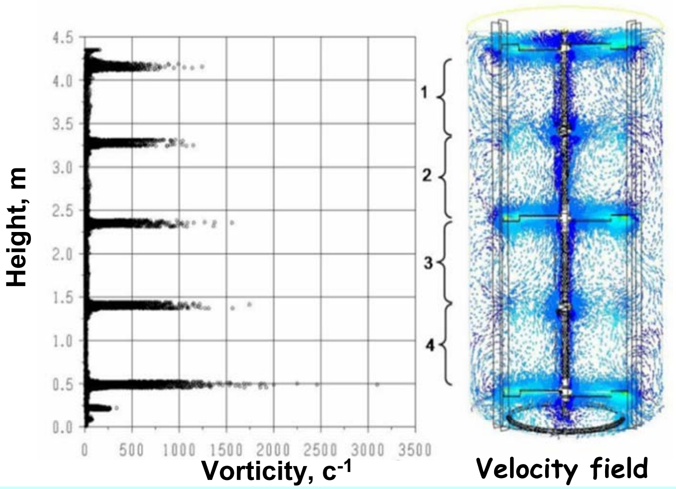
The yield and selectivity to HAS of catalysts 0.5%Pt/Grafite decreases with an increase in the content of coarsely dispersed (> 5 nm) component. Optimization of some parameters of the catalyst preparation/regeneration procedure to decrease the proportion of coarse metal particles led to significant improvement of the performance of the industrial process for hydroxylamine production on KOAO "AZOT"

Fig. 63

DEVELOPMENT OF ENGINEERING BASES FOR APPLICATION OF PALLADIUM CONTAINING CATALYSTS

1. CFD methods were used to study spatial distribution of turbulization degree of oil in an industrial reactor with stacked mixer

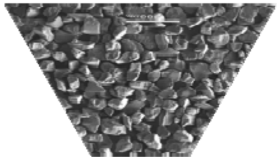
2. A kinetic model of hydrogenation of sunflower oil over a Pd-catalyst was developed

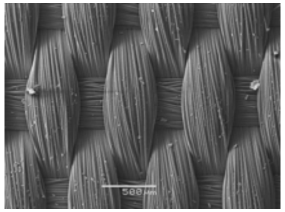


Vorticity, c^{-1} Velocity field

3. Efficiency of purification of hydrogenation products from disperse catalysts

Catalyst Pd/C





Textile filter

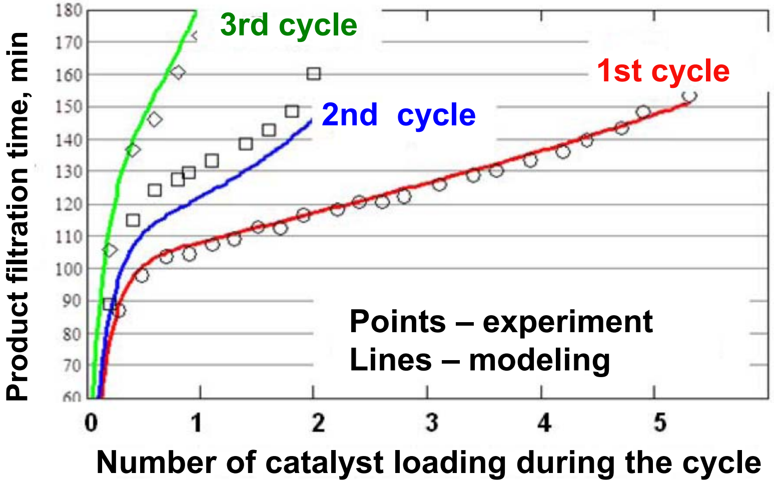


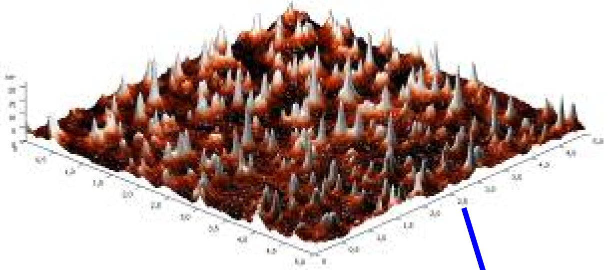
Fig. 64

SYNTHESIS OF TiO_2-NANOPARTICLES FOR SUPPLYING THERAPEUTIC COMPONENTS INTO CELLS

$Ti(OPr)_4$+P123(F127)+$C_2H_5OH+H^+$

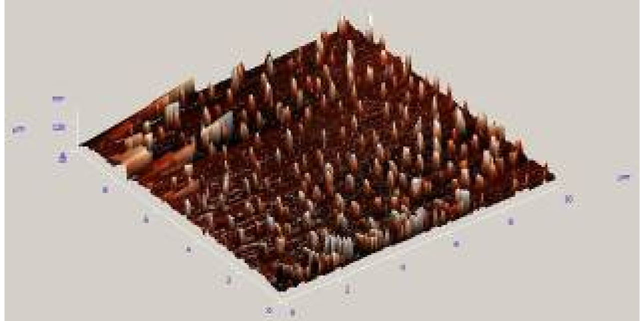
H^+ - HNO_3, H_2SO_4, H_3PO_4

H^+ - HNO_3



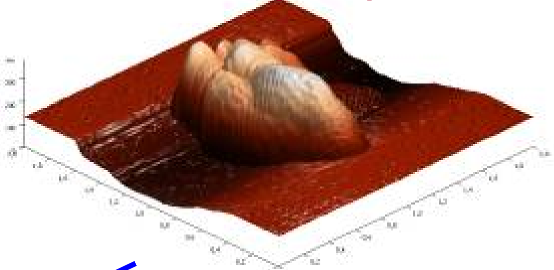
TiO_2- 12-15 nm

H^+ - H_2SO_4

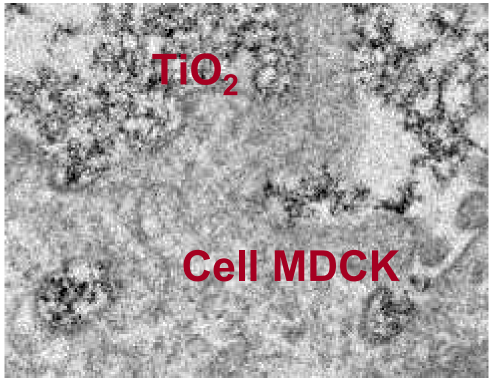


TiO_2- 50-80 nm

H^+ - H_3PO_4



TiO_2- 250-300 nm

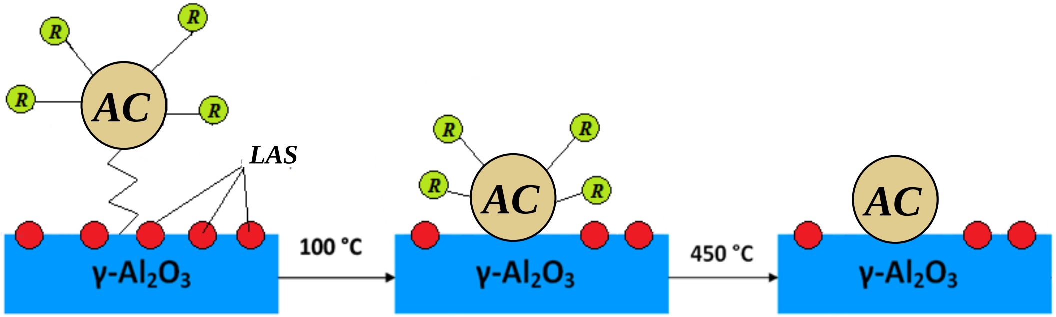


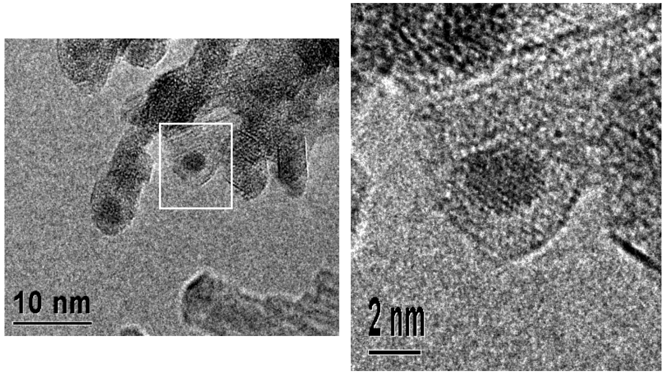
TiO_2-nanoparticles for supplying therapeutic components into cells are no more than 15 nm in size

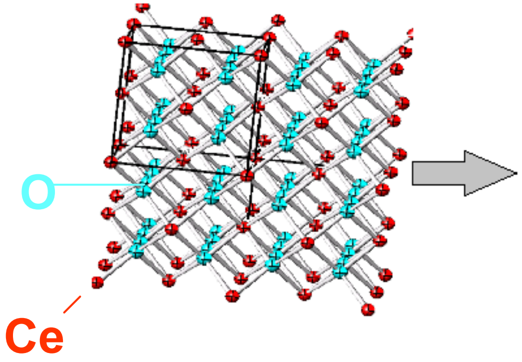
Fig. 65

SYNTHESIS OF NANOSIZED MIXED COBALT AND CERIUM OXIDES ON THE SURFACE OF γ-ALUMINA

A new method for deliberate synthesis of nanosized mixed cobalt and cerium oxides (≤5 nm) on the surface of γ-alumina is developed







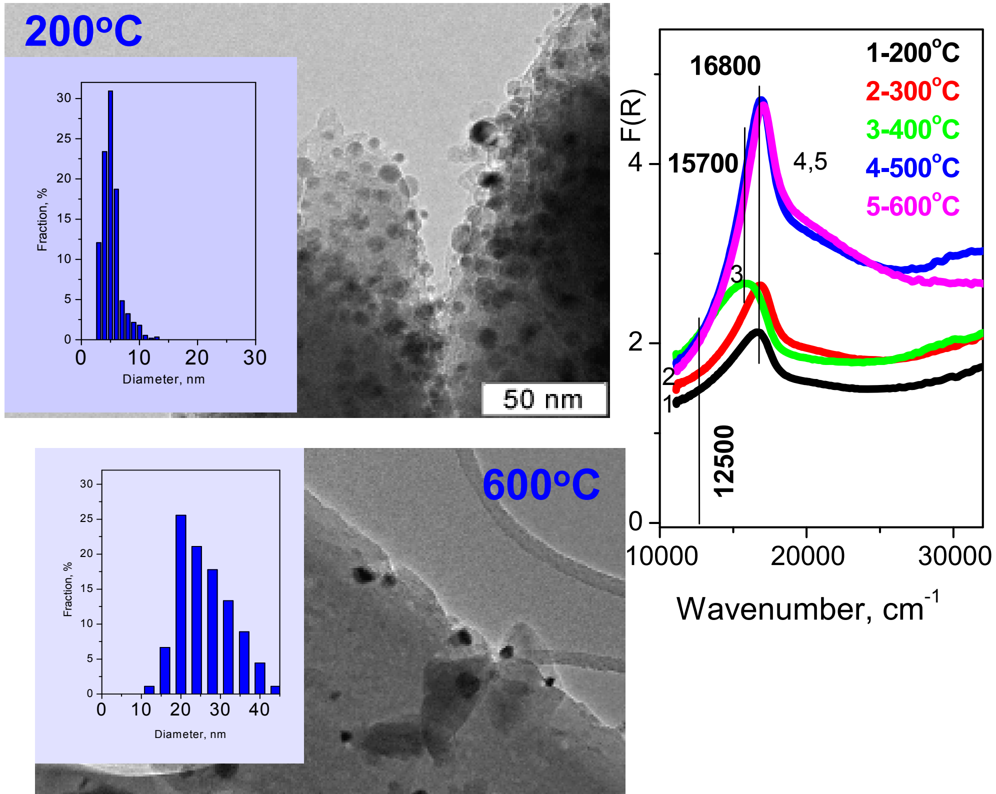
AC – active component

AC – active component - mixed nanooxide CoO-CeO_2, which is formed by substitution of cerium atoms by cobalt atoms in the structure of CeO_2 of fluorite type

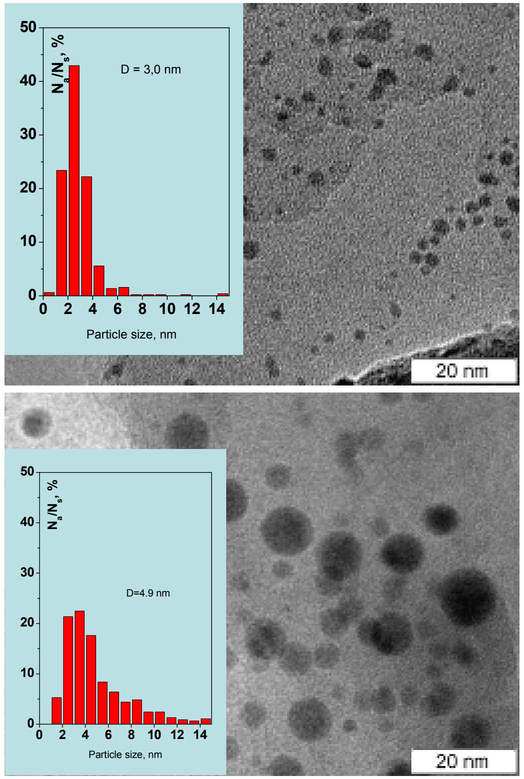
LAS – Lewis acid sites

Fig. 66

FORMATION OF NANOSIZED 1D-3D PARTICLES OF Cu, Pt AND Pd IN THE CHANNELS OF HIGH SILICA ZEOLITES AND OXIDE MESOPOROUS MATERIALS



Cu⁰/H-ZSM-5



Sulfur content in hydrogenate after HDS at 280°C, 1.5 h^{-1}

30 ppm

60 ppm

Pd(Pt)⁰/H-ZSM-5

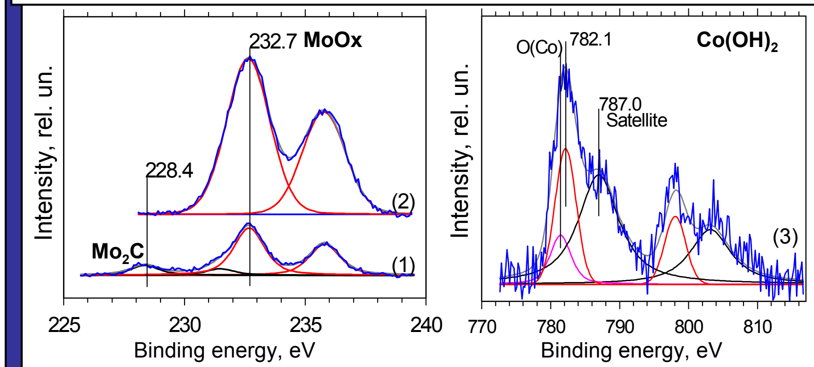
Aluminosilica matrices with a strictly organized micro- and mesopore systems are shown to be applicable for stabilization of nanosize particles of metals Cu^0, Pt^0, Pd^0 etc. Regularity of nanoparticles (1D-2D-3D) and their location (in channels and on the surface) along with chemical (electronic) properties of element determine physicochemical and catalytic properties, stability to oxidation and deactivation in reaction conditions

Fig. 67

GENESIS OF STRUCTURE AND COMPOSITION OF METAL NANOPARTICLES Mo-Me

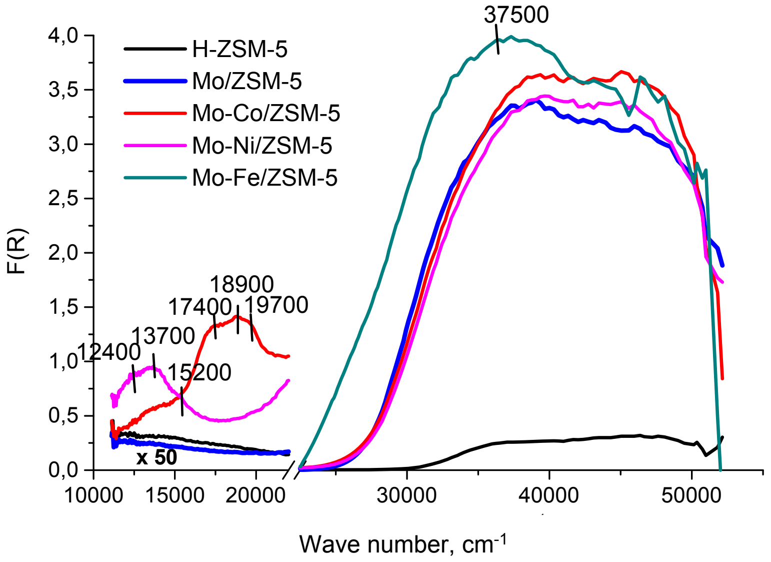
The genesis of the structure and composition of metal-containing nanoparticles (Mo-Me, Me = Fe, Co, Ni), stabilized in zeolite matrix H-ZSM-5, was investigated depending on synthesis conditions (thermal treatment in O_2, Ar, CH_4) and molar ratio Me/Mo (0.04-1.0) by a complex of physicochemical methods (XRD, EPR, ESDR, TEM, EDX, XPS)

XPS data on Mo/ZSM-5 (1) after thermal treatment in CH_4 at 720°C, Mo/ZSM-5 (2) and Mo-Co/ZSM-5 (3) after thermal treatment in O_2 at 500°C



Sample	2Mo0.1Co	2Mo0.5Co	2Mo1.0Co
Co/Mo	0.08	0.4	0.8
Mo_2C/MoOx	0.18	0.22	0.47

UV-VIS DR data on H-ZSM-5 zeolite , Mo/ZSM-5 and Mo-Me/ZSM-5 (Me = Co, Ni, Fe) after thermal treatment in O_2 at 500°C



HRTEM and XPS data indicate changes in the valence state of metals and the formation of carbon deposits after thermal treatment of Mo-Me/ZSM-5 samples in CH_4 at 720°C.

It is established that the ratio of carbide and oxide Mo species depends on the Me/Mo ratio. It equals ~0.2 at Co/Mo = 0.08–0.4 and ~0.5 at Co/Mo = 0.8

UV-VIS DR data on Mo-Me/ZSN-5 composition after treatment in O_2 at 500°C show that the stabilized metal species depend on the sample composition.

It is shown that cations Fe^{3+} and Co^{2+} are stabilized as oxide clusters on the surface of H-ZSM-5 zeolite, and cations Ni^{2+} are in the octahedral oxygen coordination and stabilized in the ion-exchange positions of H-ZSM-5 zeolite

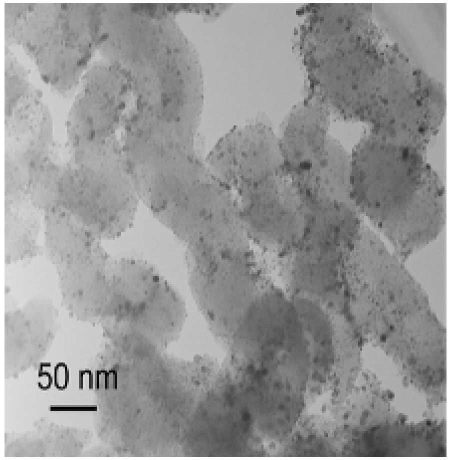
Fig. 68

METAL NANOPARTICLES IN THE STRUCTURE OF MICRO- AND MESOPOROUS CARBON NANOMATERIALS

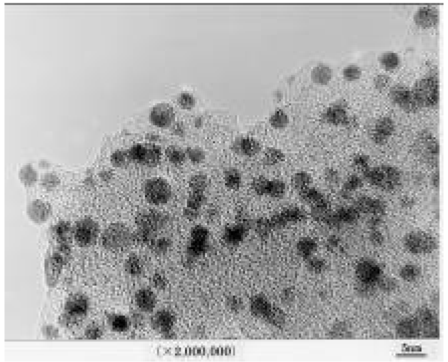
Pt nanoparticles (3–4 nm) on carbon nanofibers (a) and microporous carbon (b) prepared from chlorine-free precursors of Pt

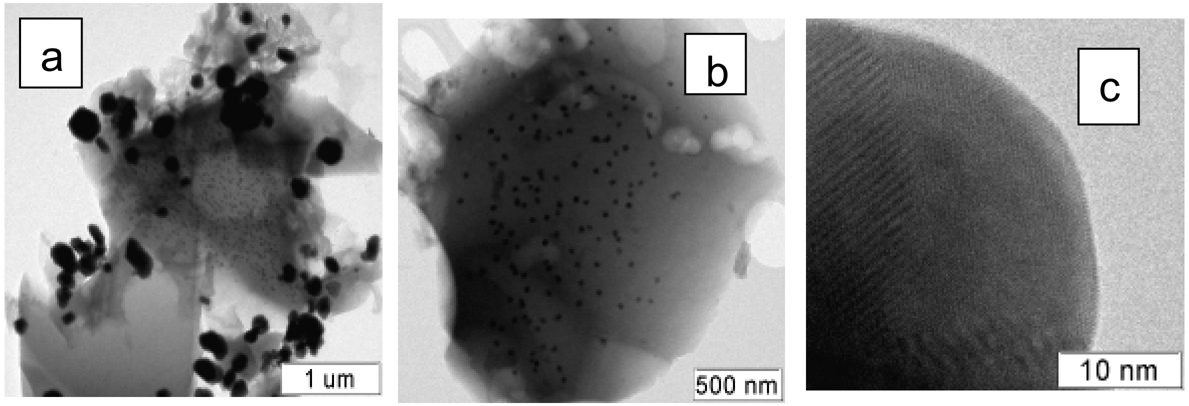
Co particles on nitrogen-doped microporous carbon material are polidisperse: 10–50 nm to 300 nm (a). After acid washing, the sample contains only particles of 10–50 nm in size (b,c)

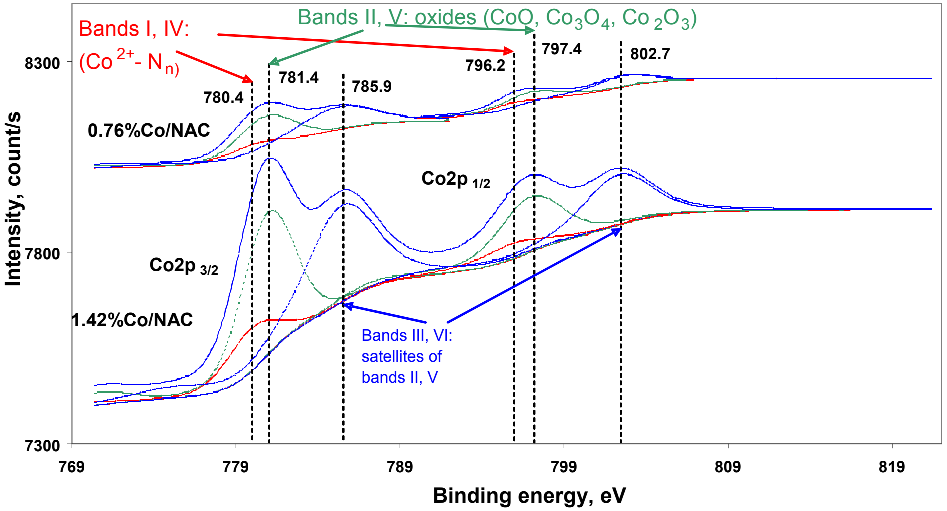
a)



b)



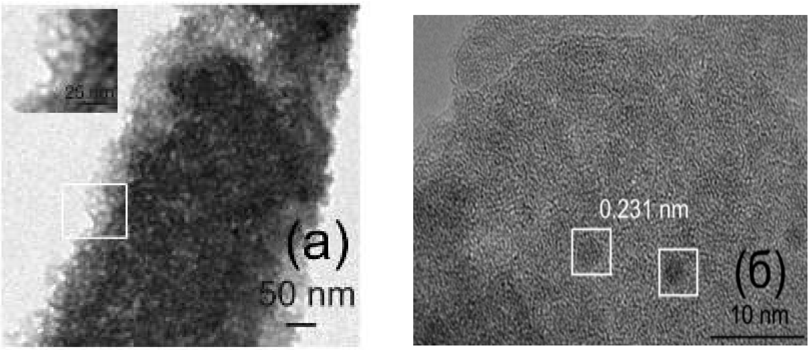




XPS data indicate the presence of cobalt nanoparticles and Co^{2+} ions bound to nitrogen

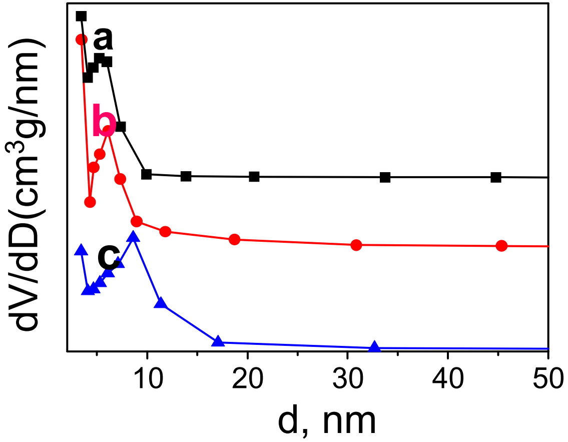
Fig. 69

SYNTHESIS OF MESOPOROUS COATING ON THE INNER SURFACE OF THE QUARTZ CAPILLARY



The capillary coating synthesized by the dip coating method is 300 nm in thickness. A quasihexagonal structure of pores (4.4 nm in average pore size) is observed. There are bimetal particles of Pd, PdZn and $PdZn_2$ (2.0 nm in average size) in the samples

Control of coating porous structure

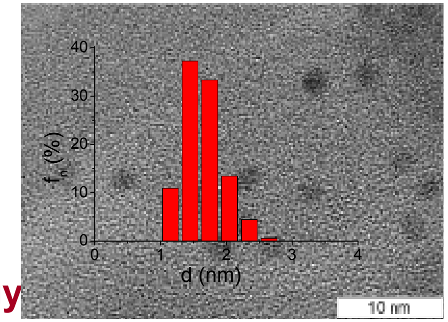


In mesoporous titanium, the pore size can be controlled by adding an organic surfactant – butanol. The pore size increases from 4.9 to 6.8 nm at an increase in the molar butanol/solvent ratio from 0 to 0.2

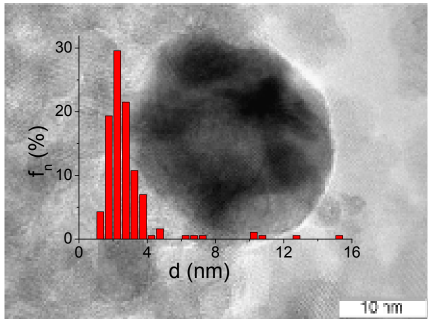
Control of particles composition at the activation stage

Conditions of activation	d_s, n,	atomic, %		wt.%	
		Pd	Zn	Pd	Zn
$Pd\text{-}Zn/TiO_2$ drying at RT	2.1	62.7	37.3	0.96	0.58
$Pd\text{-}Zn/TiO_2$-H	1.8	64.5	35.5	0.96	0.56
$Pd\text{-}Zn/TiO_2$-A	6.6	94.3	5.7	0.99	0.44

Low temperature treatment in vacuum at 300°C, 13 mbar, 2 h



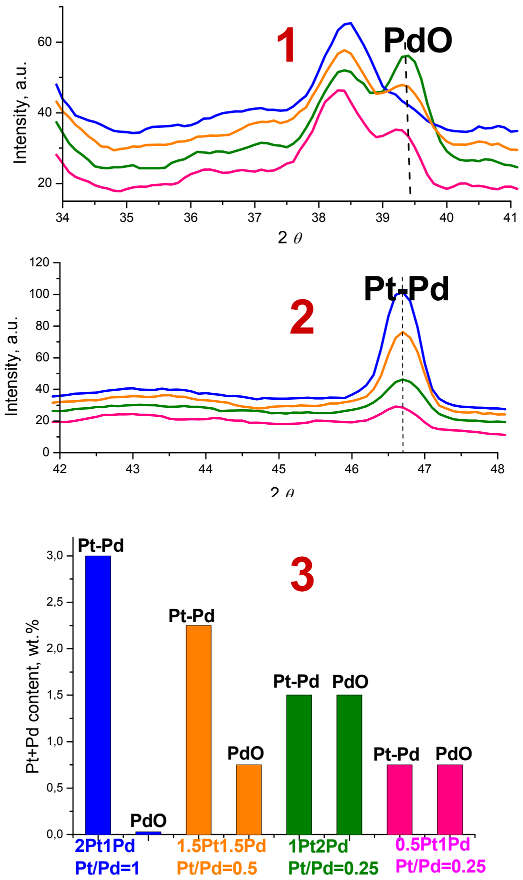
High temperature treatment in air at 400°C - 2 h and in 30%H_2/Ar at 400°C - 2 h



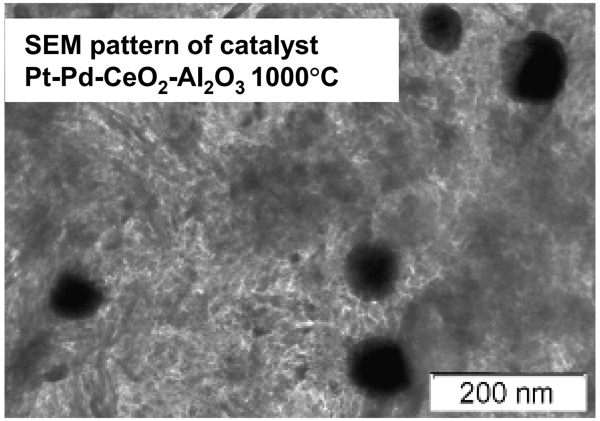
Thermal treatment leads to changes in morphology and composition of nanoparticles

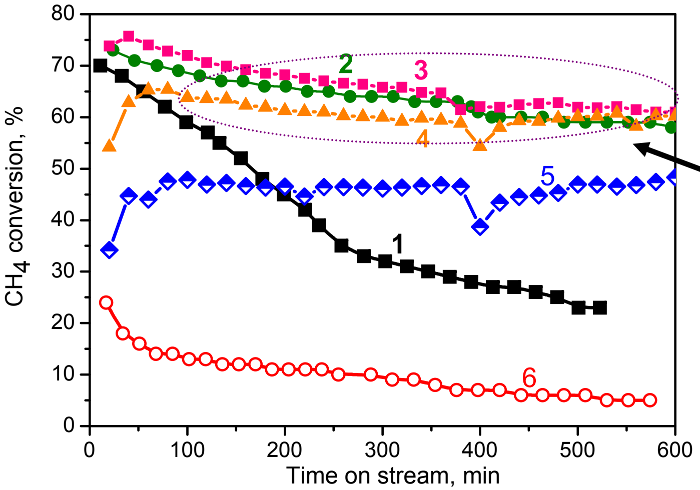
Fig. 70

NANOSIZE Pd- AND Pt-Pd CATALYSTS OVER ALUMINA SUPPORTS



Relative amount of PdO phases and Pt-Pd alloy in catalysts in dependence of ratio Pt/Pd
1,2 - X-ray data, 3 – design data





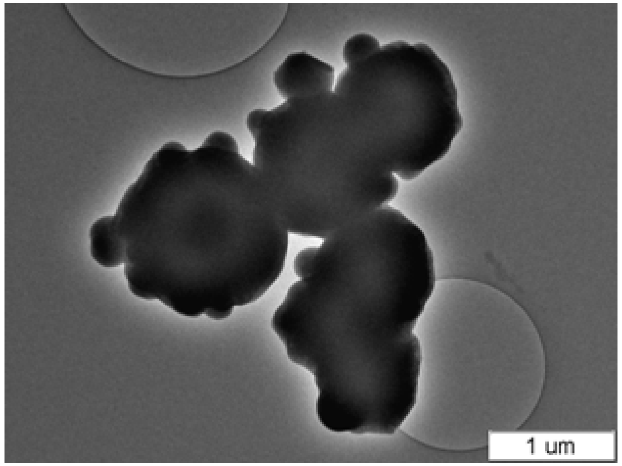
State of active component in catalysts in dependence of weight (atomic) ratio:

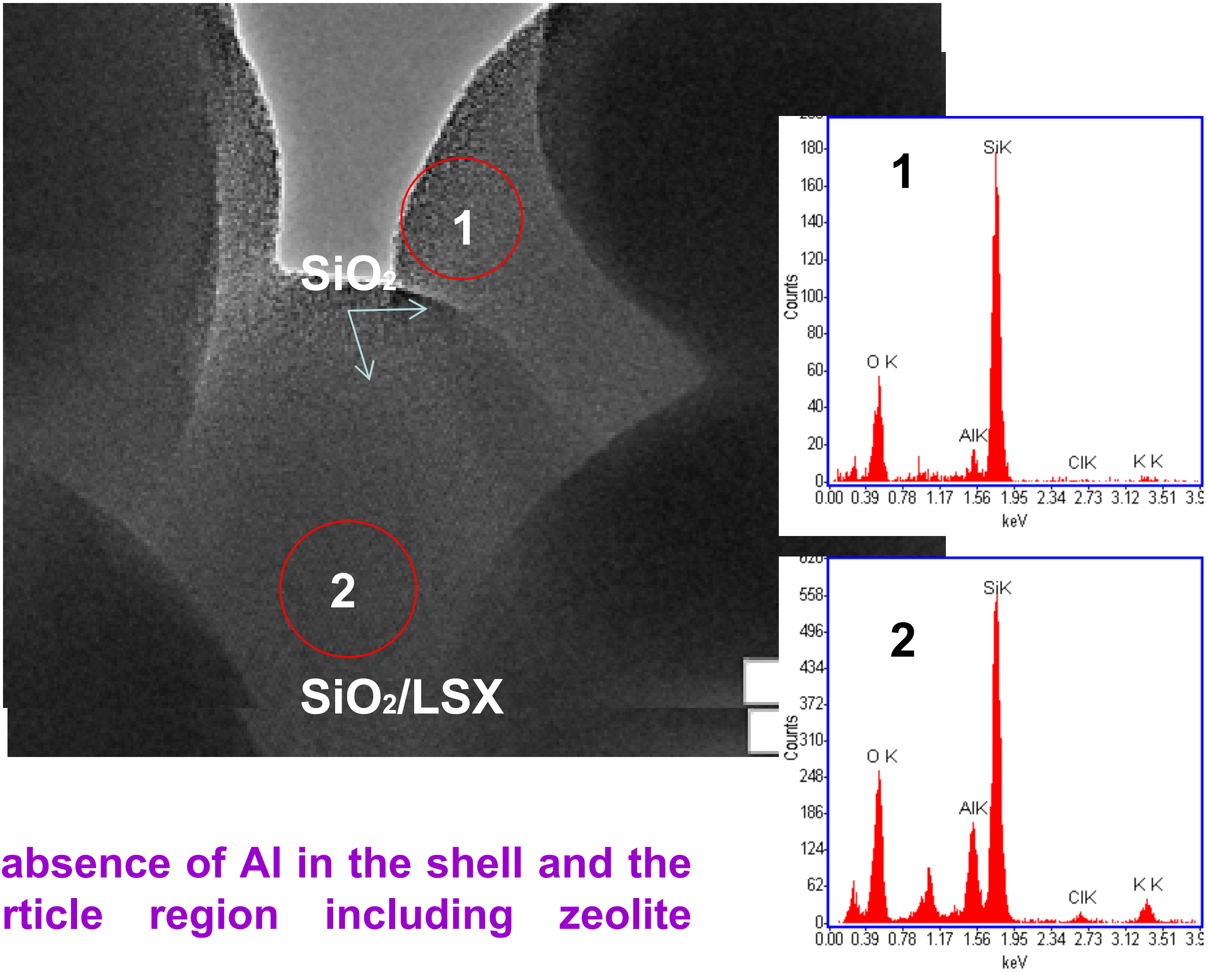
- **0Pt2Pd (Pt/Pd=0) – PdO**
- **2Pt1Pd (Pt/Pd=1) – PtPd-alloy**
- **1Pt2Pd (Pt/Pd=0.25) PdO, Pt_2O_3, PtPd-alloy**

At atomic ratio Pt/Pd=0.25-0.55 catalysts demonstrate high activity and stability in reaction of methane oxidation (GHSV = 250 000 h^{-1}, α = 10.5, C_{CH4} = 1.0 vol.%)

Fig. 71

FORMATION OF MESOPOROUS SILICATE SHELL AROUND LSX ZEOLITE MICROSEEDS





The possibility of formation of mesoporous shell with thickness of 50-150 nm was shown; the shell has no visible breaks at the thickness more than 100 nm

EDX spectra show almost total absence of Al in the shell and the presence of Al in the particle region including zeolite microparticle

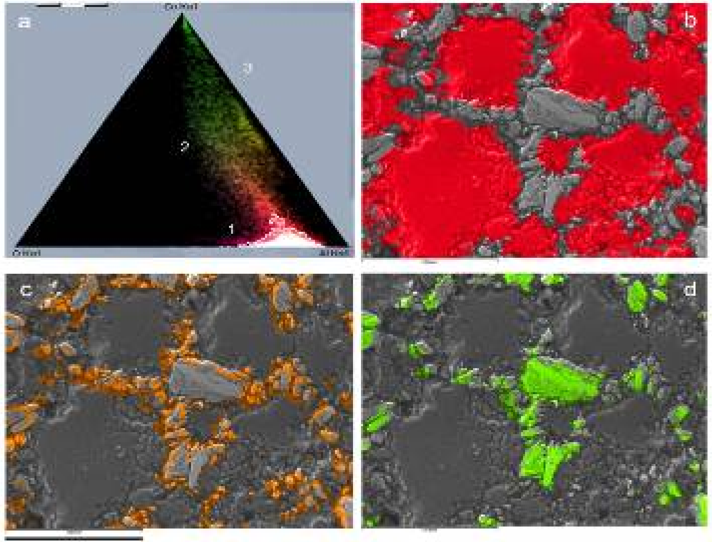
Formation of porous shell around zeolite microparticles opens wide opportunities for using such materials in medicine and toxicology due to decreasing mechanical effect of zeolite on living tissue

Fig. 72

DESIGN OF CERAMOMETAL DEHYDROGENATION CATALYST

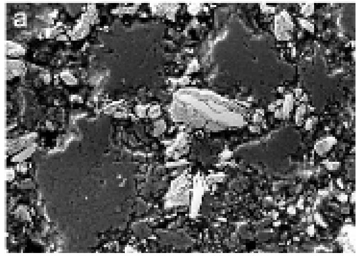
Al_2O_3 aggregates in ceramometal matrix CoAlO/CoAl

Porous Al_2O_3 (1)



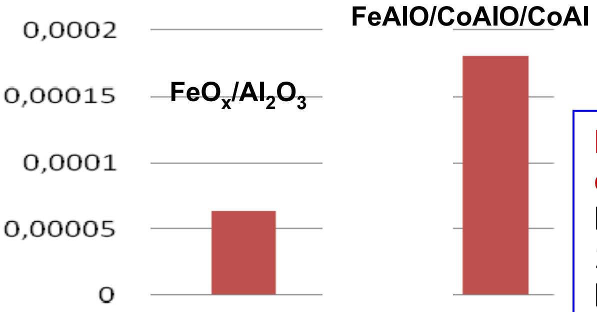
Al-Co-O interface (2) **Co и $CoAl_x$ nuclei (3)**

SEM Al_2O_3/CoAlO/CoAl



Efficiency of solid fuel combustion in the fluidized bed of inert material in the presence of ceramometal honeycomb catalysts is close to that of the granulated aluminocopper chromium catalyst (IC-12-70)

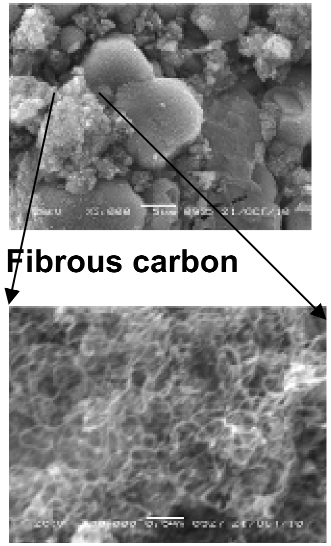
Average rate of C_6H_6 and C_6H_{12} generation (mg/sec)



Advantage:

No attrition of the catalytic units after 100 hours of testing

Dehydrogenation conditions:
MW adsorption –
120 V/g;
hexane flow –
15 vol.% in Ar.

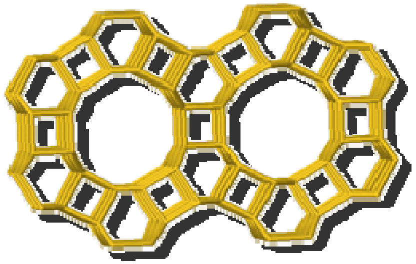


Fibrous carbon

Benzene, hexene and fibrous carbon are produced. Ceramometal catalysts reveals high activity in comparison with ceramic one

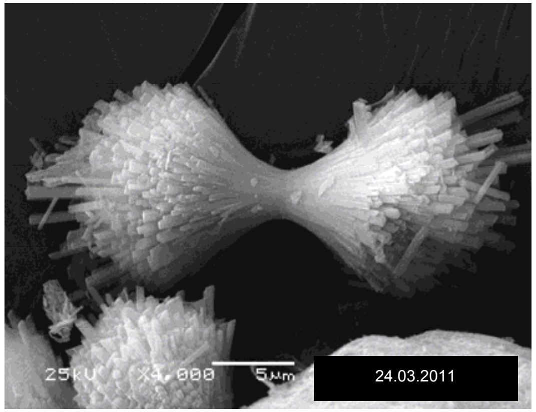
Fig. 73

CATALYST FOR *n*-ALKANE HYDROISOMERIZATION BASED ON SILICOALUMINOPHOSPHATE *SAPO-31*


SAPO-31 (5,4 x 5,4 Å)

For the first time it is shown that properties of silicoaluminophosphates SAPO-31 are determined by many factors, the master are:

- **Time of hydrothermal treatment;**
- **Template type and reagents nature;**
- **Silicon content**

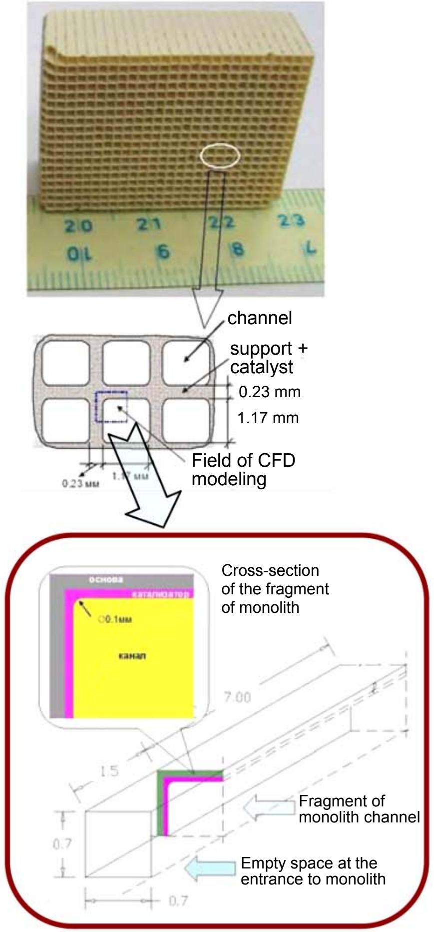


Comparison of the results obtained with the developed catalyst and industrial sample ICR-404

Catalyst	ICR-404 (1% Pt/SAPO-11) Chevron Co.	1% Pt/SAPO-31 BIC
Hydrotransformation of diesel fraction		
$T_{freez. Init.}$, °C	-3	-20
$T_{freez fin.}$, °C	-35	-(44-50)
Yield, %	94	99
Hydrotransformation of oil fraction		
$T_{freez. Init.}$, °C	42	56
$T_{freez fin.}$, °C	-15	-5
Yield, %	55-60	70-75

Fig. 74

APPLICATION OF CFD MODELING FOR DEVELOPMENT OF THE THEORY OF STRUCTURED HIGH-TEMPERATURE CATALYTIC SYSTEMS



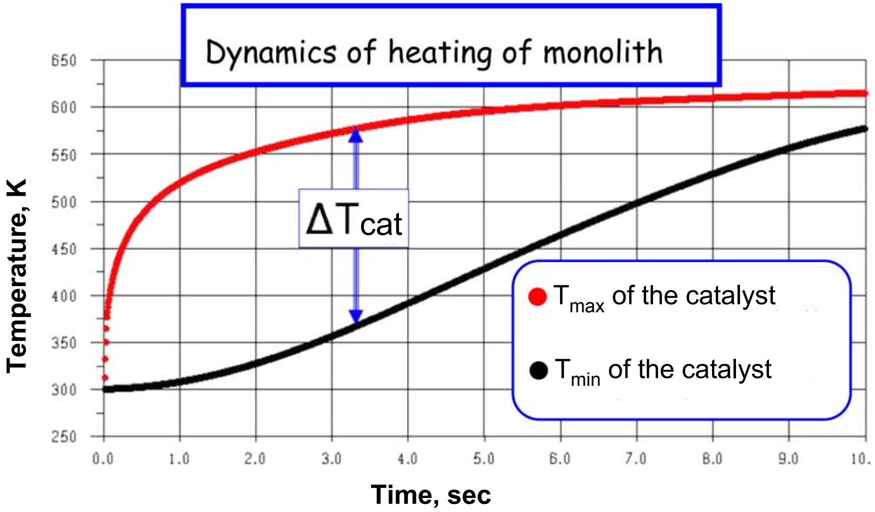
Model reaction of CO oxidation

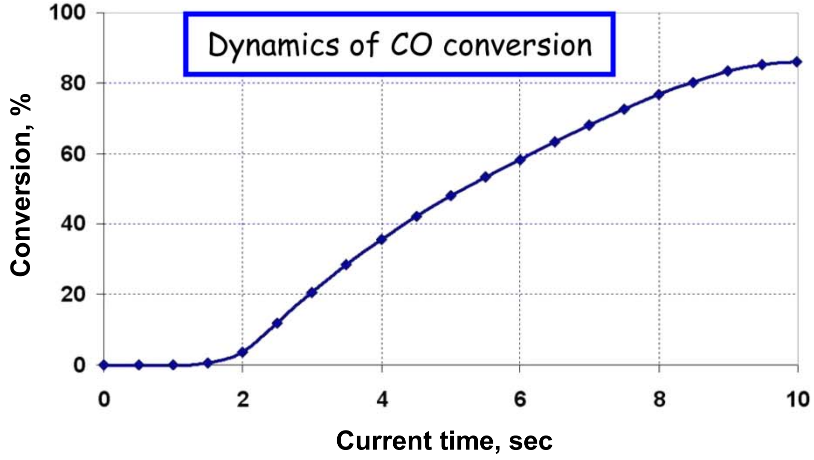
$$CO + 0.5O_2 = CO_2$$

$$r_{CO} = kC_{CO} \qquad k = k_0 \exp\left(\frac{E}{RT}\right)$$

$k_0 = 7.0 \cdot 10^{14}$, $E = 1.17 \cdot 10^{8}$ J/kg mol

Studying initial loading on “cold” catalyst





Heating of monolith is characterized by time and volume nonuniformity

Difference between the maximum and minimum temperatures ΔT_{cat} is more than 200° for the investigated regime at $0.6 \leq \tau \leq 4.0$ s.

Duration of transient processes with hypoconversion is 10-15 sec.

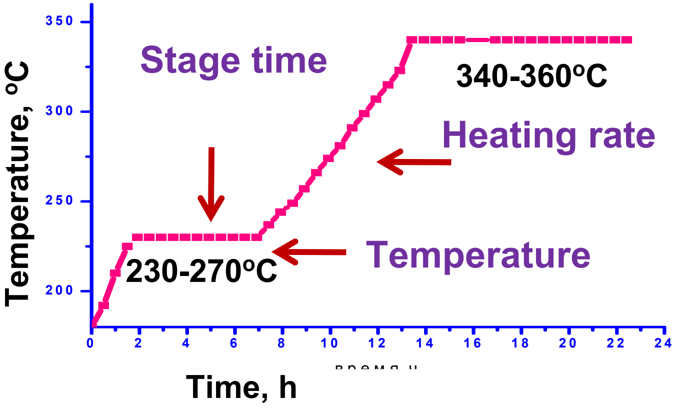
Fig. 75

ACTIVITY OF SULFIDE NiMo AND NiW CATALYSTS OVER ZEOLITE-CONTAINING SUPPORTS IN REACTION OF TETRALIN TRANSFORMATION

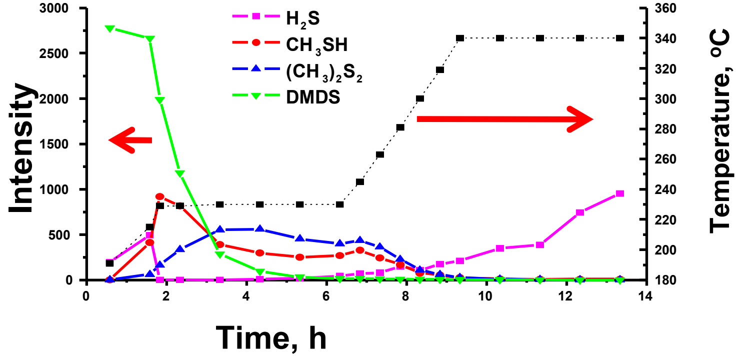
Catalysts:

- **$NiMo/Al_2O_3$ - zeolite β (10,20,30 mass.%)**
- **NiW/Al_2O_3 - zeolite β (10,20,30 mass.%)**
- **NiW/Al_2O_3 - zeolite Y (10,20,30 mass.%)**

Optimization of sufidizing conditions



Dynamics of DMDS decomposition products change upon sulfidizing :



- **DMDS decomposition with generation of H_2S in the presence of zeolite starts at lower temperature**
- **For sulfidizing of NiW system higher temperature is necessary**

The used method of preparation together with optimized sulfidizing procedure provides formation of highly disperse particles

$NiMo/Al_2O_3$-β-10

Activity in reaction of tetraline transformation

(hydrogen pressure 5,0 Mpa; H_2/raw mat. – 800 nm^3/m^3,T – 340°C)

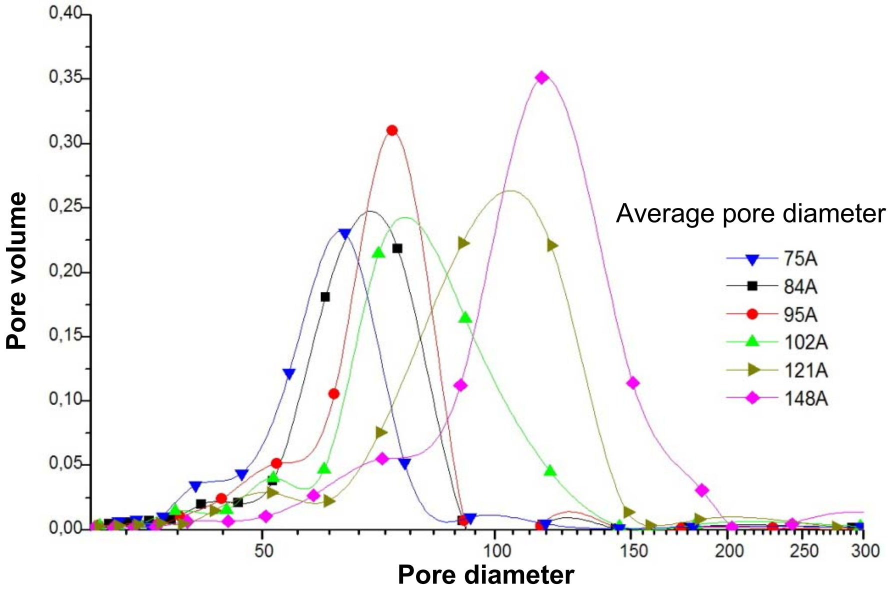
	X tetr., %	Yield $\sum C_{10}$, %	Selectivity, %	
			Decahydro-naphthalene	C_{10}
$NiMo/Al_2O_3$	43	100	100	0
NiW/Al_2O_3	49	100	100	0
$NiMo/Al_2O_3$-β-10	44	100	74	26
NiW/Al_2O_3-β-10	46	100	71	29
NiW/Al_2O_3-β-20	43	75	Formation of gaseous products	
NiW/Al_2O_3-Y-10	46	70		

Fig. 76

PREPARATION OF OPTIMAL SUPPORTS FOR HYDROTREATING CATALYSTS

Components of the methods:

1. Industrial powders of AlOOH with given grain composition and crystal morphology
2. Optimum compositions and rheologic characteristics of molding pastes
3. Optimum conditions of molding
4. Optimum conditions of drying and calcination of supports
5. Conditions of supporting which provide the structure of initial bimetal Co-Mo complexes preservation



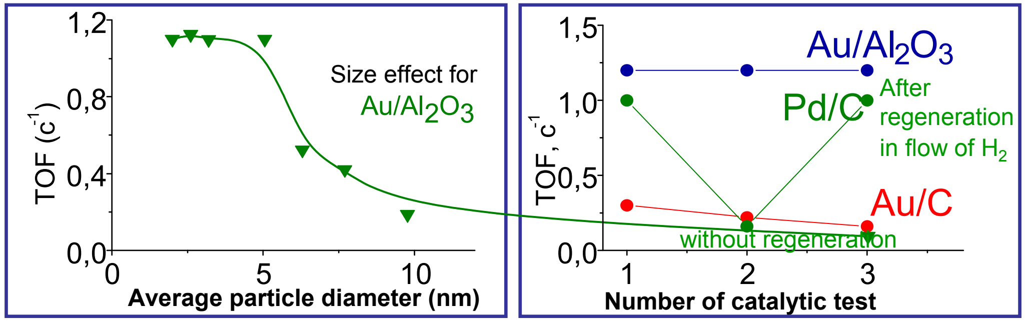
Main results:

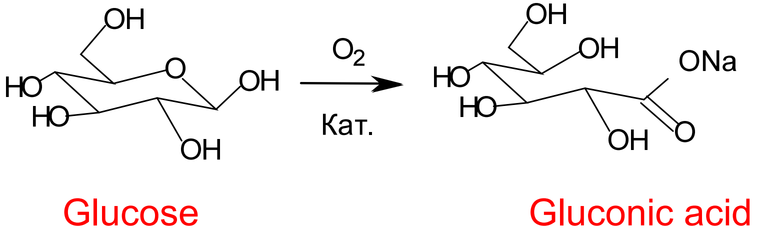
1. The supports are obtained with the required pore size distribution at a large specific surface area and pore volume ($S_{sp.}$=210±10 m^2/g, V_{por}=0,7±0,05 cm^3/g).
2. The morphology of crystals of initial powder and preparation conditions are defined which provide obtaining of extrudates in the form of trefoil with diameter 1,3 mm and bulk strength by Shell SMS 1471 method 0,6-0,8 MPa
3. Procedure conditions are determined which provide the structure preservation of initial bimetal complex compounds in the target catalyst

Fig. 77

COMMON FEATURES OF THE OXIDATION OF ALDOSUGARS OVER MONOMETAL CATALYSTS

Stability of **Pd** and **Au** catalysts in the reaction of glucose oxidation

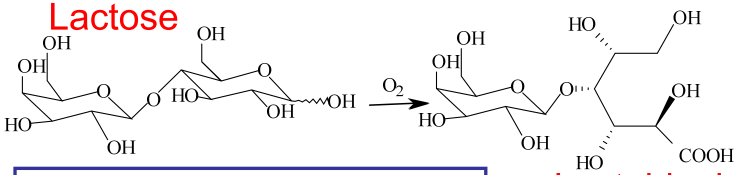




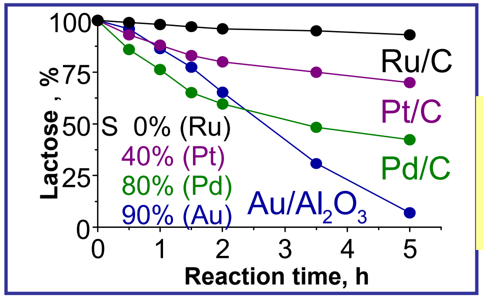
- The **Pd/C** catalyst **is deactivated** under the reaction conditions due to oxidation of the Pd particles but regenerated completely via reduction in flowing H_2
- The **Au/C** catalyst **is deactivated** irreversibly due to aggregation of the Au particles
- The **Au/Al_2O_3** catalyst is **very stable** for at least 15 hour reaction
- It is determined that the optimal Au particles are 1 to 5 nm in diameter in the **Au/Al_2O_3** catalyst

Selective lactose oxidation

Lactose



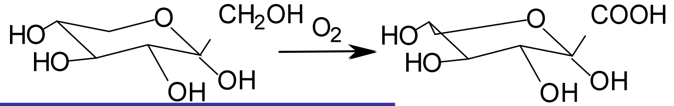
Lactobionic acid



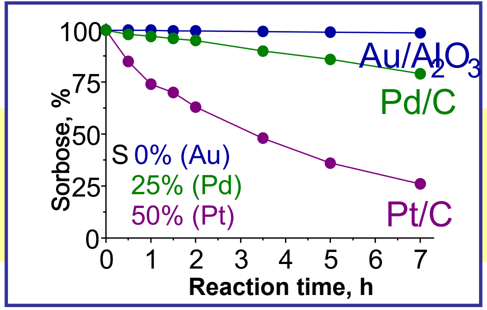
Activity for aldo-sugars (glucose and lactose))
Ru<Pt<Pd<Au

Selective sorbose oxidation

Sorbose



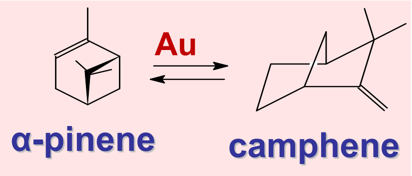
2-Ketogulonic acid



Activity for keto-sugar sorbose
Au<Pd<Pt

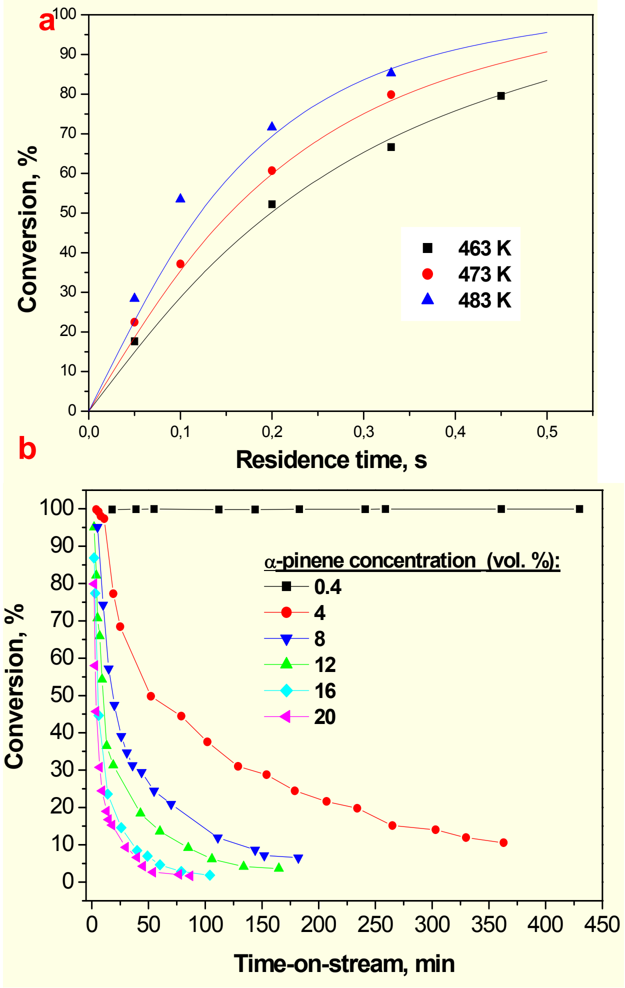
Fig. 78

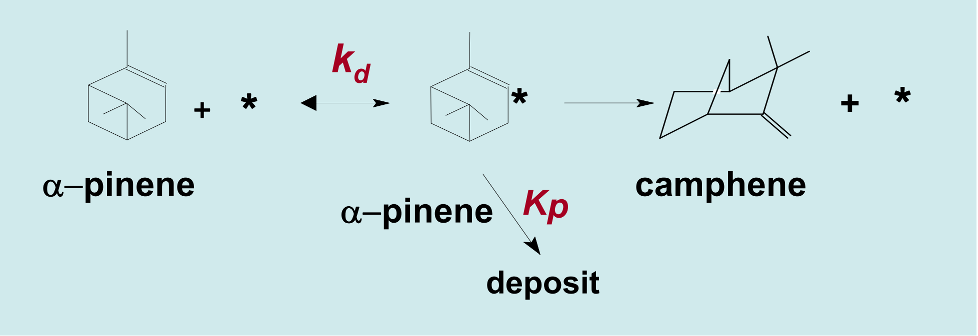
STABILITY AND DEACTIVATION OF GOLD CATALYSTS IN α-PINENE TO CAMPHENE ISOMERIZATION



***Stage 1.* The effect of temperature (a) and initial concentration of α-pinene (b) on the stability of Au/Al$_2$O$_3$ catalyst was identified**

***Stage 2.* The deactivation function was defined , the kinetic modeling of deactivation was carried out**





$$\frac{d\theta_{deposit}}{dt} = k_d\theta^2_{pinene} = k_d K_p^2 C^2 \theta_v^{\;2}$$

$$\theta_v \approx 1-\theta_{deposit}$$

$$\frac{d\theta_{deposit}}{dt} = k_d\theta^2_{pinene} = k_d K_p^2 C^2 (1-\theta_{deposit})^2$$

$$a = (1-\theta_{deposit})$$

$$-\frac{da}{dt} = k_d K_p^2 C^2 a^2$$

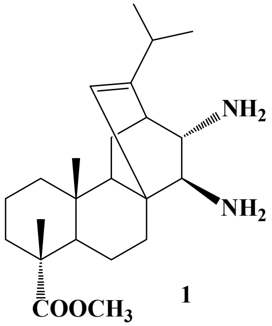
The deactivation function *a* was defined after integration with boundary conditions (t=0, a=1)

$$a = \frac{1}{1+k_d K_p^2 C_o^2 t}$$

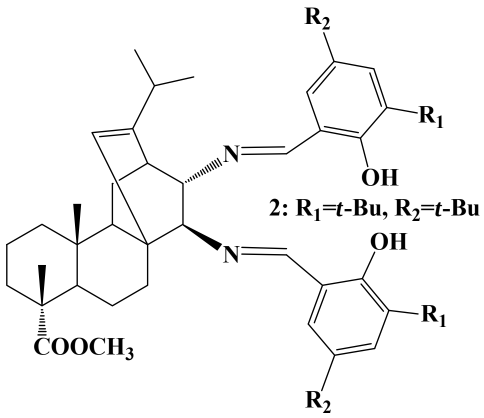
Fig. 79

METAL COMPLEX CATALYSTS FOR HOMOGENEOUS AND PHASE-TRANSFER ASYMMETRIC REACTIONS

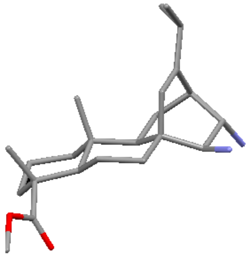
X-Ray data on the structure of the obtained organic catalysts (1) and (2)



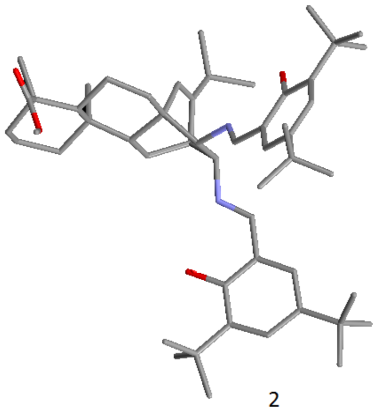
1



2: R_1=t-Bu, R_2=t-Bu

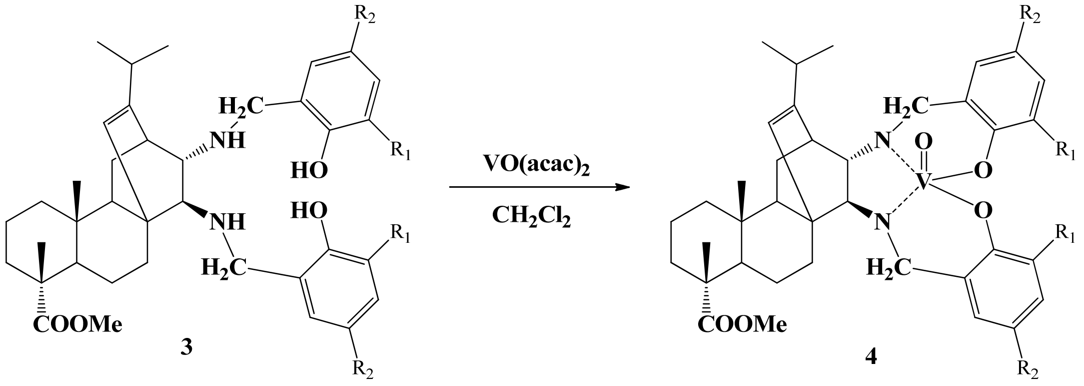


1



2

Synthesis of oxidation catalysts with chiral inductors based on diterpenes



R_1=H, R_2=H
R_1=OCH_3, R_2=H
R_1=NO_2, R_2=NO_2
R_1=t-Bu, R_2=t-Bu

Fig. 80

STUDIES ON GLYCEROL COFERMENTATION WITH GLUCOSE

Molar ratio of fermentation products after 48 fermentations of *Klebsiella pneumoniae* W18 in the presence of glucose and glycerol

Substrate	Glucose, g/l	Glycerol, g/l		
		30	60	90
[1,3 propanediol]/[glyceroll]mol/mol	0	0,43	0,59	0,72
	10	0,53	0,66	0,27
Dry weight of cells, g/l	0	1,7	1,05	0,97
	10	2,3	1,23	0,76

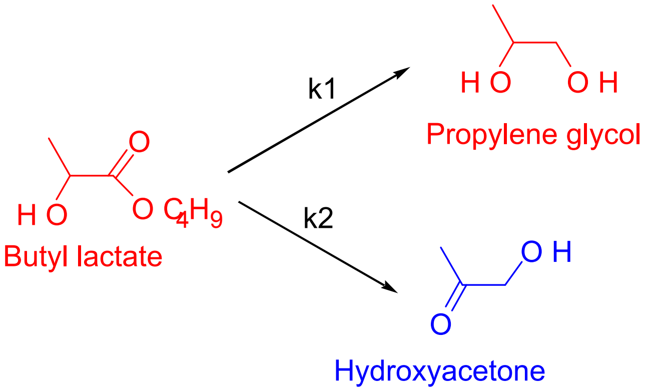
- **Glycerol (60 g/l) cofermentation with glucose by Klebsiella pneumoniae W18 showed a 13 % increase in the 1,3-propanediol yield**

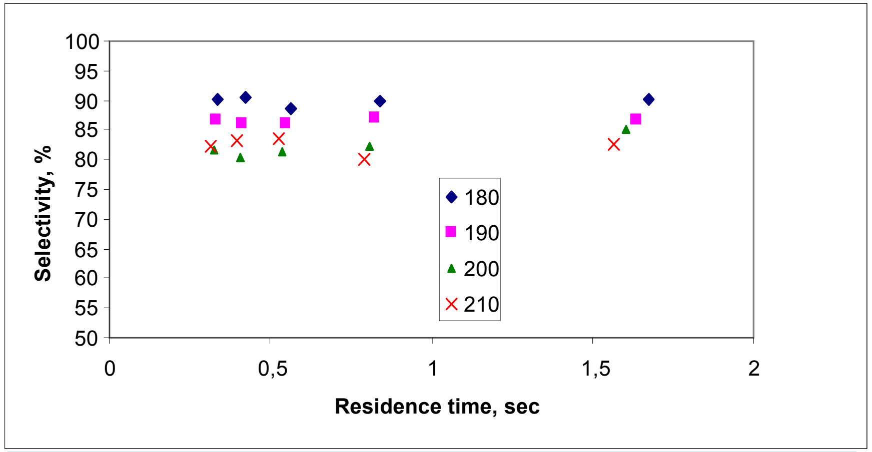
- **An increase in the glycerol concentration under identical conditions resulted in inhibiting the production of 1,3-propanediol**

- **It was established that the expression of genes responsible for transformation of glycerol into 1,3-propanediol relates directly to the anaerobic state of the cell (gene activation by transcriptional factors arcA and OxyR)**

Fig. 81

KINETIC PECULIARITIES OF HYDROGENOLYSIS OF BUTYL LACTATE





Influence of residence time on selectivity at various temperatures. 45,5 wt.% Cu/SiO$_2$, T=180°C, P(H$_2$)= 1 atm, (butyl lactate : H$_2$) = 1 : 70.

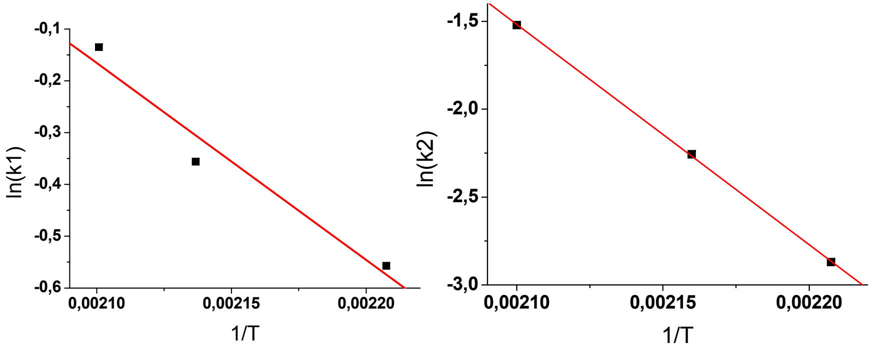
Calculating rate constants and E_a

For reaction of first order to butyl lactate dependence of conversion X on residence time τ:

$$x = 1 - e^{-k\tau} \quad k = -\frac{\ln(1-x)}{\tau} \qquad \frac{k_1}{k_2} = \frac{S_1}{S_2}$$

$$k = k_0 \cdot e^{-E_a/RT} = k_1 + k_2 = k_{10} \cdot e^{-E_{a1}/RT} + k_{20} e^{-E_{a2}/RT}$$

k_{1o}=2.5×10^3 s^{-1}, E_{a1}=32 kJ **k_{2o}=6.0×10^{10} s^{-1}, E_{a2}=104 kJ**



Dependence k_{ef} of rate constants of propylene glycol and hydroxyacetone generation on temperature in Arrhenius coordinates

Fig. 82

CATALYTIC SYNTHESIS OF BIODEGRADABLE POLYMERS

Lactic acid based polymers

Direct polycondensation:

$LA + R(COOH)_2 + R^{'}(OH)_2 \longrightarrow$ **Degradation of probability of depolymerization**

Comonomers (8-12 mol.%): siccine acid, adipi(ni)c acid, hydroxiacetic acid; ethylene glycol, 1,3-propanediol ("corn-diol"), 1,4-butanediol, 2,3-butanediol, 1,6-hexanediamine → Specific weight, T melting, T vitrification ↓

Water extraction by the inert gas flow → Absence of special equipment, solvents

Putting the dehydrator to reaction media → Drastic increase of molecular weight

$M_n > 20000$

Decreasing of synthesis temperature up to ~200 °C → Decrease of lactate formation, increase of polymer yield

Chain extender → $M_n \uparrow$ ~60000

Fig. 83

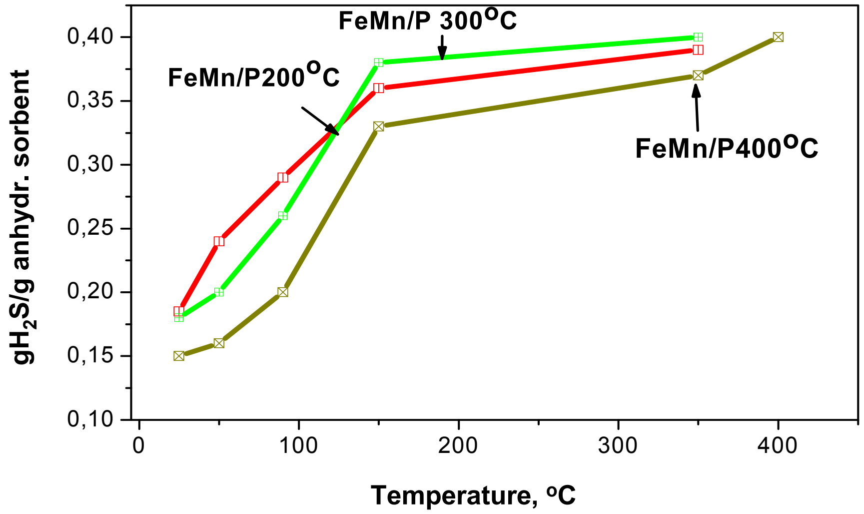
CATALYST AND ADSORBENTS FOR DIRECT OXIDATION OF HYDROGEN SULFIDE

1. **Based on the investigation of a series of supported catalysts:**

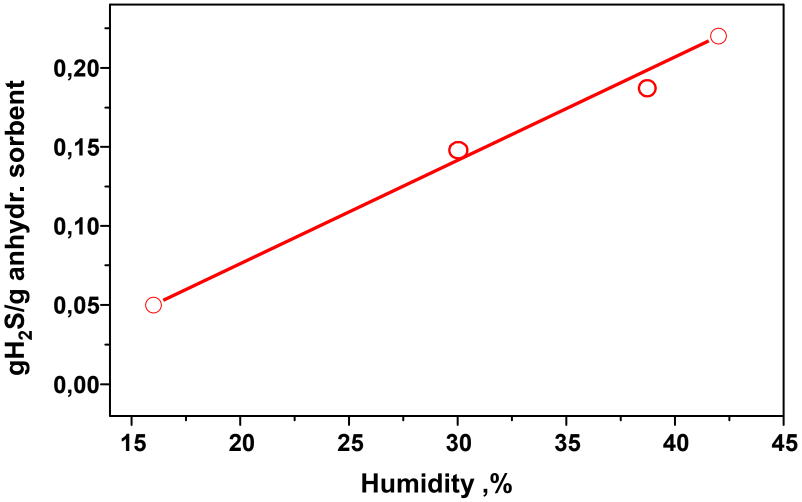
$$Co_3O_4 \geq \text{MX-sphere} > V_2O_5 > \text{Fe-O} = \text{Cr-O} > \text{Mn-O} > \gamma\text{-}Al_2O_3$$

the composition of the catalyst for direct hydrogen sulfide oxidation was developed, providing sulfur yield ≥ 90 % in temperature range 230-300°C

2. Compositions of multifunctional adsorbents based on manganese-iron mixed oxides, providing sulfur capacity more than 20 % both for H_2S and SO_2 were developed



Dependence of sorptive capacity of FeMn/P samples to H_2S in dependence of calcination temperature of FeMn/P



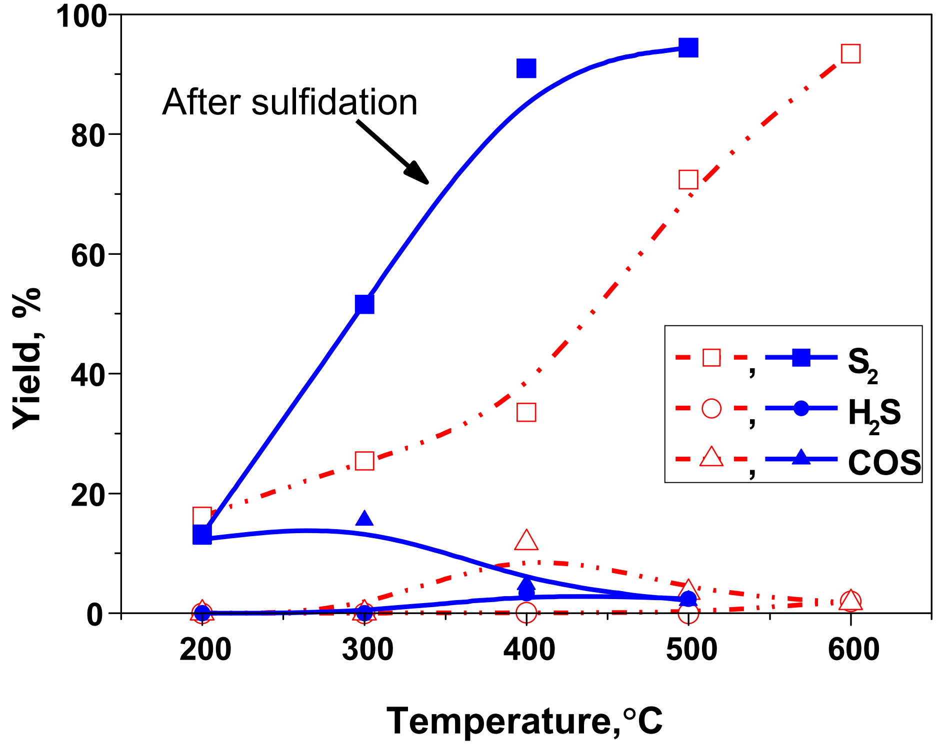
Change of sorption capacity of Fe-Mn samples to sulfur dioxide upon wetting

Fig. 84

DEVELOPMENT OF A CATALYST FOR LOW-TEMPERATURE SULFUR DIOXIDE REDUCTION

Studies of the catalytic activity in low-temperature reduction of sulfur dioxide with synthesis gas revealed that the developed Fe-Mn catalysts provide the sulfur yield no less than 90 % at 550°C.

Pretreatment of initial samples with hydrogen sulfide (sulfidation) improves substantially their catalytic performance. Sulfur yield ≥ 90% is reached at temperature 400°C.



Effect of presulfidation on catalytic characteristics of Fe-Mn catalysts in reaction of sulfur dioxide reduction with synthesis gas: open symbols – sample in oxide form, solid symbols – sample in sulfide form

Fig. 85

A CATALYST FOR THE EFFICIENT PROTECTIVE BED IN A CLAUS REACTOR

Previous result: Requirement for producing of efficient catalyst for protective bed is formation of FeS_2 /Al_2O_3

Purpose: To clarify the effect of treatment temperature and composition of promoters on formation of Fe sulfide (reactor for Claus process is preheated in the flow of smoke fumes at 200-250°C)

- Elevation of drying temperature of Fe/Al_2O_3 samples from 100 up to 250°C increases the stability to sulfidation and prevents synthesis of active catalyst for the protective bed directly in reactor
- Introduction of additional component – Ni – provides the formation of sulfide phases independently of drying temperature

Activity in reaction of COS hydrolysis

(T- 280°C; composition of the mixture, vol.%: H_2S – 3, COS - 1,

Catalyst	Initial salt	Drying temperature, °C	COS conversion,%	
			1 h	6 h
Fe/Al_2O_3	$FeSO_4$	110	59	61
Fe/Al_2O_3	$FeSO_4$	250	12	11
Ni/Al_2O_3	$Ni(NO_3)_2$	250	43	40
Fe-Ni/Al_2O_3	$NiSO_4$	$NiSO_4$	57	56

The chemical composition of the efficient catalyst for protective bed, providing formation of active phase directly in reactor was developed

Formation of the active component of the catalyst for protective bed:

- impregnation of Al_2O_3 granules with Fe, Co, Ni salts;
- drying in air at 110 or 250°C;
- treatment under conditions of the second catalytic converter:

T - 220°C; composition of the mixture, vol.%: H_2S - 3, SO_2 – 1.5; H_2O - 30

Dependence of O_2 and H_2S conversion on interaction time with reaction mixture

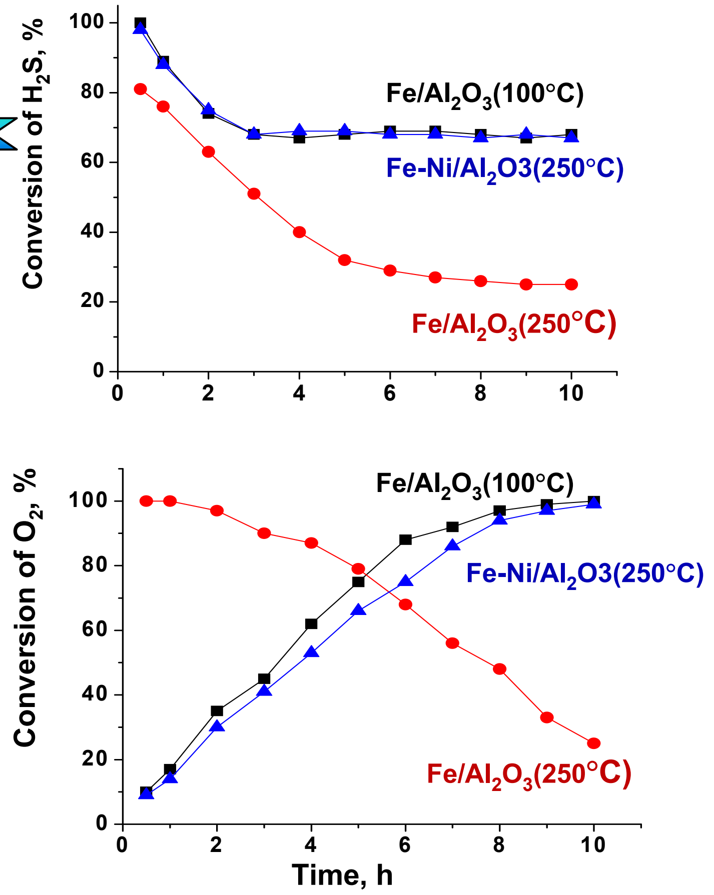


Fig. 86

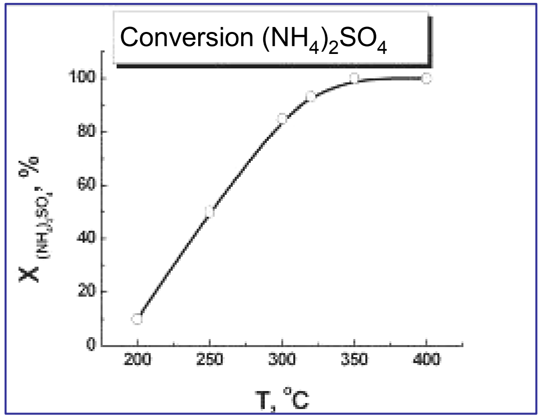
DEVELOPMENT OF A PROCESS FOR FINE PURIFICATION OF GASES FROM SULFUR DIOXIDE TO GIVE ELEMENTAL SULFUR

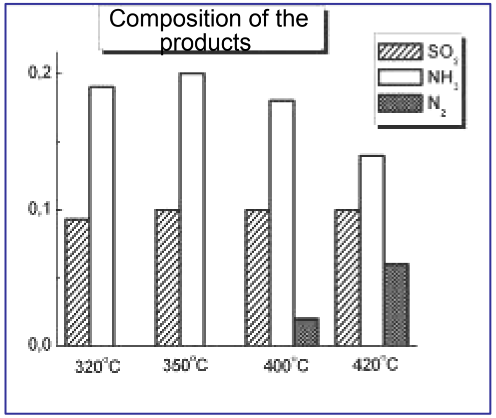
Thermal decomposition of $(NH_4)_2SO_4$ solution in the presence of CO

- $(NH_4)_2SO_4 \rightarrow NH_4HSO_4 + NH_3$
- $NH_4HSO_4 + CO \rightarrow NH_3 + SO_2 + CO_2 + H_2O$
- $3NH_4HSO_4 \rightarrow NH_3 + 3SO_2 + 6H_2O + N_2$

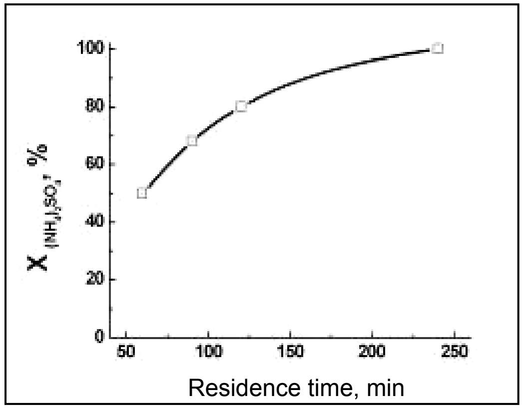
Temperature region – 300-400°C
Molar ratio $CO/(NH_4)_2SO_4 \geq 1$;
Residence time – not less than 240 min

Effect of temperature





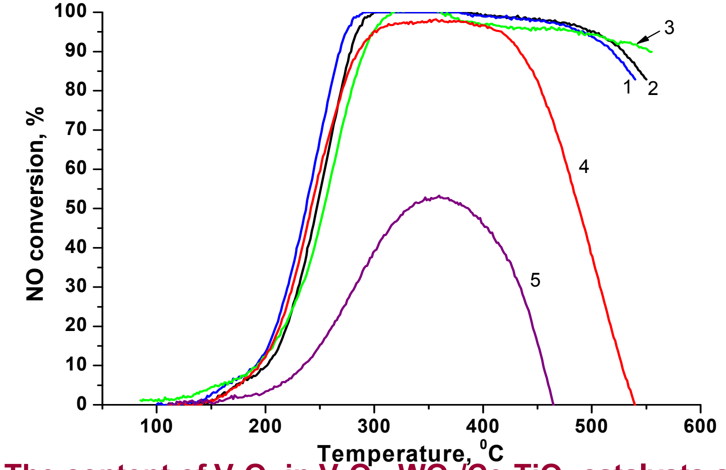
Effect of concentration

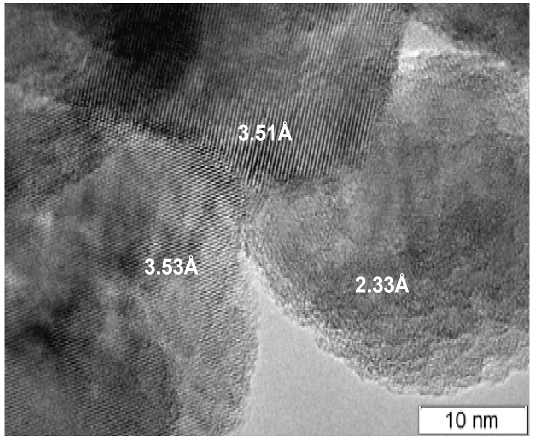


- ❑ Conditions were determined to ensure complete conversion of NH_4HSO_4 and close to stoichiometric yield of ammonia
- ❑ It was shown that the thermal decomposition of concentrated $(NH_4)_2SO_4$ solutions can be used as the stage of regeneration of absorption solution in the process of fine purification of gases from sulfur dioxide while preserving NH_3, which can be reused in the process of absorption of sulfur oxides

Fig. 87

CATALYTIC PROPERTIES AND STRUCTURE OF V_2O_5, WO_3/Ce-TiO_2, V_2O_5, WO_3/Y-TiO_2 CATALYSTS IN THE deNOx REACTION WITH AMMONIA





The structure of V_2O_5, WO_3/Ce-TiO_2 catalyst is nanocrystalline with surface forms of vanadium oxide, stabilized at the interblock boundaries formed by anatase crystallites

The content of V_2O_5 in V_2O_5, WO_3/Ce-TiO_2 catalysts affects the catalytic activity: the activity at 1–2 wt % V_2O_5 (1–3), 5 wt % V_2O_5 (4) and 10 wt % V_2O_5 (5).

The catalysts containing 1–3 wt % V_2O_5 are highly active and thermostable in the reaction medium at high temperature (X = 97% at 500°C)

(Composition of the reaction mixture: *80000 h^{-1}, [NO] - 500 ppm, [NH_3] - 500 ppm, [O_2] -10% vol., [H_2O] -. 5,0% vol, [He] – the rest*)

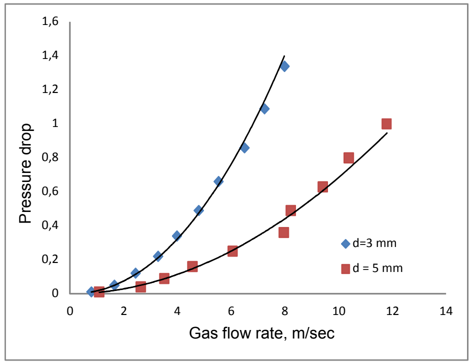
Effect of vanadium content on phase composition and catalyst structure

Catalyst, wt%	Phase composition	ACD, nm	Spacing parameter of anatase, A		S, m²/g
			a	*c*	
1% V_2O_5 3-5%WO_3/Ce-TiO_2	Anatse	15	3,783	9,506	47-52
1% V_2O_5 5%WO_3 /Y-TiO_2	Anatse	17	3.781	9.507	51
2% V_2O_5 5%WO_3 /Ce-TiO_2	Anatse	20	3,785	9,507	42
5% V_2O_5 5%WO_3 /Ce-TiO_2	Anatse, $CeVO_4$	20	3,787	9,507	41
10% V_2O_5 5%WO_3 /Ce-TiO_2	Anatse, rutile,V_2O_5	45	3,787	9,507	9

Fig. 88

TECHNOLOGICAL APPROACH TO OXIDATION OF SO_2 IN THE REVERSE-FLOW REGIME

Pressure drop in glass-fiber catalyst cartridges was studied experimentally. The obtained empirical dependences allow the pressure drop to be predicted for various type packages of microfibrous catalyst over a wide range of conditions



A 500 W fuel cell for gas fuel (propane-butane) was designed based on a platinum glass-fiber catalyst with an extra alumina support (IHP SB RAS), assembled and tested successfully

A reverse-process based on a platinum glass-fiber catalyst on a Zr-Si support was proposed for oxidation of SO_2 in the presence of CO. The process allows the conversion of SO_2 to be increased considerably and the process stability to be improved at treatment of metallurgical waste gases with variable CO content

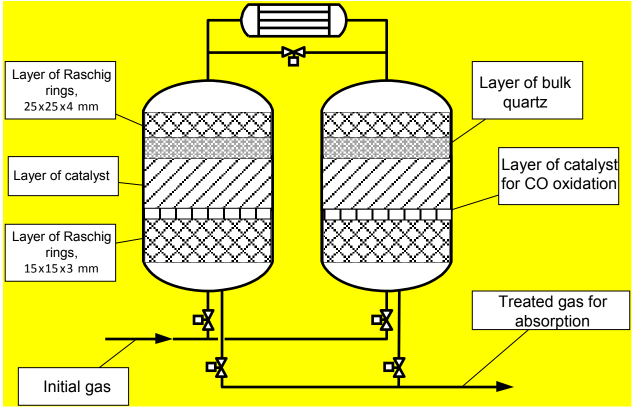
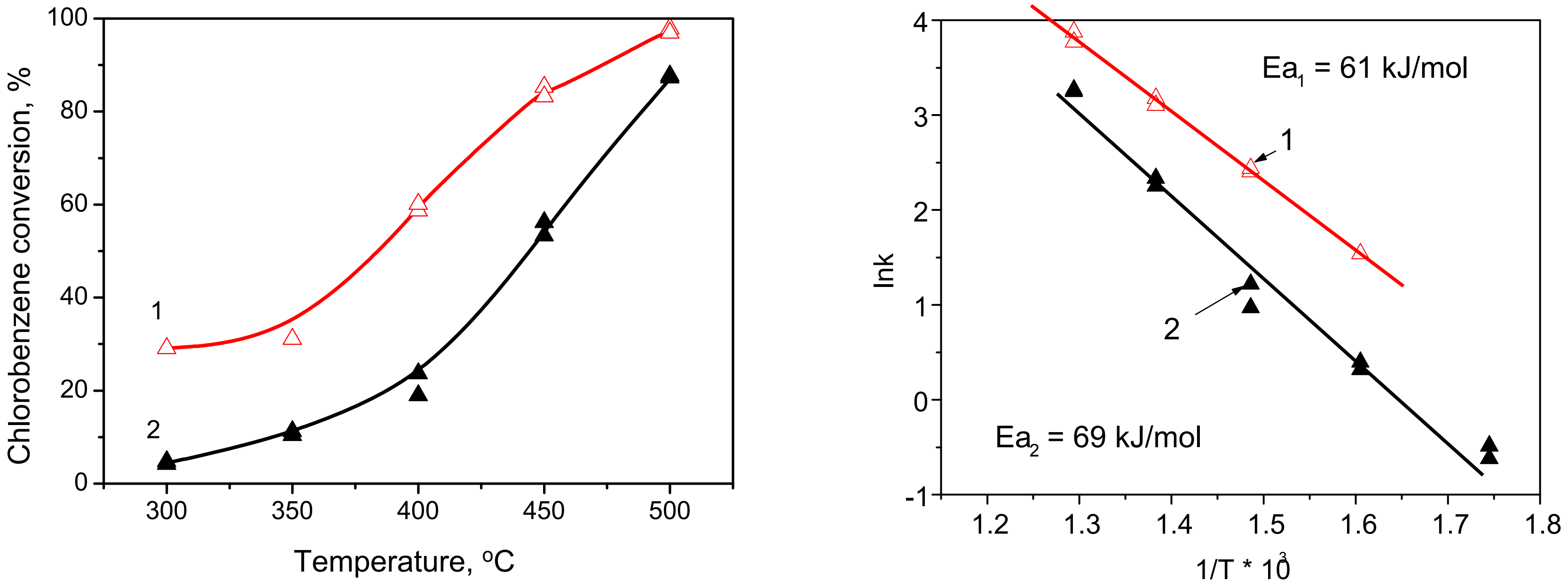


Fig. 89

STUDY OF NOVEL HIGH EFFICIENT CATALYSTS BASED ON URANIUM-CONTAINING COMPOUNDS

The influence of preparation conditions on the properties of Cr-U-Al_2O_3 catalysts in the reaction of chlorobenzene oxidation



	Catalyst	Phase composition	Ssp., m^2/g
1. Incipient wetness impregnation	$7Cr/7U/Al_2O_3$ impregnated	-γ-Al_2O_3 -$Cr_2U_2O_9$ -$UCrO_4$	97
2. Solid-phase mixing	$7Cr/7U/Al_2O_3$ solid phase	-γ-Al_2O_3	175

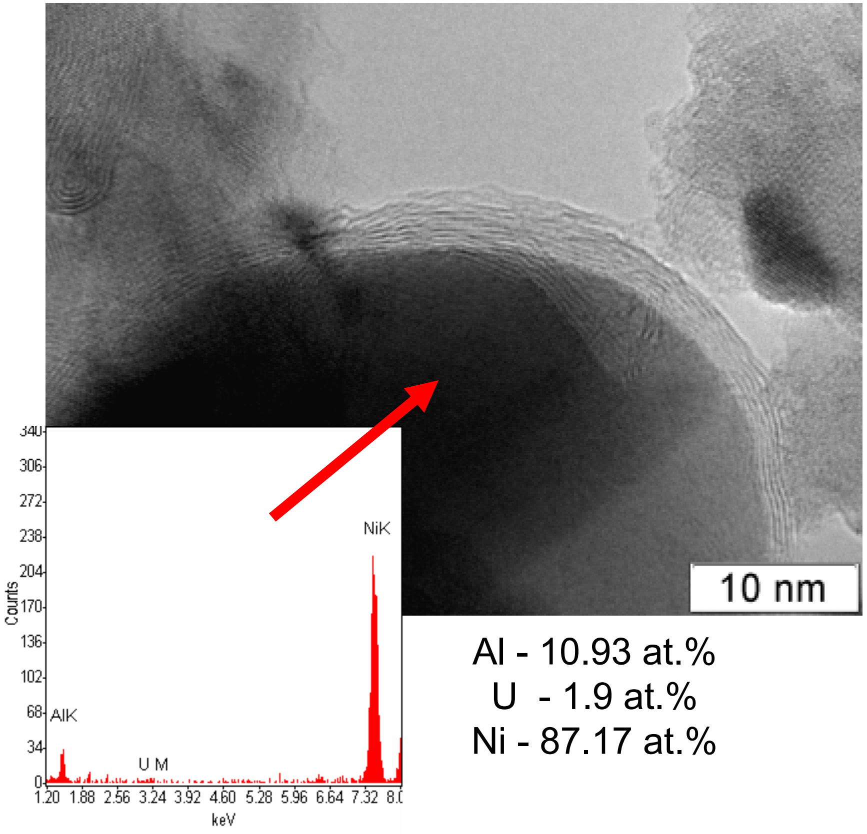
Conditions: chlorobenzene concentration – 2 g/m^3,
volumetric flow rate – 45000 h^{-1}

Fig. 90

STUDY OF NOVEL HIGH EFFICIENT CATALYSTS BASED ON URANIUM-CONTAINING COMPOUNDS

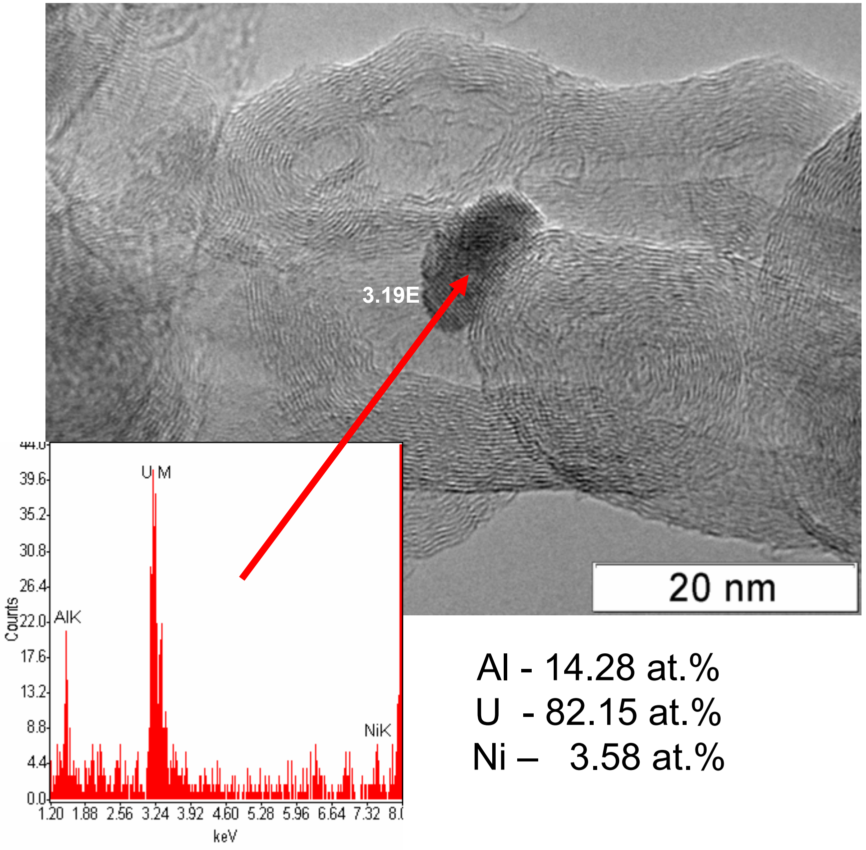
Micrographs of 10Ni-15U-Al_2O_3 catalyst after reaction of steam methane conversion

Metal Ni particle covered with carbon layers



Al - 10.93 at.%
U - 1.9 at.%
Ni - 87.17 at.%

Uranium oxide particle preserves stable catalytic activity

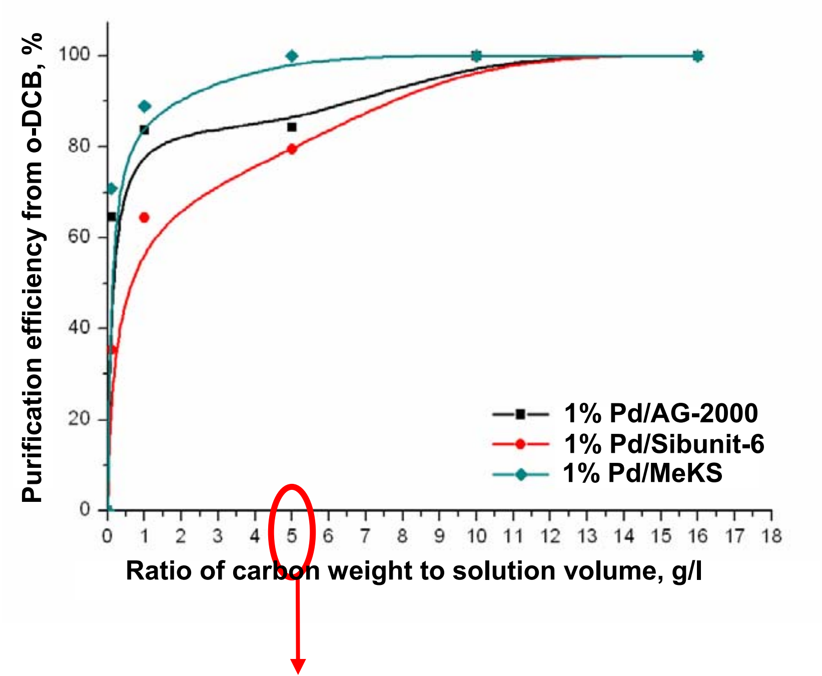


Al - 14.28 at.%
U - 82.15 at.%
Ni – 3.58 at.%

Fig. 91

REGENERATION OF CARBON-BASED CATALYSTS-ADSORBENTS BY HYDRODECHLORINATION

Study of adsorption conditions of o-DCB on the recovery rate from water

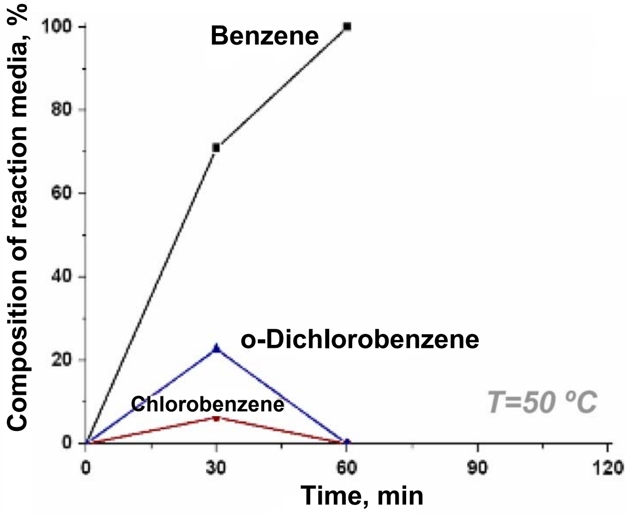


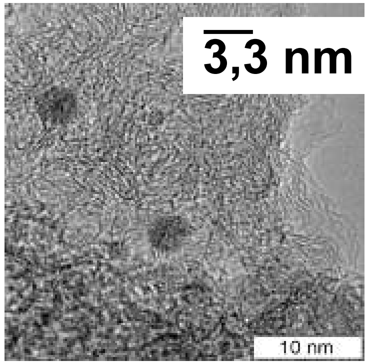
Adsorption time, min	Purification efficiency, %		
	AG-2000	Sibunit-6	MeKS
1	99,3	98,9	99,5
5	99,4	98,5	99,1
20	99,3	98,0	99,1
60	99,1	97,4	98,2

Regeneration of catalysts-adsorbents by hydrodechlorination of adsorbed o-DCB

1% Pd/MeKS

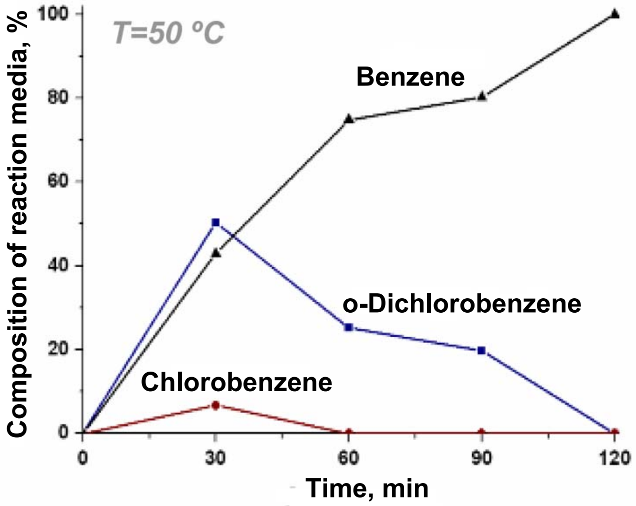
with 0,299 $cm^3_{o\text{-}DCB}/g_{cat}$





1% Pd/Sibunit-6

with 0.289 $cm^3_{o\text{-}DCB}/g_{cat}$



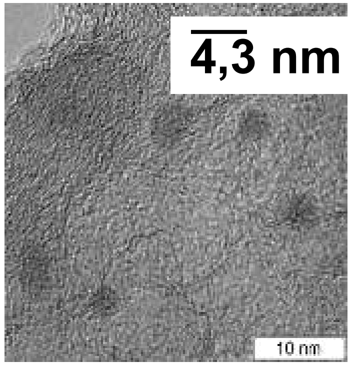
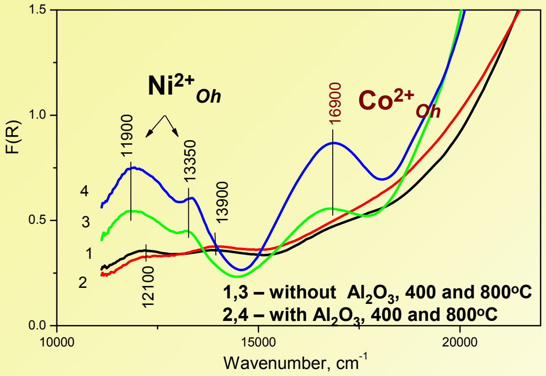


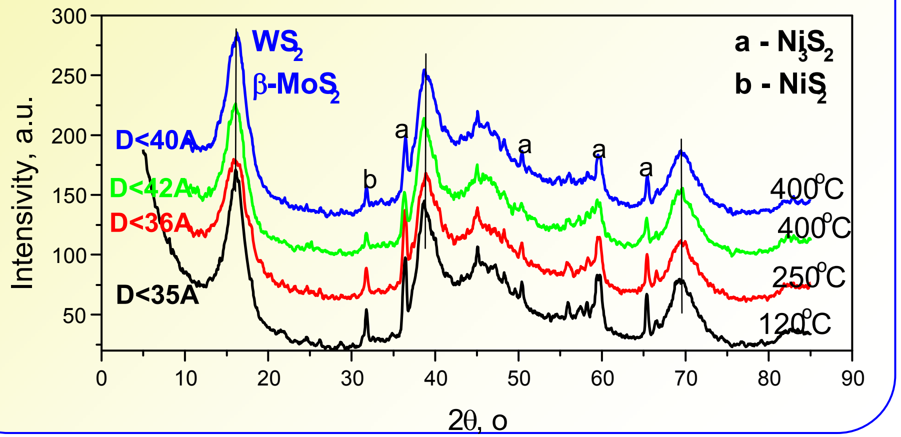
Fig. 92

DELIBERATE SYNTHESIS OF NANOSTRUCTURED CATALYSTS BASED ON MOLYBDENUM SULFIDE

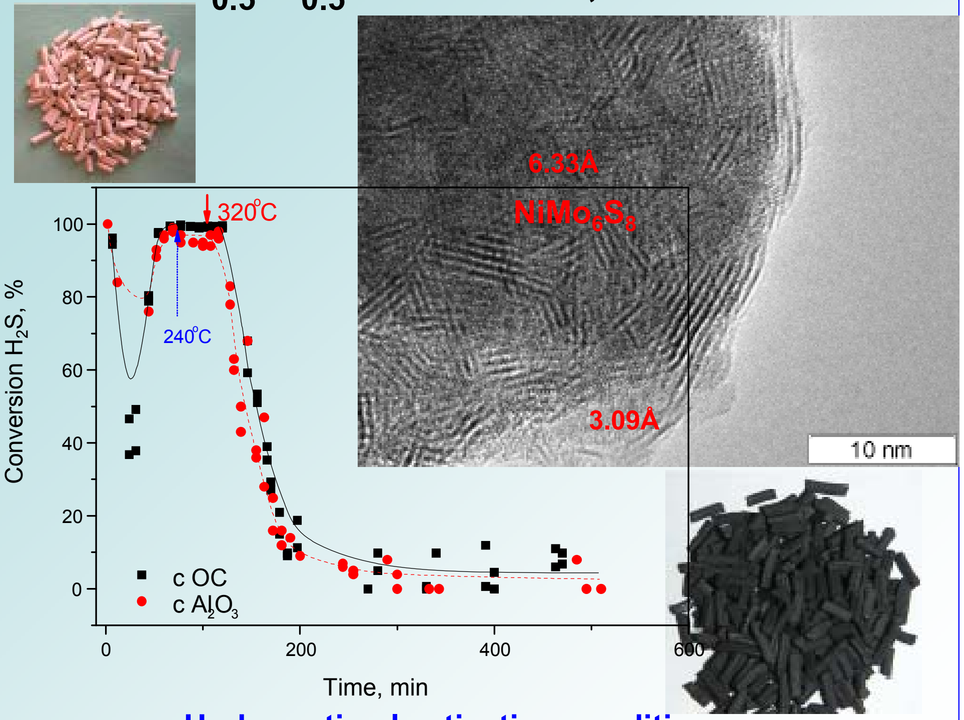


The conditions of extrusion and oxidative treatment were chosen to prevent the formation of $NiAl_2O_3$ and $CoAl_2O_4$

Crystallogram of extrudates Mo(W)-Ni with organic binding agent (curves 1-3) and Al_2O_3 (curve 4), activated at 400°C. Temperature of oxidative treatment is shown



$NiMo_{0.5}W_{0.5}$- sulfide form, 320°C



Under optimal activation conditions:

Mo(W)-Ni-S particles 5-10 nm in size, OKD < 4 nm

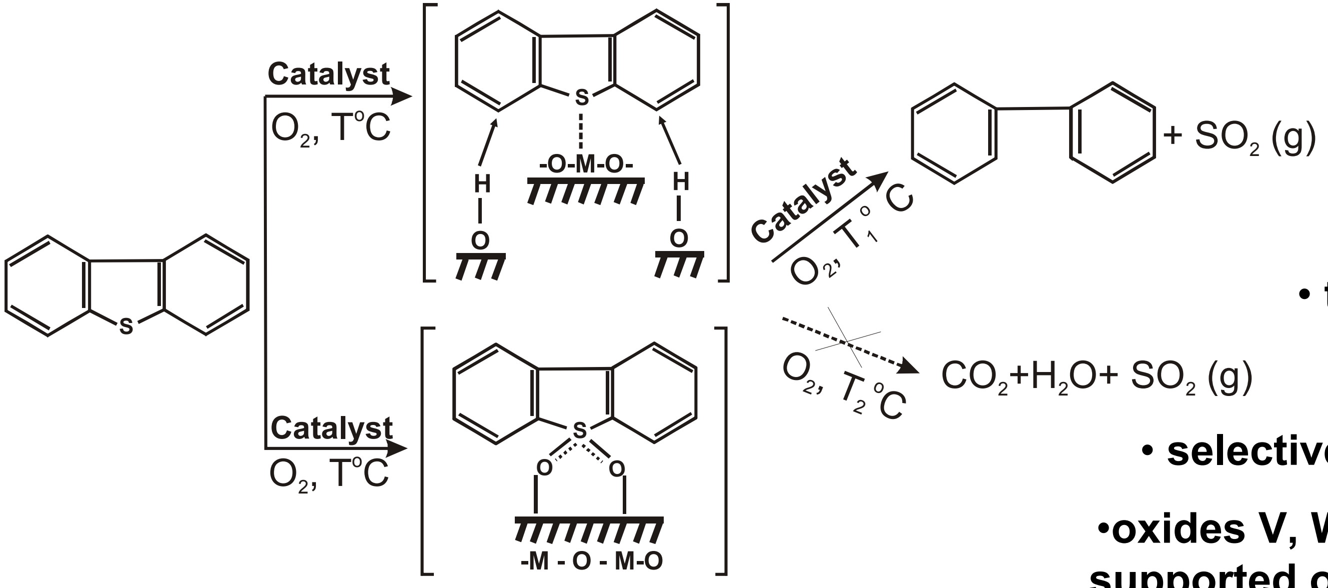
Structure is close to MoS_2 with d/n = 6.23-6.41 A

Surface area – 7-22 and 40-50 m²/g without and with Al_2O_3 bond

In the extrudates, the chemical composition, structure and size of Ni-doped Mo(W)S_2 nanoparticles are influenced by conditions of Mo(W)-Ni synthesis, temperatures of oxidative treatment and sulfide activation, while the textural and strength characteristics depend on the nature and proportion of the binder

Fig. 93

STUDIES OF OXIDATIVE DESULFURIZATION OF HYDROCARBON FUELS



Reaction conditions:

- **atmospheric pressure**
- **temperatures 180 - 400°C**
- **oxidants O_2, O_3, air**
- **selective heterogeneous catalyst**
- **oxides V, W, Mo, Mn, Co, Fe, Cu, Ce supported on Al_2O_3, SiO_2, TiO_2, ZrO_2**

Advantages:

Alkyl-substituted dibenzothiophenes are more readily oxidized

Disadvantages:

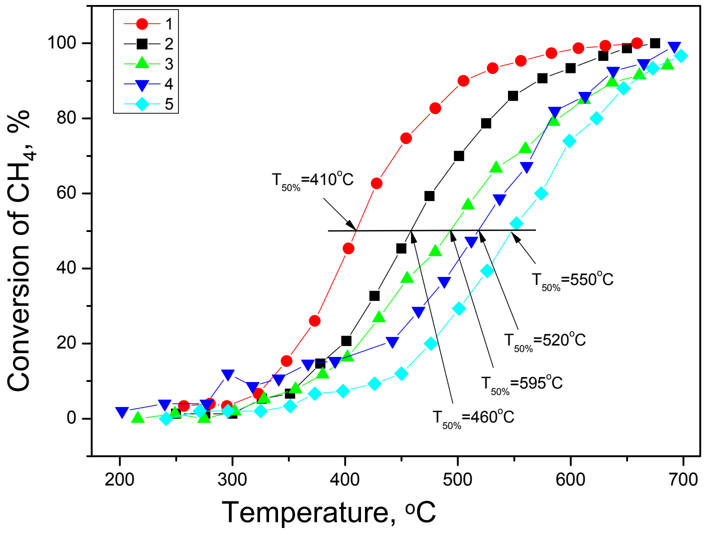
There are side reactions of hydrocarbon oxidation which can be eliminated through the process and catalyst optimization:

$O_2/C = 0.003\text{-}0.1$; $O_2/S = 20 – 150$; GHSV = 5000 – 20000 h^{-1}

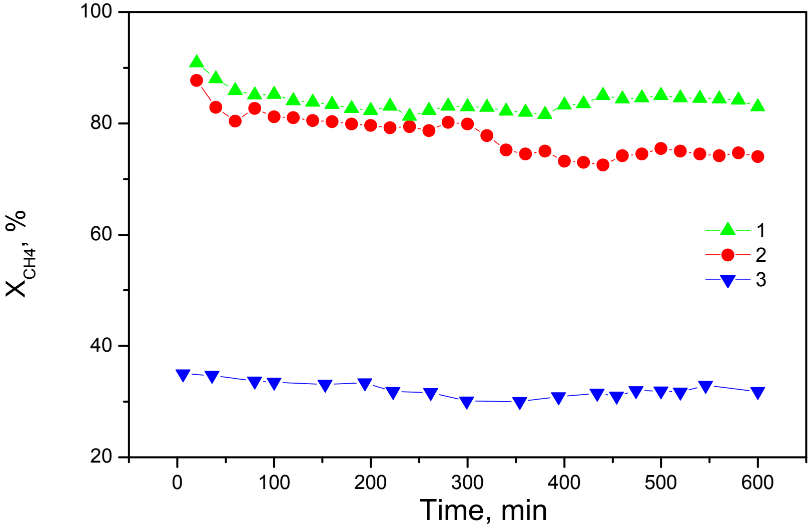
Fig. 94

STABILITY OF BIMETAL Pt-Pd-CATALYSTS BASED ON MnO$_x$, MnLaAl$_{11}$O$_{19}$ IN THE REACTION OF METHANE OXIDATION

1 об.% CH$_4$, V=24000 h^{-1}



1 об.% CH$_4$, V=250 000 h^{-1}



Catalysts Pt-Pd-MnLaAl$_{11}$O$_{19}$ 1000°C

1 – from nitrate Pt/Pd=0.1
2 – from nitrate Pt/Pd=0.5
3 – from chloride Pt/Pd=0.05
4 – from chloride Pt/Pd=0.5
5 – from chloride Pt/Pd=1

- Increasing activity

Catalyst Pt-Pd-MnLaAl$_{11}$O$_{19}$ Pt/Pd=0.1

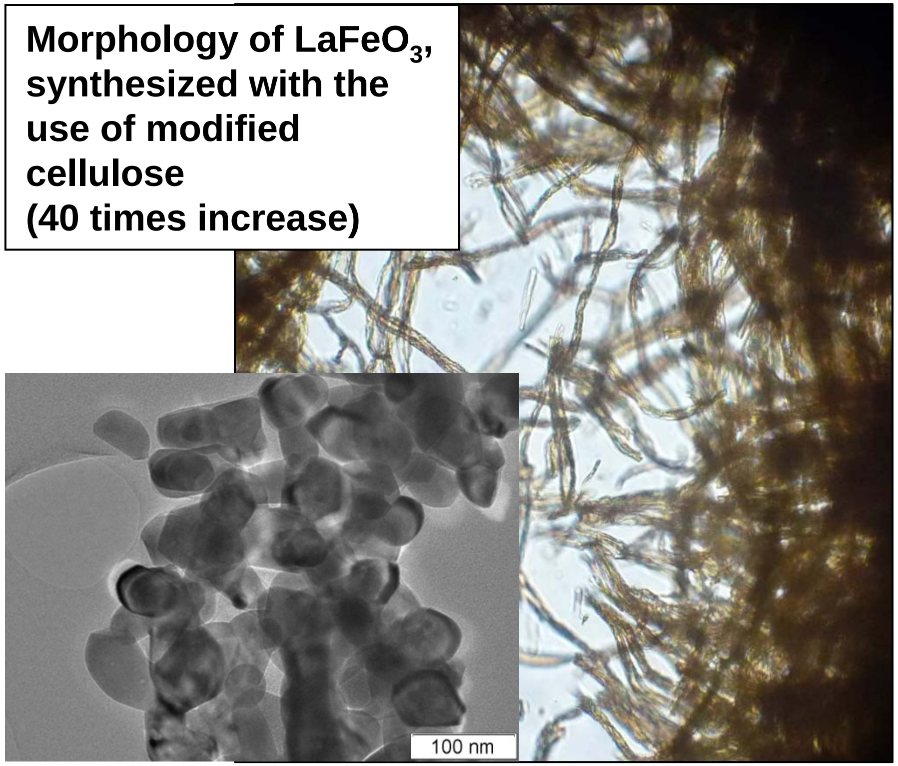
1 — from nitrate 900°C
2 — from chloride 900°C
3 — from nitrate 1000°C

Fig. 95

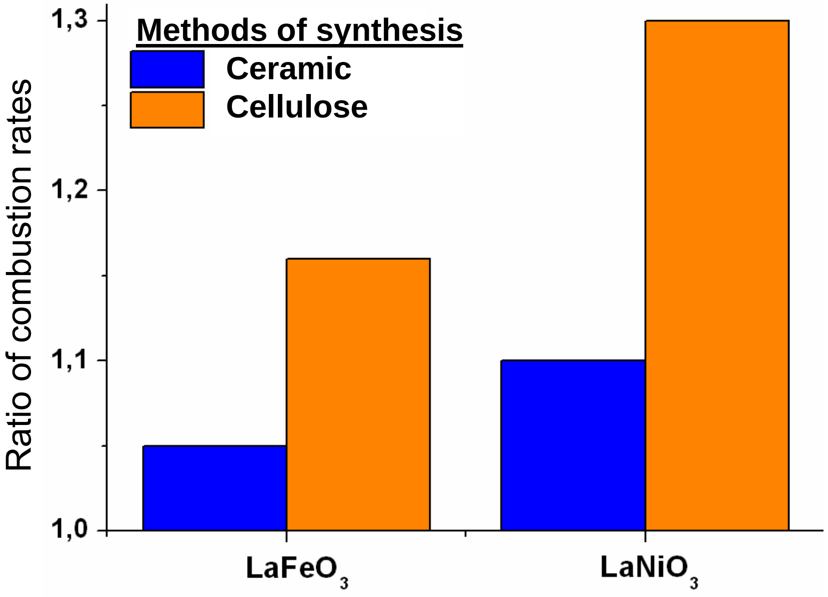
SYNTHESIS OF PEROVSKITE CATALYSTS WITH MODIFIED CELLULOSE USED AS A STRUCTURE-FORMING AGENT

A method for synthesis of perovskite catalysts was developed with modified cellulose used as a structure-forming agent that prevent aggregation and sintering of the perovskite particles

An increase in dispersion of perovskites leads to a significant increase in the combustion rate of model high-energy compounds at atmospheric pressure



Morphology of $LaFeO_3$, synthesized with the use of modified cellulose (40 times increase)



The factors that influence the rate of gas generation during thermolysis of ammonia borane based compositions were revealed

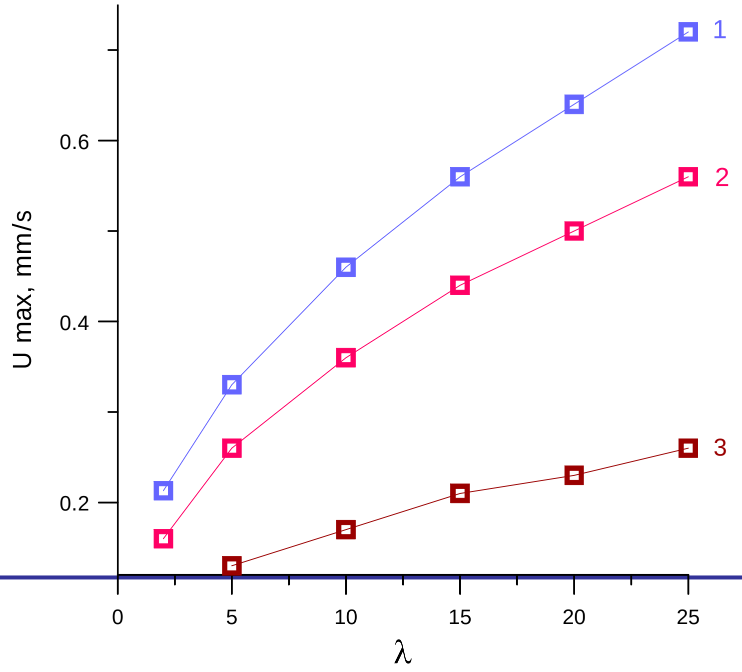
Fig. 96

SIMULATING THE CATALYTIC PROCESS OF GAS GENERATION FROM SOLID FUEL MATERIALS

New mathematical models were developed for predicting possibility of catalytic methods for controlling the processes of burning and thermal decomposition of solid fuel by contact catalysis

It was shown that the maximal achievable rate of the monolith motion depends on its heat conductivity and shape

Maximal achievable rate of the monolith motion U upon gas generation as function of heat conductivity λ [W/(m K)] for various monoliths



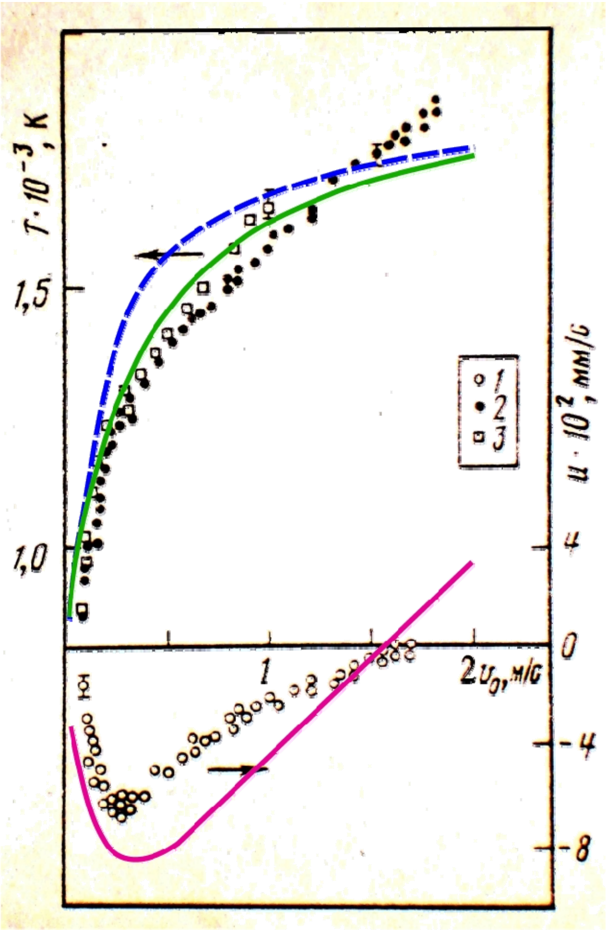
<u>Monolith 1</u> – channel diameter – 1.2 mm, wall thickness – 0.255 mm

<u>Monolith 2</u> – channel diameter – 2 mm, wall thickness – 0.8 mm

<u>Monolith 3</u> – channel diameter – 5 mm, wall thickness – 2 mm

Fig. 97

MATHEMATICAL SIMULATION OF COMBUSTION PROCESSES IN THE CATALYST FIXED-BED



HYBRID AUTOWAVES

Dependence of wave velocity, maximal gas and catalyst temperature on filtration gas rate. Mixture 3% of propane in air

Literature data

Babkin V.S., Barannik G.B., Ismagilov Z.R., Laevskii Yu.M., Potytnyakov S.I. Hybrid heat wave upon filtration gas combustion // Doklady AN SSSR. - 1989. -V. 304. -№ 3. - P. 630-633.

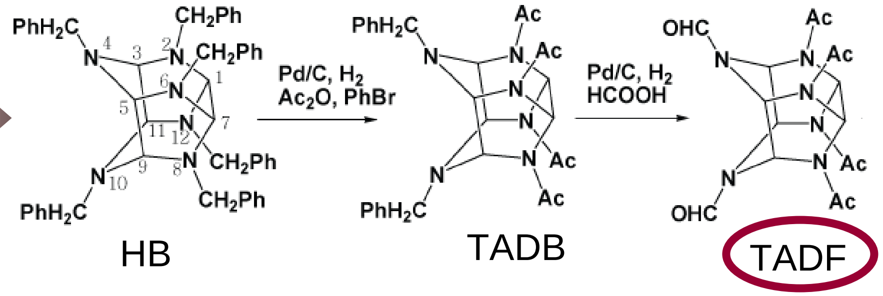
Design data, according to selected model

1 – Wave velocity (*u*), unbroken red curve
2 - T_{max} catalyst, unbroken green curve
3 - T_{max} gas, dotted blue curve

Fig. 98

SYNTHESIS OF NANODISPERSED Pd-CONTAINING CATALYST STABLE TO DEACTIVATION

Schematic of 2-step catalytic synthesis of TADF



Stage 1. Synthesis of catalyst series A and B:

A. **Pre-supporting of a metal as a ‘heat sink’ to weaken heat stress of the active centers of the TADF synthesis catalysts due to an increase in the heat transfer towards the catalyst bulk:**

5% Cu + 6% Pd B/ Sibunit
5% Sn + 6% Pd B/ Sibunit
5% Ag + 5% Pd B/ Sibunit
5% Ag + 8% Pd B/ Sibunit

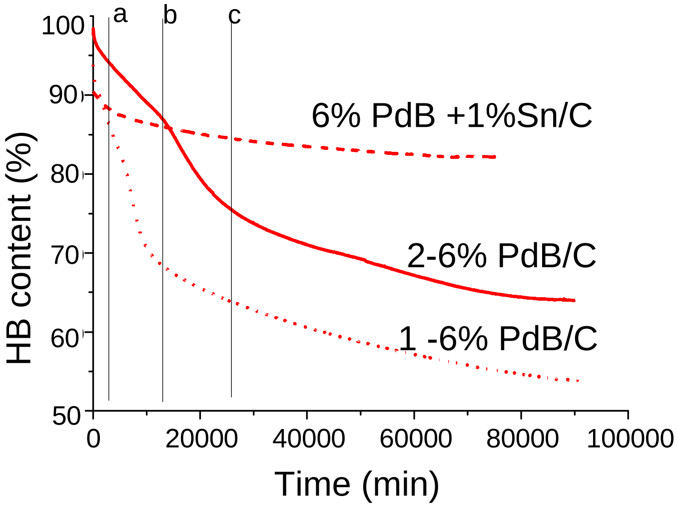
B. **Supporting of heteroatoms on the prepared Pd B/ Sibunit matrix to weaken heat stress of the active centers of the TADF synthesis catalysts due to an increase in the heat transfer to the solution:**

6% Pd – B + 1% Cu/ Sibunit
5% Pd – B + 1% Sn/ Sibunit

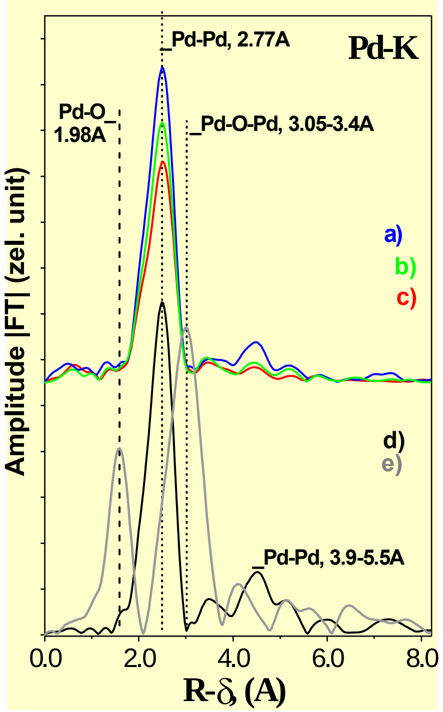
When high heat-conducting metals are introduced in the active component of Pd/C catalysts, they provide heat extraction from the active palladium atoms; as a result, processes of NADF synthesis are inhibited. A supposed reason for such an effect is the impossibility of the formation of soluble bromated palladium carbonyls at low reaction temperatures.

Fig. 99

Stage 2.



The product yields are shown to decrease over active PdB/C catalysts. The cycle-by-cycle increase in the induction period (indicated by curves *a* and *b* for cycles 1 and 2, respectively) is accompanied by a decrease in the yield of the target product



EXAFS

PPA (RDFs) local palladium surrounding (EXAFS spectra):

a) sample PdN

b) samplePdC

c) sample PdB

d) Pd foil

e) PdO

Summary

- Changes of the peak intensities in relevant EXAFS spectra indicate a decrease in the crystal ordering of the active centers structures at an increase in the catalyst stability in the series:

PdN>PdC>PdB

- The most stable TADF synthesis catalysts are Pd–B compositions containing, supposedly, palladium metal glass as the active component.

- A change in the catalytic activity of PdC and PdB observed upon introduction of high heat conducting components (Ag, Cu, Sn) is an evidence that the reaction of TADF synthesis proceeds under conditions of overheating of the catalyst active centers.

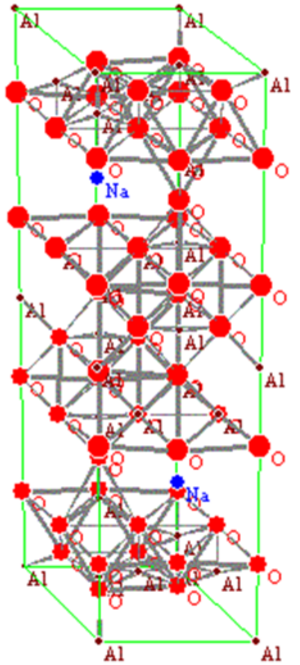
Fig. 100

Ba-CONTAINING CATALYSTS FOR TRANSESTERIFICATION OF RAPESEED OIL

Comparative activities of various heterogeneous catalysts for interesterification in flow conditions

Catalyst	oil (TG FA)	T, ºC	P, atm	alcohol : TG FA molar ratio	Conversion of TG FA, %	Ref.
WO_3/ZrO_2	soy	250	1	(methanol) 40:1	90	1
TiO_2	soy	360	170	methanol) 33:1	88	2
$CaCO_3$	soy	260	35	(ethanol) 6:1	95	3
MnO	sunflower	260	89	(methanol) 30:1	98	4
Ba-Al-O	colza	228	30	(methanol) 9:1	90	Native results

Crystal structure of barium hexaaluminate (Ba-Al-O) – magnetoblumbite and β-Al_2O_3



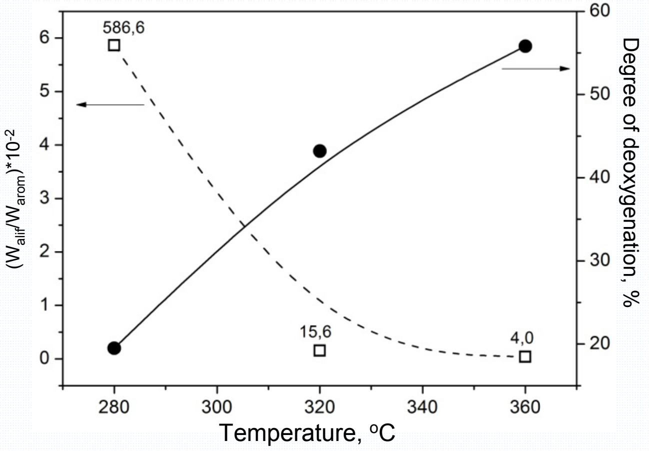
The $BaAl_{12}O_{19}$ catalyst kepts its activity for 60 h. After regeneration (calcination at 500°C in O_2-containing gas mixture) the catalyst kept its activity during the next 50 h. XPS, BET and X-ray studies of the regenerated catalyst do not reveal any changes in the catalyst structure and surface composition

Fig. 101

DEOXYGENATION OF LIQUID PRODUCTS OF BIOMASS PYROLYSIS

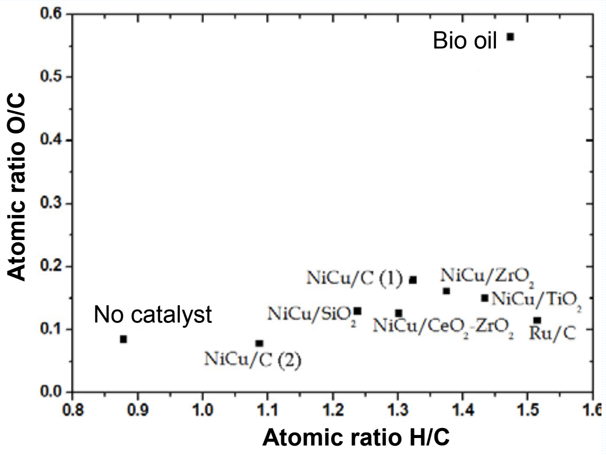
Kinetic peculiarities and the reaciton mechanism of deoxygenation of liquid products of biomass pyrolysis:

The effect of temperature on the products yield of guaiacol hydrodeoxygenation ($W_{Aliphatic}/W_{Aromatic}$) (□) and degree of HDO, % (●). Reaction time – 35 min., P(T_{react}) = 17 MPa.



The effect of the support nature on the activity and selectivity of the catalysts in the reaction of deoxygenation and their stability to leaching:

Van Krevelen diagram for the products of bio oil HDO over NiCu catalysts at pressure 11 MPa and temperature 150°C (1 hour) and 350°C (3 hours)



The effect of the active component composition on the activity and selectivity:

With an increase in the Ni content in $NiCu/Al_2O_3$ the ratio H/C and O/C in the reaction products of bio oil HDO increases. An increase in the H/C ratio is an evidence for the increasing activity to hydrogenation, the same effect was observed at hydrodeoxygenation of anisole.

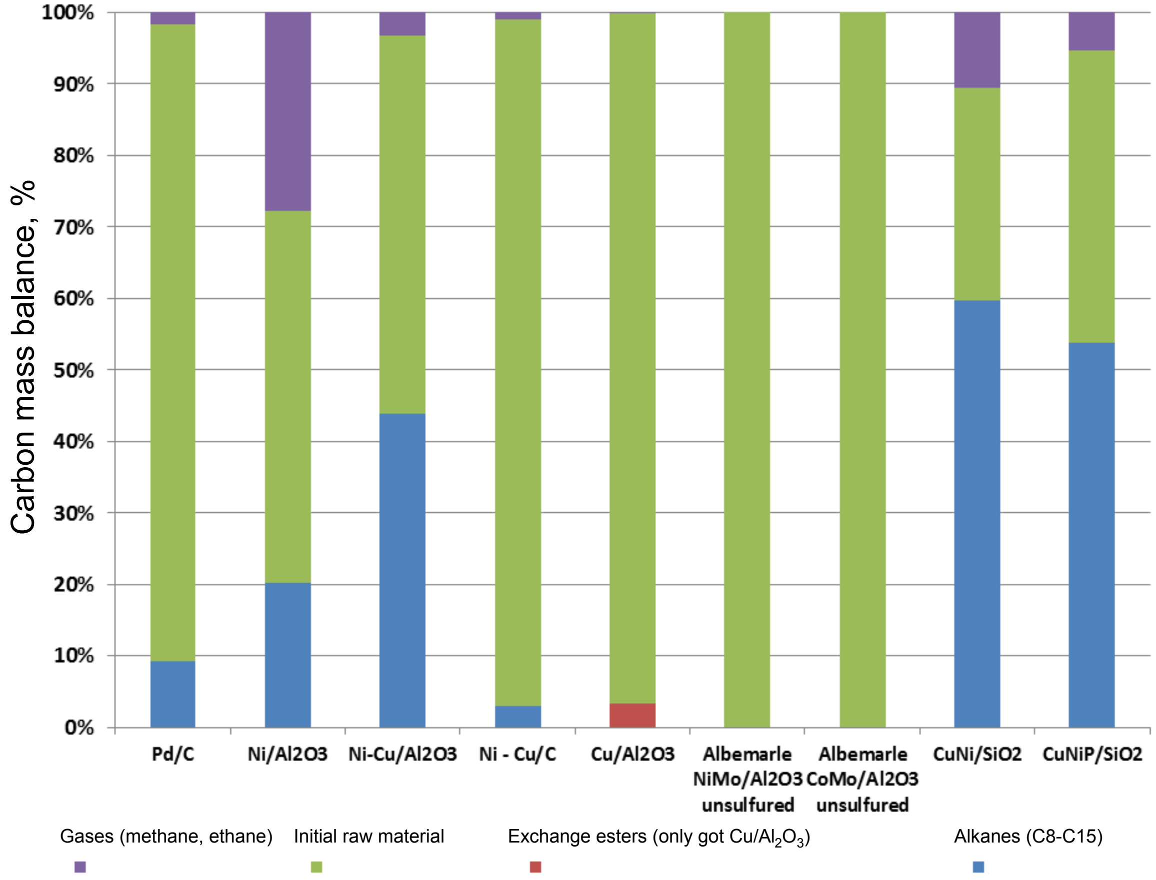
The effect of th eactive component composition on the stability to leaching:

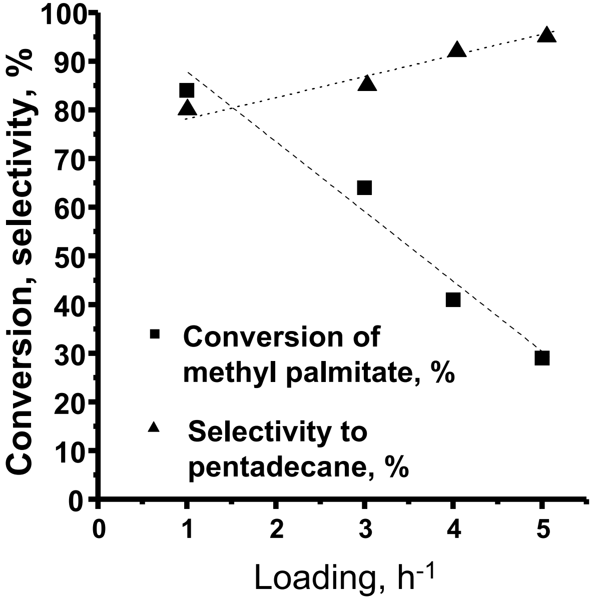
	Degree of leaching (% wt)	
	Ni	Cu
*20.8*Ni	0.5	0
*16*Ni2Cu	0.3	0
*13.8*Ni*6.83*Cu	0.6	0.3
*13.3*Ni*11.8*Cu	0.8	0.5
*5.92*Ni*18.2*Cu	2.9	1.1
*24.5*Cu	0	0

Fig. 102

DEVELOPMENT OF SYSTEM FOR SCREENING AND ISOLATION OF PROSPECTIVE MICROALGAE STRAINS

Catalysts were tested in the reaction with model compounds and under the effect of glacial acetic acid. CuNi/SiO_2 possesses optimal properties: active enough, the mass lost after treatment with acetic acid is minimal



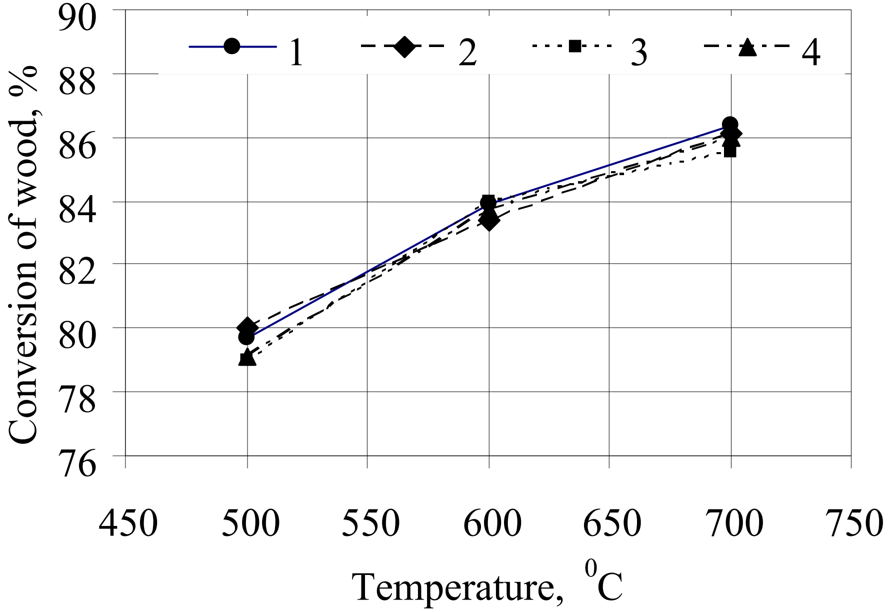


Upon variation of loading in the range 1-5 h^{-1} decrease of methyl palmitate conversion is observed, but selectivity to pentadecane increases

Experiments on hydrocracking of lipid fraction of microalgae (*Botryococcus braunii*) in the presence of catalyst NiCuP/SiO_2 were conducted in an autoclave at temperature 250^0C and initial hydrogen pressure 80 atm. After the experiments the reaction products were analyzed using chromato-mass-spectrometry. Normal alkanes C14–C18 were obtained

Fig. 103

THERMAL OXIDATIVE PROCESSING OF MUNICIPAL SLUDGE, HYDROLYSIS AND PULP AND PAPER INDUSTRY



Wood conversion into gaseous products (gas fuel, water, resins)

1 – catalyst IC-12-73;
2 – catalyst IC-12-72;
3 - γ-Al_2O_3; 4 – sand

An experimental bench for studying the gasification process was assembled and started-up. The bench includes of a gasification reactor, solid fuel supplying system, waste gas cleaning system, cyclone re-burner, control system, air feeding systems, steam feeding system

The rate of wood thermal decomposition:

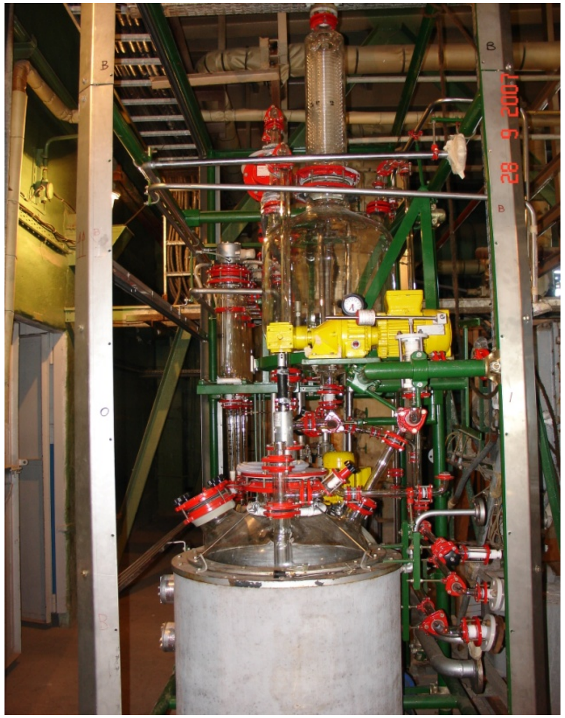
$$R = \frac{X}{t} = k \cdot (1 - X) \qquad k = A \cdot e^{-E_a / R \cdot T}$$

R –rate of pyrolysis; *X* – wood conversion;

k – constant rate; *t* – time of pine sawdust pyrolysis in reactor

Fig. 104

THERMODYNAMIC AND KINETIC REGULARITIES OF OXIDATION PROCESSES OF ALCOHOLS OVER BIFUNCTIONAL CATALYSTS



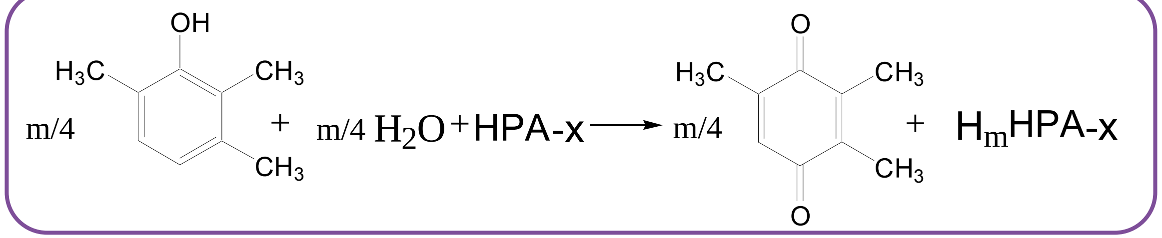
Glass reactor for conducting periodic processes Y 3000 of modular unit “Ufa 2”

Extraction and rectification of 2-acetonyloxy-3,4-difluoro nitrobenzene prototypes was realized in the “clean” facilities of Volgograd Division of BIC

Enameled reactor for conducting periodic processes Y 2900 B of modular unit “Ufa 2”

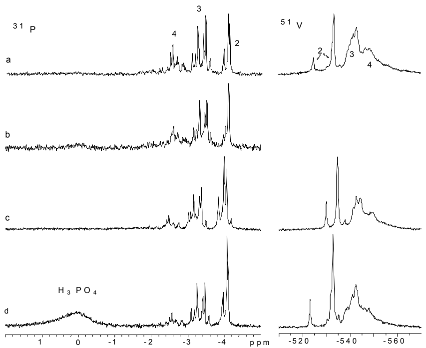
Fig. 105

KINETIC FEATURES OF TRIMETHYLPHENOL TO TRIMETHYLBENZOQUINONE OXIDATION



The best samples of modified HPA-catalysts:

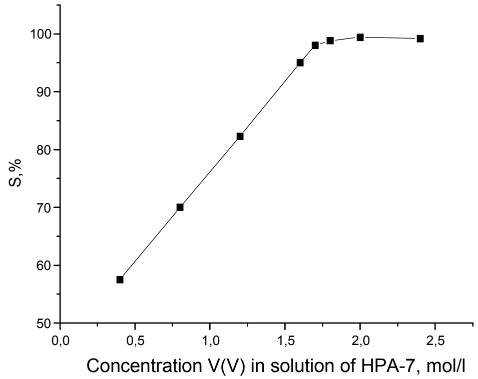
$H_{11}P_4Mo_{18}V_7O_{87}$ (HPA-7') and $H_{17}P_3Mo_{16}V_{10}O_{89}$ (HPA-10')



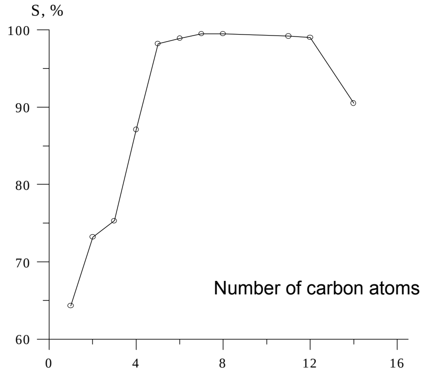
NMR ^{31}P and ^{51}V spectra of solutions of HPA-4 (0,1 (a) and 0,02 M (в)) and HPA-10' (0,1 (c) and 0,01 M (d))

In the presence of various solvents the selectivity decreases in the row: ***alcohols > n-carboxylic acids > esters, ketones > ethers.*** **Upper bound of S (>98%) is reached upon use of** ***primary non-branched alcohols***

Solutions of modified (non-Keggin) Mo-V-P HPA possess high hydrolytic stability, that permits their rapid regeneration at 170-180°C. This opens up possibilities for synthesis of high-technology catalysts for oxidation of TMP into TMQ



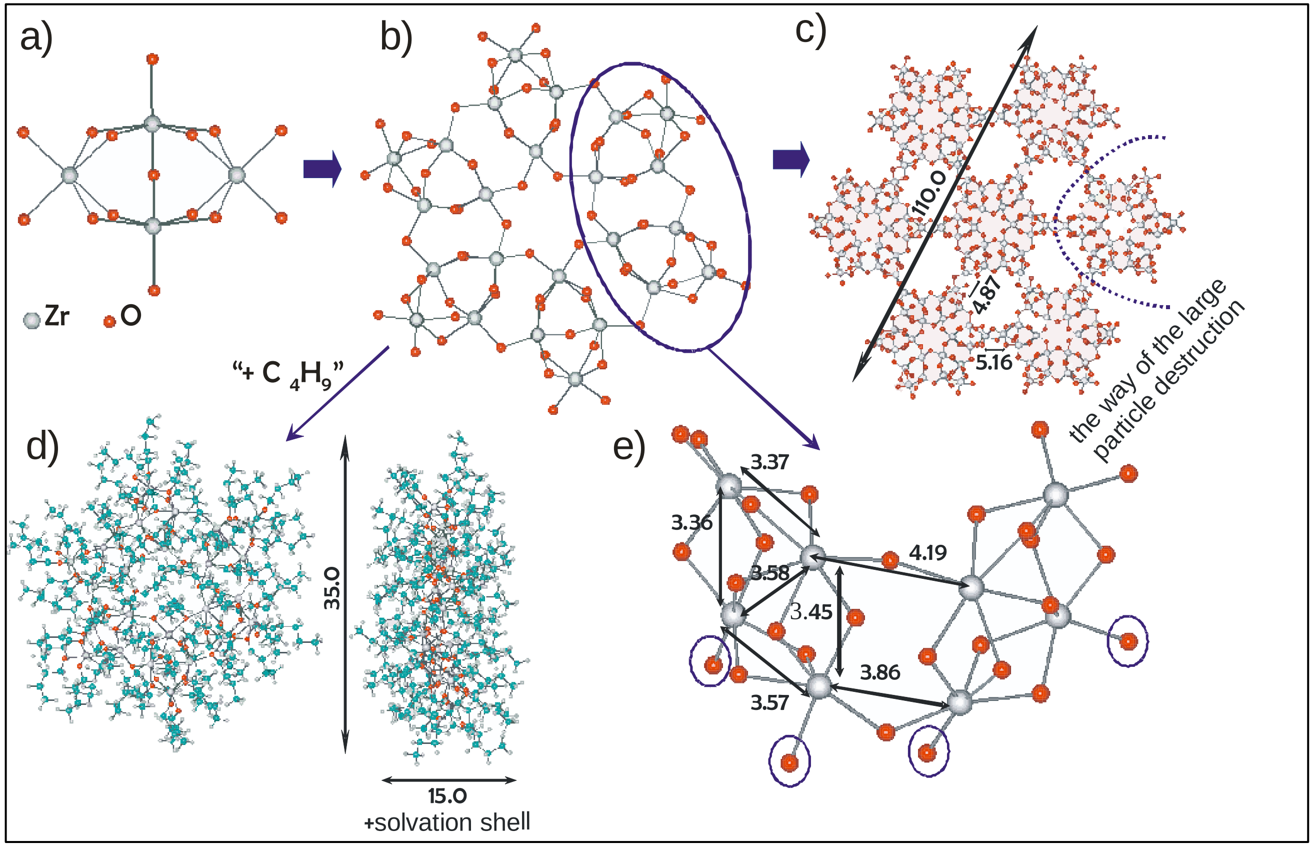
Dependence of selectivity of TMP oxidation to TMQ on concentration V(V) in solution of HPA-7'



Effect of number of C atoms in initial alcohol on selectivity TMP to TMQ oxidation at 60°C, in oxygen; HPA-8]/[TMP]=5

Fig. 106

REGULARITIES OF THE STRUCTURE OF SOLUTIONS OF ZIRCONIUM ALKOXIDE COMPLEXES



Complexes:

- $Zr(OEt)_4$
- $Zr(O^iPr)_4$
- $Zr(O^nPr)_4$
- $Zr(O^nBu)_4$

Solvents:

- ^iPrOH, ^nPrOH, ^nBuOH, ^iBuOH, ^2BuOH, ^3BuOH, Benzene, Hexane

Diameter:

a) 6 Å
b) 30 Å
c) 110 Å

- Tetramer is the primary structure (a)
- Tetramer sextet (b) is the main structural unit of all the initial compounds, solvents and concentrations under study
- Complexes of Zr alcoxides are enclosed in a dense solvate envelope in the alcohol solutions
- Associates (c) are formed depending on the concentration, compound nature and solvent

Fig. 107

RESEARCH ACTIVITY

Quantum-Chemical Investigations

MODELING OF THE MECHANISM OF ONE-ELECTRON TRANSFER FROM THE PERYLENE MOLECULE TO THE OXYGEN MOLECULE $^3O_2$ IN THE HF MEDIUM

I.V. Kuz'min*, V.N. Solkan*, G.M. Zhidomirov, V.B. Kazanskii* (**Zelinsky Institute of Organic Chemistry, Moscow, Russia)*

Kinet. Catal.,
52(2) (2011) pp. 192-196.

The thermodynamic parameters of the formation of the perylene radical cation in anhydrous hydrogen fluoride containing dissolved dioxygen were calculated by the *ab initio* method MP2. The protonated product of HF autoprotolysis was modeled as the $H(FH)_3^+$ cluster. The $^3O_2$ molecule was found to bind to the linear $H(FH)_3^+$ cluster via a hydrogen bond. As the charge and multiplicity of the system change upon the capture of an electron, the oxygen-hydrogen fluoride cluster complex undergoes rearrangement to yield the hydroperoxyl radical OOH incorporated in a cycle formed by HF molecules. The free energy of electron transfer from the perylene molecule to the $^3O_2$ molecule in the HF medium is about −38 kcal/mol.

A QUANTUM-CHEMICAL MODEL OF THE INHIBITION MECHANISM

G.A. Yuldasheva*, G.M. Zhidomirov, A.I. Ilin* (**Anti-Infective Drug Research Center, Almaty, Kazakhstan*)

Nat. Sci.,
3(7) (2011) pp. 573-579.

The interaction of molecular iodine with virus DNA nucleotide is studied by *ab initio* RHF/3-21G** method. Formation of the nucleoprotein complex of the HIV DNA, molecular iodine and the HIV-1 integrase co-factor is considered to cause the inhibition action of the integrase enzyme. Experimental data on the anti-HIV effect of the molecular iodine complex compounds and the results of calculations suggest that molecular iodine contained in iodine polymer complexes may be considered as a compound inhibiting the catalytic center of the integrase enzyme. Unlike the known integrase inhibitors, molecular iodine also changes the virus DNA structure and produces the N-I bond in the purine bases of adenosine and guanosine nucleotides.

OXIDE CLUSTERS AS SOURCE OF THE THIRD OXYGEN ATOM FOR THE FORMATION OF CARBONATES IN ALKALINE EARTH DEHYDRATED ZEOLITES

A.V. Larin*, A.A. Rybakov*, G.M. Zhidomirov, A. Mace, A. Laaksonen**, D.P. Vercauteren***** (**Moscow Lomonosov State University, Moscow, Russia; **University of Stockholm, Stockholm, Sweden; ***University of Namur, Namur, Belgium*)

J. Catal.,
281(2) (2011) pp. 212-221.

It is shown that carbonates can be formed with almost no energetic barrier from CO_2 and metal-oxide binuclear MO_xM species (M = Mg, Ca, Sr, Ba, with $X = 1–4$, depending on the cation) in alkaline earth zeolites, mordenite (MOR) and phillipsite (PHI), on the basis of quantum mechanical density functional theory (DFT) calculations at both isolated cluster and 3D periodic levels. The participation of MO_xM species ($X = 1$ and 3) explains the source of the third O atom in CO_3 species in dehydrated zeolites, on the basis of a good agreement between the calculated and experimental positions of the asymmetric and symmetric CO_3 vibration bands, of the ratio of their intensities, and of the weak dependence *versus* the cation and framework type. The reaction of formation of dimethylcarbonate from $CaCO_3Ca$ in the 8-membered (8R) ring of MOR and methanol has also been considered, suggesting the carbonate activity as the source of CO_2 at elevated temperatures.

DFT INVESTIGATION OF CO OXIDATION OVER Mg EXCHANGED PERIODIC ZEOLITE MODELS

A.A. Rybakov*, A.V. Larin*, G.M. Zhidomirov, D.N. Trubnikov*, D.P. Vercauteren** (**Moscow Lomonosov State University, Moscow, Russia; **University of Namur, Namur, Belgium*)

Comput. Theor. Chem.,
964(1-3) (2011) pp. 108-115.

A new CO oxidation mechanism occurring at $(MgO_2Mg)^{2+}$ oxide clusters in different zeolites is modeled at both the periodic DFT (PDFT) level for Mg-phillipsite and with the cluster approach for zeolite Y and mordenite. Using PDFT, the authors obtained a value of reaction activation energy (15.3 kcal/mol) that is lower than the one obtained using the isolated cluster approach (35 kcal/mol).

The main reason of the lower barrier is the strong CO chemisorption, which was not obtained with the cluster approach. The lower oxidation activity of the Mg zeolite forms is due to the smaller number of active singlet MgO_xMg species compared to those in the other alkaline earth zeolites.

Cu(II)-Alkyl CHLOROCOMPLEXES: STABLE COMPOUNDS OR TRANSIENTS? DFT PREDICTION OF THEIR STRUCTURE AND EPR PARAMETERS

E.N. Golubeva*, O.I. Gromov*, G.M. Zhidomirov (**Moscow Lomonosov State University, Moscow, Russia*)

J. Phys. Chem. A,
115(28) (2011) pp. 8147-8154.

DFT calculations were used for studying the structure and reactivity of organocuprates(II) usually considered as intermediates with very weak Cu-C bond. It was found that calculated principal g-tensor values of model compounds $RCu(II)Cl^{2-}$ are similar to the experimentally found values for organocopper product of photolysis of quaternary ammonium tetrachlorocuprates. The calculations confirm that the most of organocuprates(II) could be stable at ambient conditions, and short lifetimes of organocuprates(II) in solutions or soft matrices are caused by their high reactivity in various bimolecular processes; the rate of those may be close to the rate of diffusion controlled reactions. The charges, spin densities, and d-orbital populations of the Cu atom in them are typical for bivalent copper complexes. Natural bond orbital analysis of organochlorocuprates(II) confirms the formation of polar σ-bond between copper and carbon atoms.

ROLE OF THE SURFACE HYDROXYL GROUPS OF MODIFIED TITANIUM OXIDE IN CATALYTIC ETHYLENE OXIDE HYDRATION

D.E. Zavelev*, M.V. Tsodikov*, G.M. Zhidomirov, R.A. Kozlovskii* (**Topchiev Institute of Petrochemical Synthesis, Moscow, Russia*)

Kinet. Catal.,
52(5) (2011) pp. 659-671.

A quantum-chemical study of the mechanism of ethylene oxide hydration on titanium oxide (anatase) modified with phosphorus additives was performed. It was demonstrated that the hydroxyl groups of the anatase surface are of importance for the activation interaction of ethylene oxide with the catalyst surface. The activation of the ethylene oxide molecule and proton transfer occurs with the participation of these hydroxyl groups. It was found that the modification of the titanium oxide surface with phosphorus additives plays a crucial role in proton transfer.

EFFECT OF LATTICE STRAIN ON HYDROGEN DIFFUSION IN Pd: A DENSITY FUNCTIONAL THEORY STUDY

H. Gronbeck*, V.P. Zhdanov (**Chalmers University of Technology, Göteborg, Sweden*)

Phys. Rev. B: Condens. Matter,
84(5) (2011) 052301 (4 pp.)

The density functional theory (DFT) is used to study the effect of lattice strain on hydrogen diffusion in Pd. The activation energy for this process is found to increase dramatically with increasing compressive lattice strain. In particular, the activation energy is close to double for an isotropic compression of 5% both in the alpha and beta phases. For tensile strain, the activation energy is instead decreased. This finding has important consequences for the interpretation of various kinetic processes occurring with participation of hydrogen and other interstitial atoms in macroscopic solid samples and nanoparticles.

DFT STUDIES OF PALLADIUM MODEL CATALYSTS: STRUCTURE AND SIZE EFFECTS

I.V. Yudanov, A. Genest*, N. Rösch* (**Technische Universität München, Garching, Germany*)

J. Clust. Sci.,
22(3) (2011) pp. 433-448.

An important task for theory is the multi-scale modeling of catalytic properties of nanocrystallites with sizes ranging from clusters of few metal atoms to particles consisting of 10^3–10^4 atoms. To explore catalytic properties of nanosized metal catalysts, the authors developed an approach based on three-dimensional symmetric model clusters of 1–2 nm (~100 metal atoms) with fcc structure, terminated by low-index surfaces. With this modeling technique one is able to describe at an accurate DFT level various catalytic and adsorption properties of metal nanoparticles in quantitative agreement with experimental studies of model catalysts deposited on thin oxide films. Metal nanocrystallites exhibit properties that can significantly vary with their size and shape.

MOLECULAR MECHANISM OF THE FORMIC ACID DECOMPOSITION ON V_2O_5/TiO_2 CATALYSTS:
A PERIODIC DFT ANALYSIS

V.I. Avdeev, V.N. Parmon

J. Phys. Chem. C,
115(44) (2011) pp. 21755-21762.

Molecular and dissociative forms of formic acid adsorption on the V_2O_5/TiO_2 model surface, possible intermediates, and transition states along of the dehydrogenation (HCOOH → CO_2 + H_2) and dehydration (HCOOH → CO + H_2O) pathways have been studied by the periodic density functional theory. The CI-NEB analysis of the reaction pathways showed that two types of molecular adsorbed HCOOH species initiate two completely different reaction channels. The first more stable adsorbed form is transformed into the surface formates, which decompose according to the “formate mechanism” to yield products of dehydrogenation, whereas the second weakly adsorbed molecular form decomposes, releasing CO and forming surface hydroxyls. Recombination of two surface hydroxyl groups V–OH to form adsorbed H_2O, followed by water desorption, completes the catalytic dehydration cycle without participation of the formate species. Comparison of the reaction pathways demonstrates that both dehydrogenation and dehydration of formic acid may occur over VO_x/TiO_2 model catalysts with the preferable dehydration pathway.

ADSORPTION ENERGY OF THE As ATOM ON THE Pd(111) SURFACE ACCORDING TO THE DENSITY FUNCTIONAL THEORY DATA

S.E. Malykhin, M.Yu. Burylin*, S.Yu. Burylin*, I.L. Zilberberg (**Kuban State University, Krasnodar, Russia*)

J. Struct. Chem.,
52(6) (2011) pp. 1098-1101.

Density functional theory in the plane wave basis set is used to study As adsorption on the Pd(111) surface in order to determine the action of a palladium chemical modifier used in electrothermal atomic absorption spectrometry (ETAAS). The calculated heat of desorption of the arsenic atom is 435 kJ/mole, which corresponds to the activation energy of arsenic atomization of 439 kJ/mole (in the range of high temperatures $T > 1828$ K), obtained by ETAAS. Based on the calculated data, the action of the palladium modifier for the determination of As is assumed to be controlled by the process of chemisorption.

AN *ab initio* STUDY OF ELECTROCHEMICAL vs. ELECTROMECHANICAL PROPERTIES: THE CASE OF CO ADSORBED ON A Pt(111) SURFACE

M.I. Mamatkulov, J.-S. Filhol* (**Université Montpellier, Montpellier Cedex, France*)

Phys. Chem. Chem. Phys.,
13(17) (2011) pp. 7675-7684.

The authors have studied electrochemical vibrational and energy properties of CO/Pt(111) in the framework of periodic density functional theory (DFT) calculations. The authors have used a modified version of the previously developed Filhol-Neurock method to correct the unphysical contributions arising from homogeneous background countercharge in the case of thick metallic slabs. The stability of different CO adsorption sites on Pt(111) (Top, Bridge, Hcp, Fcc) has been studied at constant electric field. The energies are dominated by the surface dipole interaction with the external electric field: a strong positive electric field favors the surfaces with the lower dipole moment (that correspond to the ones with the lower coordination). The Stark tuning slope of the CO stretching frequency for a Top site was calculated for different surface coverages in very good agreement with both experimental and other theoretical results. Finally, an analysis of the origin of Stark shifts showing that the total Stark effect can be split into two competing components have been performed. The first one corresponds to the direct effect of charging on the C-O chemical bond: it is referred as an electrochemical effect. The second is the consequence of the surface dipole interaction with the applied electric field that modifies the C-O distance, inducing a change of the C-O force constant because of C-O bond anharmonicity: it is referred as the electromechanical effect. In the CO/Pt(111) case, the dominant contribution is electromechanical. The electrochemical contribution is very small because the electronic system involved in the surface charging is mostly non-bonding as analyzed by looking at the surface Fukui function.

Monte-Carlo Simulations to Study Physicochemical Processes

ARE THE COMPLEX DISTRIBUTED GENETIC NETWORKS INHERENTLY OSCILLATORY AND CHAOTIC?

V.P. Zhdanov

JETP Lett.,
93(1) (2011) pp. 41-45.

Complex mRNA-protein networks with distributed regulation of gene transcription are often mimicked by random Boolean networks. According to this mapping, the gene-expression kinetics are expected to depend strongly on the network connectivity, m. Specifically, the kinetics are predicted to be oscillatory or chaotic for $m > 2$. The authors analyze this problem in more detail by using an accurate model explicitly describing the mRNA-protein interplay with randomly organized transcriptional regulation. Contrary to the expectations, mean-field calculations and Monte Carlo simulations performed for $m = 1$, 2 and 4 show that oscillations and chaos are lacking irrespective of m.

KINETIC MODELS OF GENE EXPRESSION INCLUDING NON-CODING RNAs

V.P. Zhdanov

Phys. Rep.-Rev. Sec. Phys. Lett.,
500(1) (2011) pp. 1-42.

In cells, genes are transcribed into mRNAs, and the latter are translated into proteins. Due to the feedbacks between these processes, the kinetics of gene expression may be complex even in the simplest genetic networks. The corresponding models have already been reviewed in the literature. A new avenue in this field is related to the recognition that the conventional scenario of gene expression is fully applicable only to prokaryotes whose genomes consist of tightly packed protein-coding sequences. In eukaryotic cells, in contrast, such sequences are relatively rare, and the rest of the genome includes numerous transcript units representing non-coding RNAs (ncRNAs). During the past decade, it has become clear that such RNAs play a crucial role in gene expression and accordingly influence a multitude of cellular processes both in the normal state and during diseases. The numerous biological functions of ncRNAs are based primarily on their abilities to silence genes via pairing with a target mRNA and subsequently preventing its translation or facilitating degradation of the mRNA-ncRNA complex. Many other abilities of ncRNAs have been discovered as well. The review is focused on the available kinetic models describing the mRNA, ncRNA and protein interplay. In particular, the authors systematically present the simplest models without kinetic feedbacks, models containing feedbacks and predicting bistability and oscillations in simple genetic networks, and models describing the effect of ncRNAs on complex genetic networks. Mathematically, the presentation is based primarily on temporal mean-field kinetic equations. The stochastic and spatio-temporal effects are also briefly discussed.

PERIODIC PERTURBATION OF THE BISTABLE KINETICS OF GENE EXPRESSION

V.P. Zhdanov

Physica A,
390(1) (2011) pp. 57-64.

Kinetics of gene expression may be bistable or oscillatory due to the feedbacks between the RNA and protein synthesis. In complex genetic networks, kinetic oscillations may influence bistability. Following this line, the authors have performed a mean-field analysis and Monte Carlo simulations of periodic perturbation of the bistable kinetics of expression of two genes with mutual suppression of the mRNA production due to negative regulation of the gene transcription by protein. The perturbation is realized via modulation of the rate of the mRNA formation. In the mean-field kinetics, the mRNA and protein concentrations repeat themselves during each period. In the stochastic kinetics, this is also the case, provided that the modulation amplitude is small. If the modulation is appreciable, the latter kinetics exhibit new features. Specifically, the model predicts stochastic intermittence of the states of the genes. If the modulation amplitude is close to maximum, the change of the gene states during subsequent perturbation periods occurs fully at random. Taking into account that the model the authors use is generic, the results obtained are expected to be of interest far beyond the biophysics and biochemistry of gene expression.

GROWTH AND GLOBAL GENE EXPRESSION OF EUCARYOTIC CELLS

V.P. Zhdanov

Biophys. Rev. Lett.,
6(1-2) (2011) pp. 1-12.

The authors present a kinetic model describing the growth of eukaryotic cells or, more specifically, the dependence of the cell volume on time in terms of the global interplay of the mRNA and protein synthesis and degradation and lipid synthesis. Addressing two long-standing questions in this interdisciplinary field, the authors explain why the average protein concentration in growing cells is nearly constant and the growth can accurately be fitted by using a bilinear or exponential function.

NON-CODING RNAs AND COMPLEX DISTRIBUTED GENETIC NETWORKS

V.P. Zhdanov

Central Eur. J. Phys.,
9(4) (2011) pp. 909-918.

In eukaryotic cells, the mRNA-protein interplay can be dramatically influenced by non-coding RNAs (ncRNAs). Although this new paradigm is now widely accepted, an understanding of the effect of ncRNAs on complex genetic networks is lacking. To clarify what may happen in this case, a mean-field kinetic model was proposed describing the influence of ncRNA on a complex genetic network with a distributed architecture including mutual protein-mediated regulation of many genes transcribed into mRNAs. ncRNA is considered to associate with mRNAs and inhibit their translation and/or facilitate degradation. Results are indicative of the richness of the kinetics under consideration. The main complex features are found to be bistability and oscillations. One could expect to find kinetic chaos as well. The latter feature has however not been observed in calculations. In addition, the authors illustrate the difference in the regulation of distributed networks by mRNA and ncRNA.

KINETIC MODELS OF THE INTERFERENCE OF GENE TRANSCRIPTION TO ncRNA AND mRNA

V.P. Zhdanov

Chaos,
21(2) (2011) 023135 (7 pp.).

The experiments indicate that the transcription of genes into ncRNA can positively or negatively interfere with transcription into mRNA. Two kinetic models are proposed describing this effect. The first model is focused on the ncRNA-induced chromatin modification facilitating the transcription of the downstream gene into mRNA. The second model includes the competition between the transcription into ncRNA and the binding of activator to a regulatory site of the downstream gene transcribed into mRNA. The analysis based on the mean-field kinetic equations and Monte Carlo simulations shows the likely dependences of the transcription rate on RNA polymerase concentration in situations with different rate-limiting steps. The models can also be used to scrutinize the dependence of the transcription rate on other kinetic parameters. Kinetic Monte Carlo simulations show that the first model predicts stochastic bursts in the mRNA formation provided that the transcription into ncRNA is slow, while the second model predicts in addition anti-phase stochastic bursts in the mRNA and ncRNA formation provided that that the protein attachment to and detachment from a regulatory site is slow.

INTERPLAY OF VIRAL miRNAs AND HOST mRNAs AND PROTEINS

V.P. Zhdanov

Central Eur. J. Phys.,
9(5) (2011) pp. 1366-1371.

Recent experiments indicate that several viruses may encode microRNAs (miRNAs) in cells. Such RNAs may interfere with the host mRNAs and proteins. A kinetic analysis of this interplay is presented. The viral miRNA is considered to be able to associate with the host mRNA with subsequent degradation. This process may result in a decline of the mRNA population and also in a decline of the population of the protein encoded by this mRNA. With these ingredients, it was first shown the types of the corresponding steady-state kinetics in the cases of positive and negative regulation of the miRNA synthesis by the protein. In addition, the authors scrutinize the situation when the protein regulates the virion replication or, in other words, provides a feedback for the replication. For the negative feedback, the replication rate is found to increase with increasing the intracellular virion population. For the positive feedback, the replication rate first increases and then drops. These features may determine the stability of steady states.

FROM STICKING TO SLIPPING CONDITIONS IN QCM-D

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Chem. Phys. Lett.,
513(1-3) (2011) pp. 124-126.

Supported lipid bilayers are often studied by using quartz crystal microbalance with dissipation monitoring (QCM-D). The interpretation of the QCM-D data usually implies the no-slip boundary condition at the substrate (QCM) surface. Under certain circumstances, the oscillations of the QCM crystal may however result in the transition to slipping conditions. Employing the Frenkel-Kontorova model, the authors show that during this transition the amplitude of the bilayer vibrations drops in a stepwise fashion, i.e., the process can be classified as a first-order kinetic phase transition. The model allows also to scrutinize the corresponding changes in the force between the bilayer and support and dissipation of energy.

A KINETIC MODEL OF STANDARD SELECTIVE CATALYTIC REDUCTION OF NO BY NH_3 ON SINGLE SITES

V.P. Zhdanov

React. Kinet. Mech. Catal.,
103(1) (2011) pp. 11-18.

Reduction of NO by NH_3 in the presence of O_2 may occur on single Fe or Cu atoms or dimers incorporated into the inner walls of a zeolite. Although this process is of considerable intrinsic interest as an example of complex reactions running on single sites and is also important from the perspective of environmental chemistry, its mechanism is still open for debate. One of the likely schemes of the process implies the formation of N_2 and H_2O via the reaction of gas-phase NO and adsorbed NH_3. The author presents a detailed analysis of the steady-state kinetics corresponding to this scheme. The model employed includes eleven elementary steps. The results obtained allow one to interpret the apparent reaction orders observed experimentally.

A KINETIC MODEL OF STANDARD SELECTIVE CATALYTIC REDUCTION OF NO BY NH_3 ON TWO SITES

V.P. Zhdanov

React. Kinet. Mech. Catal.,
104(2) (2011) pp. 267-272.

Reduction of NO by NH_3 in the presence of O_2 may occur on single Fe or Cu atoms or dimers incorporated into the inner walls of zeolite. One of the likely schemes of this reaction implies the formation of N_2 and H_2O through the reaction of gas-phase NO and adsorbed NH_3. The steady-state kinetics corresponding to this scheme was recently analyzed by the author assuming that the reaction runs on single metal atoms. In this work, the author presents a model including two metal atoms. Under the practically important conditions, the kinetics predicted by the one- and two-site models are demonstrated to be similar. In particular, both models allow one to interpret the apparent reaction orders observed experimentally.

KINETICS OF CELL-TO-CELL SPREAD OF VIRUSES¶

V.P. Zhdanov

JETP Lett.,
93(9) (2011) pp. 551-554.

Recent experiments indicate that many viruses can move between cells directly via the cell–cell contacts without diffusing through the extracellular environment. The first generic kinetic model is presented describing intracellular viral kinetics in combination with this mode of spread of virions. Monte Carlo simulations show the specifics of the propagation of the infection front in this case.

INTERACTION OF SINGLE VIRUS-LIKE PARTICLES WITH VESICLES CONTAINING GLYCOSPHINGOLIPIDS

M. Bally*, A. Gunnarsson*, L. Svensson, G. Larson***, V.P. Zhdanov, F. Hook*** (**Chalmers University of Technology, Göteborg, Sweden; **University of Linköping, Linköping, Sweden; ***University of Gothenburg, Göteborg, Sweden*)

Phys. Rev. Lett.,
107(18) (2011) 188103 (5 pp.).

Glycosphingolipids are involved in the first steps of virus-cell interaction, where they mediate specific recognition of the host cell membrane. The authors have employed total-internal-reflection fluorescence microscopy to explore the interaction kinetics between individual unlabeled noroviruslike particles, which are attached to a glycosphingolipid-containing lipid bilayer, and fluorescent vesicles containing different types and concentrations of glycosphingolipids. Under association equilibrium, the vesicle-binding rate is found to be kinetically limited, yielding information on the corresponding activation energy. The dissociation kinetics are logarithmic over a wide range of time. The latter is explained by the vesicle-size-related distribution of the dissociation activation energy. The biological, pharmaceutical, and diagnostic relevance of the study is briefly discussed.

DISSOLUTION AND REDEPOSITION ON Pt NANOPARTICLES UNDER ELECTROCHEMICAL CONDITIONS

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Chem. Phys. Lett.,
509(4-6) (2011) pp. 134-137.

A Schottky-type model describing Pt^{2+} dissolution and redeposition on Pt nanoparticles in polymer electrolyte fuel cells is presented. The charge transfer is considered to occur near the surface of nanoparticles so that the potential barrier for the reaction is formed by the double-layer potential and the image interaction. With increasing electrode potential, the transfer coefficient for dissolution is found to decrease from 0.6-0.7 down to 0.3-0.4. Its dependence on the effective dielectric constant of the double layer is appreciable while the dependence on the particle size is weak.

POTENTIAL PROFILES NEAR THE SCHOTTKY NANOCONTACTS

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Physica E,
43(8) (2011) pp. 1486-1489.

The conventional Schottky model describes in the mean-field approximation the electrostatic potential appearing in a doped semiconductor during its flat contact with a metal. More recently, the Schottky model has been used to describe the mean-field potential profile near a metallic nanosphere surrounded by or located on the surface of a semiconductor. The authors present the corresponding results for a metallic nanowire. In these three cases, the shape of the potential profiles and their scalings are very different. In particular, the full width at half maximum of the potential barrier dramatically shrinks if the geometry changes from linear to cylindrical and then to spherical. In addition, the authors scrutinize the effect of the discreteness of the dopant charges on the potential near a metallic nanosphere.

Studying of Active Sites, Mechanism and Reaction Kinetics

INFLUENCE OF THE MOBILITY OF OXYGEN ON THE REACTIVITY OF $La_{1-x}Sr_xMnO_3$ PEROVSKITES IN METHANE OXIDATION

D.V. Ivanov, L.G. Pinaeva, E.M. Sadovskaya, L.A. Isupova

Kinet. Catal.,
52(3) (2011) pp. 401-408.

Radically different dependences of the activity of $La_{1-x}Sr_xMnO_3$ (x = 0–0.5) perovskites in methane oxidation on the degree of substitution of strontium for lanthanum are observed for low and high temperatures. Unsubstituted $LaMnO_3$ exhibits the highest activity in the temperature range from 300 to 500°C, while the sample with the maximum degree of substitution ($La_{0.5}Sr_{0.5}MnO_3$) shows the highest activity at higher temperatures of 700–900°C. In the low temperature region, the activity of $La_{1-x}Sr_xMnO_3$ is determined by the amount of weakly bound (overstoichiometric) oxygen, which is formed in cation-deficient lattices and is characterized by a thermal desorption peak with T_{max} = 705°C. At higher temperatures (800–900°C), the strongly bound oxygen of the catalyst lattice is involved in the formation of the reaction products under both unsteady- and steady-state conditions. As a consequence, the catalytic activity in methane oxidation correlates with the apparent rate constant of oxygen diffusion in the oxide bulk.

INSIGHTS INTO THE REACTIVITY OF $La_{1-x}Sr_xMnO_3$ (x = 0 ÷ 0.7) IN HIGH TEMPERATURE N_2O DECOMPOSITION

D.V. Ivanov, L.G. Pinaeva, L.A. Isupova, A.N. Nadeev, I.P. Prosvirin, L.S. Dovlitova

Catal. Lett.,
141(2) (2011) pp. 322-331.

In this paper a wide range of $La_{1-x}Sr_xMnO_3$ (x = 0–0.7) perovskites was synthesized by Pechini route, characterized by XRD (including high temperature measurements), XPS, differential dissolution phase analysis, TPR H_2, oxygen exchange and tested in N_2O decomposition at 900°C. At low degree of Sr substitution for La ($x \leq 0.3$), high catalytic activity was found for perovskites with hexagonal structure ($x = 0.1–0.2$) and can be related to fast oxygen mobility caused by the lattice disordering during polymorphic phase transition from the hexagonal to cubic structure. For multiphase samples ($x > 0.3$) increase of activity and oxygen mobility can be attributed to the formation of the layer structured perovskite – $LaSrMnO_4$ on the surface.

MECHANISM OF 1,2-DICHLOROETHANE DEHYDROCHLORINATION ON THE ACID SITES OF OXIDE CATALYSTS AS STUDIED BY IR SPECTROSCOPY

A.S. Shalygin, L.V. Malysheva, E.A. Paukshtis

Kinet. Catal.,
52(2) (2011) pp. 305-315.

The adsorption of 1,2-dichloroethane on zeolite HZSM-5 and γ-Al_2O_3 at temperatures from 25 to 400°C was studied by Fourier transform IR spectroscopy. The forms of adsorbed 1,2-dichloroethane and the products of its conversion at the Brønsted and Lewis acid sites of catalysts were identified. The kinetics of 1,2-dichloroethane conversion on the surface of catalysts was studied by *in situ* Fourier transform IR spectroscopy. It was demonstrated that 1,2-dichloroethane was dehydrochlorinated at the Lewis sites of γ-Al_2O_3 even at 100°C, whereas the reaction came into play at the Brønsted sites of zeolite HZSM-5 only at 200°C. It was found that, at the Lewis acid sites of catalysts, the resulting vinyl chloride underwent oligomerization with the intermediate formation of a dimer (1,3-dichloro-2-butene), whereas the formation of 1,3-dichloro-2-butene at the Brønsted sites of zeolite HZSM-5 was not observed. The mechanisms of 1,2-dichloroethane conversions at Lewis and Brønsted acid sites were proposed.

EFFECT OF THE ELECTRONIC STATE AND COPPER LOCALIZATION IN ZSM-5 PORES ON PERFORMANCE IN NO SELECTIVE CATALYTIC REDUCTION BY PROPANE

O.P. Krivoruchko, T.V. Larina, R.A. Shutilov, V.Yu. Gavrilov, S.A. Yashnik, V.A. Sazonov, I.Yu. Molina, Z.R. Ismagilov

Appl. Catal., B,
103(1-2) (2011) pp. 1-10.

This study was devoted to determination of localization of the individual copper species in the pores of ZSM-5 zeolite after post-synthetic zeolite modification by incipient wetness impregnation with $CuCl_2$ solution followed by hydrolytic polycondensation of the ions in the pores. A series of Cu(*n*)ZSM-5 samples, where *n* is the copper concentration varied from 0.5 to 5.0 wt%, were synthesized using this method. A commercial HZSM-5 zeolite having Si/Al = 17 was used for the synthesis of the catalysts. After modification the Cu(*n*)ZSM-5 samples were dried and calcined in air at 110 and 450°C, respectively. The samples were studied by UV–vis–NIR DR spectroscopy, XRD and by measuring and processing the low-temperature (77 K) adsorption of nitrogen and hydrogen. It was shown for the first time that at the concentration of 1.0 wt% or lower copper was localized in the form of isolated Cu^{2+}_{Oh} cations in the ion-exchange positions in the zeolite micro- and mesopores as well as on oxygen complexes of extraframework aluminum in thin mesopores with $D < 3.2$ nm in the form of superficial spinel-like structures in octahedral oxygen coordination Cu^{2+}_{Oh}. At the copper concentration above 1.0 wt% linear associates of weakly bound Cu^{2+}_{Oh} ions with unusual orbital ordering were formed in addition to the two forms discussed above. These associates existing in the forms of one- and two-dimensional nanohydroxocompounds were localized partially in the zeolite micropores but mostly in thin mesopores.

The effect of the individual copper species on the catalytic properties of Cu(*n*)ZSM-5 samples in selective catalytic reduction of NO by propane was also studied. It was found that isolated Cu^{2+}_{Oh} cations in the ion-exchange positions and Cu^{2+}_{Oh} cations localized on the oxygen complexes of extraframework aluminum had the highest catalytic activity in NO SCR by propane. The weakly bound linear associates of Cu^{2+}_{Oh} ions had lower catalytic activity, compared with isolated Cu^{2+}_{Oh} ions. When their amount was high, they caused steric hindrance for contact of the reagents with the more active sites. The Cu^{2+}_{Oh} ion associates were found to transform to nanodispersed $Cu_2(OH)_3Cl$ during catalytic experiments.

LOCATION, STABILITY, AND REACTIVITY OF OXYGEN SPECIES GENERATED BY N_2O DECOMPOSITION OVER Fe-ZSM-5 AND Fe-Beta ZEOLITES

V.I. Sobolev, K.Yu. Koltunov

J. Mol. Catal. A: Chem.,
347(1-2) (2011) pp. 22-27.

Reactivity of oxygen species generated by N_2O decomposition over Fe-ZSM-5 and Fe-Beta zeolites was investigated using oxygen isotopic exchange as test reaction. The generated species are very stable up to 300°C in the absence of the organic traces or residual N_2O in the gas phase. The reactivity of the oxygen species towards organics depends on the size of the organic molecules and their ability to penetrate into the zeolite pores. For example, in case of Fe-ZSM-5 zeolite, the oxygen species react readily with toluene, but stay intact with more bulky 1,3,5-trimethylbenzene.

MoVNbTe MIXED OXIDES AS EFFICIENT CATALYST FOR SELECTIVE OXIDATION OF ETHANOL TO ACETIC ACID

V.I. Sobolev, K.Yu. Koltunov

ChemCatChem,
3(7) (2011) pp. 1143-1145.

Results from a comparative study of the catalytic activity of MoVNb, MoVTe, and MoVNbTe mixed oxides in the gas phase oxidation of ethanol are reported. Multi-component MoVNbTe mixed oxides, analogous to those, which are used in the propane (amm)oxidation), in contrast to three-component MoVNb and MoVTe oxides show exclusive efficiency in selective oxidation of ethanol by molecular oxygen to obtain acetic acid.

GENERATION OF REACTIVE OXYGEN SPECIES ON Au/TiO_2 AFTER TREATMENT WITH HYDROGEN: TESTING THE LINK TO ETHANOL LOW-TEMPERATURE OXIDATION

V.I. Sobolev, O.A. Simakova, K.Yu. Koltunov

ChemCatChem,
3(9) (2011) pp. 1422-1425.

In the present work, the efforts were focused on the role of hydrogen in the catalytic activity of gold supported on TiO_2, Al_2O_3, and SiO_2 matrixes to provide insights into the different profiles of ethanol oxidation.

JOINT AROMATIZATION OF BUTANE AND HEXANE ON ALUMINA–PLATINUM CATALYSTS

V.V. Pashkov*, D.V. Golinsky*, I.E. Udras*, E.A. Paukshtis, A.S. Belyi* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Pet. Chem.,
51(4) (2011) pp. 286-292.

It has been found that the joint aromatization of C_4 and C_6 alkanes proceeds during the conversion of a butane and hexane mixture on alumina–platinum catalysts. It has been shown that a necessary condition for realization of the joint aromatization is the presence of highly dispersed platinum as ionic species (Pt^{σ}) and "hard" Lewis acid sites (L_z) of a catalyst. It has been determined that an optimum L_z/Pt^{σ} ratio for joint conversion reaction of light alkanes is from 1 to 2.

ROLE OF DIFFERENT ACTIVE SITES IN HETEROGENEOUS ALKENE HYDROGENATION ON PLATINUM CATALYSTS REVEALED BY MEANS OF PARAHYDROGEN-INDUCED POLARIZATION

V.V. Zhivonitko*, K.V. Kovtunov*, I.E. Beck, A.B. Ayupov, V.I. Bukhtiyarov, I.V. Koptyug* (**International Tomography Center, Novosibirsk, Russia*)

J. Phys. Chem. C,
115(27) (2011) pp. 13386-13391.

Substantial NMR signal enhancements provided by parahydrogen-induced polarization (PHIP) are associated with the ability of a catalyst to incorporate both H atoms of a dihydrogen molecule into the same product molecule. Therefore, PHIP can provide valuable information about the mechanisms and kinetics of catalytic hydrogenation reactions as well as produce hyperpolarized molecules for sensitivity enhancement in NMR. In this work, the PHIP technique was applied to study the structure sensitivity and the support effects on the degree of pairwise H_2 addition in propene hydrogenation over supported platinum catalysts. Four series of Pt catalysts supported on Al_2O_3, SiO_2, ZrO_2, and TiO_2 were examined. A nontrivial dependence of the selectivity toward pairwise H_2 addition on the Pt particle size was found. Its analysis indicates that at least three types of different active sites coexist on the catalysts surface. Among them, the major one is responsible for the nonpairwise H_2 addition to the double bond, whereas pairwise addition can proceed on the other two minor active sites. An explanation of the nature of these active sites is proposed. A substantial increase in the pairwise addition selectivity was found for Pt/TiO_2 catalysts as compared to other catalyst series, possibly due to a strong metal—support interaction taking place even after low temperature catalyst reduction.

CHARACTERIZATION OF ACTIVE SITES OF Pd/Al_2O_3 MODEL CATALYSTS WITH LOW Pd CONTENT BY LUMINESCENCE, EPR AND ETHANE HYDROGENOLYSIS

A.A. Vedyagin, A.M. Volodin, V.O. Stoyanovskii, D.A. Medvedev, A.S. Noskov

Appl. Catal., B,
103(3-4) (2011) pp. 397-403.

Spectroscopic (laser-induced luminescence (LIL) and EPR) and catalytic (ethane hydrogenolysis) techniques were used for characterization of the active sites of Pd/Al_2O_3 catalysts. These techniques have high sensitivity and make it possible to study the catalysts with Pd concentrations as low as 0.02–0.03 wt%. It was found by EPR using spin probes that the electron donor sites of the support are modified by the deposited palladium. It was found by LIL that the Pd deposition has a substantial effect on the state of hydroxyls on the Al_2O_3 surface. The obtained results indicate that at Pd concentrations 0.5 wt% or lower supported Pd does not form PdO phase. Instead, it is stabilized in the form of atomically dispersed ion clusters. The possible role of the Al_2O_3 donor sites in stabilization of such clusters is discussed.

STRUCTURAL AND CHEMICAL STATES OF PALLADIUM IN Pd/Al_2O_3 CATALYSTS UNDER SELF-SUSTAINED OSCILLATIONS IN REACTION OF CO OXIDATION

E.M. Slavinskaya, O.A. Stonkus, R.V. Gulyaev, A.S. Ivanova, V.I. Zaikovsky, P.A. Kuznetsov, A.I. Boronin

Appl. Catal., A,
401(1-2) (2011) pp. 83-97.

Pd/Al_2O_3 supported catalysts, differed in the initial structural and chemical states of palladium, were examined for the possible existence of self-sustained oscillations in the reaction of CO oxidation under temperature-programmed and isothermal modes using plug flow reactor at ambient pressure and CO and O_2 concentration of 0.2 and 1.0 vol.%, respectively. The supported samples after the action of reaction mixture were characterized using the HRTEM and XPS methods. The catalysts, calcined at relatively low temperatures 450°C, cannot induce the self-sustained oscillation phenomena in the reaction of CO oxidation. The calcination at 800°C yields highly dispersed particles of Pd^0 and PdO in the catalysts with sizes varying between 2–3 and 10–20 nm, respectively. In this case self-sustained oscillations (SO) of the CO oxidation appeared in the region of middle CO conversions. In the catalyst calcined at 1000°C, PdO is formed as large particles with sizes 20–100 nm. During prolonged self-sustained oscillations under isothermal conditions with varying CO concentrations in the reaction mixture, particles with “core–shell” structures are formed, where the cores are PdO and the shells are a Pd^0 clusters ordered along a specific direction due to an epitaxy on PdO. Calcination at 1200°C results in the formation of large Pd^0 particles with sizes ≥200 nm. During prolonged self-sustained oscillations with varying CO concentrations under isothermal conditions, the reaction mixture causes destruction of the above particles to yield palladium particles with core–shell structures; in this case the cores are Pd^0, and the shells are PdO layers.

LOW-TEMPERATURE OXIDATION OF CARBON MONOXIDE ON Pd(Pt)/CeO$_2$ CATALYSTS PREPARED FROM COMPLEX SALTS

E.M. Slavinskaya, R.V. Gulyaev, O.A. Stonkus, A.V. Zadesenets*, P.E. Plyusnin*, Yu.V. Shubin*, S.V. Korenev*, A.S. Ivanova, V.I. Zaikovsky, I.G. Danilova, A.I. Boronin (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Kinet. Catal.,
52(2) (2011) pp. 282-295.

Catalysts containing cerium oxide as a support and platinum and palladium as active components for the low-temperature oxidation of carbon monoxide were studied. The catalysts were synthesized in accordance with original procedures with the use of palladium and platinum complex salts. Regardless of preparation procedure, the samples prepared with the use of only platinum precursors did not exhibit activity at a low temperature because only metal and oxide (PtO, PtO$_2$) nanoparticles were formed on the surface of CeO$_2$. Unlike platinum, palladium can be dispersed on the surface of CeO$_2$ to a maximum extent up to an almost an ionic (atomic) state, and it forms mixed surface phases with cerium oxide. In a mixed palladium-platinum catalyst, the ability of platinum to undergo dispersion under the action of palladium also increased; as a result, a combined surface phase with the formula $Pd_xPt_yCeO_{2-\delta}$, which exhibits catalytic activity at low temperatures, was formed.

SYNERGETIC EFFECT IN PdAu/CeO$_2$ CATALYSTS FOR THE LOW-TEMPERATURE OXIDATION OF CO

R.V. Gulyaev, L.S. Kibis, O.A. Stonkus, A.V. Zadesenets*, P.E. Plyusnin*, Yu.V. Shubin*, S.V. Korenev*, A.S. Ivanova, E.M. Slavinskaya, V.I. Zaikovsky, I.G. Danilova, A.I. Boronin
(**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Struct. Chem.,
52(suppl.) (2011) pp. 123-136.

Gold-palladium catalysts supported on cerium oxide were synthesized with the double complex salts. X-ray photoelectron spectroscopy (XPS) and other physicochemical methods (TEM, TPR) were used to demonstrate that synthesis of highly active palladium catalysts requires the oxidative treatment stimulating the formation of a catalytically active surface solid solution $Pd_xCe_{1-x}O_2$, which is responsible for the low-temperature activity (LTA) in the reaction CO + O$_2$. In the case of gold catalysts, active sites for the low-temperature oxidation of CO are represented by gold nanoparticles and its cationic interface species. Simultaneous deposition of two metals increases the catalyst LTA due to interaction of both gold and palladium with the support surface to form a $Pd_{1-x}Ce_xO_2$ solid solution and cationic interface species of palladium and gold on the boundary of Pd-Au alloy particles anchored on the solid solution surface.

DYNAMIC Cu/Zn INTERACTION IN SiO$_2$ SUPPORTED METHANOL SYNTHESIS CATALYSTS UNRAVELED BY *in situ* XAFS

D. Grandjean*,, V.V. Pelipenko, E.D. Batyrev***, J.C. van den Heuvel***, A.A. Khassin, T.M. Yurieva, B.M. Weckhuysen****
(**Laboratory of Solid State Physics and Magnetism & INPAC, Leuven, Belgium; **Utrecht University, Utrecht, The Netherlands; ***University of Amsterdam, Amsterdam, The Netherlands*)

J. Phys. Chem. C,
115(41) (2011) pp. 20175-20191.

In situ X-ray absorption spectroscopy XAFS at the Cu and Zn K-edge has been used to unravel the Cu/Zn interaction and identify the possible active site of Cu-based methanol synthesis catalysts in the Cu/ZnO/SiO$_2$ ternary system. These highly dispersed silica supported catalysts, whose activity increases sharply as a function of the reduction temperature, were studied calcined, reduced at 200, 300, and 400°C, and for each reduction temperature under passivation/rereduction and methanol synthesis conditions. Results showed that the calcined form consists mainly of a mixed Cu/Zn hydrosilicate that is progressively transformed as the reduction temperature increases into (i) Cu metal particles, (ii) increasingly dispersed ZnO species on SiO$_2$, and (iii) finally a Zn metallic phase forming segregated bimetallic Cu–Zn α-brass alloy particles. These different structures and Cu/Zn interfaces may correspond to different active phases and activities in methanol synthesis. After reduction at 200 and 300°C, Cu^0 is likely composing most of the active phase, whereas above 300°C, the sharp increase in the number Zn^0-based sites formed as a function of the reduction temperature could explain the major role played by this parameter in controlling the activity of these catalysts. The dynamic Cu/Zn interaction as a function of the temperature and gas environment pointed out in this ternary system may be at the origin of the existence of different and sometimes contradictory models to account for the mechanisms of the methanol synthesis.

CHARACTERIZATION OF THE ACTIVE SITES ON THE SURFACE OF Al_2O_3 ETHANOL DEHYDRATION CATALYSTS BY EPR USING SPIN PROBES

R.A. Zotov, V.V. Molchanov, A.M. Volodin, A.F. Bedilo

J. Catal.,
278(1) (2011) pp. 71-77.

Several pure and doped alumina samples were characterized by EPR using spin probes and tested in ethanol dehydration. It was found that the concentrations of the electron acceptor sites and the catalytic activity increased when alumina was modified with chlorides and sulfates. Meanwhile, the number of the electron donor sites decreased. A very good correlation between the concentration of the weak acceptor sites and the catalytic activity of the acid-modified catalysts almost passing through the origin of the coordinates was obtained for all the studied samples. Alumina poisoning with sodium resulted in the decrease in the catalytic activity and the concentration of the weak acceptor sites. Therefore, it appears that the weak acceptor sites tested using anthracene are related to the sites active in the ethanol dehydration reaction.

INVESTIGATION OF OXYGEN STATES AND REACTIVITIES ON A NANOSTRUCTURED CUPRIC OXIDE SURFACE

D.A. Svintsitskiy, A.I. Stadnichenko, D.V. Demidov, S.V. Koshcheev, A.I. Boronin

Appl. Surf. Sci.,
257(20) (2011) pp. 8542-8549.

Nanostructured copper (II) oxide was formed on clean copper foil at room temperature using activated oxygen produced by RF discharge. CuO particles of approximately 10-20 nm were observed on the surface by Scanning Tunneling Microscopy (STM). The copper states and oxygen species of the model cupric oxide were studied by means of X-ray Photoelectron Spectroscopy (XPS). These oxide particles demonstrated abnormally high reactivity with carbon monoxide (CO) at temperatures below 100°C. The XPS data showed that the interaction of CO with the nanostructured cupric oxide resulted in reduction of the CuO particles to Cu_2O species. The reactivity of the nanostructured cupric oxide to CO was studied at 80°C using XPS in step-by-step mode. The initial reactivity was estimated to be 5×10^{-5} and was steadily reduced down to 5×10^{-9} as the exposure was increased. O1s spectral analysis allowed to propose that the high initial reactivity was caused by the presence of non-lattice oxygen states on the surface of the nanostructured CuO. It was established that reoxidation of the partially reduced nanostructured cupric oxide by molecular oxygen O_2 restored the highly reactive oxygen form on the surface. These results allowed to propose that the nanostructured cupric oxide could be used for low temperature catalytic CO oxidation. Some hypotheses concerning the nature of the non-lattice oxygen species with high reactivity are also discussed.

Fe-CONTAINING NICKEL PHOSPHATE MOLECULAR SIEVES AS HETEROGENEOUS CATALYSTS FOR PHENOL OXIDATION AND HYDROXYLATION WITH H_2O_2

M.N. Timofeeva, Z. Hasan*, A.Yu. Orlov, V.N. Panchenko, Yu.A. Chesalov, I.E. Soshnikov, Sung H. Jhung* (**Kyungpook National University, Taegu, South Korea*)

Appl. Catal., B,
107(1-2) (2011) pp. 197-204.

Fe-containing nickel phosphate molecular sieves (Fe-VSB-5) were hydrothermally synthesized in weak basic conditions under microwave irradiation and characterized by SEM, XRD, N_2-adsorption/desorption, DRS-UV–vis, and FT-IR spectroscopy using PhCN and $CDCl_3$ as probe molecules. The catalytic activity of Fe-VSB-5 was tested for the phenol hydroxylation and wet phenol oxidation with H_2O_2. The increase in iron content in Fe-VSB-5 leds to an increase in the reaction rates. The increases in activity can be explained by the role of the Fe species, which increases the generation of radicals. The Fe-VSB-5 samples were stable against the leaching out of Fe ions. The catalytic activity of Fe-VSB-5 was compared to the catalytic activity of traditional Fe-containing materials.

CATALYTIC ROLE OF $O^{\bullet-}$ RADICALS IN THE LOW-TEMPERATURE ISOTOPIC EXCHANGE IN DIOXYGEN

E.V. Starokon, M.V. Parfenov, S.E. Malykhin, G.I. Panov

J. Phys. Chem. C.,
115(25) (2011) pp. 12554-12559.

In spite of a long investigation history, the low-temperature isotopic exchange in dioxygen taking place without involvement of the catalyst oxygen (R_0 exchange) is still an exotic and poorly understood phenomenon in heterogeneous catalysis. Although very strong bonds are to be cleft in O_2 molecules (118 kcal/mol), over some metal oxides R_0 can be observed even at the temperature of liquid nitrogen. In this work, the authors studied the R_0 exchange over a FeZSM-5 zeolite at 233 K and discovered for the first time a linear dependence of the R_0 rate on the concentration of $O^{\bullet-}$ radicals (α-oxygen), which identifies a catalytic role of these species. Upon transition to cryogenic temperatures, $O^{\bullet-}$ species lose the ability to exchange themselves with dioxygen, but start functioning as a principal part of unique active sites capable of catalyzing a very smooth redistribution of the oxygen–oxygen bonds in adsorbed O_2 molecules. Running by a highly concerted mechanism, this remarkable process leads to the R_0 exchange with almost zero activation energy (0.2 kcal/mol). The catalytic role of $O^{\bullet-}$ radicals well explains all previous results obtained for the R_0 exchange in the literature. Possible models of active sites comprising $O^{\bullet-}$ species are discussed.

ROOM-TEMPERATURE OXIDATION OF METHANE BY α-OXYGEN AND EXTRACTION OF PRODUCTS FROM THE FeZSM-5 SURFACE

E.V. Starokon, M.V. Parfenov, L.V. Piryutko, S.I. Abornev, G.I. Panov

J. Phys. Chem. C,
115(5) (2011) pp. 2155-2161.

Room-temperature oxidation of methane to methanol by α-oxygen is of great mechanistic interest for both conventional and biomimetic oxidation catalysis. This work was carried out using new-generation FeZSM-5 samples that have the O_α concentration of 100 μmol/g. This value exceeds 3−15 times the O_α concentration on the earlier studied samples, thus providing more precise quantitative measurements related to the reaction mechanism. Fourier transform infrared spectroscopy data confirmed an earlier conclusion that $CH_4 + O_\alpha$ surface reaction proceeds by the hydrogen abstraction mechanism. This mechanism leads to hydroxy and methoxy groups residing on α-sites. The methanol formation takes place by hydrolysis of $(Fe\text{-}OCH_3)_\alpha$ groups at the step of extraction. For the first time dimethyl ether (DME) was identified in the reaction products, its amount comprising 6−7% of the methane reacted. In distinction to methanol, DME is readily extracted both by dry solvents (acetonitrile, tetrahydrofuran, ethanol) and their mixtures with water. A reliable extraction procedure was developed, which provides a 75% recovery of the methane oxidation products (methanol + DME). The missing products are shown to remain on the catalyst surface and can be quantitatively recovered in the form of CO_x at heating the sample. A mechanism involving $CH_3^{\bullet}$ radicals formed in the H-abstraction step is suggested to explain the reaction stoichiometry $CH_4:O_\alpha = 1:1.75$ and a deficit of the carbon balance at extraction.

KINETICS AND MECHANISM OF THE HOMOGENEOUS OXIDATION OF *n*-BUTENES TO METHYL ETHYL KETONE IN A SOLUTION OF Mo-V-PHOSPHORIC HETEROPOLY ACID IN THE PRESENCE OF PALLADIUM PYRIDINE-2,6-DICARBOXYLATE

V.F. Odyakov, E.G. Zhizhina

Kinet. Catal.,
52(6) (2011) pp. 828-834.

In catalytic two-step *n*-butene oxidation with dioxygen to methyl ethyl ketone, the first step is the oxidation of $n\text{-}C_4H_8$ with an aqueous solution of Mo–V–P heteropoly acid in the presence of Pd(II) complexes. The kinetics of *n*-butene oxidation with solutions of $H_7PV_4Mo_8O_{40}$ (HPA-4) in the presence of the Pd(II) dipicolinate complex $(H_2O)Pd^{II}$(dipic) (**I**), where $dipic^{2-}$ is the tridentate ligand $2,6\text{-}NC_5H_3(COO^-)_2$, is studied. Calculation shows that, at the ratio $dipic^{2-}$: Pd(II) = 1 : 1, the ligand decreases the redox potential of the Pd(II)/Pd_{met} system from 0.92 to 0.73–0.77, due to which Pd(II) is stabilized in reduced solutions of HPA-4. The reaction is first-order with respect to $n\text{-}C_4H_8$. Its order with respect to Pd(II) is slightly below unity, and its order with respect to HPA-4 is relatively low (~0.63). The activation energy of but-1-ene oxidation in the temperature range from

40 to 80°C is 49.0 kJ/mol, and that of the oxidation of but-2-ene is 55.6 kJ/mol. The mechanism of the reaction involving the *cis*-diaqua complex $[(H_2O)_2Pd^{II}(Hdipic)]^+$, which forms reversibly from complex **I**, is proposed. The reaction rate is shown to increase with an increase in the HPA-4 concentration due to an increase in the acidity of the solution.

PARTIAL OXIDATION OF METHANE ON Pt-SUPPORTED LANTHANIDE DOPED CERIA–ZIRCONIA OXIDES: EFFECT OF THE SURFACE/LATTICE OXYGEN MOBILITY ON CATALYTIC PERFORMANCE

V.A. Sadykov, N.N. Sazonova, A.S. Bobin, V.S. Muzykantov, E.L. Gubanova*, G.M. Alikina, A.I. Lukashevich, V.A. Rogov, E.N. Ermakova, E.M. Sadovskaya, N.V. Mezentseva, E.G. Zevak, S.A. Veniaminov, M. Muhler*, C. Mirodatos, Y. Schuurman**, A.C. van Veen*****

(**Ruhr-Universität Bochum, Bochum, Germany; **Institut de Recherches sur la Catalyse et L'environnement de Lyon, Villeurbanne Cedex, France*)

Catal. Today,
169(1) (2011) pp. 125-137.

Partial oxidation of methane into syngas at short contact times (5–15 ms) was studied in both steady-state and transient modes at temperatures up to 850°C in realistic feeds (CH_4 content up to 20%, $CH_4/O_2 = 2$) with a minimum impact of mass and heat transfer for structured catalysts carrying $Pt/Ln_{0.3}Ce_{0.35}Zr_{0.35}O_{2-y}$ (Ln = La, Pr, Gd) as thin layers on walls of corundum channel substrates. Oxygen mobility and reactivity of the active phase were characterized by oxygen isotope heteroexchange, temperature-programmed O_2 desorption and CH_4 reduction, isothermal pulse reduction by methane with wide variation of CH_4 concentrations and TAP pulse studies. Experimental data point towards a selective oxidation of methane into syngas via a direct route with oxygen-assisted methane activation. This mechanistic feature is related to the strong Pt-support interaction stabilizing highly dispersed oxidic Pt species less active in CH_4 and syngas combustion than metallic Pt clusters. Support activates O_2 molecules and supplies active oxygen species to Pt sites. A high rate of oxygen diffusion on the surface and in the bulk of the support and Pt-support oxygen spillover stabilizes Pt in a well dispersed partially oxidized state while preventing coking at high concentrations of CH_4 in the feed.

DRY REFORMING OF METHANE OVER Pt/PrCeZrO CATALYST: KINETIC AND MECHANISTIC FEATURES BY TRANSIENT STUDIES AND THEIR MODELING

V.A. Sadykov, E.L. Gubanova, N.N. Sazonova, S.A. Pokrovskaya, N.A. Chumakova, N.V. Mezentseva, A.S. Bobin, R.V. Gulyaev, A.V. Ishchenko, T.A. Krieger, C. Mirodatos*

(**Institut de Recherches sur la Catalyse et L'environnement de Lyon, Villeurbanne Cedex, France*)

Catal. Today,
171(1) (2011) pp. 140-149.

The effect of pretreatment and Pt content on the catalytic properties as well as mechanistic features of DR were investigated for structured catalysts comprised of Pt supported on CeO_2-ZrO_2 oxide doped by Pr. Progressive reduction of cationic Pt species by the reaction feed lowers the activity in CH_4 dry reforming while accelerating the reverse water gas shift reaction catalyzed only by Pt(0), which then decreases progressively the H_2/CO ratio in the effluent. This process is counteracted by the mobility of surface oxygen supplying oxygen atoms to reduced Pt centers thus ensuring their reoxidation and generating in parallel surface oxygen vacancies for the dissociation of CO_2.

A mathematical model and software were developed for numerically studying the transients of the complex catalytic reactions. The processing of experimental data was fulfilled taking into account the importance of cationic forms of Pt, reactivity of carbonate complexes coordinated to these cations and oxygen surface/bulk diffusion. A quantitative evaluation of the density of catalyst's active sites and their coverage by reactive species was accomplished and the rates both of the lattice oxygen diffusion and main stages of the catalytic reaction were estimated.

DRY REFORMING OF METHANE OVER $LnFe_{0.7}Ni_{0.3}O_{3-\delta}$ PEROVSKITES: INFLUENCE OF Ln NATURE

L.G. Kapokova, S.N. Pavlova, R.V. Bunina, G.M. Alikina, T.A. Krieger, A.V. Ishchenko, V.A. Rogov, V.A. Sadykov

Catal. Today,
164(1) (2011) pp. 227-233.

$LnFe_{0.7}Ni_{0.3}O_{3-\delta}$ (Ln = La, Pr, Sm) perovskites synthesized via Pechini method have been studied as catalysts of methane dry reforming (MDR). Effects of pretreatment and type of Ln cation on the structural and redox properties of perovskites and their catalytic performance have been elucidated. The most active catalysts are obtained by keeping perovskites in the reaction feed at high temperatures due to the formation of Ni–Fe alloy particles released from the perovskite lattice and stabilized on its surface. $PrFe_{0.7}Ni_{0.3}O_{3-\delta}$ was found to be the most active and stable catalyst due to the optimal composition of segregated Ni–Fe alloy particles and redox properties of oxide matrix.

FORMATION OF PLATINUM SITES ON LAYERED DOUBLE HYDROXIDES TYPE BASIC SUPPORTS: I. EFFECT OF THE NATURE OF THE INTERLAYER ANION ON THE STRUCTURE CHARACTERISTICS OF THE LAYERED ALUMINUM–MAGNESIUM HYDROXIDE AND THE FORMATION OF AN OXIDE PHASE

O.B. Belskaya*,, N.N. Leont'eva*,**
T.I. Gulyaeva*, V.A. Drozdov*,,**
V.P. Doronin*,, V.I. Zaikovsky,**
V.A. Likholobov* (**Institute of Hydrocarbons Processing, Omsk, Russia; **Omsk State Technical University, Omsk, Russia*)

Kinet. Catal.,
52(5) (2011) pp. 761-769.

A layered aluminum–magnesium hydroxide of the hydrotalcite type containing interlayer carbonate counterions (HT-CO_3) and activated hydrotalcite containing interlayer OH^- ions (HT-OH) were studied for the subsequent use as the precursors of supports for platinum catalysts. It was found that the nature of an interlayer anion in the composition of an aluminum–magnesium layered hydroxide is an important factor affecting both the formation of the oxide support and its texture characteristics. The replacement of the interlayer anion by OH^- resulted in changes in the structural parameters of the initial double hydroxide: a decrease in the interlayer distance with the retention of the Mg/Al ratio and an increase in the imperfection of the layered material. X-ray diffraction studies in the temperature range of 30–900°C showed that HT-OH is characterized by the ability to form low-temperature spinel at 375°C. As a result, two types of aluminum–magnesium oxide supports, which were characterized by different pore space organizations at the same Mg : Al ratio, were obtained from the given layered hydroxides.

HYDROISOMERIZATION OF BENZENE-CONTAINING GASOLINE FRACTIONS ON A Pt/SO_4^{2-}–ZrO_2–Al_2O_3 CATALYST: II. EFFECT OF CHEMICAL COMPOSITION ON ACIDIC AND HYDROGENATING AND THE OCCURRENCE OF MODEL ISOMERIZATION REACTIONS

M.O. Kazakov*, A.V. Lavrenov*, I.G. Danilova, O.B. Belskaya*, V.K. Duplyakin* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Kinet. Catal.,
52(4) (2011) pp. 573-578.

The acidic and hydrogenating of Pt/SO_4^{2-}–ZrO_2–Al_2O_3 samples containing from 18.8 to 67.8 wt% Al_2O_3 as a support constituent were studied by the IR spectroscopy of adsorbed CO and pyridine, and the model reactions of *n*-heptane and cyclohexane isomerization on these catalysts were examined. The total catalyst activity in the conversion of *n*-heptane decreased with the concentration of Al_2O_3; this manifested itself in an increase in the temperature of 50% *n*-heptane conversion from 112 to 266°C and in an increase in the selectivity of isomerization to 94.2%. In this case, the maximum yield of isoheptanes was 47.1 wt%, which was reached on a sample whose support contained 67.8 wt% Al_2O_3. A maximum yield (69.6 wt%) and selectivity (93.7%) for methylcyclopentane formation from cyclohexane were also reached on the above catalyst sample. This can be explained by lower concentrations of Lewis and Bronsted acid sites in the Pt/SO_4^{2-}–ZrO_2–Al_2O_3 system, as compared with those in Pt/SO_4^{2-}–ZrO_2. The experimental results allowed to make a preliminary conclusion that the Pt/SO_4^{2-}–ZrO_2–Al_2O_3 catalyst whose support contains 67.8 wt% Al_2O_3 is promising for use in the selective hydroisomerization of benzene-containing gasoline fractions in the thermodynamically favorable process temperature range of 250–300°C.

FORMATION OF PLATINUM SITES ON LAYERED DOUBLE HYDROXIDE TYPE BASIC SUPPORTS: II. EFFECT OF THE NATURE OF THE INTERLAYER ANION OF THE LAYERED ALUMINUM-MAGNESIUM HYDROXIDES ON PLATINUM BINDING AND Pt/MgAlO$_x$ FORMATION

O.B. Belskaya*, T.I. Gulyaeva*, N.N. Leont'eva*, V.I. Zaikovsky, T.V. Larina, T.V. Kireeva*, V.P. Doronin*, V.A. Likholobov* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Kinet. Catal.,
52(6) (2011) pp. 876-885.

The interaction of aqueous H_2PtCl_6 solutions with hydrotalcite-type aluminum–magnesium hydroxides differing in the nature of their interlayer anion is reported. In the case of CO_3^{2-} as the interlayer anion, the introduction of the platinum(IV) chloro complex does exerts no significant effect on the structural properties of the support, on its thermal decomposition dynamics, and on the textural characteristics of the resulting oxide phase. The binding of the platinum complexes to "activated hydrotalcite" with interlayer OH^- anions increases the interplanar spacing and enhances the thermal stability of the layered structure. This is accompanied by marked changes in textural characteristics of the material, leading to the formation of a nearly monodisperse mixed oxide phase. In the Pt/MgAlO$_x$ samples obtained by reductive treatment, a considerable proportion of platinum is in the form of planar particles, and this corroborates the hypothesis that the metal complex at the sorption stage is mainly localized in the interlayer space of this support. Platinum binds to the support as chloro complexes via rapid anion exchange, and these bound platinum species are characterized by a higher reduction temperature.

COBALT OXIDE CATALYST FOR HYDROLYSIS OF SODIUM BOROHYDRIDE AND AMMONIA BORANE

V.I. Simagina, O.V. Komova, A.M. Ozerova, O.V. Netskina, G.V. Odegova, D.G. Kellerman*, O.A. Bulavchenko, A.V. Ishchenko (**Institute of Solid State Chemistry, Yekaterinburg, Russia*)

Appl. Catal., A,
394(1-2) (2011) pp. 86-92.

The catalytic properties of Co_3O_4 in $NaBH_4$ and NH_3BH_3 hydrolysis have been studied. Experiments were carried out at 20–40°C using 0.12 M hydride solution. According to magnetic susceptibility measurements, FTIR, XRD, and TEM studies, Co_3O_4 is reduced to the ferromagnetic catalytically active Co_2B phase under the action of the $NaBH_4$ hydrolysis reaction medium. A correlation was found between the content of the cobalt boride phase formed *in situ* and catalyst activity. The reduction of Co_3O_4 in NH_3BH_3 proceeds at slower rate than in $NaBH_4$. The addition to a solution of NH_3BH_3 of even a small amount of $NaBH_4$ increases considerably the reduction rate of Co_3O_4. Using a Co_3O_4-based precursor instead of the widely used $CoCl_2$ leads to the formation of a stable catalytically active phase of cobalt boride.

LOW-TEMPERATURE DECOMPOSITION OF AMMONIA BORANE IN THE PRESENCE OF TITANIA

O.V. Komova, V.I. Simagina, G.V. Odegova, Yu.A. Chesalov, O.V. Netskina, A.M. Ozerova

Inorg. Mater.,
47(10) (2011) pp. 1101-1107.

In the presence of anatase, the thermal decomposition of ammonia borane (AB) begins at a lower temperature, which enables AB dehydrogenation at a temperature as low as 80°C. The reduction in the AB decomposition temperature depends on the AB content of the mixture. *In situ* IR spectroscopy data demonstrate that, in the presence of TiO_2, the structural destabilization of AB occurs during heating and is accompanied by the formation of an oxygen-containing boron phase and partial reduction of the titania, which is supported by diffuse reflectance spectroscopy data.

EFFECT OF THE REACTION MEDIUM ON THE STRUCTURE OF THE $La_{1-x}Ca_xMnO_3$ (x = 0–1) SOLID SOLUTIONS PREPARED BY THE PECHINI METHOD

L.A. Isupova, E.Yu. Gerasimov, V.I. Zaikovsky, S.V. Tsybulya

Kinet. Catal.,
52(1) (2011) pp. 104-110.

The phase composition and microstructure of $La_{1-x}Ca_xMnO_3$ (x = 0–1) materials prepared by the Pechini method from polymer-salt stocks were studied after testing these materials in methane oxidation. According to X-ray diffraction data, the reaction medium causes no significant changes in the samples, while high-resolution transmission electron microscopy indicates that the x > 0.3 samples are unstable. Under the action of the reaction medium, the perovskite structure of these samples undergoes partial decomposition accompanied by the formation of planar defects having a lower manganese content. The number and degree of segregation of these defects increase with increasing calcium content. The calcium oxide and manganese oxide phases as segregated nanoparticles are observed on the particle surface. These changes are caused by the decrease in the oxygen content of the manganites under the action of the reaction medium (T, PO_2), by the formation of vacancies, and by the variation of the charge of the manganese cations, as well as by the charge ordering tendency of the manganese cations. Therefore, the observed changes in catalytic activity under the action of the reaction medium for $x > 0.3$ can be due to perovskite decomposition accompanied by the formation of planar defects, the release of the manganese oxide and calcium oxide phases, and their subsequent sintering.

INTERACTION OF HYDROGEN AND WATER WITH OXYGEN ADSORBED ON SILVER

E.V. Dokuchits, A.V. Khasin, A.A. Khassin

React. Kinet. Mech. Catal.,
103(2) (2011) pp. 261-266.

The identity of surface silver hydroxides produced by hydrogenation or hydration of surface silver oxide was demonstrated. A two-route mechanism of hydrogen interaction with oxygen adsorbed on silver was suggested. The first route includes two consecutive-parallel steps: formation of adsorbed hydroxyl groups and their interaction with hydrogen; the second route consists of two consecutive steps: formation of adsorbed hydroxyl groups and their disproportionation yielding water and adsorbed oxygen.

COMPOSITION AND PROPERTIES OF FUNCTIONAL GROUPS ON SURFACE OF CARBON SORBENTS MODIFIED BY AMINOCAPROIC ACID

V.A. Likholobov*, L.G. P'yanova*, A.I. Boronin, S.V. Koshcheev, A.N. Salanov, O.N. Baklanova*, O.A. Knyazheva*, A.V. Veselovskaya* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Prot. Met. Phys. Chem. Surf.,
47(2) (2011) pp. 181-190.

The composition and properties of functional groups on the surface of carbon sorbents modified with aqueous solutions of aminocaproic acid of different concentrations were studied using physicochemical analysis methods including: acid-base titration, the Kjeldahl method, scanning electron microscopy, X-ray microanalysis, and X-ray photoelectron spectroscopy. The initial carbon sorbent was shown to have almost no functional groups on its surface. It was ascertained that the surface functionalization of carbon sorbent results in a change in microstructure and an increase in the amount of oxygen- and nitrogen-containing groups with increasing concentration of the modifying agent followed by its further polycondensation on the surface. According to the XPS data, the formation of the bond between aminocaproic acid and the carbon surface of sorbents occurs via a carboxylic group.

IDENTIFICATION OF NITROGEN-CONTAINING SPECIES OBTAINED BY NITRIC OXIDE ADSORPTION ON THE SURFACE OF MODEL GOLD CATALYSTS

A.V. Bukhtiyarov, A.V. Nartova, R.I. Kvon

Kinet. Catal.,
52(5) (2011) pp. 756-760.

Nitric oxide adsorption at 300–500 K on gold particles supported on an alumina film has been investigated for the first time by *in situ* X-ray photoelectron spectroscopy. Two nitrogen-containing adsorption species can form on the surface of gold particles. By test experiments on NO adsorption on the stepped face (533) of a gold single crystal, these species have been identified as adsorbed nitrogen atoms (which are detected throughout the temperature range examined) and a surface complex with N_2O stoichiometry (which is stable in a narrow temperature range of 325–425 K).

AN XPS AND STM STUDY OF THE SIZE EFFECT IN NO ADSORPTION ON GOLD NANOPARTICLES

A.V. Bukhtiyarov, A.V. Nartova, R.I. Kvon, V.I. Bukhtiyarov

Russ. Chem. Bull.,
60(10) (2011) pp. 1977-1984.

The effect of the gold particle size, temperature of the model gold catalyst, and NO pressure on the composition of the adsorption layer was studied by *in situ* XPS and STM methods. Adsorption of nitric oxide was carried out on gold nanoparticles with a mean size of 2–7 nm prepared on the thin film surface of alumina. In high-vacuum conditions ($P_{NO} \approx 10^{-5}$ Pa), only atomically adsorbed nitrogen is formed on the surface of gold nanoparticles. At about 1 Pa pressure of NO and in the temperature range from 325 to 475 K, atomically adsorbed nitrogen coexists with the N_2O adsorption complex. The surface concentration of the adsorbed species changes with a change in both the mean gold particle size and adsorption temperature. The saturation coverage of the surface with the nitrogen-containing complexes is observed for the sample with a mean size of gold particles of 4 nm. The surface of these samples is mainly covered with atomically adsorbed nitrogen, the saturation coverage of adsorbed nitrogen of about ~0.6 monolayer is attained at $T = 473$ K. The change in the composition of the adsorption layer with temperature of the catalysts agrees with the literature data on the corresponding temperature dependence of the selectivity of N_2 formation observed in the catalytic reduction of NO with carbon monoxide on the Au/Al_2O_3 catalyst. The dependences of the composition of the adsorption layer on the mean size of Au nanoparticles (size effect) and temperature of the catalyst are explained by the sensitivity of NO adsorption to specific features of the gold surface.

MECHANISM OF H_2-PROMOTED OXIDATION OF NITROGEN MONOXIDE OVER Ag/Al_2O_3

N.A. Sadokhina*, A.V. Bukhtiyarov,
A.I. Mytareva*, R.I. Kvon, V.I. Bukhtiyarov,
A.Yu. Stakheev* (**Zelinsky Institute of Organic Chemistry, Moscow, Russia*)

Mendeleev Commun.,
21(5) 2011 pp. 274-276.

H_2-promoted oxidation of NO to NO_2 over Ag/Al_2O_3 proceeds via two-step mechanism: (1) formation of surface nitrate species, and (2) reduction of this species with NO. Hydrogen plays a crucial role at the first step.

H_2-INDUCED NO_x ADSORPTION/ DESORPTION OVER Ag/Al_2O_3: TRANSIENT EXPERIMENTS AND TPD STUDY

N.A. Sadokhina*, D.E. Doronkin*,
P.V. Pributkov*, V.I. Bukhtiyarov, R.I. Kvon,
A.Yu. Stakheev* (**Zelinsky Institute of Organic Chemistry, Moscow, Russia*)

Top. Catal.,
54(16-18) (2011) pp. 1190-1196.

NO adsorption/desorption over 1 wt% Ag/Al_2O_3 was studied by a combination of isothermal transient adsorption/desorption and NO_x temperature-programmed desorption (NO_x-TPD) methods. NO_x-TPD profiles obtained for Ag/Al_2O_3 were identified by comparison with decomposition profiles of “model” $AgNO_3/Al_2O_3$ and $Al(NO_3)_3/Al_2O_3$ prepared by impregnation of Al_2O_3 with individual $AgNO_3$ and $Al(NO_3)_3$ compounds. The data obtained indicate that H_2-induced NO adsorption leads to the formation of surface Ag and Al-nitrates. Their accumulation on the catalyst surface is accompanied by an intensive NO_2 evolution, which proceeds primarily via reaction of surface nitrates with NO. Thus, NO_2 formation appears to result from an intrinsic stage of the H_2-induced NO_x adsorption process, rather than from the direct oxidation of NO by gaseous oxygen catalyzed by Ag.

CONCENTRATION HYSTERESIS IN METHANE OXIDATION ON NANOSIZED PLATINUM PARTICLES

I.Yu. Pakharukov, I.E. Beck, M.M. Matrosova,
V.I. Bukhtiyarov, V.N. Parmon

Doklady Phys. Chem.,
439(1) (2011) pp. 131–134.

Study of hysteresis is an efficient tool for investigating the catalytic process mechanism. In the work it was for the first time detected the concentration hysteresis in low-temperature methane oxidation on a dispersed $Pt/\gamma\text{-}Al_2O_3$ catalyst with an average platinum particle size of 2 nm.

GAS PHASE NITRIDATION OF SILICATE FIBER GLASS MATERIALS WITH AMMONIA: THREE CASE STUDIES

Yu.K. Gulyaeva, A.P. Suknev, E.A. Paukshtis, B.S. Bal'zhinimaev,

J. Non-Cryst. Solids,
357(18) (2011) pp. 3338-3344.

Three types of the leached fiber glass materials of silicate origin modified with Zr, Al and rare earth metals (REM) were nitridated with ammonia at temperatures ranging from 673 to 973 K. DRIFTS (Diffuse Reflectance Infrared Fourier-Transform Spectroscopy) and H/D exchange using ND_3 were applied for characterization of the formed NH species. Along with nitridation of silanol groups their dehydroxylation as well as hydrolysis of NH_x species take place. *In situ* DRIFTS study showed that the limiting steps are slow chemical reactions, but not a diffusion of NH_3 or H_2O molecules in the bulk of glasses. The concept on strained siloxane bridges formed due to dehydroxylation of two adjacent silanol groups was used for explanation of the reaction kinetics features.

CARBONYLATION OF DIMETHYL ETHER ON SOLID Rh-PROMOTED Cs-SALT OF KEGGIN 12-$H_3PW_{12}O_{40}$: A SOLID-STATE NMR STUDY OF THE REACTION MECHANISM

M.V. Luzgin, M.S. Kazantsev, G.G. Volkova, W. Wang*, A.G. Stepanov (**Lanzhou University, Gansu, PR China*)

J. Catal.,
277(1) (2011) pp. 72-79.

The carbonylation of dimethyl ether (DME) with carbon monoxide on Rh-promoted cesium salt of 12-tungstophosphoric acid, $Rh/Cs_2HPW_{12}O_{40}$ (HPA), has been studied with ^{13}C solid-state NMR. The bi-functional character of $Rh/Cs_2HPW_{12}O_{40}$ catalyst in halide-free carbonylation of DME has been directly demonstrated. The activation of the C–O bond of DME proceeds on Brønsted acid sites of HPA with the formation of the methyl group attached to the surface of HPA (methoxy species), whereas the role of rhodium consists in trapping carbon monoxide from gaseous phase and a transfer of CO to the center of DME activation, acidic OH-group of the catalyst, in the form of rhodium carbonyls. The lattice of $Cs_2HPW_{12}O_{40}$ makes it possible to locate these two different active centers in close proximity to each other, e.g., on two adjacent oxygen atoms, terminal and bridging, of one Keggin anion, thus facilitating the insertion of carbon monoxide from rhodium carbonyl into the C–O bond of methoxy-group to produce the acetate group bound to the Keggin anion. The latter offers finally methyl acetate under the interaction with DME, the intermediate surface methoxy-groups being restored.

HYDROGEN H/D EXCHANGE AND ACTIVATION OF C_1-*n*-C_4 ALKANES ON Ga-MODIFIED ZEOLITE BEA STUDIED WITH ^{1}H MAGIC ANGLE SPINNING NUCLEAR MAGNETIC RESONANCE *in situ*

A.A. Gabrienko, S.S. Arzumanov, A.V. Toktarev, D. Freude*, J. Haase*, A.G. Stepanov (**University of Leipzig, Leipzig, Germany*)

J. Phys. Chem.,
115(28) (2011) pp. 13877-13886.

Kinetics of H/D hydrogen exchange between C_1-*n*-C_4 alkanes and Bronsted acid sites (BAS) of both the pure acid-form zeolite BRA (H-BRA) and Ga-modified zeolite BRA (Ga/H-BEA) was monitored by ^{1}H MAS NMR spectroscopy *in situ* at 423-563 K. Comparative analysis of the rates of the exchange for H-BRA and Ga/H-BRA zeolites reveals a remarkable increase of the rate by 1-2 orders of magnitude, decrease of activation energy, and an appearance of regioselectivity of the exchange into the methyl groups of C_3-*n*-C_4 alkanes upon modification of H-BEA zeolite with gallium. These data identify an evident promoting effect of Ga on activation of alkane C-H bonds by BAS. The effect has been rationalized by preliminary dissociative adsorption of alkanes on gallium(III) oxide species inside zeolite pores to form gallium-alkyl species, which are further involved in the exchange with neighbor BAS. Involvement of both BAS and Ga species in alkane activation accounts for earlier suggested synergistic effect (Buckles, G., et al. Catal. Lett. 1991, 11, 89) of both BAS and gallium species in alkane activation and aromatization on Ga-modified high silica zeolites.

CATALYTIC ENANTIOSELECTIVE OXIDATION OF BULKY ALKYL ARYL THIOETHERS WITH H_2O_2 OVER TITANIUM-SALAN CATALYSTS

K.P. Brylyakov, E.P. Talsi

Eur. J. Org. Chem.,
24 (2011) pp. 4693-4698.

A simple and efficient catalytic procedure for the oxidation of bulky (preferably aryl benzyl substituted) thioethers with hydrogen peroxide in good to high yields and enantioselectivities (up to 98.5 % *ee*) is reported. The high optical yields are achieved in a tandem stereoconvergent enantioselective oxidation and kinetic resolution process. A reasonable balance between the sulfoxide yield and enantioselectivity could be found by varying the concentration and temperature. An improved synthesis of the titanium-salan catalysts for the preparation of a more stereoselective catalyst is reported.

NON-HEME MANGANESE COMPLEXES CATALYZED ASYMMETRIC EPOXIDATION OF OLEFINS BY PERACETIC ACID AND HYDROGEN PEROXIDE

R.V. Ottenbacher, K.P. Brylyakov, E.P. Talsi

Adv. Synth. Catal.,
353(6) (2011) pp. 885-889.

Chiral non-heme aminopyridine manganese complexes catalyze the enantioselective epoxidation of olefins with peracetic acid or hydrogen peroxide with moderate to high yields and *ee* values up to 89% (peracetic acid, AcOOH) and 84% (hydrogen peroxide, H_2O_2), performing as many as 1000 turnovers.

EPR, ^1H AND ^2H NMR, AND REACTIVITY STUDIES OF THE IRON–OXYGEN INTERMEDIATES IN BIOINSPIRED CATALYST SYSTEMS

O.Yu. Lyakin, K.P. Brylyakov, E.P. Talsi

Inorg. Chem.,
50(12) (2011) pp. 5526–5538.

Complexes $[(BPMEN)Fe^{II}(CH_3CN)_2](ClO_4)_2$ (**1**, BPMEN = *N,N'*-dimethyl-*N,N'*-bis(2-pyridylmethyl)-1,2-diaminoethane) and $[(TPA)Fe^{II}(CH_3CN)_2](ClO_4)_2$ (**2**, TPA = tris(2-pyridylmethyl)amine) are among the best nonheme iron-based catalysts for bioinspired oxidation of hydrocarbons. Using EPR and ^1H and ^2H NMR spectroscopy, the iron–oxygen intermediates formed in the catalyst systems **1**,**2**/H_2O_2; **1**,**2**/H_2O_2/CH_3COOH; **1**,**2**/CH_3CO_3H; **1**,**2**/*m*-CPBA; **1**,**2**/PhIO; **1**,**2**/^{t}BuOOH; and **1**,**2**/^{t}BuOOH/CH_3COOH have been studied (*m*-CPBA is *m*-chloroperbenzoic acid). The following intermediates have been observed: $[(L)Fe^{III}(OOR)(S)]^{2+}$, $[(L)Fe^{IV}{=}O(S)]^{2+}$ (L = BPMEN or TPA, R = H or ^{t}Bu, S = CH_3CN or H_2O), and the iron–oxygen species **1c** (L = BPMEN) and **2c** (L = TPA). It has been shown that **1c** and **2c** directly react with cyclohexene to yield cyclohexene oxide, whereas $[(L)Fe^{IV}{=}O(S)]^{2+}$ react with cyclohexene to yield mainly products of allylic oxidation. $[(L)Fe^{III}(OOR)(S)]^{2+}$ are inert in this reaction. The analysis of EPR and reactivity data shows that only those catalyst systems which display EPR spectra of **1c** and **2c** are able to selectively epoxidize cyclohexene, thus bearing strong evidence in favor of the key role of **1c** and **2c** in selective epoxidation. **1c** and **2c** were tentatively assigned to the oxoiron(V) intermediates.

HOMOCHIRAL POROUS METAL-ORGANIC FRAMEWORKS: A STEP TO THE FUTURE OF STEREOSELECTIVE RECOGNITION AND CATALYSIS

K.P. Brylyakov, E.P. Talsi

In “*Chemical Physics Research and Developments*”,
Nova Science Publishers, NY, 2011, pp. 47-59.

In this commentary, the authors present an overview of known homochiral metal-organic materials capable of stereoselective recognition, sorption and separation of guest molecules and those promoting asymmetric catalytic processes inside the chiral pores.

ELECTRICAL CONDUCTIVITY OF MAGNESIUM OXIDE AS A CATALYST FOR RADICAL CHAIN HYDROCARBON PYROLYSIS REACTIONS

N.A. Vasilieva, N.F. Uvarov* (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Kinet. Catal.,
52(1) (2011) pp. 98-103.

The electrical conductivity of polycrystalline MgO between 350 and 750°C is determined by the transport of surface electronic and hole defects and depends on the applied voltage. Near 620°C at low applied voltages, the conductivity decreases by 1–2 orders of magnitude in a narrow temperature range (ΔT = 75°C), and this is accompanied by a change of the sign of the surface charge carriers. The “ignition” of the catalytic activity of magnesium oxide in free radical generation in radical chain hydrocarbon pyrolysis is observed in the same temperature range. It is assumed that the change of the sign of the charge carriers is due to the existence of an isoelectric temperature T_i and that, at $T > T_i$, $O_O^{\cdot}$ defects come out to the magnesium oxide surface.

AMMONIA SYNTHESIS FROM DINITROGEN AND DIHYDROGEN OVER THE CATALYSTS BASED ON SUPPORTED MONONUCLEAR POTASSIUM CARBONYL RUTHENATE. PROMOTING EFFECT OF ALKYLLITHIUM COMPOUNDS

S.M. Yunusov*, E.S. Kalyuzhnaya*, B.L. Moroz, A.S. Ivanova, V.B. Shur* (**Nesmeyanov Institute of Organoelement Compounds, Moscow, Russia*)

Russ. Chem. Bull.,
60(9) (2011) pp. 1842-1847.

New catalysts for the ammonia synthesis from dinitrogen and dihydrogen based on supported mononuclear potassium carbonyl ruthenate $K_2Ru[(CO)_4]$ as a precursor of catalytically active particles have been developed. Magnesium oxide and graphite-like active carbon Sibunit were used as supports, while aliphatic organolithium compounds (Bu^nLi and Bu^tLi) were employed as electron promoters in these catalysts. The systems with MgO as a support are the most efficient. The introduction of RLi into these systems allows one to considerably increase the ammonia synthesis rate. When using carbon Sibunit, the promoting effect of organolithium compounds is much weaker but the activity of such catalysts can be essentially increased by the introduction of an additional electron promoter, *viz.*, metallic potassium, into the system. All the catalysts tested are active in the ammonia synthesis at atmospheric pressure and temperatures ≥250°C.

Application of Physicochemical Methods for Characterization of Catalysts, Supports, Synthesized Substances and Matertials

X-RAY DIFFRACTION STRUCTURE DIAGNOSTICS OF NANOMATERIALS

E.M. Moroz

Russ. Chem. Rev.,
80(4) (2011) pp. 293-312.

The review concerns the development and applications of the X-ray diffraction method of the radial electron density distribution based on the integral analysis of X-ray diffraction in studies of nanomaterials, in particular, oxide supports for catalysts. The method provides information on the interatomic distances and coordination numbers in the structure and allows one to detect and estimate the size of nanostructures (phases) less than 3 nm in size, which cannot be detected by conventional powder X-ray diffraction analysis. The method is sensitive to the changes in the local structure measuring 1-3 unit cells; therefore, it is successfully used to identify various defects in nanoobjects of any chemical composition. The bibliography includes 124 references.

STUDY OF PHASE COMPOSITION OF NANOMATERIALS

E.M. Moroz

Nanoeng.,
5 (2011) pp. 26-32.

The possibilities of X-ray techniques to determine the phase composition of typical nanomaterials and nanostructures - catalysts and carriers for them - are considered. For supported catalysts it is shown that besides phases characteristic for support and active component, there are always present the phase formed as a result of interaction between support and active component. Metastable phases are identified for oxide systems. Examples of investigation of defective nanostructures are considered.

POSSIBILITIES OF X-RAY DIFFRACTION STRUCTURE DIAGNOSTICS OF NANOMATERIALS

E.M. Moroz

Nanoeng.,
4 (2011) pp. 3-21.

In this work the data on the development and use of radial electron distribution function or pair distribution function method based on integral analysis of X-ray scattering curve are presented. The method gives information about interatomic distances and coordination numbers and it is used for detection of nanospecies (phases) with sizes lower than 3 nm and estimation of their sizes. Such highly dispersed species are not detected by conventional X-ray phase analysis based on consideration of interplanar spacings. The method is sensitive to changes in local structure (short range arrangement of atoms in the range of 1...3 elementary cells), so it is used successfully for determination of defects in the nanomaterials.

A STUDY OF THE LOCAL STRUCTURE OF ALUMINAS OBTAINED BY DIFFERENT METHODS

E.M. Moroz, K.I. Shefer, D.A. Zyuzin, A.N. Shmakov

J. Struct. Chem., 52(2) (2011) pp. 326-329.

The local structure of aluminas obtained from hydroxides (pseudo-boehmites) synthesized by different methods is studied using the radial density distribution function. The occupancy of the cation sites of different types (tetrahedral and octahedral, spinel and non-spinel) in the structure of the studied oxides is analyzed.

Pt-IMPLANTED INTERMETALLIDES AS THE CATALYSTS FOR CH_4-CO_2 REFORMING

L.A. Arkatova*, O.V. Pakhnutov*, A.N. Shmakov, Yu.S. Naiborodenko, N.G. Kasatsky***** (**Tomsk V.V. Kuibyshev State University, Tomsk, Russia; **Tomsk Scientific Center, Tomsk, Russia*)

Catal. Today, 171(1) (2011) pp. 156-167.

A new type of catalytic system on the base of Ni_3Al intermetallic compound was proposed for CO_2 reforming of methane. Several catalysts were prepared by self-propagating high temperature synthesis and characterized by XRD (*in situ* and *ex situ*), DTA-TG, SEM + EDS, HRTEM + EDS and XPS. Ion implantation was used as a method of catalyst surface modification. Activity testing has been performed in the fixed bed reactor at the temperatures of 600–900°C under atmospheric pressure and the reactant molar ratio of 1. The structure and morphology of different types of carbon deposits obtained on the surface of unmodified Ni_3Al were investigated. The results indicated that the addition of a low amount (less than 0.1 wt%) of Pt to the Ni_3Al intermetallide leads to a decrease in carbon deposition and Pt-implanted catalysts were stable for a long period of time. The evidence suggests that the differences in the stabilities may be due to the following reasons: (1) Pt prevents Ni phase sintering by avoiding particle coalescence, which is the main sintering process under severe CH_4–CO_2 reforming conditions, (2) Pt hinders deactivating carbon formation by limiting bulk nickel carbide and therefore carbon filament formation, which may lead to reactor plugging and/or particle fragmentation, and by suppressing encapsulating carbon formation which limits access of reactant to the active nickel phase.

ACTIVITY OF COPPER–CERIUM–ZIRCONIUM CATALYSTS IN OXIDATION OF HYDROGEN

A.V. Gural'skii*, G.R. Kosmambetova*, E.M. Moroz, V.I. Gritsenko*, P.E. Strizhak*
(**Pisarzhevskii Institute of Physical Chemistry, Kiev, Ukraine*)

Theor. Exp. Chem., 47(4) (2011) pp. 251-256.

The authors have studied the catalytic properties in oxidation of hydrogen for copper–cerium oxide systems deposited on supports obtained by calcination of yttrium-stabilized zirconium dioxide at 300–100°C. The authors have shown that the catalytic activity of the samples obtained depends on the specific surface area of the original supports and the amount of reduced copper within the composition of the catalyst. In samples whose support has high specific surface area, the content of reduced metallic copper is greater and the catalytic activity is higher.

LOW TEMPERATURE HYDROGEN PURIFICATION FROM CO FOR FUEL CELL APPLICATION OVER COPPER-CERIA CATALYSTS SUPPORTED ON DIFFERENT OXIDES

G.R. Kosmambetova*, E.M. Moroz, A.V. Guralsky*, V.P. Pakharukova, A.I. Boronin, T.S. Ivashchenko*, V.I. Gritsenko*, P.E. Strizhak* (**Pisarzhevskii Institute of Physical Chemistry, Kiev, Ukraine*)

Int. J. Hydrogen Energy, 36(1) (2011) pp. 1271-1275.

The CuO–CeO_2–MeO_x (Me = Zr, Ti, Mn, Al; $x = 1.5$–2) solids were tested in the preferential CO oxidation reaction in hydrogen-rich gas mixtures (PROX). The authors study an effect of a support (MeO_x) on the CO conversion and selectivity in the PROX reaction showing that monoclinic zirconia (*m*-zirconia) with low surface area is the most effective support. The optimal catalyst composition was determined by varying copper and ceria loadings over *m*-zirconia. XRD and XPS studies indicate that a good catalytic performance of *m*-zirconia supported copper–ceria catalysts may be attributed to the presence of dispersed Cu-containing species that interact with CeO_2 and ZrO_2.

EFFECTS OF SPATIAL ORDERING OF QUANTUM DOT ARRAYS FROM SMALL-ANGLE X-RAY DIFFRACTION DATA UNDER VARIATION OF GROWTH PARAMETERS

L.M. Plyasova, I.Yu. Molina, N.P. Stepina*, A.F. Zinov'eva*, A.V. Dvurechenskii* (**Institute of Semiconductor Physics, Novosibirsk, Russia*)

J. Surf. Invest. - X-Ray Synchrotron Neutron Techn., 5(1) (2011) pp. 120-125.

The small angle X-ray diffraction method is applied to the system of germanium quantum dots in the silicon matrix prepared by molecular-beam epitaxy in self-organization mode using the Stranski-Krastanov technique. Depending on the growth mode, the specific distances between Ge quantum dots and deviations from their correlated distribution are determined. The results are in agreement with the scanning tunneling microscopy data.

ELECTRODEPOSITED OXOTUNGSTATE FILMS: TOWARDS THE MOLECULAR NATURE OF RECHARGING PROCESSES

V.K. Laurinavichute*, S.Yu. Vassiliev*, A.A. Khokhlov*, L.M. Plyasova, I.Yu. Molina, G.A. Tsirlina* (**Moscow Lomonosov State University, Moscow, Russia*)

Electrochim. Acta, 56(10) (2011) pp. 3530-3536.

In situ Raman spectroscopy is applied to supplement voltammetric, spectroelectrochemical, and XRD data on redox transformations of electrodeposited oxotungstate films. These films undergo electrochromic transition at rather positive potentials, as compared to usual sputtered tungsten oxides. The depth of electroreduction for the films conditioned in acidic solutions under open circuit is about 0.11 e^- per W atom. Coloration of the films correlates with the decrease of Raman band, corresponding to the terminal W(VI)$=$O vibration in the hydrated phase of highly defective tungstic acid (hydrated tungsten oxide). The data allow to state the absence of oxotungstate octahedra rearrangement in the course of reduction at positive RHE potentials, and to assume that slightly deeper reduction up to 0.15 W(V)/[W(V) + W(VI)] ratio is possible at more negative potentials. The authors also demonstrate that the gas phase reduction is less reversible as compared to electrochemical reduction in solution. The most possible nature of films degradation in the gas phase is their partial dehydration in the course of reduction.

HIGH-TEMPERATURE XRD INVESTIGATION OF SPINEL $Mn_{1.5}Al_{1.5}O_4$ DECOMPOSITION

O.A. Bulavchenko, S.V. Tsybulya, E.Yu. Gerasimov, S.V. Cherepanova, T.N. Afonasenko*, P.G. Tsyrulnikov* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Z. Kristallogr. Proc., 1 (2011) pp. 325-330.

This article describes a study of behaviour of cubic $Mn_{1.5}Al_{1.5}O_4$ spinel during heating and cooling under air. High-temperature XRD and TEM were used to investigate structure transformations and sample microstructure. XRD data show spinel decomposition during cooling and heating under air at 500-700°C. The products of decomposition consist of nanocrystalline tetragonal phase (with particle size of 20 nm) and cubic spinel (50 nm). Cubic spinel composition changes by various ways on the initial step during the heating and cooling. Thus, the structure mechanisms of decomposition are different. But the final decomposition products are the same.

PRODUCING OF Cu/ZrO_2 COMPOSITES BY COMBINING MECHANICAL ACTIVATION AND SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS

T.F. Grigor'eva*, A.I. Letsko, T.L. Talako**, S.V. Tsybulya, I.A. Vorsina*, A.P. Barinova*, A.F. Il'yushchenko**, N.Z. Lyakhov*** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of Powder Metallurgy NAS Belarus*)

Combust. Explosion Shock Waves, 47(2) (2011) pp. 174-178.

The possibility of producing Cu/ZrO_2 composites by combining mechanical activation and self-propagating high-temperature synthesis (SHS) is studied using X-ray diffraction and electron microscopy. It is shown that Cu/ZrO_2 composites are formed in SHS using CuO/Cu/Zr mechanocomposite as a precursor.

INFLUENCE OF Al IONS ON THE REDUCTION OF $Co_{3-x}Al_xO_4$: *in situ* XRD INVESTIGATION

**S.V. Cherepanova, O.A. Bulavchenko,
I.I. Simentsova, E.Yu. Gerasimov, A.A. Khassin**

Z. Kristallogr. Proc.,
1 (2011) pp. 331-336.

The addition of small amounts of Al ions to nanocrystalline Co_3O_4 leads to considerable changes in its reduction. *In situ* XRD and TPR show that Al ions affect the extent of cobalt reduction achieved in a hydrogen flow. Co_3O_4 is fully reduced to metallic cobalt at a temperature of ca. 200°C. As for Al-modified samples $Co_{3-x}Al_xO_4$ (x = 0.05, 0.1, 0.2), they contain CoO even after reduction at 350°C. The higher is the Al content; the lower is the Co/CoO ratio. At 350°C, metallic particles in all cases consist of platelet domains having the hcp and fcc structure. In the case of metallic cobalt reduced from Co_3O_4, the fcc domains are twice thinner as compared to hcp ones, their average thicknesses being ca. 0.9 nm and 1.8 nm, respectively. In metallic cobalt reduced from $Co_{3-x}Al_xO_4$ (x = 0.05, 0.1, 0.2), the fcc and hcp domains have almost equal average thicknesses of ca. 1.4 nm.

ANIONIC COMPOSITION OF PRECURSORS OF THE Co/Al_2O_3 CATALYSTS FOR THE FISCHER-TROPSCH SYNTHESIS

**I.I. Simentsova, A.A. Khassin, G.A. Filonenko,
G.K. Chermashentseva, O.A. Bulavchenko,
S.V. Cherepanova, T.M. Yurieva**

Russ. Chem. Bull.,
60(9) (2011) pp. 1827-1834.

Cobalt and aluminum hydroxo compounds with the hydrotalcite-type structure containing nitrate, carbonate, and hydroxyl groups are formed due to the deposition by precipitation of cobalt cations from a nitrate solution on δ- and γ-Al_2O_3 under the conditions of urea hydrolysis. The influence of the method of preparation on the anionic composition of the hydroxo compounds (precursors of the Co-Al catalyst) was studied. A correlation between the anionic composition of the precursor compound and the catalytic properties of the catalysts in the Fischer-Tropsch synthesis was established.

SYNTHESIS, CRYSTAL STRUCTURE AND THERMAL PROPERTIES OF $[Co(NH_3)_5Cl]MO_4$ (M = Mo, W)

**E.A. Shusharina*, S.P. Khranenko*,
P.E. Plusnin*, T.Yu. Kardash, S.A. Gromilov***
(**Nikolaev Institute of Inorganic Chemistry,
Novosibirsk, Russia*)

J. Struct. Chem.,
52(5) (2011) pp. 918-923.

Crystal structures of $[Co(NH_3)_5Cl]MoO_4$ and $[Co(NH_3)_5Cl]WO_4$ complex salts are determined by single crystal X-ray diffraction. It is demonstrated for both salts that within the temperature range T = –123-20°C there is a negative thermal expansion (about 0.26%) towards the c axis of the orthorhombic unit cell (Pnma space group). Thermal properties of the salts are investigated. The phase composition of the products obtained on heating the salts in different gas atmospheres is studied.

CRYSTAL STRUCTURE AND THERMAL PROPERTIES OF $[Au(en)_2]_2[Cu(C_2O_4)_2]_3\cdot 8H_2O$

**E.V. Makotchenko*, E.A. Bykova*,
E.Yu. Semitut*, Yu.V. Shubin*, P.V. Snytnikov,
P.E. Plyusnin*** (**Nikolaev Institute of Inorganic
Chemistry, Novosibirsk, Russia*)

J. Struct. Chem.,
52(5) (2011) pp. 924-929.

The crystal structure of a double complex salt of the composition $[Au(en)_2]_2[Cu(C_2O_4)_2]_3\cdot 8H_2O$ (en = ethylenediamine) at 150 K is determined by single crystal X-ray diffraction. The crystal data for $C_{20}H_{48}Au_2Cu_3N_8O_{32}$ are: a = 9.1761(3) Å, b = 16.9749(6) Å, c = 13.4475(5) Å, β = 104.333(1)°, V = 2029.43(12) Å^3, $P2_{1/c}$ space group, Z = 2, d_x = 2.450 g/cm^3. It is demonstrated that the thermal decomposition of the double complex salt in a helium or hydrogen atmosphere affords the solid solution $Au_{0.4}Cu_{0.6}$.

MICROPOROUS SENSOR: GAS SORPTION, GUEST EXCHANGE AND GUEST-DEPENDANT LUMINESCENCE OF METAL-ORGANIC FRAMEWORK

S.A. Sapchenko*, D.G. Samsonenko*, D.N. Dybtsev*, **, M.S. Melgunov, V.P. Fedin*
(**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia;* ***Division of the Advanced Materials Science, POSTECH, Hyojadong, Pohang, Republic of Korea*)

Dalton Trans.,
40(10) (2011) pp. 2196-2203.

Zn(II)-containing metal–organic framework (MOF) $[Zn_4(dmf)(ur)_2(ndc)_4]$ (ndc^{2-} = 2,6-naphtalenedicarboxylate, ur = urotropin, dmf = N,N′-dimethylformamide) was synthesized and characterized by X-ray crystallography and gas sorption analysis. Host MOF retains its crystallinity after guest removal and exchange. Single-crystal to single-crystal formation of different host–guest systems with benzene and ferrocene was investigated. Interesting guest-depended luminescence properties of the porous host framework were observed.

XPS FOR *in situ* STUDY OF THE MECHANISMS OF HETEROGENEOUS CATALYTIC REACTIONS

V.V. Kaichev, I.P. Prosvirin, V.I. Bukhtiyarov

J. Struct. Chem.,
52(suppl.) (2011) pp. 90-101.

The possibility to use X-ray photoelectron spectroscopy (XPS) for *in situ* studies of the mechanisms of heterogeneous catalytic reactions over the pressure range from ultrahigh vacuum to 100 mbar is considered. The application of this method to investigation of CO adsorption and hydrogenation as well as kinetics and mechanism of methanol transformation on the palladium surface at pressures of 10^{-6} mbar to 0.1 mbar is reported.

A STUDY OF THE STRUCTURE OF $(HfO_2)_x(Al_2O_3)_{1-x}$/Si FILMS BY X-RAY PHOTOELECTRON SPECTROSCOPY

V.V. Kaichev, Yu.V. Dubinin, T.P. Smirnova*, M.S. Lebedev* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Struct. Chem.,
52(3) (2011) pp. 480-487.

By X-ray photoelectron spectroscopy (XPS), using the technique of layer-by-layer analysis, the films of $(HfO_2)_x(Al_2O_3)_{1-x}$ solid solutions synthesized by chemical vapor deposition are studied. The possibility to determine the structure of solid binary solutions based on the analysis of the XPS spectra is demonstrated.

X-RAY PHOTOELECTRON SPECTROSCOPY DEPTH PROFILING OF La_2O_3/Si THIN FILMS DEPOSITED BY REACTIVE MAGNETRON SPUTTERING

C.V. Ramana*, R.S. Vemuri*, V.V. Kaichev, V.A. Kochubey, A.A. Saraev, V.V. Atuchin****
(**University of Texas at El Paso, El Paso, Texas, USA;* ***Institute of Semiconductor Physics, Novosibirsk, Russia*)

ACS Appl. Mater. Interfaces,
3(11) (2011) pp. 4370-4373.

The La_2O_3/Si thin films have been deposited by reactive DC magnetron sputtering. Amorphous state of La_2O_3 layer has been shown by RHEED observation. Top surface chemistry of the *a*-La_2O_3 has been evaluated with layer-by-layer depth profiling by ion bombardment and XPS measurements. It was found by core level spectroscopy that the top surface of the *a*-La_2O_3 film consists of hydrocarbon admixture, lanthanum carbonate, and hydroxides that formed as a result of contact with air atmosphere. Thickness of this top surface modified layer is below 1 nm for a contact time of ~ 1.5 h with air at normal conditions.

ELECTRONIC STRUCTURE OF δ-Ta_2O_5 WITH OXYGEN VACANCY: *ab initio* CALCULATIONS AND COMPARISON WITH EXPERIMENT

M.V. Ivanov*, T.V. Perevalov*, V.S. Aliev*, V.A. Gritsenko*, V.V. Kaichev (**Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia*)

J. Appl. Phys.,
110(2) (2011) pp. 024115 (5 pp).

Electronic structure of oxygen vacancies in Ta_2O_5 have been studied theoretically by first-principles calculations and experimentally by X-ray photoelectron spectroscopy. Calculations of δ-Ta_2O_5 were performed using density functional theory within gradient-corrected approximation with the +U approach. Results indicate that the oxygen vacancy causes a defect level in the energy gap at 1.2 eV above the top of the valence band. To produce oxygen vacancies, amorphous films of Ta_2O_5 were bombarded with Ar^+ ions. XPS results indicate that the Ar-ion bombardment leads to the generation of the oxygen vacancies in Ta_2O_5 that characterize the peak at 2 eV above the valence band. The calculated spectrum of crystalline δ-Ta_2O_5 demonstrates qualitative correspondence with the XPS spectrum of the amorphous Ta_2O_5 film after Ar-ion bombardment.

Ab initio SIMULATION OF THE ELECTRONIC STRUCTURE OF δ-Ta_2O_5 WITH OXYGEN VACANCY AND COMPARISON WITH EXPERIMENT

M.V. Ivanov*, T.V. Perevalov*, V.Sh. Aliev*, V.A. Gritsenko*, V.V. Kaichev (**Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia*)

J. Exp. Theor. Phys.,
112(6) (2011) pp. 1035-1041.

The electronic structure of a Ta_2O_5 insulator with oxygen vacancies is studied theoretically and experimentally. The *ab initio* calculations of δ-Ta_2O_5 are performed in terms of density functional theory using the generalized gradient (GGA) and GGA + U approximations. The electronic structure of Ta_2O_5 is experimentally studied by X-ray photoelectron spectroscopy (XPS). To study oxygen vacancies, an amorphous Ta_2O_5 film is irradiated by argon ions. The calculated XPS spectra of the valence band of δ-Ta_2O_5 agree satisfactorily with the corresponding experimental spectra of the amorphous films. The oxygen vacancy in δ-Ta_2O_5 is found to be a trap for holes and electrons. The minimum and maximum effective masses of electrons and holes in δ-Ta_2O_5 are calculated.

NEW TECHNIQUE FOR HETEROGENEOUS VAPOR-PHASE SYNTHESIS OF NANOSTRUCTURED METAL LAYERS FROM LOW-DIMENSIONAL VOLATILE METAL COMPLEXES

A.M. Badalyan*, L.F. Bakhturova*, V.V. Kaichev, O.V. Polyakov*, O.P. Pchelyakov, G.I. Smirnov**** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institute of Semiconductor Physics, Novosibirsk, Russia*)

Tech. Phys.,
56(9) (2011) pp. 1333-1338.

A new technique for depositing thin nanostructured layers on semiconductor and insulating substrates that is based on heterogeneous gas-phase synthesis from low-dimensional volatile metal complexes is suggested and tried out. Thin nanostructured copper layers are deposited on silicon and quartz substrates from low-dimensional formate complexes using a combined synthesis-mass transport process. It is found that copper in layers thus deposited is largely in a metal state (Cu_0) and has the form of closely packed nanograins with a characteristic structure.

FROM 'CORE–SHELL' TO COMPOSITE MIXED CATHODE MATERIALS FOR RECHARGEABLE LITHIUM BATTERIES BY MECHANOCHEMICAL PROCESS

N.V. Kosova*, E.T. Devyatkina*, V.V. Kaichev, A.B. Slobodyuk** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of Chemistry, Vladivostok, Russia*)

Solid State Ionics,
192(1) (2011) pp. 284-288.

Solid state mechanical activation method was applied for surface modification of $LiMn_2O_4$ by Li–M–O (M = Co, Co+Ni) and for preparation of composite mixed $LiMn_2O_4/LiCoO_2$ cathode materials. Pristine $LiMn_2O_4$ was ground with correspondent precursors (for coating) or with $LiCoO_2$ (for composites) in high-energy planetary mills and then heat treated at different temperatures. As prepared materials were studied by XRD, ^7Li MAS NMR spectroscopy, XPS, SEM and electrochemical cycling. It has been shown that both 'core–shell' and composite materials prepared by mechanochemical process are characterized by superior electrochemical performance due to smaller particles and chemical modification of $LiMn_2O_4$.

XPS STUDY OF PHARMACOLOGICAL SUBSTANCES MECHANOCHEMICALLY IMMOBILIZED ON THE SURFACE OF ALUMINA

A.I. Nizovskii, A.V. Kalinkin, T.P. Shakhtshneider*, M.A. Dyakonova*, S.A. Myz*, E.V. Boldyreva*, R. Kumar** (**Institute of Solid-State Chemistry and Mechanochemistry, Novosibirsk, Russia; **National Metallurgical Laboratory, Jamshedpur, Bihar, India*)

J. Struct. Chem.,
52(suppl.) (2011) pp. 137-144.

Piroxicam and meloxicam nanocomposites with alumina were synthesized by mechanochemical treatment of medicinal substances mixed with the oxide. X-ray photoelectron spectroscopy demonstrated that interaction of the components during mechanical activation proceeds via binding the amide and sulfate groups in the molecules of medicinal substances with the active sites of alumina surface. XPS studies confirmed the formation of "core-shell" composites with the shell represented by medicinal substances distributed over the support surface.

MECHANOCHEMICAL PREPARATION OF ORGANIC-INORGANIC HYBRID MATERIALS OF DRUGS WITH INORGANIC OXIDES

T.P. Shakhtshneider*, S.A. Myz*, M.A. Dyakonova*, V.V. Boldyrev*, E.V. Boldyreva*, A.I. Nizovskii, A.V. Kalinkin, R. Kumar** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **National Metallurgical Laboratory, Jamshedpur, Bihar, India*)

Acta Phys. Pol., A,
120(2) (2011) pp. 272-278.

The nanocomposites of piroxicam and meloxicam with alumina were obtained by ball-milling as a result of distribution of the drugs at the surface of oxide with formation of the stable composites. The observed changes in the IR spectra of the ball-milled mixtures suggested the interaction of the drugs with the alumina active surface sites. The functional groups in molecules of piroxicam and meloxicam involved into formation of bonds between the drugs and the surface of the oxide were determined, they are amide, sulfate, enol groups, and pyridyl/thiazolyl nitrogen atoms. It appears that the formation of the new bonds at the contacts of particles in the composite leads to the stabilization of the drugs in metastable state inhibiting their transformation into initial crystalline form.

USE OF THE DIFFERENTIAL CHARGING EFFECT IN XPS TO DETERMINE THE NATURE OF SURFACE COMPOUNDS RESULTING FROM THE INTERACTION OF A Pt/($BaCO_3$ + CeO_2) MODEL CATALYST WITH SO_x

M.Yu. Smirnov, A.V. Kalinkin, A.A. Dubkov*, E.I. Vovk, A.M. Sorokin, A.I. Nizovskii, B. Carberry*, V.I. Bukhtiyarov (**Ford Forschungszentrum, Aachen, Germany*)

Kinet. Catal.,
52(4) (2011) pp. 595-604.

Changes in the chemical composition of the surface of a Pt/($BaCO_3$ + CeO_2) model NO_x storage-reduction catalyst upon its interaction with SO_x (SO_2 (260 Pa) + O_2 (2600 Pa) + H_2O (525 Pa)) followed by regeneration in a mixture of CO (2100 Pa) with H_2O (525 Pa) were studied by X-ray photoelectron spectroscopy (XPS). Model catalyst samples were prepared as a thin film (about several hundreds of angstrom units in thickness) on the surface of tantalum foil coated with a layer of aluminum oxide (~100 Å). It was found that the Pt/$BaCO_3$ and Pt/CeO_2 catalyst constituents acquired different surface charges (differential charging) in the course of photoelectron emission; because of this, it was possible to determine the nature of surface compounds formed as a result of the interaction of the catalyst with a reaction atmosphere. It was found that barium carbonate was converted into barium sulfate as a result of reaction with SO_x on the surface of $BaCO_3$ at 150°C. As the treatment temperature in SO_x was increased to 300°C, the formation of sulfate on the surface of CeO_2 was observed. The sulfatization of CeO_2 was accompanied by the reduction of Ce(IV) to Ce(III). The regeneration reaction of the catalyst treated in SO_x at 300°C resulted in the consecutive decomposition of cerium(III) sulfate at ≤500°C and then barium sulfate at 600–700°C. Upon the decomposition of $BaSO_4$, a portion of sulfur was converted into a sulfide state, probably, because of the formation of BaS.

SPECTROSCOPIC ELLIPSOMETRY AND X-RAY PHOTOELECTRON SPECTROSCOPY OF La_2O_3 THIN FILMS DEPOSITED BY REACTIVE MAGNETRON SPUTTERING

V.V. Atuchin*, A.V. Kalinkin, V.A. Kochubey*, V.N. Kruchinin*, R.S. Vemuri, C.V. Ramana**** (**Institute of Semiconductor Physics, Novosibirsk, Russia; **University of Texas at El Paso, El Paso, Texas, USA*)

J. Vac. Sci. Technol., A,
29(2) (2011) 021004 (5 pp.).

Lanthanum oxide (La_2O_3) films were grown by the reactive dc magnetron sputtering and studied their structural, chemical and optical parameters. La_2O_3 films were deposited onto Si substrates by sputtering La-metal in a reactive gas (Ar+O_2) mixture at a substrate temperature of 200°C. Reflection high-energy electron diffraction measurements confirm the amorphous state of La_2O_3 films. Chemical analysis of the top-surface layers evaluated with X-ray photoelectron spectroscopy indicates the presence of a layer modified by hydroxylation due to interaction with atmosphere. Optical parameters of α-La_2O_3 were determined with spectroscopic ellipsometry (SE). There is no optical absorption over spectral range λ = 250–1100 nm. Dispersion of refractive index of α-La_2O_3 was defined by fitting of SE parameters over λ = 250–1100 nm.

A DIRECT EVIDENCE FOR THE INSTABILITY AND DEACTIVATION OF MIXED-OXIDE SYSTEMS: INFLUENCE OF SURFACE SEGREGATION AND SUBSURFACE DIFFUSION

E. Emmez*, E.I. Vovk, V.I. Bukhtiyarov,
E. Ozensoy* (**Bilkent University, Bilkent, Ankara, Turkey*)

J. Phys. Chem. C,
115(45) (2011) pp. 22438-22443.

In the current contribution, a direct demonstration is provided of the thermally induced surface structural transformations of an alkaline-earth oxide/transition metal oxide interface that is detrimental to the essential catalytic functionality of such mixed-oxide systems toward particular reactants. The $BaO_x/TiO_2/Pt(111)$ surface was chosen as a model interfacial system where the enrichment of the surface elemental composition with Ti atoms and the facile diffusion of Ba atoms into the underlying TiO_2 matrix within 523–873 K leads to the formation of perovskite type surface species ($BaTiO_3/Ba_2TiO_4/Ba_xTi_yO_z$). At elevated temperatures ($T > 973$ K), excessive surface segregation of Ti atoms results in an exclusively TiO_2/TiO_x-terminated surface which is almost free of Ba species. Although the freshly prepared $BaO_x/TiO_2/Pt(111)$ surface can strongly adsorb ubiquitous catalytic adsorbates such as NO_2 and CO_2, a thermally deactivated surface at $T > 973$ K practically loses all of its NO_2/CO_2 adsorption capacity due to the deficiency of surface BaO_x domains.

ROLE OF THE EXPOSED Pt ACTIVE SITES AND BaO_2 FORMATION IN NO_x STORAGE REDUCTION SYSTEMS: A MODEL CATALYST STUDY ON $BaO_x/Pt(111)$

E.I. Vovk, E. Emmez*, M. Erbudak,**
V.I. Bukhtiyarov, E. Ozensoy* (**Bilkent University, Bilkent, Ankara, Turkey; **Laboratorium für Festkörperphysik, ETH Zurich, Zurich, Switzerland*)

J. Phys. Chem. C,
115(49) (2011) pp. 24256-24266.

BaO_x (0.5 MLE - 10 MLE)/Pt(111) (MLE: monolayer equivalent) surfaces were synthesized as model NO_x storage reduction (NSR) catalysts. Chemical structure, surface morphology, and the nature of the adsorbed species on $BaO_x/Pt(111)$ surfaces were studied via X-ray photoelectron spectroscopy (XPS), temperature-programmed desorption (TPD), and low-energy electron diffraction (LEED). For $\theta_{BaOx} < 1$ MLE, (2 × 2) or (1 × 2) ordered overlayer structures were observed on Pt(111), whereas BaO(110) surface termination was detected for $\theta_{BaOx} = 1.5$ MLE. Thicker films ($\theta_{BaOx} \geq 2.5$ MLE) were found to be amorphous. Extensive NO_2 adsorption on BaO_x(10 MLE)/Pt(111) yields predominantly nitrate species that decompose at higher temperatures through the formation of nitrites. Nitrate decomposition occurs on BaO_x(10 MLE)/Pt(111) in two successive steps: (1) NO(g) evolution and BaO_2 formation at 650 K and (2) NO(g) + O_2(g) evolution at 700 K. O_2(g) treatment of the BaO_x(10 MLE)/Pt(111) surface at 873 K facilitates the BaO_2 formation and results in the agglomeration of BaO_x domains leading to the generation of exposed Pt(111) surface sites. BaO_2 formed on BaO_x(10 MLE)/Pt(111) is stable even after annealing at 1073 K, whereas on thinner films ($\theta_{BaOx} = 2.5$ MLE), BaO_2 partially decomposes into BaO, indicating that small BaO_2 clusters in close proximity of the exposed Pt(111) sites are prone to decomposition. Nitrate decomposition temperature decreases monotonically from 550 to 375 K with decreasing BaO_x coverage within $\theta_{BaOx} = 0.5$ to 1.0 MLE. Nitrate decomposition occurs at a rather constant temperature range of 650-700 K for thicker BaO_x overlayers (2.5 MLE < θ_{BaOx} < 10 MLE). These two distinctly characteristic BaO_x-coverage-dependent nitrate decomposition regimes are in very good agreement with the observation of the so-called "surface" and "bulk" barium nitrates previously reported for realistic NSR catalysts, clearly demonstrating the strong dependence of the nitrate thermal stability on the NO_x storage domain size.

X-RAY PHOTOELECTRON INVESTIGATION OF CHARGE DISTRIBUTION IN COPPER(II) PHTHALOCYANINE COMPLEXES

R.V. Gulyaev, N.A. Kryuchkova*, L.N. Mazalov*,
A.I. Boronin, T.V. Basova*, V.A. Plyashkevich*
(**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Surf. Invest. -
X-Ray Synchrotron Neutron Techn.,
5(1) (2011) pp. 48-56.

The charged states of atoms in unsubstituted copper(II) phthalocyanine ($CuPcH_{16}$) and hexadecafluorinated copper(II) phthalocyanine ($CuPcF_{16}$) complexes and in thin films of them deposited on silicon substrates by vacuum thermal evaporation are investigated by X-ray photoelectron spectroscopy (XPS). The C(1*s*), N(1*s*), Cu(2*p*) core level energies and the charged states of atoms in the studied complexes are calculated using the DFT method. The performed experimental study and theoretical calculations show that the introduction of electron acceptor substituents into benzene rings mostly affects the atoms of benzene rings and insignificantly affects the charge state of nitrogen atoms in the pyrrole ring.

MICELLAR SYNTHESIS AND CHARACTERIZATION OF ULTRAFINE SILVER POWDERS

M.G. Demidova*, A.I. Bulavchenko*, T.Yu. Podlipskaya*, A.I. Boronin, L.S. Kibis, V.I. Zaikovsky (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Russ. J. Inorg. Chem.,
56(8) (2011) pp. 1199-1207.

Methods for the synthesis and coagulation of ultrafine silver powders in the water-Triton N-42-decane inverted-micellar system were developed. Varying $AgNO_3$ concentration (1–5 mol/L), the type of reducing agent (hydrazine or potassium borohydride), and the coagulation method (spontaneous or induced by acetone or water addition) allowed to select the parameters that provide powders containing about 98% silver and having particle sizes of 15–80 nm. The authors propose methodology for characterizing ultrafine silver powders comprising the determination of the total and surface composition and the charge state of impurities using atomic absorption spectroscopy (AAS), atomic emission spectroscopy (AES), microanalysis, FTIR spectroscopy, and X-ray photoelectron spectroscopy. The impurity composition of the nanomaterial is found to depend on the type of reducing agent, the synthesis parameters, and coagulation conditions.

XES AND QUANTUM CHEMICAL INVESTIGATION OF THE ELECTRONIC STRUCTURE OF PHTHALOCYANINE COMPLEXES MPCH$_{16}$ AND MPCF$_{16}$ WITH M = Cu, Co

G.I. Semushkina*, L.N. Mazalov*, N.A. Kryuchkova*, A.I. Boronin, R.V. Gulyaev, T.V. Basova*, V.A. Plyashkevich* (**Nikolaev Institute of Inorganic Chmestry, Novosibirsk, Russia*)

J. Struct. Chem.,
52(suppl.) (2011) pp. 21-35.

The X-ray spectroscopy and X-ray electron study of the electronic structure of unsubstituted phthalocyanines $MPcH_{16}$ and hexadecafluorophthalocyanines $MPcF_{16}$ with M = Cu, Co is reported. Quantum-chemical calculation of the electronic structure of these compounds was performed. The calculation was used to analyze the metal-ligand electronic interaction in the complexes. The theoretically calculated energy position and composition of the highest occupied molecular orbitals were compared with experimental data obtained from X-ray fluorescence spectra.

MOBILITY OF SOLID TERT-BUTYL ALCOHOL STUDIED BY DEUTERIUM NMR

A.M. Nishchenko, D.I. Kolokolov, A.G. Stepanov

J. Phys. Chem. A,
115(26) (2011) pp. 7428-7436.

The molecular mobility of solid deuterated tert-butyl alcohol (TBA) has been studied over a broad temperature range (103-283 K) by means of solid-state ^{2}H NMR spectroscopy, including both line shape and anisotropy of spin—lattice relaxation analyses. It has been found that, while the hydroxyl group of the TBA molecule is immobile on the ^{2}H NMR time scale ($\tau_C > 10^{-5}$ s), its butyl group is highly mobile. The mobility is represented by the rotation of the methyl [CD_3] groups about their 3-fold axes (C_3 rotational axis) and the rotation of the entire butyl [$(CD_3)_3$-C] fragment about its 3-fold axis (C_3' rotational axis). Numerical simulations of spectra line shapes reveal that the methyl groups and the butyl fragment exhibit three-site jump rotations about their symmetry axes C_3 and C_3' in the temperature range of 103-133 K, with the activation energies and preexponential factors $E_1 = 21 \pm 2$ kJ/mol, $f_{01} = (2.6 \pm 0.5) \times 10^{12}$ s^{-1} and $E_2 = 16 \pm 2$ kJ/mol, $k_{02} = (1 \pm 0.2) \times 10^{12}$ s^{-1}, respectively. Analysis of the anisotropy of spin—lattice relaxation has demonstrated that the reorientation mechanism of the butyl fragment changes to a free diffusion rotational mechanism above 173 K, while the rotational mechanism of the methyl groups remains the same. The values of the activation barriers for both rotations at T > 173 K have the values, which are similar to those at 103—133 K. This indicates that the interaction potential defining these motions remains unchanged. The obtained data demonstrate that the detailed analysis of both line shape and anisotropy of spin-lattice relaxation represents a powerful tool to follow the evolution of the molecular reorientation mechanisms in organic solids.

QUADRUPOLAR METAL NMR OF OXIDE MATERIALS INCLUDING CATALYSTS

O.B. Lapina, V.V. Terskikh

Encyclopedia of Magnetic Resonance,
Eds. R.K Harris, R.E Wasylishen,
John Wiley & Sons, Ltd, 2011.

In this work, the authors review the basic methodology and recent applications of quadrupolar metal solid-state NMR spectroscopy in oxide systems with emphasis on materials science and catalysis. Three typical quadrupolar metal nuclei, ^{51}V, ^{93}Nb, and ^{95}Mo, are discussed in detail to illustrate the complex interplay between the quadrupolar and chemical shielding interactions in oxides. In the first part, a systematic overview is given of the metal coordination environments in oxides and their corresponding NMR parameters. The importance of quantum chemical calculations in correlating experimental NMR results with a molecular level oxide structure is highlighted. In the second part, examples of quadrupolar metal NMR in materials science are presented, including paramagnetic oxide systems, layered materials, ferroelectrics, silicates, and glasses. The final section is dedicated to the latest applications of NMR in heterogeneous oxide catalysis.

MULTINUCLEAR NMR STUDY OF SILICA FIBERGLASS MODIFIED WITH ZIRCONIA

O.B. Lapina, D.F. Khabibulin, V.V. Terskikh

Solid State Nucl. Magn. Reson.,
39(3-4) (2011) pp. 47-57.

Silica fiberglass textiles are emerging as uniquely suited supports in catalysis which offer unprecedented flexibility in designing advanced catalytic systems for chemical and auto industries. During manufacturing fiberglass materials are often modified with additives of various nature to improve glass properties. Glass network formers, such as zirconia and alumina, are known to provide the glass fibers with higher strength and to slow down undesirable devitrification processes. In this work multinuclear ^{1}H, ^{23}Na, ^{29}Si, and ^{91}Zr NMR spectroscopy was used to characterize the effect of zirconia on the molecular-level fiberglass structure. ^{29}Si NMR results help in understanding why zirconia-modified fiberglass is more stable towards devitrification comparing with pure silica glass. Internal void spaces formed in zirconia-silica glass fibers after acidic leaching correlate with sodium and water distributions in the starting bulk glass as probed by ^{23}Na and ^{1}H NMR. These voids spaces are important for stabilization of catalytically active species in the supported catalysts. Potentials of high-field ^{91}Zr NMR spectroscopy to study zirconia-containing glasses and similarly disordered systems are illustrated.

MECHANOCHEMICAL SYNTHESIS OF γ-LiAlO$_2$ STUDIED BY ^{6}Li AND ^{27}Al NMR AND SYNCHROTRON X-RAY DIFFRACTION

V.P. Isupov*, O.A. Kharlamova*,
L.E. Chupakhina*, M.R. Sharafutdinov*,
D.F. Khabibulin, O.B. Lapina (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Inorg. Mater.,
47(7) (2011) pp. 763-767.

The structural transformations accompanying the mechanochemical synthesis of fine-particle γ-LiAlO$_2$ have been studied by ^{6}Li and ^{27}Al NMR and *in situ* X-ray diffraction. Mechanical activation of a mixture of aluminum hydroxide and lithium carbonate in an AGO-2 planetary mill results not only in size reduction, intermixing, and partial amorphization of the starting materials but also in the mechanochemical synthesis of a carbonate form of aluminum lithium hydroxide. Subsequent heat treatment of the mechanically activated mixture leads to the release of water and carbon dioxide molecules and the formation of an X-ray amorphous phase containing aluminum in octahedral and tetrahedral oxygen coordination. The X-ray amorphous material converts to gamma lithium aluminate through an intermediate phase.

BOROTUNGSTATE POLYOXOMETALATES: MULTINUCLEAR NMR STRUCTURAL CHARACTERIZATION AND CONVERSIONS IN SOLUTIONS

R.I. Maksimovskaya, G.M. Maksimov

Inorg. Chem.,
50(11) (2011) pp. 4725-4731.

The unique heteropolyanion $[H_3BW_{13}O_{46}]^{8-}$ (**BW$_{13}$**), previously suggested on the basis of indirect evidence, and protonated lacunary heteropolyanion $[HBW_{11}O_{39}]^{8-}$ (**BW$_{11}$**) have been identified in aqueous solutions at pH 5–7.5 from NMR spectra. The pattern of tungsten–tungsten connectivities based on the analysis of the $^{2}J_{W-O-W}$ coupling satellites in the ^{183}W NMR spectrum of BW$_{11}$, containing six peaks of relative intensities ~2:2:2:1:2:2, indicates that the latter is the α isomer. The ^{17}O NMR spectrum confirms the protonated state of the polyanion with the proton delocalized on two out of four terminal O atoms surrounding the tungsten vacancy. The ^{183}W NMR spectrum of $\mathbf{BW_{13}}$ contains seven peaks of relative intensities ~2:1:2:2:2:2:2 with additional large couplings due to the connectivity between $\mathbf{BW_{11}}$ and $[W_2O_7]^{2-}$ fragments. According to the ^{17}O NMR spectrum, two protons of $[BW_{13}O_{46}H_3]^{8-}$ are delocalized on the two terminal trans O atoms of the dimeric fragment while the third one is linked to its bridging O atom. The conversions of $\mathbf{BW_{11}}$ and $\mathbf{BW_{13}}$ in solution were followed by using ^{183}W NMR spectra at a “fingerprint” level. In the pH range from ~7.5 to 6, $\mathbf{BW_{11}}$ transforms to $\mathbf{BW_{13}}$, transforming further to $[BW_{12}O_{40}]^{5-}$ ($\mathbf{BW_{12}}$) and $[B_3W_{39}O_{132}H_n]^{n-21}$ ($\mathbf{B_3W_{39}}$) in different ratios. Conversion of $\mathbf{BW_{13}}$ to $\mathbf{BW_{12}}$ proceeds through an intermediate complex of suggested composition $[BW_{11}O_{39}{\cdot}WO_2]^{7-}$. At high acidity (pH ~0), $\mathbf{B_3W_{39}}$ gradually decomposes into tungstic acid, $\mathbf{BW_{12}}$ and H_3BO_3. Polyanion $\mathbf{BW_{12}}$ persists in the pH range ~0–7.5.

A STUDY OF THE HYDROLYSIS OF ZrF_6^{2-} AND THE STRUCTURE OF INTERMEDIATE HYDROLYSIS PRODUCTS BY ^{19}F AND ^{91}Zr NMR IN THE 9.4 T FIELD

M.A. Fedotov, A.V. Belyaev* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Struct. Chem.,
52(1) (2011) pp. 69-74.

The high-field ^{19}F and ^{91}Zr NMR method is used to study the hydrolysis and polycondensation of hexafluorozirconate ZrF_6^{2-} in aqueous and water-peroxide solutions. During hydrolysis in aqueous solutions only ZrF_6^{2-} and F^- ions were observed by NMR, however, in the water-peroxide medium, an intermediate product of hydrolysis ($[F_5Zr\text{-}OO\text{-}ZrF_5]^{4-}$ dimer) was detected. The dimer structure is confirmed by ^{19}F and ^{91}Zr NMR. In high fields (^{19}F NMR frequency > 200 MHz), the fluorine exchange between ZrF_6^{2-} and F^- is slow in the ^{19}F NMR scale and has a multisite character.

SOLID-PHASE CONDENSATION OF RHODIUM(III) AQUA SULFATES

S.N. Vorob'eva*, A.V. Belyaev*, M.A. Fedotov, I.V. Yushina*, T.I. Nedoseikina* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Russ. J. Inorg. Chem.,
56(10) (2011) pp. 1609-616.

Solid-phase condensation of rhodium(III) aqua sulfates yielding oligomeric rhodium(III) aqua sulfate complexes was revealed. The isothermal dehydration of rhodium(III) aqua sulfates under thermal diffusion conditions in the temperature range 100–130°C was studied, and effective rate constants and activation energies were determined. The solid phases of dehydration products were studied by X-ray powder diffraction and IR spectroscopy, and solutions of polymeric phases were studied by ^{103}Rh and ^{17}O NMR, electronic absorption spectroscopy, chromatography, and electrophoresis.

PLATINUM(IV) COMPLEXATION WITH THE NITRATE ION IN AQUEOUS SOLUTIONS ACCORDING TO ^{195}Pt, ^{15}N, ^{14}N, AND ^{17}O NMR DATA

A.V. Belyaev*, M.A. Fedotov, S.N. Vorobieva*
(**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Russ. J. Coord. Chem.,
37(4) (2011) pp. 281-287.

Solutions of platinum(IV) nitrate were studied by ^{195}Pt, ^{15}N, ^{14}N, and ^{17}O NMR and IR and Raman spectroscopy. It was found that in nitric acid, two interrelated systems of nitrate complexes, mono- and polynuclear ones, coexist. The complexes predominating in concentrated solutions are $[Pt_2(\mu\text{-}OH)(\mu\text{-}NO_3)(NO_3)_2(H_2O)_{6-x}(OH)_x]^{(4-x)+}$, $[Pt_4(\mu\text{-}OH)_3(\mu\text{-}NO_3)_3(NO_3)_3(H_2O)_{9-x}(OH)_x]^{(7-x)+}$, $[Pt_4(\mu\text{-}OH)_4(\mu\text{-}NO_3)_2(NO_3)_4(H_2O)_{8-x}(OH)_x]^{(6-x)+}$, and $[Pt_4(\mu\text{-}OH)_6(NO_3)_3(H_2O)_{16-x}(OH)_x]^{(7-x)+}$.

THE INFLUENCE OF AN EXOTHERMIC REACTION ON THE SPATIAL DISTRIBUTION OF THE LIQUID PHASE IN A TRICKLE BED REACTOR: DIRECT EVIDENCE PROVIDED BY NMR IMAGING

A.A. Lysova, A. Von Garnier*, E.H. Hardy, R. Reimert*, I.V. Koptyug***** (**Karlsruhe Institute of Technology, Karlsruhe, Germany; **International Tomography Center, Novosibirsk, Russia*)

Chem. Eng. J.,
173(2) (2011) pp. 552-563.

In this paper, NMR imaging was applied to study the distribution of the liquid phase in a fixed catalyst bed of an operating multiphase reactor with a cocurrent gas-liquid flow under conditions when the heterogeneous catalytic hydrogenation of 1-octene was taking place in the reactor. The 2D maps of the spatial distribution of the external and internal liquid holdups in the various regimes of the catalyst bed operation have been obtained for the first time in the course of the reaction. It was shown by a direct *in situ* method that an exothermic reaction taking place in a trickle bed reactor dramatically affected the distribution of the liquid phase in the catalyst bed. In particular, in the presence of the reaction, the catalyst bed was characterized by a non-uniform distribution of the liquid phase, as revealed by evaluating the external and internal liquid holdups. In the absence of the reaction, the bed was largely filled with the liquid phase.

PROBING THE DYNAMICS OF CO_2 AND CH_4 WITHIN THE POROUS ZIRCONIUM TEREPHTHALATE UiO-66(Zr): A SYNERGIC COMBINATION OF NEUTRON SCATTERING MEASUREMENTS AND MOLECULAR SIMULATIONS

Q. Yang*,**, H. Jobic**, F. Salles*, D.I. Kolokolov, V. Guillerm***, Ch. Serre***, G. Maurin*** (**Institut Charles Gerhardt Montpellier, Universit Montpellier II, Montpellier CEDEX, France; **Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Villeurbanne, France; ***Institut Lavoisier, Versailles, France; ****Beijing University of Chemical Technology, Beijing, P.R. China*)

Chem. Eur. J.,
17(32) (2011) pp. 8882-8889.

Quasi-elastic neutron scattering (QENS) measurements combined with molecular dynamics (MD) simulations were conducted to deeply understand the concentration dependence of the self- and transport diffusivities of CH_4 and CO_2, respectively, in the humidity-resistant metal–organic framework UiO-66(Zr). The QENS measurements show that the self-diffusivity profile for CH_4 exhibits a maximum, while the transport diffusivity for CO_2 increases continuously at the loadings explored in this study. MD simulations can reproduce fairly well both the magnitude and the concentration dependence of each measured diffusivity. The flexibility of the framework implemented by deriving a new forcefield for UiO-66(Zr) has a significant impact on the diffusivity of the two species. Methane diffuses faster than CO_2 over a broad range of loading, and this is in contrast to zeolites with narrow windows, for which opposite trends were observed. Further analysis of the MD trajectories indicates that the global microscopic diffusion mechanism involves a combination of intracage motions and jump sequences between tetrahedral and octahedral cages.

NMR IMAGING OF HEAVY CRUDE OIL FOR SOFTENING DETECTION UNDER HEAT TREATMENT

E.V. Morozov*, O.N. Martyanov, N.V. Volkov*, O.V. Falaleev* (**Kirensky Institute of Physics, Krasnoyarsk, Russia*)

J. Mater. Sci. Eng. A,
1 (2011) pp. 545-551.

NMR imaging results of Mongolian heavy crude oil samples subjected to heat treatment are presented in this work. Abundance of dotted inhomogeneities related with high paraffinicity of heavy oil was obtained during imaging investigation. Behavior of heavy oil subjected to heat treatment, dotted inhomogeneities changes, softening and dynamic of melting front were visualized by means of imaging techniques based on both gradient and spin echo. Softening forestalling over the melting front are demonstrated using artificial mark in the form of water drop deposited on the oil surface. In results the NMR imaging proved to be highly effective for investigation of impurity agglomerates in heavy oil engineering development.

ELECTRON SPIN RESONANCE OF VO^{2+} RADICAL-ION IN SUB- AND SUPERCRITICAL WATER

S.N. Trukhan, V.F. Yudanov, O.N. Martyanov

J. Supercrit. Fluids,
57(3) (2011) pp. 247-250.

Electron spin resonance (ESR) spectra of VO^{2+} radical-ions in sub- and supercritical water are observed. Upon increasing the temperature from 20 to 100°C, the fine structure line widths in the ESR spectra of the vanadyl ion are observed to be reduced that is associated with the effective averaging of the *g*-factor anisotropy and the hyperfine interaction. With further increasing the temperature, the spectrum components of the hyperfine structure are broadened significantly resulting in the unresolved low-intensity line in supercritical water with $\Delta H_{pp} \sim 300$ G. The data obtained allow behavior peculiarities of the paramagnetic VO^{2+} ions in sub- and supercritical water including rotational dynamics and spin exchange between the radicals to be elucidated. The registration of the unresolved low-intensity line in supercritical conditions points to an increase in the local ion concentration in the system that can be an initial stage for the formation of vanadium-based particles in supercritical conditions. The study demonstrates that ESR is the powerful tool to investigate properties of sub- and supercritical water *in situ*.

THE CHARACTERISTICS OF NEW PERMANENT SORBENT–MODIFIERS FOR THE HYDRIDE ATOMIC ABSORPTION SPECTROMETRIC DETERMINATION OF ARSENIC WITH TRAPPING OF THE ARSINE IN A GRAPHITE FURNACE

M.Yu. Burylin*, V.I. Zaikovsky, K.A. Romanovsky*, P.R. Arushanian* (**Kuban State University, Krasnodar, Russia*)

Anal. & Control,
15(1) (2011) pp. 23-36.

The characteristics of new Zr–Ir and W–Ir permanent sorbent–modifiers on the carbonized basis for the determination of arsenic by electrothermal atomic absorption spectrometry (ETAAS) with trapping within a graphite (GF) furnace were studied. The results of the electron microscopic investigation, local X-ray elemental analysis and electron microdiffraction corroborated zirconium and tungsten carbide's formation. The particle sizes of these compounds are from 50 to 200 nm. The iridium component presents as nanoparticles (5-10 nm) of condensed systems with the carbide forming metal. There is even distribution of the particles on the basis. Achievement of necessary purity's level of the permanent systems during their synthesis in a graphite furnace is confirmed. The parameters of the stage of arsine trapping by new sorbent-modifiers and arsenic's atomization stage are studied: temperature of trapping stage, velocity of reagent's entering, time of trapping stage, temperature of atomization stage. The optimized conditions were used for the determination of As in natural surface-water. The limits of detection were 7 ng/l and 5 ng/l for the Zr-Ir modifier and W-Ir modifier respectively.

METHANE CONVERSION INTO AROMATIC HYDROCARBONS OVER Ag–Mo/ZSM-5 CATALYSTS

A.V. Vosmerikov*, V.I. Zaikovsky, L.L. Korobitsyna*, V.V. Kozlov*, N.V. Arbuzova*, S.P. Zhuravkov** (**Institute of Petroleum Chemistry, Tomsk, Russia; **Tomsk Polytechnic University, Tomsk, Russia*)

Kinet. Catal.,
52(3) (2011) pp. 427-433.

Nonoxidative methane conversion into aromatic hydrocarbons over ZSM-5-type high-silica zeolites modified with nanosized powders of molybdenum (4.0 wt%) and silver (0.1–0.5 wt%) is reported. The acidic properties of the catalysts have been investigated by temperature-programmed ammonia desorption. The microstructure and composition of the Ag-Mo/ZSM-5 catalytic systems have been studied by high-resolution transmission electron microscopy and energy-dispersive X-ray spectroscopy. The doping of the Mo containing zeolite with silver enhances its activity and stability in nonoxidative methane conversion into aromatic hydrocarbons.

SUBMICROMETER INTERMEDIATES IN THE CITRATE SYNTHESIS OF GOLD NANOPARTICLES: NEW INSIGHTS INTO THE NUCLEATION AND CRYSTAL GROWTH MECHANISMS

Yu.L. Mikhlin*, A.A. Karacharov*, M.N. Likhatski*, T.Yu. Podlipskaya, Ya.V. Zubavichus***, A.A. Veligzhanin***, V.I. Zaikovsky** (**Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia; **Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; ***National Research Centre "Kurchatov Institute", Moscow, Russia*)

J. Colloid Interf. Sci.,
362(2) (2011) pp. 330-336.

The reduction of tetrachloroaurate by citrate ions in aqueous solutions yielding gold nanoparticles (GNPs) has been studied using *in situ* tapping mode atomic force microscopy (AFM), UV-vis absorption and dynamic light scattering (DLS) spectroscopies, small-angle X-ray scattering (SAXS) along with *ex situ* TEM, EDX and XPS. Special attention is given to mesoscale intermediates responsible for the intense coloring of the transient solutions and their role in nucleation and crystal growth. AFM detects liquid droplet-like domains, globules 30-50 nm in diameter arranged in submicrometer aggregates in the gray and blue solutions, and well separated individual particles in the final red sols. DLS shows abrupt appearance of species about 30 nm and larger but not growing Au nanoparticles, while SAXS reveals gradually increasing nanoparticles and no aggregates. The mesoscale structures observed in TEM become looser as the reaction proceeds; they contain signatures of oxidized Au and other solutes. The results are interpreted in terms of decomposition of supersaturated solutions to afford domains ("dense droplets") enriched by gold, and then, after nucleation and coalescence of Au nuclei inside them, rather slow growth of gold nanoparticles within the associated globules; the color changes of the transient solutions are due to increasing interparticle distances.

KINETICS AND MECHANISM OF THE GROWTH OF GOLD NANOPARTICLES BY REDUCTION OF TETRACHLOROAURIC ACID BY HYDRAZINE IN Triton N-42 REVERSE MICELLES

V.V. Tatarchuk*, A.P. Sergievskaya*, I.A. Druzhinina*, V.I. Zaikovsky (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Nanopart. Res.,
13(10) (2011) pp. 4997-5007.

The kinetics of the growth of gold nanoparticles during the reduction of tetrachloroauric acid by hydrazine in dispersed aqueous solution encapsulated by reverse micelles of Triton N-42 surfactant (with decane as dispersion medium) was studied by means of spectrophotometry. According to DLS data, at a set value of solubilization capacity $V_s/V_o = 0.005$ initial micelles have an aqueous core hydrodynamic diameter $d_c = 3.6\pm0.2$ nm. The final particles obtained after full reduction of Au^{III} have a metallic core of defect-free single-crystalline gold with a narrow size distribution and average core diameter $d_{Au} = 7.7 \pm 1.4$ nm as shown by TEM. The rate of the particle growth is limited by the rate of gold reduction. The process kinetics corresponds to the model consisting of two stages of reduction $Au^{III} \rightarrow Au^{I} \rightarrow Au^{0}$. The stages involve the formation and redox decay of the intermediate complexes $Au(N_2H_4)Cl_3$ and $Au(N_2H_4)Cl$, and each stage proceeds via two routes: (1) homogeneous in the dispersed aqueous phase, and (2) heterogeneous on the particle surfaces. Reactions taking route (2) are autocatalytic because they proceed with participation of the surface atoms of particles as the final products of Au^{III} reduction. The dependencies of observed rate constants on reagent concentrations, temperature, and solubilization capacity of the micellar solution are studied.

THE AGEING OF SILICA GELS AFFECTED BY HYDROTHERMAL TREATMENT

W. Lutz*, M. Weber, R. Bertram***,**
R. Kurzhals**, G.N. Kryukova**
(**Brandenburgische Technische Universität Cottbus, Berlin, Germany; **SCW Process Technology Development GmbH, Berlin, Germany; ***Leibniz-Institut für Kristallzüchtung, Berlin, Germany; ****Süd-Chemie Zeolites GmbH, Bitterfeld-Wolfen, Germany*)

Z. Anorg. Allg. Chem.,
637(3-4) (2011) pp. 421-425.

Commercial silica gels of the pyrogenic and precipitated types were hydrothermally treated for 72 hours at temperatures between 90°C and 210°C in water of autogenous pressure. The samples were characterised by IR spectroscopy, water and nitrogen adsorption. Stability and sorption capacity run similarly. The more Q^4 ($Si(OSi)_4$) building units the framework of a silica gel contained, the lower was its sorption capacity. Sorption capacity increased with rising number of structural defects characterised by the presence of Q^3 ($Si(OSi)_3OH$) and Q^2 ($Si(OSi)_2(OH)_2$) groups. Simultaneously, the hydrothermal stability of the silica material dropped off.

REACTIVITY OF EXTRA-FRAMEWORK SPECIES OF USY ZEOLITES IN ALKALINE MEDIUM

W. Lutz*, R. Bertram, D. Heidemann***,**
R. Kurzhals**, C. Ruscher*****,**
G.N. Kryukova (**Lehrstuhl fur Luftchemie und Luftreinhaltung Brandenburgische Technische Universitat Cottbus, Berlin, Germany; **Leibniz-Institut fur Kristallzuchtung, Berlin, Germany; ***Institut fur Chemie Humboldt-Universitat zu Berlin, Berlin, Germany; ****Sud-Chemie Zeolites GmbH, Bitterfeld-Wolfen, Germany; *****Universitat Hannover, Hannover, German*y)

Z. Anorg. Allg. Chem.,
637(1) (2011) pp. 75-82.

Zeolites of type USY (ultra-stable Y) were obtained by steaming of NH_4NaY modification. Samples were modified by subsequent alkaline treatment in KOH solution. USY and USY-KOH were characterised by chemical element analysis, XRD, IR, ^{29}Al and ^{29}Si MAS NMR spectroscopic measurements. Correct silicon to aluminium ratios (Si/Al) were determined by XRD and IR (double ring vibration w_{DR}) data whereas values calculated according to data of ^{29}Si MAS NMR and IR spectroscopy (asymmetrical TOT valence vibration w_{TOT}) appeared to be too high.

In the latter case, the signals of the zeolite framework were strongly superimposed by that of extra-framework silica gel (EFSi) formed during steaming. It was found that alkaline leaching induces desilication of silicon-rich area of the zeolite framework and partial dissolution of EFSi. Silicate ions of both react with likewise dissolved extra-framework aluminium (EFAl) to form X-ray amorphous aluminosilicate. Consequently, the superposition of the ^{29}Si MAS NMR signals of the zeolite framework by silica gel was reduced for $Q^4(0Al)$ but increased for Q^4 (2Al) and $Q^4(3Al)$ structure units. A reinsertion of EFAl into the zeolite framework has not been observed.

LIGHT SCATTERING IN A SURFACE GLASS LAYER PRODUCED BY A SURFACE ION EXCHANGE PROCESS AND COATED WITH THIN GOLD LAYERS

O.N. Sidel'nikova*, G.A. Pozdnyakov,**
A.N. Serkova, A.N. Salanov (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Khristianovich Institute of Theoretical and Applied Mechanics, Novosibirsk, Russia*)

Glass Technol.,
52(1) (2011) pp. 15-22.

The morphology and optical properties of a glass surface treated by a surface ion exchange process and coated with a thin surface gold layer are investigated. It was found by SEM that the modified surface layer consists of a system of microblocks and microcracks. In addition the thin gold layer consists of nanosized hemispherical gold nucleation centers of volume growth (diameters ~100-500 nm), three-dimensional gold aggregates and pendant "cornice". The investigated optical properties (light scattering, depolarization, light loss characteristics and effectiveness of light propagation) differ significantly from the analogous optical data previously reported for glass surface modified by the same surface ion exchange process but lacking the thin gold layer. The results are also compared with results obtained from a chemically etched glass surface. The obtained data may be important and useful in glass illumination engineering, light decoration and others fields.

METHOD OF SPECTRAL SUBTRACTION OF GAS-PHASE FOURIER TRANSFORM INFRARED (FT-IR) SPECTRA BY MINIMIZING THE SPECTRUM LENGTH

D.V. Kozlov, A.S. Besov

Appl. Spectrosc.,
65(8) (2011) pp. 918-923.

A new method of spectral subtraction for gas-phase Fourier transform infrared (FT-IR) spectra was developed for long-path gas measurements. The method is based on minimization of the length of the spectrum that results from subtracting the spectrum of an individual component of a gas mixture (water, CO_2, etc.) from the experimental spectrum of the mixture. For this purpose a subtraction coefficient (k_{min}) is found for which the length of the resulting spectrum is minimized. A mathematical simulation with two Lorentzian absorption bands was conducted and the limits of application for the proposed method were determined. Two experimental examples demonstrate that a successful result could be achieved in the case when the subtrahend spectrum contains a number of narrow absorption bands (such as the spectrum of water vapor).

In situ FTIR STUDY OF β-PICOLINE TRANSFORMATIONS ON V–Ti–O CATALYSTS

G.B. Chernobay, Yu.A. Chesalov, V.P. Baltakhinov, G.Ya. Popova, T.V. Andrushkevich

Catal. Today,
164(1) (2011) pp. 58-61.

Surface complexes formed during β-picoline transformations on V–Ti–O catalysts in the temperature range of 120–300°C were studied using *in situ* FTIR spectroscopy. Two vanadia–titania catalysts with several kinds of vanadia species were used in experiments. FTIR spectra have revealed differences in composition of surface complexes under different coverage, which could be related to different ways of transformations of intermediate pyridine-3-carbaldehyde.

O^- RADICAL ANIONS ON OXIDE CATALYSTS: FORMATION, PROPERTIES, AND REACTIONS

A.M. Volodin, S.E. Malykhin, G.M. Zhidomirov

Kinet. Catal.,
52(4) (2011) pp. 605-619.

A systematic *in situ* EPR study of processes yielding O^- radical anions on the surface of oxide dielectrics (MgO, CaO), semiconductors (ZnO, TiO_2), supported systems (V/SiO_2), and zeolite FeZSM-5 is reported. Methodological approaches to the study of O^- radical anions are considered for the cases in which these species are directly undetectable by EPR. Particular attention is focused on the development of methods of investigation of so-called α-oxygen on the FeZSM-5 surface, which is an O^- radical anion stabilized on the paramagnetic ion Fe^{3+}. The reactions involving α-oxygen and the analogous reactions known for O^- radical anions stabilized on the oxide surface are demonstrated to occur in similar ways. The photostimulated formation of spatially separated electron and hole centers on the surface of oxide systems is most likely due not to charge separation, but to the spatial separation of the radicals resulting from the homolytic photodissociation of chemisorbed water. A scheme is suggested for this process on the partially hydroxylated MgO surface.

EXPLORING BY PULSED EPR THE ELECTRONIC STRUCTURE OF UBISEMIQUINONE BOUND AT THE Q_H SITE OF CYTOCHROME bo_3 FROM ESCHERICHIA COLI WITH in vivo ^{13}C-LABELED METHYL AND METHOXY SUBSTITUENTS

M.T. Lin*, A.A. Shubin, R.I. Samoilova, K.V. Narasimhulu*, A. Baldansuren*, R.B. Gennis*, S.A. Dikanov** (**University of Illinois at Urbana-Champaign, Urbana, Illinois; **Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*)

J. Biol. Chem.,
286(12) (2011) pp. 10105-10114.

The cytochrome bo_3 ubiquinol oxidase from Escherichia coli resides in the bacterial cytoplasmic membrane and catalyzes the two-electron oxidation of ubiquinol-8 and four-electron reduction of O_2 to water. The one-electron reduced semiquinone forms transiently during the reaction, and the enzyme has been demonstrated to stabilize the semiquinone. The semiquinone is also formed in the D75E mutant, where the mutation has little influence on the catalytic activity, and in the D75H mutant, which is virtually inactive. In this work, wild-type cytochrome bo_3 as well as the D75E and D75H mutant proteins were prepared with ubiquinone-8 ^{13}C-labeled selectively at the methyl and two methoxy groups. This was accomplished by expressing the proteins in a methionine auxotroph in the presence of l-methionine with the side chain methyl group ^{13}C-labeled. The ^{13}C-labeled quinone isolated from cytochrome bo_3 was also used for the generation of model anion radicals in alcohol. Two-dimensional pulsed EPR and ENDOR were used for the study of the ^{13}C methyl and methoxy hyperfine couplings in the semiquinone generated in the three proteins indicated above and in the model system. The data were used to characterize the transferred unpaired spin densities on the methyl and methoxy substituents and the conformations of the methoxy groups. In the wild type and D75E mutant, the constraints on the configurations of the methoxy side chains are similar, but the D75H mutant appears to have altered methoxy configurations, which could be related to the perturbed electron distribution in the semiquinone and the loss of enzymatic activity.

SIZE-DEPENDENT EFFECTS IN EPR AND LUMINESCENCE SPECTRA OF NH_4BPh_4 EXCITED STATES: FROM BULK TO NANOPARTICLES

O.V. Antonova*, V.A. Nadolinny*, E.A. Il'inchik*, M.K. Kovalev, A.P. Yelisseyev** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia;* ***Institute of Geology & Mineralogy, Novosibirsk, Russia*)

Appl. Magn. Reson.,
40(4) (2011) pp. 459-469.

Photoexcited states of NH_4BPh_4 (TPhBA) particles embedded in mesoporous frameworks of different pore sizes were studied by combined electron paramagnetic resonance (EPR), optical and photoluminescence techniques. A distribution of triplet states with short and long electron-hole distances was found. While EPR studies on TPhBA bulk sample suggested that the formation of electron-hole pairs upon the excitation was caused by electron capture on electron traps, the samples in mesoporous frameworks exhibit two ways of the pair formation. The first one is attributed to the capture on phenyl rings and another one is to be thought as the capture of electrons on adsorbed oxygen molecules. These results are also consistent with the thermoluminescence spectra and EPR studies of the photoexcited samples during annealing.

EFFECT OF Cs^+ PROMOTER IN Ru/MgO CATALYSTS

Yu.V. Larichev

J. Phys. Chem. C,
115(3) (2011) pp. 631-635.

Ru/MgO and Ru–Cs^+/MgO catalysts were prepared from $Ru(OH)Cl_3$ and were studied by XPS, TEM, CO chemisorption, and EXAFS. An explanation for the large differences in sizes of Ru particles measured by TEM and XRD compared to those determined by CO chemisorption is proposed. This explanation is based on the XPS data that the initial catalyst Ru/MgO consists of Ru^0 metal particles and RuO_2 clusters. The latter are not measured by CO chemisorption and have high stability due to RuO_2–MgO interaction. A new feature of Cs^+ promoter influence on the Ru/MgO catalyst was found. The addition of Cs^+ to the Ru/MgO catalyst, which contains Ru partly in the oxidized form, does not lead to the formation of any cesium ruthenates. Instead, the cesium promoter reduces the RuO_2 clusters, which are stabilized by epitaxy interaction with the support, to form the Ru^0 particles. This new feature of Cs^+ promoter results in the increase of supported Ru useful ratio and Ru-specific surface area in these catalysts.

ELECTRONIC STATE OF RUTHENIUM DEPOSITED ONTO OXIDE SUPPORTS: AN XPS STUDY TAKING INTO ACCOUNT THE FINAL STATE EFFECTS

Yu.V. Larichev, B.L. Moroz, V.I. Bukhtiyarov

Appl. Surf. Sci.,
258(4) (2011) pp. 1541-1550.

The electronic state of ruthenium in the supported Ru/EO_x (EO_x = MgO, Al_2O_3 or SiO_2) catalysts prepared with the use of $Ru(OH)Cl_3$ or $Ru(acac)_3$ (acac = acetylacetonate) and reduced with H_2 at 723 K is characterized by X-ray photoelectron spectroscopy (XPS) in the Ru 3d, Cl 2p and O 1s regions. The influence of the final state effects (the differential charging and variation of the relaxation energy) on the binding energy (BE) of Ru $3d_{5/2}$ core level measured for supported Ru nanoparticles is estimated by comparison of the Fermi levels and the modified Auger parameters determined for the Ru/EO$_x$ samples with the corresponding characteristics of the bulk Ru metal. It is found that the negative shift of the Ru 3d$_{5/2}$ peak which is observed in the spectrum of ruthenium deposited onto MgO (BE = 279.5–279.7 eV) with respect to that of Ru black (BE = 280.2 eV) or ruthenium supported on γ-Al_2O_3 and SiO_2 (BE = 280.4 eV) is caused not by the transfer of electron density from basic sites of MgO, as considered earlier, but by the differential charging of the supported Ru particles compared with the support surface. Correction for the differential charging value reveals that the initial state energies of ruthenium in the Ru/EO$_x$ systems are almost identical (BE = 280.5 ± 0.1 eV) irrespectively of acid–base properties of the support, the mean size of supported Ru crystallites (within the range of 2–10 nm) and the surface Cl content. The results obtained suggest that the difference in ammonia synthesis activity between the Ru catalysts supported on MgO and on the acidic supports is accounted for by not different electronic state of ruthenium on the surface of these oxides but by some other reasons.

SMALL-ANGLE SCATTERING STUDY OF COLLOIDAL PARTICLES IN HEAVY CRUDE OILS

F.V. Tuzikov, Yu.V. Larichev, L.S. Borisova*, I.V. Kozhevnikov, O.N. Martyanov (**Trofimuk Institute of Petroleum Geology and Geophysics, Novosibirsk, Russia*)

Pet. Chem.,
51(4) (2011) pp. 281-285.

The structural and dispersion characteristics of samples of heavy crude oils and fractions isolated from them have been studied. A method of *in situ* analysis of the aggregation of asphaltenes directly in crude oils on the basis of small-angle X-ray scattering is proposed. It has been shown that the maximum size of scattering particles in all crude oil samples is limited to the value on the order of 8.0 nm; the average diameter is ~2.0 nm. It has been found that the fraction with sizes of 0.8–2.5 nm is mostly composed of resins. Asphaltenes in crude oils form larger aggregated particles with a size up to 8 nm. A comparative study of model dilute solutions of asphaltenes in toluene (0.23 wt%) has shown that the major part of asphaltenes in the liquid (~94%) is in the form of individual molecules with a size of 0.4–1.2 nm, and only an insignificant remaining part (~6%) occurs in the form of large aggregates.

INFLUENCE OF ATORVASTATIN ON SERUM LIPIDS ON MICE WITH LIPEMIA

V.M. Loginova*, F.V. Tuzikov, N.A. Tuzikova, M.S. Cherkanova*, E.E. Filyushina*, T.A. Korolenko* (**Institute of Physiology, Novosibirsk, Russia*)

Bull. SB RAMS,
31(2) (2011) pp. 133-137.

Atorvastatin (75 mg/kg) was administered twice in ICR mice with acute lipemia induced with a single injection of Triton WR 1339 (500 mg/kg). A novel small-angle X-ray scattering (SAXS) method for the determination of fractional and subfractional composition of C-LP was used. In Triton WR 1339-treated animals, there was a drastic increase of atherogenic low-density C-LP (C-LDL) fraction, intermediate density lipoprotein-cholesterol (C-IDL) subfraction, and very low-density C-LP (C-VLDL) fractions (C-VLDL$_{3\text{-}5}$ subfraction), with an increase of the C-HDL$_3$ subfraction. Atorvastatin treatment of lipemia was followed a decrease in the total C and, especially, a decrease in the TG concentration, by normalization of atherogenic C-LDL fraction, C-IDL subfraction, and a decrease of C-VLDL (C-VLDL$_{3\text{-}5}$ subfraction).

INFLUENCE OF ATORVASTATIN ON FRACTIONAL AND SUBFRACTIONAL COMPOSITION OF SERUM LIPOPROTEINS AND MMP ACTIVITY IN MICE WITH TRITON WR 1339-INDUCED LIPAEMIA

T.A. Korolenko*, M.S. Cherkanova*, F.V. Tuzikov, T.P. Johnston, N.A. Tuzikova, V.M. Loginova*, V.I. Kaledin*** (**Institute of Physiology, Novosibirsk, Russia; **University of Missouri-Kansas City, Kansas City, Missouri, USA*)

J. Pharm. Pharmacol.,
63(6) (2011) pp. 833-839.

The effects of atorvastatin on the atherogenic and anti-atherogenic lipoprotein-cholesterol (C-LP) and lipoprotein-triglyceride (TG-LP) fractions and subfractions at the early stage of murine acute hyperlipidaemia, and its pleiotropic anti-inflammatory effects via the activity of matrix metalloproteinases (MMPs) were studied.

Atorvastatin (75 mg/kg) was administered to ICR mice with acute lipaemia induced by a single injection of Triton WR 1339 (500 mg/kg). A novel small-angle X-ray scattering (SAXS) method was used for the determination of the fractional and subfractional composition of C-LP and TG-LP.

In Triton WR 1339-treated mice, there was a drastic increase in the atherogenic low-density C-LP (C-LDL) fraction, intermediate density lipoprotein-cholesterol (C-IDL) subfraction, and very low-density C-LP (C-VLDL) fractions (C-VLDL(3-5) subfraction). Additionally, there was an increase in the C-HDL(3) subfraction. Treatment of lipaemia with atorvastatin resulted in the normalization of the atherogenic C-LDL fraction and the C-IDL subfraction. A decrease in C-VLDL (C-VLDL(3-5) subfraction), total cholesterol and, especially, triglyceride (TG) concentrations was also demonstrated. Similar results were obtained with the TG-LP fractions and subfractions. Additionally, atorvastatin treatment resulted in an increase in the serum and liver MMP activity.

STUDY OF CdSe/CdS QUANTUM DOTS IN SOLUTIONS AND GELS BY SMALL-ANGLE X-RAY SCATTERING

N.B. Simonova*, F.V. Tuzikov, R.N. Khramov*, N.A. Tuzikova, M.F. Tuzikov*, M.S. Vakshtein**
(**Institute of Theoretical and Experimental Biophysics, Pushchino, Moscow oblast, Russia; **Federal State Unitary Association Research Institute of Applied Acoustics, Dubna, Moscow oblast, Russia*)

J. Surf. Invest. - X-Ray Synchrotron Neutron Techn.,
5(1) (2011) pp. 126-133.

The sizes of semiconductor nanocrystals of CdSe/CdS quantum dots (QDs) synthesized by the colloidal method were estimated using small-angle X-ray scattering. The distribution of QD nanocrystals in organic solvents of different polarities and in polymer gels and matrices is studied. Structural invariants of scattering QD particles (heterogeneities of the electron density) — namely, inertia radii and sizes, forms, and dispersive composition of particles — are determined. The contribution of scattering by QDs in solutions and gels is calculated. The effective sizes of particles and their aggregates are determined, and the parameters of the distribution over the QD sizes in organic solvents and polymer matrices are estimated. The typical distance between particles in samples is determined. The position of the maximum at the beginning of the small-angle scattering curves corresponds to the distance $d_m = 2\pi/h_0$ between the planes (here, h_0 is the position of the maximum on the scale h). It is 74–76.9 Å for solutions, 60 Å for gels, and 99 Å for polymer matrices with concentrations of up to 0.15% and 77 Å for those with the concentrations exceeding 0.15%, which is close to the estimation of the sizes of separate CdSe QDs that was obtained from the distribution histograms (60–80 Å). This result shows that CdSe/CdS QDs introduced in the polymer matrices disperse to form either separate particles or small aggregates and located at a distance on the order of 80 Å from each other.

SPECIFIC FEATURES OF ASSOCIATION OF Cu^{2+} IONS IN CONCENTRATED AQUEOUS AMMONIA SOLUTIONS OF COPPER NITRATE AS PROBED BY ESR

V.F. Anufrienko, G.A. Zenkovets, R.A. Shutilov, V.Yu. Gavrilov, N.T. Vasenin, A.A. Shubin, Z.R. Ismagilov, V.N. Parmon

Doklady Phys. Chem.,
440(2) (2011) pp. 194-197.

In this work, self-association of Cu^{2+} ions in aqueous ammonia solutions of copper nitrate was revealed for the first time.

It was shown that, in aqueous ammonia solutions of copper nitrate containing 10 g/L Cu in a wide range of ammonium ion concentrations, different types of Cu^{2+} associates with specific orbital ordering were formed. The ammonium concentration in a solution has a decisive effect on the type of orbital ordering of Cu^{2+} ions in associates. In all cases, copper ion ordering in associates is caused by the presence of bridging OH groups in the axial or equatorial position of $[Cu(NH_3)_n(H_2O)_{6-n}]^{2+}$ complexes ($n < 6$).

BIMETALLIC Pd–M (M = Co, Ni, Zn, Ag) NANOPARTICLES CONTAINING TRANSITION METALS: SYNTHESIS, CHARACTERIZATION, AND CATALYTIC PERFORMANCE

B.G. Ershov*, A.V. Anan'ev*, E.V. Abkhalimov*, D.I. Kochubei, V.V. Kriventsov, L.M. Plyasova, I.Yu. Molina, N.Yu. Kozitsyna, S.E. Nefedov**, M.N. Vargaftik**, I.I. Moiseev**** (**Frumkin Institute of Physical Chemistry and Electrochemistry, Moscow, Russia; **Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia*)

Nanotechn. Russia,
6(5-6) (2011) pp. 323-329.

The reductive thermolysis of $Pd(OOCMe)_4M(OH_2)$ (M = NiII, CoII, ZnII) and

$Pd(OOCMe)_4Ag_2(HOOCMe)_4$ molecular complexes results in the generation of bimetallic Pd-based Pd–M (M = Co, Ni, Zn, Ag) nanoparticles. The composition and morphology of nanoparticles and the electron state of metal atoms were characterized using electron microscopy, elemental ICP analysis, X-ray diffraction, and XAFS (XANES/EXAFS) techniques. The catalytic performance of nanoparticles was studied using the example of reactions of catalytic hydrazine decomposition and U(VI) reduction to U(IV) by hydrazine and formic acid. The catalytic performance of Pd–Ni nanoparticles is superior to that of the standard supported Pd/SiO_2 catalyst containing a similar amount of Pd atoms, while Pd–Co, Pd–Zn, and Pd–Ag Nanoparticles do not catalyze the studied reactions.

NOVEL HETEROMETALLIC PALLADIUM-SILVER COMPLEX

N.Yu. Kozitsyna*, S.E. Nefedov*, A.P. Klyagina*, A.A. Markov*, Zh.V. Dobrokhotova*, Yu.A. Velikodny, D.I. Kochubey, T.S. Zyubina***, A.E. Gekhman*, M.N. Vargaftik*, I.I. Moiseev*** (**Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Institute for New Chemical Problems, Moscow Region, Chernogolovka, Russia*)

Inorg. Chim. Acta,
370(1) (2011) pp. 382-387.

The reaction between $Pd_3(OOCMe)_6$ and $Ag_2(OOCMe)_2$ afforded the first palladium–silver heterometallic acetate-bridged complex $Pd^{II}[(\mu\text{-}OOCMe)_2Ag^{I}(HOOCMe)_2]_2$ (**1**). The molecular geometry and electronic structure of **1** were studied by single-crystal XRD and quantum-chemical DFT calculations. Thermal transformations of **1** *in vacuo* and under Ar, H_2 produced PdAg alloy nanoparticles characterized with powder XRD and EXAFS.

COCATALYTIC EFFECT OF PALLADIUM AND ZINC IN THE CONDENSATION OF ALCOHOL CARBON BACKBONES INTO HYDROCARBONS

A.V. Chistyakov*, M.V. Tsodikov*, V.Yu. Murzin*, F.A. Yandieva*, Ya.V. Zubavichus, N.Yu. Kozitsyna***, A.E. Gekhman***, V.V. Kriventsov, I.I. Moiseev***
(**Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; **Kurchatov Institute Russian Research Center, Moscow, Russia; ***Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia*)

Kinet. Catal.,
52(2) (2011) pp. 258-272.

The results of the direct conversion of ethanol and its mixture with glycerol into a C_4–C_{10}^+ alkane and olefin fraction in the presence of Pd-, Zn-, and Pd–Zn-containing catalysts, which were prepared by supporting homo- and heterometallic acetate complexes onto the surface of γ-Al_2O_3, are reported. It was found that, in the presence of mono- and bicomponent Pd–ZnO (Pd; ZnO)/γ-Al_2O_3 systems, selectivity in the formation of alkanes, olefins, or their mixtures in the target fraction can be controlled as a result of the cocatalytic effect of active components that are responsible for the catalyst activity in condensation and hydrogenation reactions. The structures of the active components were studied and the genesis of the catalytic systems was characterized using XAFS, XPS, and XRD analysis. It was found that the addition of glycerol considerably increased the yield of the target hydrocarbon fraction.

STERIC FACTOR IN LIGAND DISPLACEMENT OF ZIRCONIUM ALKOXIDES DISSOLVED IN ALCOHOLS

V.V. Kanazhevskii, Yu.A. Chesalov, N.S. Kotsarenko, D.I. Kochubey

J. Organomet. Chem.,
696(9) (2011) pp. 1879-1886.

The present study indicates EXAFS direct structural data obtained for zirconium ethoxide, iso- and *n*-propoxide are alike those for zirconium *n*-butoxide complexes. This is evident for agreement of structural units of above mentioned alkoxides complexes. The structural model of *n*-butoxide was developed earlier. Six interconnected tetramers assemble a structural unit of the alkoxides under study. The tetramers build of zirconium atoms in the highly flattened pyramid corners. Four zirconium atoms are bonded in series by double bridges through oxygen atoms of alkoxide ligands. Two of the four zirconium atoms are bias bonded by single ligand bridges. The distances between pairs of zirconium atoms inside the tetramer are 3.3 and 3.5 angstrom. Tetramers are linked together also by a single ligand bridges. The distance between zirconium atoms of the two neighbor tetramers is 3.9 angstrom. Primary particles (tetramer sextet) form aggregates in a solution. Possible shapes of the anisotropically sized aggregates is a large diameter cylinder with small height (a disk), or a small diameter cylinder with large height (a rod). Primary particles composed through ligands. The distance between the neighbor zirconium atoms of different primary particles is 4.8 or 5.1 angstrom depending on the coordination nature and the neighboring particles number.

A HIERARCHIC STRUCTURE IN ZIRCONIUM BUTOXIDE COMPLEXES IN *n*-BUTANOL SOLUTIONS

V.V. Kanazhevskii, N.S. Kotsarenko,
V.N. Kolomiichuk, D.I. Kochubey

J. Struct. Chem.,
52(1) (2011) pp. 75-82.

The structure of particles in zirconium *n*-butoxide solutions in *n*-butyl alcohol is determined by means of EXAFS, SAXS, and molecular mechanics modeling. Zirconium atoms are found to be bonded to each other via the oxygen atom and to form large anisotropic particles in the solution. Primary particles have a shape close to spherical; their diameter together with the solvate shell is 28.9 Å. These particles then aggregate into anisotropic structures. During solution aging under normal conditions without contact with the atmosphere, the particle anisotropy increases because of the aggregation of complexes. When the solution concentration decreases, the particles are divided into primary spherical particles with a characteristic size of 28.9 Å. The described changes are confirmed by a decrease in the number of Zr-Zr distances of 4.8 Å and 5.1 Å, which according to the EXAFS data, correspond to the bonds between the primary particles. The characteristic maximum sizes of particles in solutions with concentrations from 0.1 g to 0.003 g ZrO_2/ml are 160–80 Å.

TRANSPORT AND THERMAL CHARACTERISTICS OF $Cs_{1-x}Rb_xH_2PO_4$

V.G. Ponomareva*, V.V. Martsinkevich*,
Yu.A. Chesalov (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Russ. J. Electrochem.,
47(5) (2011) pp. 605-612.

The transport and thermal properties of $Cs_{1-x}Rb_xH_2PO_4$ in a wide range of compositions were studied. The binary salts $Cs_{1-x}Rb_xH_2PO_4$ ($x = 0$–0.9) contain solid solutions with a structure of CsH_2PO_4. The binary salts were synthesized by mechanically mixing the starting components and growing crystals by isothermal evaporation from aqueous solutions. The properties of $Cs_{1-x}Rb_xH_2PO_4$ salts obtained by different procedures were found to differ considerably. At higher rubidium contents in compounds obtained by mechanical mixing, the superionic transition temperature raised insignificantly, the high-temperature phase conductivity decreased twofold, the low-temperature conductivity increased within the limits of the order of magnitude, and the system of hydrogen bonds was slightly weakened. In $Cs_{1-x}Rb_xH_2PO_4$ crystals grown from solutions, the temperature of the superionic transition decreased along with its slowing down, and the low-temperature conductivity increased by more than three orders of magnitude because of the higher contents of residual acid aqueous centers in the structure of the salt. These systems are characterized by increased thermal stability.

VIBRATIONAL SPECTRA OF $WO_3 \cdot nH_2O$ AND WO_3 POLYMORPHS

G.N. Kustova, Yu.A. Chesalov, L.M. Plyasova,
I.Yu. Molina, A.I. Nizovskii

Vib. Spectrosc.,
55(2) (2011) pp. 235-240.

Vibrational spectra of polycrystalline WO_3 hydrates and polymorphs were measured and analyzed. The effect of sampling techniques on IR spectra has been demonstrated. The phase transition into triclinic polymorph ($C^5_{2h} \rightarrow C^1_i$) has been revealed for the sample of monoclinic WO_3 prepared as KBr pellet. Using the deuteration method *in situ* has shown that cubic WO_3 is non-stoichiometric oxide stabilized by residual OH groups of $WO_3 \cdot H_2O$ precursor.

INELASTIC ELECTRON SCATTERING IN THE ADSORBED SYSTEM

A.R. Cholach, N.N. Bulgakov, V.M. Tapilin

J. Struct. Chem.,
52(suppl.) (2011) pp. S13-S20.

The study revealed additional channels of inelastic electron scattering, which accompany the threshold excitation of the substrate Pt4*d* level — ionization of the valent states of adsorbed particles chemically bonded to the excited atom, and excitation of the surface plasmon vibrations. The conjugate excitation of this type shows up as a series of typical satellites in the spectra of disappearance potentials, which reflects the structure of valent states of adsorbed particles. Analysis of the satellite structure revealed the intermediate formation of $NH_{x,ads}$ particles in the reaction $NO_{gas} + H_{ads}$ on the surface of Pt(100) single crystal and, taking into account the earlier data, made it possible to formulate a general mechanism of selfoscillations in the $NO + H_2$ reaction on platinum metals. Mathematical modeling of reaction kinetics on the Pt(100) surface within the suggested mechanism demonstrated the presence of regular self-oscillations of the reaction rate at invariable values of the step constants.

ADVANCED POWER OF DISAPPEARANCE POTENTIAL SPECTROSCOPY IN THE ADSORBED SPECIES IDENTIFICATION

A.R. Cholach

In "*Chemical Physics Research Developments*",
Ed. P.W. Hansen, Nova Press, 2011, ch. 6,
pp. 149-173.

The novel potentialities of Disappearance Potential Spectroscopy for fundamental studies and practical application are highlighted. Electronic structure of the adsorbed species can be characterized properly from an extended spectra processing due to following reasons. First, because of the pronounced sensitivity of this technique to precious few top sample layers exactly those are responsible for the processes of adsorption and surface reactions. Second, due to availability of the novel kind of electron-solid interaction, namely the conjugate electron excitation developed recently from the model studies. The latter phenomenon consists in ordinary substrate core level excitation accompanied by electron transition from the valence state of adsorbed particle to vacuum level. This is displayed experimentally as a set of spectral satellites localized by the respective ionization potential above the Fermi level of a given substrate component. It enables to fingerprint the electronic valence state structure and thus to ascertain the chemical nature of adsorbed species of any complexity. It also gives potentiality to determine an exact location of adsorbed particle on the composite substrate surface.

STATUS OF AEROGEL PRODUCTION IN NOVOSIBIRSK

**A.Yu. Barnyakov*, M.Yu. Barnyakov*,
K.I. Beloborodov*, V.S. Bobrovnikov*,
A.R. Buzykaev*, V.B. Golubev*, B.V. Gulevich*,
A.F. Danilyuk, S.A. Kononov*, E.A. Kravchenko*,
K.A. Martin*, A.P. Onuchin*, V.V. Porosev*,
S.I. Serednyakov*** (**Budker Institute of Nuclear Physics, Novosibirsk, Russia*)

Nucl. Instrum. Methods Phys. Res., Sect. A,
639(1) (2011) pp. 225-226.

Silica aerogel blocks are being produced for use in Cherenkov detectors by a collaboration of Boreskov Institute of Catalysis and Budker Institute of Nuclear Physics since 1986. Novosibirsk aerogel is used in several detectors; among them are KEDR, SND (BINP, Novosibirsk), LHCb (CERN, Geneva), AMS (for International Space Station mission) and others. Currently the investigations are going on in two directions: multilayer aerogels for Focusing Aerogel RICH and aerogels with high index of refraction. The authors have synthesized two-, three- and four-layer aerogel tiles with dimensions of 115 mm x 115 mm. The authors have modernized the method of pinhole drying for preparation of aerogels with refractive index in the range of 1.07-1.20.

FOCUSING AEROGEL RICH FOR PARTICLE IDENTIFICATION AND MOMENTUM MEASUREMENT

**A.Yu. Barnyakov*, M.Yu. Barnyakov*,
I.Yu. Basok*, V.E. Blinov*, V.S. Bobrovnikov*,
A.A. Borodenko*, A.R. Buzykaev*,
V.V. Gulevich*, A.F. Danilyuk, S.A. Kononov*,
E.A. Kravchenko*, I.A. Kuyanov*,
A.P. Onuchin*, I.V. Ovtin*** (**Budker Institute of Nuclear Physics, Novosibirsk, Russia*)

Nucl. Instrum. Methods Phys. Res., Sect. A,
639(1) (2011) pp. 290-293.

The work is devoted to the development of the Focusing Aerogel RICH (FARICH). The option of the forward RICH for the SuperB project in Italy is presented. It features an aerogel-NaF radiator and

MCP photodetectors. Monte Carlo simulation predicts the π/K separation at the level better than 3σ from 0.2 to 7 GeV/*c*, the μ/π separation — from 0.13 to 1.3 GeV/*c*, and the kaon momentum measurement with an accuracy of about 1% at 1 GeV/*c*. FARICH for the Super Charm-Tau Factory project in Novosibirsk is proposed. Monte Carlo simulation predicts μ/π separation at the level better than 3σ for a momentum from 0.3 to 1.7 GeV/*c*. A prototype will be tested on the new electron test beam facility at VEPP-4M collider.

STRUCTURE MODIFICATION OF DIFFERENT GRAPHITE AND GLASSY CARBON SURFACES UNDER HIGH POWER ACTION BY HYDROGEN PLASMA

A.A. Shoshin*, A.V. Arzhannikov*, A.V. Burdakov*, K.N. Kuklin*, I.A. Ivanov*, K.I. Mekler*, S.V. Polosatkin*, V.V. Postupaev*, K.S. Raspopin, A.F. Rovenskikh*, P.A. Simonov, S.L. Sinitsky*, V.N. Snytnikov (**Budker Institute of Nuclear Physics, Novosibirsk, Russia*)

Fusion Sci. Technol.,
59(1T) (2011) pp. 268-270.

The studies of exposing of targets by hot-electron plasma exhaust from the multi-mirror trap GOL-3 are carried out. The results of Raman and SEM studies of surface modification of carbon materials with different ordering range of sp2 fraction (different graphite and glassy carbon) exposed by pulsed hot hydrogen plasma with energy density up to 8 MJ/m^2 are presented. It is shown that on the depth up to ~80 nm due to this exposing there are obtained two effects – micro structural destruction of the surface and extension of crystallite size of sp2 phase, i.e. ordering of nanostructure.

DIAGNOSIS OF FUNCTIONAL MATERIALS

V.V. Malakhov

Fact. Lab. Mat. Diagnosis,
77(2) (2011) pp. 3-10.

Theoretical and experimental aspects of using chemical analytical methods in diagnostics of functional materials are considered. Currently, these methods are used to determine the gross elemental composition of materials, though the needs of diagnosis are mainly reduced to the necessity of determining the chemical composition of various manifestations of the fine structure of such objects. Presented are novel approaches associated with chemical stoichiographic methods. These methods do not need the reference samples of phases to be determined, thus providing simultaneous detection of both known and previously unknown phases, identification of phases by the stoichiometry of elemental composition and to quantitative determination of their content. The objects of analysis are dispersed powders, ceramics, crystals, thin films, hetero- and nano-structures. Examples of the using the stoichiographic methods in diagnostics of various functional materials are given.

METHODOLOGY AND PROCEDURE OF THE STOICHIOGRAPHIC ANALYSIS OF SOLID INORGANIC SUBSTANCES AND MATERIALS

V.V. Malakhov, N.N. Boldyreva, A.A. Vlasov, L.S. Dovlitova

J. Anal. Chem.,
66(5) (2011) pp. 458-464.

The technical and experimental aspects of creating the conditions of differential dissolution in a flow stoichiographic system are discussed; the scheme of the experimental apparatus, stoichiograph, is presented. The construction, operation conditions of the main units of the stoichiograph, and sample treatment issues are considered. The principles of the creation and optimization of the conditions of the dynamic differential dissolution for the analysis of compounds and materials of the known and unknown phase composition are discussed: the composition of solvents and temperature, and the principles of their variation in time, including those in the processes of stoichiographic titration.

CALCULATIONS AND INTERPRETATION OF THE RESULTS OF STOICHIOGRAPHIC ANALYSIS OF SOLID MULTI-ELEMENT MULTI-PHASE COMPOUNDS AND MATERIALS

V.V. Malakhov, A.A. Vlasov

J. Anal. Chem.,
66(3) (2011) pp. 262-268.

Methods and approaches to the calculations and interpretation of the results of stoichiographic analysis of solid multi-element multi-phase compounds and materials using the flow mode of the differential dissolution (DD) method are reported. Special features of calculationls as well as the objective reasons for the necessity of obtaining more or less precise results of stoichiographic calculations are discussed. The details of the procedure of stoichiographic calculations, refinement, and interpretation of the results are considered on an example of the DD-analysis of the Co-Ni-Fe-Bi-K-P-Mo-O/SiO_2-catalyst for the selective oxidation and oxidative ammonolysis of hydrocarbons. The specific details and methods used for the estimation of the performance characteristics of the DD analytical procedure are discussed.

DETERMINATION OF THE CHEMICAL COMPOSITION OF SUPPORTED VANADIUM-CONTAINING OXIDE CATALYSTS BY THE DIFFERENTIAL DISSOLUTION METHOD

L.S. Dovlitova, A.A. Pochtar', N.N. Boldyreva, V.V. Malakhov

J. Anal. Chem.,
66(1) (2011) pp. 88-93.

The results of the application of the stoichiographic method of differential dissolution (**DD**) in the determination of the chemical composition of vanadium-containing catalysts are presented. In the studied catalyst series, amounts of vanadium were deposited onto TiO_2, SiO_2, Al_2O_3, ZrO_2, and Nb_2O_5. The catalysts were prepared by the impregnation method or by the spray drying method and thermally treated at different temperatures. The DD method was used for the precise correction of the phase composition of the V_2O_5/TiO_2 catalyst samples in order to determine the nature of the active component of these catalysts and obtain the correct information on their structure using the NMR method.

DETERMINATION OF THE CHEMICAL COMPOSITION OF FIBERGLASS SILICATE MATERIALS BY THE DIFFERENTIAL DISSOLUTION METHOD

L.S. Dovlitova, A.A. Pochtar', N.N. Boldyreva, V.V. Malakhov

J. Anal. Chem.,
66(10) (2011) pp. 981-990.

The standardless method of differential dissolution (DD) was used for determining the chemical composition of aluminosilicate and zirconium silicate glass-fiber clothes at different stages of their preparation and modification. Conditions for the detection, identification, and quantitative determination of various forms of heterogeneity in the elemental, phase, and surface compositions of these materials are considered. The distribution of the elements that constitute the glass-fiber clothes between various forms — surface ion-exchange (Na), hydrated (Al, Si), and framework (Al, Si) species — was quantitatively determined for the first time.

CHROMATOGRAPHIC AND ADSORPTION PROPERTIES OF THE MIXED STATIONARY PHASE POLY(1-TRIMETHYLSILYL-1-PROPYNE)/POLY(1-PHENYL-1-PROPYNE)

E.Yu. Yakovleva, V.Yu. Belotserkovskaya

J. Anal. Chem.,
66(6) (2011) pp. 629-633.

Adsorption and chromatographic properties of the mixed stationary phase poly-(1-trimethylsilyl-1-propyne)/poly(1-phenyl-1-propyne) (PTMSP/PPP) composed as 97 : 3 by weight have been investigated by methods of low-temperature nitrogen adsorption and gas chromatography on packed columns. The resultant phase has uniform mesoporous structure. The chromatographic properties of the mixed phase are significantly different from the properties of the original porous polymers PTMSP and PPP. The adsorbent obtained by modifying Chromosorb P NAW with a mixture of polymers provides the selective separation of chlorosubstituted, saturated, and aromatic hydrocarbons.

CHROMATOGRAPHIC PROPERTIES OF POLY(1-TRIMETHYLSILYL-1-PROPYNE)

V.Yu. Belotserkovskaya, E.Yu. Yakovleva

Russ. J. Phys. Chem. A,
85(5) (2011) pp. 851-856.

Changes in the properties of the surface of poly(1-trimethylsilyl-1-propyne) (PTMSP) over time were studied by gas chromatography combined with adsorption under static conditions. It was ascertained that a reduction in the volume of micropores in a polymer results in the sorption-desorption processes occurring preferentially in mesopores. The formation of a more chemically uniform surface leads to a considerable increase in the symmetry of chromatographic peaks and the efficiency of a column. These changes allow to broaden the range of compounds analyzed on columns with PTMSP.

DIHYDROGEN ADSORPTION ISOTHERMS (77 K) ON CARBON NANOMATERIALS

V.Yu. Gavrilov, E.A. Ustinov* (**Ioffe Physicotechnical Institute, St. Petersburg, Russia*)

Kinet. Catal.,
52(3) (2011) pp. 459-466.

Dihydrogen adsorption at 77 K on a number of fine-particle carbon materials, activated carbons, and carbon nanotubes has been investigated. The micropore structure parameters of these materials have been determined using a volumetric comparative method and nonlocal density functional theory (NLDFT). These data processing methods lead to different values of textural parameters. This difference is attributed to the presence of specific sorption sites on the surface of real carbon materials. The pore size range in which the NLDFT method is applicable to the C-H_2 system has been determined. A comparison between the hydrogen sorption properties of different carbon nanotubes is presented.

Fundamental and Practical Approaches to Catalyst Preparation

SCIENTIFIC BASES OF CATALYST PREPARATION: INTRODUCTION INTO THEORY AND PRACTICE

N.A. Pakhomov

Eds. V.A. Sadykov, Novosibirsk,
Publishing House SB RAS, 2011, 262 pp.

The monograph focuses on problems and aims of the catalyst preparation. The role of catalyst supports and requirements to them are discussed. Requirements to materials used for the catalyst preparation are formulated. Basic methods for granulation of catalyst masses are considered. Under discussion are physicochemical aspects of catalyst preparation by traditional methods of precipitation, supporting and mechanical mixing, as well as by new nanotechnology-based methods. Physicochemical basis of the sol-gel method are considered. Fundamentals of the classical theory of crystallization of insoluble hydroxides by the mechanism of oriented growing are given. Hydroxide interaction levels at co-precipitation are classified. Methods and mechanisms of immobilization of active components on the support surface in one- and multicomponent catalysts are considered. Processes observed at catalyst thermal treatment are considered: thermal destruction, sintering, polymorphous transformations, solid-phase reactions. Factors affecting the depth of component interaction in the catalysts prepared by mixing are shown. The monograph will be useful to under- and post-graduate students, researchers engaged in development and preparation of porous solid catalysts.

POROUS CERAMIC MATRIX Al_2O_3/Al COMPOSITES AS SUPPORTS AND PRECURSORS FOR CATALYSTS AND PERMEABLE MATERIALS

S.F. Tikhov, N.A. Pakhomov, E.I. Nemykina, A.N. Salanov, V.A. Sadykov, V.E. Romanenkov*, T.E. Pietiushyk* (**Powder Metallurgy Institute, Minsk, Belarus*)

In "*Metal, Ceramic and Polymeric Composites for Various Uses*", Ed. J. Cuppoletti, INTECH, Croatia, 2011, pp. 195-210.

Hydrothermal treatment of blends with aluminum metal powders provides an efficient technique for preparation of mechanically strong monolith composite materials with developed nanopore structure along with a relatively high fraction of macropores. The developed macropore structure provides a high permeability and decreases diffusion limitations inside the porous composite. Changing the reactivity of Al powder particles allows to tune the oxide/aluminum ratio, while their shape affect the monolith permeability. These materials can be used as filters or membrane supports.

Incorporation of precursors of the nanoporous materials in a macroporous system leads to a substantial increase of the nanopore volume. Application of granulated Al_2O_3/Al composites prepared from powdered blends of aluminum and thermally activated gibbsite as catalysts supports allowed to prepare catalysts with high activity and selectivity in dehydrogenation of isobutane.

MESOPOROUS ALUMINA IN AN Al_2O_3/Al CERMET PREPARED FROM POWDERED ALUMINUM

S.F. Tikhov, D.F. Khabibulin, O.B. Lapina, A.N. Salanov, Yu.N. Bespalko, V.A. Sadykov, A.I. Ratko*, T.F. Kouznetsova*, V.E. Romanenkov*, S.I. Eremenko* (**Institute of General and Inorganic Chemistry, Minsk, Belarus; **Powder Metallurgy Institute, Minsk, Belarus*)

J. Mat. Sci. Eng.,
5 (2011) pp. 281-292.

The synthesis of the mesoporous alumina by hydrothermal oxidation of powdered aluminum with an aqueous solution of polyethylene glycole (PEG) followed by calcination was studied. The increase of the PEG concentration from 0 to 3% was found to result in an increase of the alumina BET surface area from 254 to 406 m^2/g, with the pore volume growing from 0.46 to 0.82 cm^3/g and pore diameter increasing from 4.5 to 6.2 nm. The methods for regulating the mesopore structure in the Al_2O_3/Al cermet monoliths with the crushing strength 8.6-12.3 MPa the enhanced fraction of macropores (up to ~88 vol.%) were developed. The alumina structure in the cermets was characterized by ^{27}Al MAS NMR. It was shown that aluminum oxide became more distorted in the cermets prepared with PEG and its distortion increased with the PEG concentration.

HYDROTHERMAL SYNTHESIS OF METAL OXIDE NANO- AND MICROPARTICLES IN SUPERCRITICAL WATER

V.I. Anikeev

Russ. J. Phys. Chem. A,
85(3) (2011) pp. 377-382.

Hydrothermal syntheses of nano- and microparticles of metal oxides of two types, $LiMO_n$ ($LiCoO_2$, $LiNiO_2$, $LiZnO_2$, and $LiCuO_2$) and MO_n (Ga_2O_3, CeO_2) were performed under continuous conditions in a tubular reactor with the use of supercritical water. An important role in the synthesis of nanoparticles and the reproducibility of the results was played by the conditions of mixing of supercritical water and precursor solution flows. The morphology and composition of synthesized compounds were studied by scanning electron microscopy and X-ray diffraction. The syntheses of $LiCoO_2$, $LiNiO_2$, $LiZnO_2$, $LiCuO_2$, Ga_2O_3, and CeO_2 were most successful.

EFFECT OF CALCINATION TEMPERATURE ON THE PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF $FeSO_4/SiO_2$ IN HYDROGEN SULFIDE OXIDATION

M.A. Shuvaeva, I.V. Deliy, O.N. Martyanov, O.A. Bayukov*, E.I. Osetrov, A.A. Saraev, V.V. Kaichev, N.S. Sakaeva***, G.A. Bukhtiyarova** (**Kirenskii Institute of Physics, Krasnoyarsk, Russia; **Siberian Federal University, Krasnoyarsk, Russia; ***OAO Katalizator, Novosibirsk, Russia*)

Kinet. Catal.,
52(6) (2011) pp. 896-906.

The effect of calcination temperature on the state of the active component of iron-containing catalysts prepared by the impregnation of silica gel with a solution of $FeSO_4$ and on their catalytic properties in selective H_2S oxidation to sulfur was studied. With the use of thermal analysis, XPS, and Mössbauer spectroscopy, it was found that an X-ray amorphous iron-containing compound of complex composition was formed on the catalyst surface after thermal treatment in the temperature range of 400–500°C. This compound contained Fe^{3+} cations in three nonequivalent positions characteristic of various oxy and hydroxy sulfates and oxide and sulfate groups as anions. Calcination at 600°C led to the almost complete removal of sulfate groups; as a result, the formation of an oxide structure came into play, and it was completed by the production of finely dispersed iron oxide in the ε-Fe_2O_3 modification (the average particle size of 3.2 nm) after treatment at 900°C. As the calcination temperature was increased from 500 to 700°C, an increase in the catalyst activity in hydrogen sulfide selective oxidation was observed because of a change in the state of the active component. A comparative study of the samples by temperature-programmed sulfidation made it possible to establish that an increase in the calcination temperature leads to an increase in the stability of the iron-containing catalysts to the action of a reaction atmosphere.

INFLUENCE OF HEAT TREATMENT CONDITIONS ON THE PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF A CHROMIUM-CONTAINING CATALYST FOR TETRACHLOROETHYLENE HYDROFLUORINATION TO PENTAFLUOROETHANE

L.G. Simonova, A.A. Zirka, S.I. Reshetnikov, T.V. Larina, G.S. Litvak, L.G. Pinaeva, L.A. Isupova

Kinet. Catal.,
52(3) (2011) pp. 418-426.

The physicochemical properties of coprecipitated 95% Cr_2O_3-5% Al_2O_3 oxide systems obtained by heat treatment of the precursor in nitrogen and air between 110 and 600°C and their influence on the catalytic activity in tetrachloroethylene hydrofluorination were studied by thermal and X-ray diffraction analyses, diffuse reflectance spectroscopy, and specific surface area measurements. The $CrO_{1.9}$ compounds are more active than $CrO_{1.5}$, but their preparation in the finely divided state is difficult because of the high exothermicity of the oxidation stage, which results in the decomposition of the oxides $CrO_{1.9}$ and $CrO_{1.5}$ followed by the crystallization and sintering of the decomposition products. Fine-powder and highly active chromium-containing oxides with $CrO_{1.9}$ stoichiometry can be obtained by two-stage heating of hydroxides first in nitrogen and then in air at comparatively low temperatures.

CATALYTIC COMBUSTION OF METHANE ON SUBSTITUTED STRONTIUM FERRITES

M.V. Bukhtiyarova, A.S. Ivanova, E.M. Slavinskaya, L.M. Plyasova, V.A. Rogov, V.V. Kaichev, A.S. Noskov

Fuel,
90(3) (2011) pp. 1245-1256.

Sr–hexaferrites prepared by co-precipitation method and calcined at 700–1000°C have been characterized by thermogravimetric and differential thermal analysis (TG–DTA), Fourier transformed infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), hydrogen temperature-programmed reduction (H_2-TPR), and Ar adsorption techniques. It has been shown that hexaferrite phase formed after calcination at 700°C is amorphous and its crystallization occurs at 800°C. Specific surface area (S_{BET}) of the samples calcined at 700°C is 30–60 m^2/g. Reduction in hydrogen proceeds in several steps, Fe(III) in the hexaferrite structure being practically reduced to Fe^0. Amount of hydrogen necessary for the reduction of the samples decrease in the order: $SrMn_2Fe_{10}O_{19} > SrFe_{12}O_{19} > SrMn_6Fe_6O_{19} > SrMn_2Al_{10}O_{19}$. Surface composition of the ferrites differs from bulk. According to XPS data, the surface is enriched with strontium. Sr segregation is most probably explained by the formation of surface carbonates and hydroxocarbonates. The main components on the surface are in oxidized states: Mn^{3+} and Fe^{3+}. Maximum activity in the methane oxidation is achieved for the $SrMn_xFe_{12-x}O_{19}$ ($0 \le x \le 2$) catalysts. These samples are characterized by highest amount of the hexaferrite phase, which promotes change of oxidation state $Mn(Fe)^{3+} \leftrightarrow Mn(Fe)^{2+}$.

CATALYSTS FOR PROCESSING LIGHT HYDROCARBON RAW STOCK: COMBUSTION SYNTHESIS AND CHARACTERIZATION

G.B. Aldashukurova*, N.V. Shikina, A.V. Mironenko*, Z.A. Mansurov*, Z.R. Ismagilov (**Al-Farabi National University, Almaty, Kazakhstan*)

Int. J. Self-Propag. High-Temp. Synth.,
20(2) (2011) pp. 124-127.

Fiber glass supported nanosized Co and Co-Ni catalysts were prepared by solution-combustion synthesis and characterized for their structure and catalytic activity.

PREPARATION AND CHARACTERIZATION OF BULK URANIUM OXIDES FOR CATALYSIS

Z.R. Ismagilov, S.V. Lazareva, N.V. Shikina, V.V. Kuznetsov, M.A. Kerzhentsev, Yu.V. Ostrovskii*, N.A. Rudina, V.A. Rogov, V.A. Ushakov (**Novosibirsk Branch of JSC "State Specialized Design Institute" Novosibirsky "VNIPIET"*)

Mendeleev Commun.,
21(4) (2011) pp. 209-211.

The physicochemical and catalytic properties of bulk uranium oxides prepared by the thermal decomposition of uranyl nitrate $[UO_2(NO_3)_2{\cdot}6H_2O]$ and precipitation from an aqueous solution of this salt are reported.

PREPARATION OF $CuO-CeO_2$ CATALYSTS DEPOSITED ON GLASS CLOTH BY SURFACE SELF-PROPAGATING THERMAL SYNTHESIS

I.V. Desyatykh, A.A. Vedyagin, Yu.S. Kotolevich*, P.G. Tsyrulnikov* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Combust. Explosion Shock Waves,
47(6) (2011) pp. 677-682.

$(CuO-CeO_2)$/glass cloth acting as CO oxidation catalyst was prepared by surface selfpropagating thermal synthesis. In the process of synthesis of $(CuO-CeO_2)$/glass cloth samples, the content of active components $(CuO-CeO_2)$ and fuel additives and the conditions of thermal synthesis were varied. Impact of the nature of fuel additives and salts that are precursors of active components, and their ratio on the reaction of solid-phase combustion were studied. The resulting catalysts were studied with the use of scanning electron microscopy and *in situ* time-resolved synchrotron radiation powder X-ray diffraction.

BIFUNCTIONAL CATALYSTS OF HYDROGENATION PROCESSES

O.V. Klimov

Chem. Sustain. Devel.,
19(1) (2011) pp. 59-60.

A new approach to the preparation of highly active bifunctional catalysts of hydrogenation processes providing an increase in the extent of oil processing and obtaining motor fuel in agreement with the world standards is proposed. This approach is based on the preparation of the support containing acidic components, and on purposive selective synthesis of the active component of hydrogenolysis and hydrogenation - Co(Ni)-Mo(W)-S-phase. The latter is localized in the catalyst in such a manner that it is available for all the raw material components to be transformed catalytically. The preparation procedure is based on the solution synthesis of bimetal compounds that are precursors of the active component. Within the framework of the proposed approach, highly active catalysts intended for hydrocracking and hydropurification of various oil distillates can be obtained.

SYNTHESIS OF TITANIUM OXIDE STRUCTURES ON MESOPOROUS SILICON DIOXIDE SURFACE BY MOLECULAR LAYERING

Yu.M. Koshtyal*, A.A. Malkov*, A.A. Malygin*, A.N. Shmakov, M.S. Melgunov (**St. Petersburg State Institute of Technology, St. Petersburg, Russia)*

Colloid J.,
73(4) (2011) pp. 495-503.

The formation of titanium oxide structures through the repeated successive treatment of SBA-15 mesoporous silicon dioxide with vapors of $TiCl_4$ and H_2O at 200°C is investigated. The influence of the number of synthesis cycles on the character of the buildup of the surface titanium oxide structures and changes in the adsorption and structural characteristics of modified silica is shown.

MODIFYING THE FUNCTIONAL COVER OF THE γ-Al_2O_3 SURFACE USING ORGANIC SALTS OF ALUMINUM

R.M. Mironenko*, O.B. Belskaya*, I.G. Danilova, V.P. Talzi*, V.A. Likholobov* (**Institute of Hydrocarbons Processing, Omsk, Russia*)

Kinet. Catal.,
52(4) (2011) pp. 629-636.

A method is suggested for modifying the surface properties of alumina without changing its chemical composition. The sorption of aluminum complexes with organic acid ligands on the γ-Al_2O_3 surface is reported. The thermal decomposition of the adsorbed oxalate complexes yields supported aluminum oxide compounds on the surface of the initial support. This modifies the functional cover of the γ-Al_2O_3 surface, altering the proportions of different types of surface hydroxyl groups, reducing their total number, and lowering the concentration of weak Lewis acid sites.

PREPARATION OF Ag/HOPG MODEL CATALYSTS WITH A VARIABLE PARTICLE SIZE AND AN *in situ* XPS STUDY OF THEIR CATALYTIC PROPERTIES IN ETHYLENE OXIDATION

D.V. Demidov, I.P. Prosvirin, A.M. Sorokin, T. Rocha*, A. Knop-Gericke*, V.I. Bukhtiyarov (**Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*)

Kinet. Catal.,
52(6) (2011) pp. 855-861.

The preparation of model silver catalysts supported on highly oriented pyrolytic graphite is described, and the effect of the Ag particle size on the catalytic ethylene oxidation into ethylene oxide, studied by *in situ* XPS and mass spectrometry, is considered. For a mean particle diameter of 8 nm, the adsorbed oxygen species characterized by an O 1*s* binding energy of 530.8 ± 0.2 eV (electrophilic oxygen) forms on the silver surface exposed to the ethylene–oxygen reaction mixture. Larger silver particles with a mean diameter of 40 nm additionally contain the adsorbed oxygen species characterized by an O 1*s* binding energy of 529.2± 0.2 eV (nucleophilic oxygen). The presence of both oxygen species on the surface of the larger particles ensures the formation of ethylene oxide, while the sample with the smaller silver particles is inactive in the epoxidation reaction. The O 1*s* signal at 530.8 eV is partly due to oxygen dissolved in the subsurface layers of silver.

MODEL Ag/HOPG CATALYSTS: PREPARATION AND STM/XPS STUDY

D.V. Demidov, I.P. Prosvirin, A.M. Sorokin, V.I. Bukhtiyarov

Catal. Sci. Technol.,
8 (2011) pp. 1432-1439.

Model catalysts - Ag on highly oriented pyrolytic graphite (Ag/HOPG) - have been studied using scanning tunneling microscopy (STM), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and X-ray induced Auger electron spectroscopy (XAES). Two types of catalysts were compared: Ag nanoparticles supported on sputtered and non-sputtered HOPG, and the influence of graphite surface defects on the stabilization of Ag nano-sized particles was discussed. A procedure for the preparation of stable (up to 250°C under a submillibar oxygen/ethylene pressure) silver nanoparticles is suggested. The disappearance of Ag particles in STM images after a sample treatment in the ambient conditions is explained in terms of silver penetration into graphite and the loss of conductivity due to adsorption of contaminants.

TEMPLATE SYNTHESIS OF 3-D STRUCTURED MACROPOROUS OXIDES

E.V. Parkhomchuk, K.A. Sashkina, N.A. Rudina, A.G. Okunev, V.N. Parmon

Alternative Energy Ecol.,
102(10) (2011) pp. 35-39.

The work is devoted to the producing of 3-D macroporous structure of inorganic oxides by template method. According to the literature, catalysts based on the macroporous oxides possess improved transport properties with respect to high molecular weight reagents in the most industrially important chemical processes. In this work templates for producing of 3-D macroporous structure of inorganic oxides are obtained, they consist of close packed monodispersed polystyrene spheres. The spheres size is controlled by conditions of emulsion styrene polymerization, namely is strongly depends on polymerization temperature. With the use of templates macroporous alumina, zirconia, amorphous silica and silicalite-1 are obtained. It is shown that template synthesis results in significant increase of pore volume and external area of porous oxide.

CONTROL OF METAL DISPERSION, CHEMICAL COMPOSITION AND TEXTURE OF PALLADIUM-ZINC CATALYSTS ON MESOPOROUS TITANIA

L.B. Okhlopkova, M.A. Kerzhentsev, Z.R. Ismagilov

IRECHE,
3(6) (2011) pp. 774-783.

Nanoparticle-doped mesoporous titania coatings were synthesized by incorporation of PdZn nanoparticles into support sol and deposition of the resulting sol on the inner surface of a fused silica capillary. This method allows controlling the chemical nature of the film, the porosity, metal dispersion and loading with an active species. The structural properties, chemical composition and morphology of the active component and the support were studied by means of TEM, EDS, ICP AES, X-ray diffraction and N_2 adsorption. Monodispersed PdZn bimetallic colloidal particles were prepared by polyol method in the presence of polyvinylpyrrolidone. The average particle size ranging from 1.8-4.3 nm was found to depend on the amount of PVP added and NaOH concentration. The bulk composition of nanoparticles depends on concentrations of the precursors and NaOH. The reaction mechanism is shown to involve the oxidation of ethylene glycol to mainly glyoxal and glycolic acid, while the metal Pd salts are reduced to form catalysts for Zn^{2+} ions reduction. Palladium-zinc-incorporated mesoporous TiO_2 films were synthesized by a sol-gel method using a nonionic structure-directing agent Pluronic F127. The control of the pore size of the mesoporous titania was achieved by adding co-surfactants, such as *n*-butanol. The influence of the activation conditions on crystallite size and composition of metal particles was investigated.

PLATINUM CATALYSTS ON ACTIVATED CARBON SUPPORTS PREPARED FROM MONONUCLEAR AND POLYNUCLEAR PRECURSORS. INFLUENCE OF POROUS STRUCTURE OF THE SUPPORT

L.B. Okhlopkova, S.Yu. Troitskii

In "*Activated Carbon: Classifications, Properties and Applications*", Nova Science Publishers, 2011, pp. 393-408.

A number of catalysts have been prepared by adsorption of platinum precursors on activated carbons of different origin followed by reduction in flowing hydrogen. They were characterized by CO chemisorption, TEM and liquid-phase hydrogenation of cyclohexene. Porous structure of the support and the nature of platinum precursor proved to have a profound influence on the properties of catalysts. The metal dispersion of catalysts prepared from platinum (IV) chloride can be controlled in the range from 10 to 90%. Activity of the catalysts reached a maximum in the range of intermediate metal dispersion, with the limit being dependent on the support used. It has been suggested that a part of the supported metal became inaccessible to the organic substrate due to localization of metal particles in narrow pores of the support. The extent of blocking proved to be higher for highly dispersed Pt particles and on the supports with smaller pores. An alternative route to preparing supported Pt catalysts is the synthesis of polynuclear hydroxochloride complexes from Pt(II) chloride that is followed by their deposition on carbon. The catalysts prepared from polynuclear precursor showed high activity even in the range of high metal dispersion and for microporous carbons. Structure of product of Pt(II) chloride hydrolysis was established by means of NMR ^{195}Pt, ^{17}O.

SYNTHESIS OF NANOSIZE Co–Rh SYSTEMS AND STUDY OF THEIR PROPERTIES

A.I. Gubanov*, E.M. Churakova, S.D. Badmaev, P.V. Snytnikov, E.Yu. Filatov*, P.E. Plyusnin*, N.V. Kurat'eva*, V.A. Sobyanin, S.V. Korneev*** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Novosibirsk State University, Novosibirsk, Russia*)

Russ. J. Appl. Chem.,
84(10) (2011) pp. 1677-1683.

Precursor compounds $[Co(NH_3)_6][Rh(NO_2)_6]$ and $[Co(NH_3)_6][Co(NO_2)_6]$, solid solutions $[Co(NH_3)_6]$ $[Rh(NO_2)_6]_{1-x}[Co(NO_2)_6]_x$, and solid solutions $Na_3[Rh_{1-x}Co_x(NO_2)_6]$ were synthesized and studied by IR spectroscopy and elemental, X-ray phase, X-ray diffraction, and thermogravimetric analyses. X-ray phase analysis was employed to examine products of thermal decomposition of precursors in the atmospheres of hydrogen and helium. Catalysts with a Co–Rh active system, supported by ZrO_2, were prepared and tested in the reaction of steam conversion of ethanol.

EFFECT OF YTTRIUM OXIDE ON THE FORMATION OF THE PHASE COMPOSITION AND POROUS STRUCTURE OF TITANIUM DIOXIDE

A.A. Shutilov, G.A. Zenkovets, V.Yu. Gavrilov, S.V. Tsybulya

Kinet. Catal.,
52(1) (2011) pp. 111-118.

The formation of the structure of TiO_2 (anatase) doped with 1–5 mol % Y_2O_3 is reported. The dopant changes the anatase structure from regular to nanocrystalline. The nanocrystalline structure consists of incoherently intergrown 5- to 7-nm anatase crystallites (500°C) separated by interblock boundaries accommodating yttrium ions. The formation of the nanocrystalline anatase structure stabilizes small anatase crystallites and raises the anatase-to-rutile phase transition temperature above 900°C. Owing to this structure, the developed specific surface area and fine porous texture of yttrium oxide-doped titanium dioxide survive up to higher temperatures than those of undoped titanium dioxide.

NANOCRYSTAL AEROGELS OF METAL OXIDES AS DESTRUCTIVE SORBENTS AND CATALYSTS

A.F. Bedilo, E.V. Ilyina, I.V. Mishakov, A.A. Vedyagin

Chem. Sustain. Devel.,
19(1) (2011) pp. 31-38.

The procedure of the synthesis of aerogels Al_2O_3 and VO_x/MgO with the particle size of several nanometers was developed. The specific surface of materials obtained after drying under supercritical conditions exceeded 1000 m/g. The possibility to govern the properties of aerogels through modification with acids and β-diketones of the solutions of alkoxides used as initial substances was revealed. The high activity of modified aerogel of Al_2O_3 in the processes of destructive sorption and catalytic dehydrohalogenation was demonstrated. It was shown that the aerogel VO_x/MgO exhibits high activity in the reaction of decomposition of freon CF_2Cl_2.

SYNTHESIS OF PROPYLENE GLYCOL METHYL ETHER FROM METHANOL AND PROPYLENE OXIDE OVER ALUMINA-PILLARED CLAYS

M.N. Timofeeva, V.N. Panchenko, A. Gil*, Yu.A. Chesalov, T.P. Sorokina, V.A. Likholobov**** (**Universidad Publica de Navarra, Pamplona, Spain; **Institute of Hydrocarbons Processing, Omsk, Russia*)

Appl. Catal., B,
102(3-4) (2011) pp. 433-440.

Al-pillared interlayered clays (Al-PILCs) have been synthesized by the exchange reaction between Na-clay and Al-hydroxypolycation solutions aged for 0.5–14 days and characterized by DRS-UV–vis, XRD, FT-IR and N_2-adsorption/desorption analyses, Hammett acidity titration with *n*-butylamine and FT-IR spectroscopy using PhCN and $CDCl_3$ as probe molecules. It was found that the aging time of Al-hydroxypolycation pillaring solution affects both the textural characteristics and the physicochemical properties of Al-PILCs. Al-PILCs have been tested as catalysts for synthesis of propylene glycol methyl ether from methanol and propylene oxide. Increase in Al content due to the prolonged aging time favors the increase in the activity of Al-PILCs.

EFFECT OF THE ACID–BASE PROPERTIES OF Zr,Al-PILLARED CLAYS ON THE CATALYTIC PERFORMANCES IN THE REACTION OF PROPYLENE OXIDE WITH METHANOL

M.N. Timofeeva, V.N. Panchenko, A. Gil*, V.P. Doronin, A.V. Golovin, A.S. Andreev, V.A. Likholobov**** (**Universidad Publica de Navarra, Pamplona, Spain; **Institute of Hydrocarbons Processing, Omsk, Russia*)

Appl. Catal., B,
104(1-2) (2011) pp. 54-63.

A series of Zr,Al-pillared interlayered clays (Zr,Al-PILCs) have been prepared and characterized by X-ray diffraction, elemental analysis, FT-IR and N_2-adsorption/desorption analyses, ^{27}Al NMR(MAS), FT-IR spectroscopy using pyridine, PhCN and $CDCl_3$ as probe molecules. It was found that textural and physicochemical properties of Zr,Al-PILCs depend on Zr content in clay. The relationship between the acid–base properties and catalytic performances of Zr,Al-PILCs was revealed in the synthesis of propylene glycol methyl ether from methanol and propylene oxide. The results show that the conversion of propylene oxide and the selectivity to 1-methoxy-2-propanol decrease with increasing the amount of zirconium in Zr,Al-PILCs due to the change in acid–base properties.

EFFECT OF THE NATURE OF THE ADDITIVES OF METAL CATIONS (Sr, Ba, AND La) ON THE PROPERTIES OF Co–Mo HYDRODESULFURIZATION CATALYSTS

E.V. Korneeva, A.S. Ivanova, G.A. Bukhtiyarova, P.V. Aleksandrov, V.I. Zaikovsky, I.P. Prosvirin, A.S. Noskov

Kinet. Catal.,
52(4) (2011) pp. 579-594.

The effect of the nature of the support modified with the ions of alkaline earth and rare earth elements (Sr, Ba, and La) on the properties of Co–Mo catalysts for the hydrodesulfurization of dibenzothiophene (DBT), 4-methyldibenzothiophene (4-MDBT), and 4,6-dimethyldibenzothiophene (4,6-DMDBT) was studied using a set of physicochemical and catalytic techniques. It was found that the introduction of modifying additives decreased the surface concentration of Lewis acid sites (LASs) and increased the concentration of basic sites (BSs) in aluminum-containing supports; these changes were more significant upon modification with lanthanum and strontium. The modification affected the distribution and degree of dispersion of Co–Mo–S sulfide packets. It was found that the rate constants of DBT and 4-MDBT conversion increased with decreasing total surface concentration of both LASs and BSs on the support. The highest rate constant of 4,6-DMDBT conversion was reached at an optimum concentration of weak Lewis sites on Co–Mo catalysts, whose support was modified with strontium or barium.

MICROWAVE IRRADIATION SYNTHESIS OF SAPO-31 MOLECULAR SIEVE AND ITS CHARACTERIZATION AND CATALYTIC PERFORMANCE

J. Yang*, W. Wu*, Ya. Zhou*, G. Wu*, A. Zhao*, O.V. Kikhtyanin, A.V. Toktarev, G.V. Echevsky
(**Sino-Russian Joint Laboratory for Catalysis, Heilongjiang University, Harbin, Heilongjiang, China*)

Chinese J. Catal.,
32(7) (2011) pp. 1234-1241.

$AlPO_4$-31 molecular sieve was synthesized by microwave irradiation using aluminum isopropoxide, orthophosphoric acid, and di-*n*-butylamine as sources of aluminum, phosphorus, and template, respectively. The crystallization conditions of $AlPO_4$-31 were optimized. SAPO-31 molecular sieve samples with different silicon contents were synthesized at the optimal conditions. The structure and acidity of the samples were characterized by X-ray diffraction, N_2 physical adsorption, scanning electron microscopy, ^{29}Si MAS NMR, NH_3 temperature-programmed desorption, FT-IR of adsorbed pyridine. The catalytic performance of Pd/SAPO-31 bifunctional catalyst for hydroisomerization of *n*-decane was investigated. The results indicated that the $AlPO_4$-31 and SAPO-31 molecular sieves with pure crystal phase and higher crystallinity assigned to ATO topology structure were obtained at 170°C for 2 h by microwave irradiation. The BET surface area and micropore volume were increased because of the introduction of Si to the framework of $AlPO_4$-31. The distribution of Si in the framework and the acidity of the SAPO-31 molecular sieve were varied by changing the composition of the reaction mixture. The bifunctional catalyst Pd/SAPO-31 with suitable acidity showed high activity and selectivity for hydroisomerization of *n*-decane.

FACILE SYNTHESIS OF NANOSIZED ε-Fe_2O_3 PARTICLES ON THE SILICA SUPPORT

G.A. Bukhtiyarova, M.A. Shuvaeva,
O.A. Bayukov*, S.S. Yakushkin, O.N. Martyanov
(**Kirensky Institute of Physics, Krasnoyarsk, Russia*)

J. Nanopart. Res.,
13(10) (2011) pp. 5527-5534.

An approach is suggested to synthesize the ε-Fe_2O_3 particles supported on silica with the mean size of few nanometers, narrow size distribution and no admixture of any other iron oxide polymorphs. The facile synthesis is based on the pore filling impregnation method by iron sulfate (II) water solution with the following annealing procedure at similar to 1173 K. It is shown that the ε-Fe_2O_3 nanoparticles obtained are stable up to similar to 1173 K and possess superparamagnetic behavior up to similar to 870 K.

AN INVERTED SPHERICAL MODEL OF AN OPEN-CELL FOAM STRUCTURE

O. Smorygo*, V.V. Mikutski*, A. Marukovich*,
A. Ilyushchanka*, V.A. Sadykov, A. Smirnova**
(**Powder Metallurgy Institute, Minsk, Belarus;*
***Eastern Connecticut State University, Storrs, USA*)

Acta Mater.,
59(7) (2011) pp. 2669-2678.

An inverted open-cell foam model based on hexagonal close packing symmetry is proposed for open-cell foams with different configuration of struts. The novel model predicts the properties of the broad spectrum of open-cell ceramic and metallic structures. According to the proposed model, the specific surface and hydraulic permeability can be derived from experimentally measurable parameters such as porosity and cell diameter. The calculated parameters are in good correlation with the experimental data even without introducing additional empirical coefficients.

GAS-PHASE EPOXIDATION OF BUTADIENE: INFLUENCE OF THE CONTENT AND DISTRIBUTION OF CESIUM PROMOTER ON CATALYTIC PROPERTIES Ag/α–Al_2O_3

D.S. Afanasiev, T.V. Larina, N.I. Kuznetsova

Catal. Ind.,
4(2) (2011) pp. 89-95.

Using the well-known patent methods, the authors have synthesized 1,3-butadiene epoxidation α-Al_2O_3 supported catalysts containing 15 wt% of Ag and 250–1500 ppm of Cs (Johnson Matthey, H16P07). The physicochemical properties of samples are systematically studied by varying the dispersion of supported silver, the amount of an introduced promoter, and its distribution over the surface of a catalyst. Catalytic tests of samples show that the optimum amount of a promoter depends directly on the surface of a catalyst. With optimum promotion, the steady-state activity of catalysts is determined by the dispersion of supported silver. In the course of catalytic tests, it is established that the shape of kinetic curves is governed by the excess or lack of Cs in a catalyst, thus providing a method for optimizing the concentration of the promoter. An analysis of the energy dispersion spectra (EDS) is applied for the first time to study the distribution of Cs over the surface of promoted catalysts. It is shown that thermal treatment favors the uniform distribution of a promoter over the surface of a catalyst and shortens the time required to attain its steady-state activity in catalytic tests. In the work, the steady-state productivity of catalysts reaches 0.5 g of 3,4-epoxy-1-butene per gram of the catalyst per hour, thus exceeding the claimed patent values.

MIL-101 SUPPORTED POLYOXOMETALATES: SYNTHESIS, CHARACTERIZATION, AND CATALYTIC APPLICATIONS IN SELECTIVE LIQUID-PHASE OXIDATION

N.V. Maksimchuk, O.A. Kholdeeva,
K.A. Kovalenko*, V.P. Fedin* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Israel J. Chem.,
51(2) (2011) pp. 281-289.

Recent achievements in the preparation of heterogeneous catalysts via incorporation of polyoxometalates (POMs) within cages of the mesoporous coordination polymer MIL-101, their physicochemical characterization, and application for liquidphase selective oxidation of organic compounds with green oxidants — O_2 and aqueous H_2O_2 are presented. Special attention is paid to analyze a manifestation of confinement effects and to address the issues of catalytic activity and selectivity after immobilization and after recycling, catalyst resistance to POM leaching, and the nature of catalysis. The scope and limitations of POM/MIL-101 catalysts are discussed.

IRON TETRASULFOPHTHALOCYANINE IMMOBILIZED ON METAL ORGANIC FRAMEWORK MIL-101: SYNTHESIS, CHARACTERIZATION AND CATALYTIC PROPERTIES

O.V. Zalomaeva, K.A. Kovalenko*,
Yu.A. Chesalov, M.S. Melgunov, V.I. Zaikovsky,
V.V. Kaichev, A.B. Sorokin, O.A. Kholdeeva,**
V.P. Fedin* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institut de Recherches sur la Catalyse et l'Environnement de Lyon, Villeurbanne Cedex, France*)

Dalton Trans.,
40 (2011) pp. 1441-1444.

Iron tetrasulfophthalocyanine (FePcS) has been irreversibly inserted into nanocages of the metal organic framework MIL-101 to give a hybrid material FePcS/MIL-101 which demonstrated a superior catalytic performance in the selective oxidation of aromatic substrates with ^{t}BuOOH than homogeneous FePcS.

EFFECT OF OXYGEN ADSORPTION ON THE SURFACE PLASMON RESONANCE OF OXIDE-SUPPORTED SILVER NANOPARTICLES

D.S. Afanasiev, V.F. Anufrienko, S.Ph. Ruzankin,
T.V. Larina, N.I. Kuznetsova, V.I. Bukhtiyarov

Doklady Phys. Chem.,
436(2) (2011) pp. 23–25.

In the present work, the surface plasmon resonance (SPR) of oxide-supported silver nanoparticles was studied. It was demonstrated that oxygen adsorption (formation of an oxide film) had an effect on the SPR position of fine silver nanoparticles.

Carbon and Carbon Related Materials

MODIFICATION OF NANOFIBROUS CARBON MORPHOLOGY UNDER EFFECT OF LASER ABLATION

G.G. Kuvshinov*, Yu.L. Krutskii*, I.S. Chukanov*, A.M. Orishich, Yu.V. Afonin**, V.I. Zaikovsky, D.G. Kuvshinov**** (**Novosibirsk State Technical University, Novosibirsk, Russia; **Institute of Theoretical and Applied Mechanics, Novosibirsk, Russia*)

Nanotechn. Russia,
6(9-10) (2011) pp. 607-612.

This paper presents the results of studies of carbon nanostructures obtained by the laser ablation of a nanofibrous carbon formed in the process of a catalytic decomposition of hydrocarbons in the presence of high-percentage catalysts containing the iron subgroup of metals. A continuous CO_2 laser with a radiation density of 3.4 W/cm^2 was used in the experiments. The target was placed on a cooled copper substrate in a helium medium under a pressure of 770–780 torr. Upon the impact of laser radiation, the carbon evaporated and, further, condensed on the surface of a special condenser. The samples were collected from the condenser surface and the target in the radiation-exposed area. The products were studied by high resolution transmission electron microscopy using a JEM-2010 electron microscope. A number of samples underwent a local energy dispersion X-ray microanalysis on the EDAX spectrometer. Multilayer nanotubes of diameters 14–40 nm and lengths of up to 2 μm have been found in the evaporated and condensed carbon materials. It was established that part of the nanotubes was filled by the catalyst metal. Interestingly, in the target area exposed to the radiation, the initial material comprising carbon nanofibers with the structure of inserted cones transformed into carbon nanotubes (CNTs) with an average cross-section size of 20 nm.

PALLADIUM-CONTAINING MULTIWALL NANOTUBES AS CATALYSTS FOR HYDROGENATION

N.N. Osipov*, N.A. Magdalinova*, V.V. Chesnokov, A.S. Chichkan*, M.V. Klyuev* (**Ivanovo State University, Ivanovo, Russia*)

Vestnik Ivanovskogo Gosudarstvennogo Universiteta,
2 (2011) pp. 61-63.

Palladium-containing multiwall carbon nanotubes were obtained and their catalytic activity was studied in model reaction of nitrobenzene hydrogenation. It was shown, that reaction rate is lower than for platinum analogues.

CATALYSTS BASED ON FILAMENTOUS CARBON IN THE HYDROGENATION OF AROMATIC COMPOUNDS

N.A. Zaitseva, V.V. Goidin, V.V. Molchanov, V.V. Chesnokov, R.A. Buyanov, V.A. Utkin

Kinet. Catal.,
52(5) (2011) pp. 770-773.

In order to extend the area of application of the base catalytic system metal–filamentous carbon, the catalytic properties of Ni–filamentous carbon catalysts have been tested in the hydrogenation of aromatic compounds (benzene, benzyl cyanide, benzophenone, and nitrobenzene). The selectivity of the catalysts depends on the outer faceting of the active metal particles. The benzene ring is hydrogenated on the (111) face of the metal nanoparticles, whereas the selective hydrogenation of functional groups in substituted aromatic compounds occurs on the surface of active component nanoparticles in which the (111) face is blocked.

STRUCTURE AND ELECTROPHYSICAL PROPERTIES OF MULTIWALLED CARBON NANOTUBE/POLYMETHYLMETHACRYLATE COMPOSITES PREPARED VIA COAGULATION TECHNIQUE

I.N. Mazov, V.L. Kuznetsov, S.I. Moseenkov, A.V. Ishchenko, N.A. Rudina, A.I. Romanenko*, T.I. Buryakov*, O.B. Anikeeva*, J. Macutkevic, D. Seliuta**, G. Valusis**, J. Banys***** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia;* ***Semiconductor Physics Institute, Vilnius, Lithuania;* ****University of Vilnius, Vilnius, Lithuania*)

Nanosci. Nanotechn. Lett.,
3(1) (2011) pp. 18-23.

This paper considers the formation of the conductive network in the composite system of multiwall carbon nanotubes (MWNT) and polymethylmetacrylate (PMMA) produced via coagulation technique. All stages of formation of uniform composite materials with high state of MWNT dispersion were characterized with optical microscopy, TEM, SEM along with conductivity measurements. The key stage is the formation of precipitate of polymer on the surface of MWNTs suspended in suitable solvent which provides effective wetting of MWNT surface with polymer and formation of the "polymer-NT" interface. This precipitate (powder) was used to produce composite film, which electrophysical properties were characterized with four-probe electrical conductivity measurements and by broadband dielectric spectroscopy (20 Hz-1 MHz). Both static and low-frequency analysis demonstrate low percolation threshold (lower than 1 wt%) for the produced MWNT/polymethylmetacrylate composites, whereas a much higher MWNT concentration (3～4 wt%) is needed to form a conductive network for the composite films produced by other methods, such as extrusion or solvent cast technique.

STRUCTURE AND PROPERTIES OF MULTIWALL CARBON NANOTUBES/POLYSTYRENE COMPOSITES PREPARED VIA COAGULATION PRECIPITATION TECHNIQUE

I.N. Mazov, V.L. Kuznetsov, D.V. Krasnikov, N.A. Rudina, A.I. Romanenko*, O.B. Anikeeva*, V.I. Suslyaev, E.Yu. Korovin**, V.A. Zhuravlev**** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Nanotechn.,
ID 648324 (2011) 7 pp.

Coagulation technique was applied for preparation of multiwall carbon nanotube- (MWNT-containing polystyrene (PSt) composite materials with different MWNT loading (0.5–10 wt%). Scanning and transmission electron microscopies were used for investigation of the morphology and structure of produced composites. It was shown that synthesis of MWNT/PSt composites using coagulation technique allows one to obtain high dispersion degree of MWNT in the polymer matrix. According to microscopy data, composite powder consists of the polystyrene matrix forming spherical particles with diameter ca. 100–200 nm, and the surface of MWNT is strongly wetted by the polymer forming thin layer with 5–10 nm thickness.

Electrical conductivity of MWNT/PSt composites was investigated using a four-probe technique. Observed electrical percolation threshold of composite materials is near to 10 wt%, mainly due to the insulating polymer layer deposited on the surface of nanotubes. Electromagnetic response of prepared materials was investigated in broadband region (0.01–4 and 26–36 GHz). It was found that MWNT/PSt composites are almost radiotransparent for low frequency region and possess high absorbance of EM radiation at higher frequencies.

INFLUENCE OF THE DIELECTRIC MATRIX ON THE ELECTRICAL NANOCOMPOSITES BASED ON OXIDIZED MULTI-WALLED CARBON NANOTUBES

I.V. Totosov*, A.I. Romanenko*, O.B. Anikeeva*, V.L. Kuznetsov, I.N. Mazov, S.I. Popkov, K.A. Shaichutdinov**** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Kirensky Institute of Physics, Krasnoyarsk, Russia*)

J. Siberian Federal Univ. Math. & Phys.,
4(2) (2011) pp. 175-181.

In this paper the authors consider the effect of oxidative treatments on the properties of multiwalled carbon nanotubes (MWNT). The experimental temperature dependence of electrical conductivity (in the temperature range 4,2–293 K) and field dependence of magnetoresistance (in fields up to 9 Tl at 10 K) of the samples with MWCNT modified by oxidation of the surface layers, as well as the composites based on them. It was established that the oxidation of the surface layers of MWCNTs in acid solutions leads to a change in the temperature dependence of electrical conductivity. Introduction of MWCNTs in a dielectric matrix of polymethylmethacrylate (PMMA) leads to the dependence of the conductivity close to that typical for hopping conductivity with variable hopping length, three-dimensional case.

TEMPERATURE DEPENDENCES OF CONDUCTIVITY AND MAGNETOCONDUCTIVITY OF MULTIWALL CARBON NANOTUBES ANNEALED AT DIFFERENT TEMPERATURES

S.D. Borodanov*, A.I. Romanenko*, O.B. Anikeeva*, V.L. Kuznetsov, K.V. Elumeeva, S.I. Moseenkov (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Siberian Federal Univ. Math. & Phys.,
4(2) (2011) pp. 143-148.

Temperature (in range 4.2-300 K) and magnetic field (in fields up to 10 kG at 4.2 K) dependences of the conductivity of two sets of multiwall carbon nanotubes with different average diameters (8-10 nm and 20-22 nm) heated at various temperatures (1600, 2200, 2600, 2800°C) were investigated. Temperature dependences for nanotubes with average diameter 20-22 nm is typical for quantum corrections to conductivity of the systems with interaction electrons in two dimensional conductors with local disorder. For nanotubes with average diameter 8-10 nm temperature dependences corresponds to one-dimensional variable range hopping conductivity (VRHC). The variation of annealing temperature of MWNTs influence on the contribution of corrections to conductivity and parameters of VRHC. The magnetoconductivity of MWNTs also depends on the annealing temperature and is less than that of highly oriented pyrographite. Annealed MWNTs with average diameter 20–22 nm has a positive magnetoconductivity.

MICROWAVE CHARACTERISTICS OF COMPOSITE RADIO MATERIALS ON THE BASIS OF POLYMER AND CARBON STRUCTURES

O.A. Dotsenko*, V.I. Suslyaev*, V.L. Kuznetsov, I.N. Mazov, O.A. Kochetkova* (**Tomsk State University, Tomsk, Russia*)

Doklady TIREET,
2(24) part 2, (2011) pp. 36-40.

In the paper there are given the results of research on frequency dependences of permittivity of composite radio materials on the basis of multiwall carbon nanotubes (MWCNT) in polymer matrix with different weight concentration. The measurements are completed on microwave by resonator method. The authors compared the weight concentration of MWCNT and graphite powder for composites with equal values of permittivity. It's shown that for achievement of equal values of graphite powder permittivity it is required 10–20 times more.

LASER-INDUCED DIAMAGNETISM IN SUSPENSION OF ONION-LIKE CARBON PARTICLES

G.M. Mikheev*, V.L. Kuznetsov, K.G. Mikheev*, T.N. Mogileva*, S.I. Moseenkov (**Institute of Applied Mechanics, Izhevsk, Udmurtia, Russia*)

Tech. Phys. Lett.,
37(9) (2011) pp. 831-834.

It is experimentally established that the bleached fraction of a suspension of onion-like carbon (OLC) particles in N,N-dimethylformamide (DMF), which is clarified under the action of high-power pulsed laser radiation at λ = 1064 nm, is pushed out from inhomogeneous magnetic field. By changing the spatial arrangement of a permanent magnet relative to the point of laser action on the suspension, it is possible to control the direction of motion of the bleached fraction. The observed behavior can be explained by laser-stimulated chemical reactions between OLC and DMF, which lead to the formation of a new substance with pronounced diamagnetic properties.

HYDROXYLATED DETONATION NANODIAMOND: FTIR, XPS, AND NMR STUDIES

O. Shenderova*, A.M. Panich, S.I. Moseenkov, S.C. Hens***, V.L. Kuznetsov, H.-M. Vieth*****
(**International Technology Center, North Carolina, USA; **Ben-Gurion University of the Negev, Be'er Sheva, Israel; ***Free University of Berlin, Berlin, Germany*)

J. Phys. Chem. C,
115(39) (2011) pp. 19005-19011.

Detailed and unambiguous characterization of the surface structure of detonation nanodiamond (DND) particles remains one of the most challenging tasks for the preparation of chemically functionalized nanodiamonds. In the present paper, a combination of FTIR, NMR, and XPS was used to characterize DND particles that were treated in a reduction reaction that results in the enrichment of hydroxyl and hydroxymethyl functional groups. FTIR spectra and quantum-chemistry modeling demonstrated that the vacuum treatment of the sample, with the purpose of the removing adsorbed water and other volatile contaminates, is mandatory to obtain the correct data on the nature and relative content of the −OH surface groups on DND. ^{13}C and ^{1}H NMR spectra show signals from the diamond core, hydroxyl, hydrocarbon groups, and moisture on the diamond surface. NMR data were taken for as-prepared DNDs, as well as those that were dried under vacuum conditions of 10^{-4} Torr, in order to distinguish between the NMR signal contributions due to moisture and other hydrogen-containing groups.

COMPARATIVE STUDY OF REFLECTANCE PROPERTIES OF NANODIAMONDS, ONION-LIKE CARBON AND MULTIWALLED CARBON NANOTUBES

V.L. Kuznetsov, S.I. Moseenkov, K.V. Elumeeva, T.V. Larina, V.F. Anufrienko, A.I. Romanenko*, O.B. Anikeeva*, E.N. Tkachev* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Phys. Status Solidi B,
248(11) (2011) pp. 2572-2576.

Carbon nanomaterials are the promising candidates for potential broadband limiting applications and extremely low reflectance coatings, particularly in the infrared, visible and UV spectral regions. In this paper the authors have performed the comparative study of diffuse reflectance of nanodiamond (ND), sp^2/sp^3 composites, onion-like carbon (OLC) and multiwalled carbon nanotubes (MWNTs) in visible and UV regions. ND, sp^2/sp^3 composites and OLC produced via high temperature annealing of the same set of NDs allow to vary sp^2/sp^3 carbon ratio, size of primary particle agglomerates and concentration of defects while MWNT set provides possibility to vary NT diameters and length, order/disorder degree (via high temperature MWNTS annealing). The diffuse reflectance of carbon nanomaterials depends mainly on the electronic configuration, defect concentration, size of graphene-like ordered fragments and agglomerates of nanoparticles along with their morphology.

ELECTROMAGNETIC RESPONSE OF POLYMER COMPOSITES WITH QUASI-SPHERICAL NANOCARBON INCLUSIONS: THEORY BELOW THE PERCOLATION THRESHOLD

P. Kuzhir*, A. Paddubskaya*, D. Bychanok*, G. Slepyan*, S. Maksimenko*, J. Macutkevic, D. Seliuta**, G. Valusis**, J. Banys***, V.L. Kuznetsov, S.I. Moseenkov, O. Shenderova****, Ph. Lambin******* (**Institute for Nuclear Problem, Minsk, Belarus; **Semiconductor Physics Institute, Vilnius, Lithuania; ***University of Vilnius, Vilnius, Lithuania; ****International Technology Center, Raleigh, USA; *****FUNDP – University of Namur, Namur, Belgium*)

J. Polym. Eng.,
31(2-3) (2011) pp. 167-173.

The linear electromagnetic response of polymer composite with nanocarbon inclusions was modeled for a random multi-component system with particles and clusters of different shape and size. The results of the generalized effective medium Maxwell-Garnett theory below the percolation threshold demonstrate good coincidence with the experimental data for onion-like carbon-based polyurethane composites collected in a quasi-static regime (at 129 Hz) in a broad temperature range.

CARBON ONION COMPOSITES FOR EMC APPLICATIONS

P. Kuzhir*, A. Paddubskaya*, S. Maksimenko*, V.L. Kuznetsov, S.I. Moseenkov, A. Romanenko, O. Shenderova***, J. Macutkevic****, G. Valusis****, P. Lambin******* (**Institute for Nuclear Problem, Minsk, Belarus; **Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; ***International Technology Center, Raleigh, USA; ****Semiconductor Physics Institute, Vilnius, Lithuania; *****FUNDP – University of Namur, Namur, Belgium*)

IEEE Trans. Electromagn. Capability,
54(1) (2012) pp. 6-11.

A novel lightweight onion-like carbon (OLC)-based polymer composite with high electromagnetic (EM) shielding properties is presented. OLC have been produced via the large-scale production technology based on the annealing of detonation nanodiamond under vacuum conditions (or in inert atmosphere). EM shielding effectiveness has been tested in the frequency range of 26-37 GHz. The highest EM attenuation at 36.6 GHz reaching -34 dB was observed for polymethylmethacrylate films comprising 20 wt% of OLC. The shielding effectiveness data collected for microwave frequencies were found to correlate well with the electrical resistivity measurements by four-probe method as well as conductivity measurements provided by the broadband dielectric spectroscopy (20 Hz-3 GHz). It was proved experimentally that OLC EM shielding capacity can be optimized by varying the nanoonion cluster size and nanodiamond annealing temperature so that effective EM coatings can be produced. Both the experimental observations and theoretical simulations demonstrate that even small (smaller than percolation threshold) additions of OLC particles to a polymer host can noticeably modify the composite response to EM radiation.

MESOPOROUS COMPOSITE MATERIALS FROM ACTIVATED RICE HUSK CARBON AND MONTMORILLONITE

J.M. Jandosov*, Z.A. Mansurov*, M.A. Biisenbayev*, A.R. Kerinkulova*, Z.R. Ismagilov, N.V. Shikina, I.Z. Ismagilov, I.P. Andrievskaya (**Institute of Combustion Problems, Almaty, Kazakhstan*)

Eurasian Chem.-Techn. J.,
13(1-2) (2011) pp. 105-113.

Three different carbons were prepared from rice husk by steam activation at 700°C, H_3PO_4-activation followed by desilication or desilication followed by H_3PO_4-activation at 500°C. Honeycomb monoliths were obtained by mixing of a carbon with montmorillonite followed by extrusion, curing, calcination and leaching by alkaline solution. Obtained blocks were compared in terms of their morphology and elemental composition using data of SEM/EDX-analysis. From low temperature nitrogen adsorption study results it follows that prepared monoliths are characterized by SBET up to 700 m^2/g ($V_\Sigma = 0.79\ cm^3/g$) and pore size distribution shows the maximum around 4 nm. Methylene blue number is as high as 250 mg/g.

In situ STUDY ON CHANGES IN THE PHASE COMPOSITION OF A Ni–Cu CATALYST DURING GROWTH OF NITROGEN-CONTAINING CARBON NANOFIBERS

O.Yu. Podyacheva, A.N. Shmakov, Z.R. Ismagilov, V.N. Parmon

Doklady Phys. Chem.,
439(1) (2011) pp. 127-130.

The work deals with *in situ* study of the phase changes in the Ni–Cu catalyst during the growth of N-CNFs in the process of decomposition of an ethylene–ammonia mixture with the use of a high-precision X-ray diffractometer equipped with a high-temperature camera–reactor. It was found that the formation of N-CNFs occurs through the stage of dissolution of carbon and nitrogen in particles of the Ni–Cu catalyst, but without formation of metal carbides.

STUDY OF OXYGEN GROUPS AT A POROUS CARBON SURFACE BY A NEW FAST INTERMITTENT THERMODESORPTION TECHNIQUE

F. Gaillard*, A. El Hachimi*, C. Descorme*, M. Besson*, J.-P. Joly*, E.M. Polyanskaya, O.P. Taran, V.N. Parmon (**Institut de Recherches sur la Catalyse et L'environnement de Lyon, Villeurbanne, France*)

Carbon,
49(6) (2011) pp. 2062-2073.

A threshold thermodesorption method, named fast Intermittent TPD (ITPD), was used to study the evolution of CO_2 and CO arising from the decomposition of oxygen groups at the surface of a porous carbon used in the wastewater treatment.

Applied to the as-received carbon, CO_2-ITPD provided clear evidence for six values of the apparent activation energy of oxygen group decomposition (E_{app}): 139, 168, 206, 237, 270 and 290 kJ mol^{-1}. Corresponding apparent pre-exponential factors (A_{app}) were also determined. The data (E_{app} and A_{app}) derived from ITPD for the six desorption steps allowed a successful description of the complete TPD profile, considering a Gaussian narrow distribution of E_{app} for each step. CO-ITPD also showed the presence of six (possibly seven) distinguishable steps upon CO thermal desorption and further demonstrated the interest of the fast ITPD technique for studying carbon surface chemistry.

The TPD and ITPD profiles of the carbon treated with sodium hypochlorite showed: (i) a sharp increase in the amount of desorbed species, (ii) the prevailing presence of less stable oxygen groups, mainly carboxylic acids, giving rise to CO_2 desorption at low temperature, and (iii) the progressive merging of the desorption steps detectable at low temperature upon increasing surface density of oxygen groups.

SIBUNIT-BASED CATALYTIC MATERIALS FOR THE DEEP OXIDATION OF ORGANIC ECOTOXICANTS IN AQUEOUS SOLUTIONS. II: WET PEROXIDE OXIDATION OVER OXIDIZED CARBON CATALYSTS

O.P. Taran, E.M. Polyanskaya, O.L. Ogorodnikova, C. Descorme*, M. Besson*, V.N. Parmon (**Institut de Recherches sur la Catalyse et L'environnement de Lyon, Villeurbanne, France*)

Catal. Ind.,
3(2) (2011) pp. 161-169.

The influence of the surface chemical composition of carbon catalysts prepared by oxidative treatment on the basis of the Sibunit-4 carbon material of the Sibunit family on their catalytic properties in the liquid-phase oxidation of formic acid by hydrogen peroxide was studied for the first time. Pure carbon samples were found to be active in the destruction of hydrogen peroxide and the oxidation of an organic substrate, and their activity decreased with an increase in the number of carboxyl and lactone groups on the surface of a carbon catalyst. Nevertheless, the rates of such processes on carbon catalysts are lower than in the presence of even small amounts of homogeneous Fe^{3+}. It was shown that carbon samples accelerate or (to the contrary) inhibit the Fe^{3+}-catalyzed peroxide oxidation of an organic substance, depending on the quantitative ratio of surface carboxyl and lactone groups and Fe^{3+} ions in the reaction solution. Possible acceleration and inhibition mechanisms for peroxide oxidation on carbon catalysts are discussed. The established influence of the surface chemical properties of carbon catalysts must be taken into account in the development of catalysts and processes for the oxidative purification of industrial wastewater.

MODERN APPROACHES TO THE PRODUCTION OF CARBON MATERIALS FROM VEGETABLE BIOMASS

P.M. Eletskii, V.A. Yakovlev, V.N. Parmon

Theor. Exp. Chem.,
47(3) (2011) pp. 139-154.

Recent trends in methods for the preparation of porous carbon materials (PCM) from vegetable biomass by physical and chemical activation methods are analyzed. Data on the effect of activating agents and also other parameters on the textural characteristics of PCMs were classified. A new direction for the production of PCMs was discovered in the use of high-ash biomass.

SYNTHESIS OF CATALYTIC FILAMENTOUS CARBON ON A NICKEL/GRAPHITE CATALYST AND A STUDY OF THE RESULTING CARBON–CARBON COMPOSITE MATERIALS IN MICROBIAL FUEL CELLS

G.A. Kovalenko, L.G. Tomashevskaya*, T.V. Chuenko, N.A. Rudina, L.V. Perminova, A.N. Reshetilov* (**Skryabin Institute of the Biochemistry and Physiology of Microorganisms, Pushchino, Moscow oblast, Russia*)

Kinet. Catal.,
52(4) (2011) pp. 564-572.

The carbon-carbon composite materials obtained via the synthesis of catalytic filamentous carbon (CFC) on a Ni/graphite supported catalyst in the process of the pyrolysis of C_3–C_4 alkanes in the presence of hydrogen were systematically studied. The effects of the following conditions on the catalytic activity expressed as the yield of carbon (g CFC)/(g Ni) and on the character of CFC synthesis on graphite rods were studied: procedures for supporting Ni(II) compounds (impregnation and homogeneous precipitation), the concentrations of impregnating compouds (nickel nitrate, urea, and ethyl alcohol) in solution, graphite treatment (oxidation) conditions before supporting Ni(II) compounds, and the pyrolysis temperature of C_3–C_4 alkanes in the range of 400–600°C. Optimum conditions for preparing CFC/graphite composite materials, which are promising for use as electrodes in microbial fuel cells (MFCs), were chosen. The electrochemical characteristics of an MFC designed with the use of a CFC/graphite electrode (anode) and *Gluconobacter oxydans* glycerol-oxidizing bacteria were studied. The morphology of the surfaces of graphite, synthesized CFC, and also bacterial cells adhered to the anode was studied by scanning electron microscopy.

CATALYTIC PROPERTIES OF MASSIVE IRON-SUBGROUP METALS IN DICHLOROETHANE DECOMPOSITION INTO CARBON PRODUCTS

Yu.I. Bauman, I.V. Mishakov, R.A. Buyanov, A.A. Vedyagin, A.M. Volodin

Kinet. Catal.,
52(4) (2011) pp. 547-554.

The formation of nanocarbon materials on massive nickel, nichrome, and some other alloys via the carbide cycle mechanism is reported using 1,2-dichloroethane decomposition as an example. The role of the physical stage of the carbide cycle is elucidated, and massive metal surface activation methods ensuring the realization of this stage are considered. The surface layer of massive nickel or some nickel alloys is most effectively activated by the action of chlorine resulting from the catalytic decomposition of 1,2-dichloroethane. It has been demonstrated by ferromagnetic resonance (FMR) spectroscopy that the activation of the massive metal surface in 1,2-dichloroethane decomposition to nanocarbon is due to the surface undergoing crystal chemical restructuring. The microstructuring of the surface yields fine Ni particles similar in size (0.2–0.3 μm) and shape, whose FMR spectra are anisotropic and have similar magnetic resonance parameters. Both chlorine-free and chlorinated hydrocarbons decompose over these particles via the carbide cycle mechanism. It is demonstrated that it is possible to design catalytic reactors packed with massive nickel or its alloy. The nanocarbon material obtained in such a reactor will not be contaminated by components of conventional catalyst supports (Al, Mg, etc.). The stable performance temperature of the catalyst will be increased, and this will allow the equilibrium outlet methane concentration to be reduced.

PROSPECTS OF MACRO- AND NANOCARBON FIBRES APPLICATION FOR UPDATING THE POLYETHYLENE OF PE80B MARK

L.Ya. Morova*, S.N. Popov*, E.S. Semenova*, M.E. Savvinova*, S.V. Solovyeva*, I.V. Mishakov, I.A. Streltsov (**Institute of Oil and Gas Problems, Yakutsk, Russia*)

Proceed. Samara Sci. Center RAS,
13 (1(2)) (2011) pp. 386-389.

Results of the physicomechanical characteristics of composites on the basis of pipe polyethylene of PE80B mark, which has been reinforced by dispersed macro- and nanocarbon fibres are stated. It is established that efficiency of reinforcing effect of macrocarbon fibres on polymeric matrix is defined by their superficial characteristics - specific surface and presence of microdefects. It is shown that application of carbon nanofibres allows to raise adhesive interaction between composite components.

PREPARATION METHODS OF CATALYSTS FOR SYNTHESIS OF CARBON NANOFIBERS OF DIFFERENT MORPHOLOGICAL TYPES

A.A. Vedyagin, I.V. Mishakov, I.A. Streltsov, E.A. Zhukova, R.A. Buyanov

Proceed. Inst. Higher Educ., Ser.: Chem. Chem. Techn.,
54(5) (2011) pp. 101-105.

Different preparation methods of nickel containing catalysts (co-precipitation of hydroxides, mechanochemical activation of oxides, impregnation of support and ultrasound sublimation of solutions) for CNF synthesis have been considered from viewpoint of possibility to control the diameter of obtained carbon nanofibers. The activity of catalysts in decomposition of propane as well as the morphology of obtained carbon products has been compared for different catalysts. The catalysts obtained by ultrasound sublimation have been shown to provide more thin CNF size distribution and maximum morphological homogeneity of fibers.

CARBON NANOFIBERS WITH LARGE SURFACE AREA: PECULIARITIES OF SYNTHESIS AND MORPHOLOGY

I.V. Mishakov, I.A. Streltsov, Yu.I. Bauman, A.A. Vedyagin, R.A. Buyanov

Proceed. Inst. Higher Educ., Ser.: Chem. Chem. Techn.,
54(7) (2011) pp. 107-110.

The focus is made on methods for synthesis of ‘feathery’ carbon fibers from 1. 2-dichloroethane and C_3–C_4 hydrocarbons over nickel-containing catalysts. The feathery fibers feature a kind of defect fragmentary packing of grapheme layers. As a result, they possess high specific surface area (300–400 m^2/g) and porosity (0.5–0.8 cm^3/g) that are 3 to 5 times as large as those of traditional carbon nanofibers. The reaction of methanation is supposed as the key factor determining textural and morphological characteristics of this carbon material.

URANIUM AND ITS DECAY PRODUCTS IN RADIOACTIVE ANOMALIES OF OXIDIZED BROWN COALS (WESTERN PART OF KANSKO-ACHINSK BROWN COAL BASIN)

M.S. Melgunov, V.M. Gavshin*, E.V. Lazareva*, E.A. Melgunova (**Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia*)

Radioprot.,
46(6) (2011) S371-S376.

Vertical distribution of uranium and its decay products (^{226}Ra and ^{210}Pb) in the uppermost layers of the oxidised brown coals was studied for some deposits and natural outcrops of the Western part of the Kansko-Achinsk brown-coal basin. Abnormal accumulation of the mentioned radioactive elements is observed in all studied sites. Several types of radioactive anomalies are differed by the ratio of activities of ^{238}U and ^{226}Ra: 1) Equilibrium; 2) Radium; 3) Uranium. The depletion of ^{210}Pb in the radioactive horizons of some sites indicates an active emanation of ^{222}Rn in the underlying coal layers. Uranium besides the form sorbed on coal is presented in poral solutions. It says about its potential mobility and is confirmed experimentally. Radium is actively absorbed by the plants growing on radioactive coals.

Composite Sorbents

COMPOSITES $CaCl_2$/SBA-15 FOR ADSORPTIVE TRANSFORMATION OF LOW TEMPERATURE HEAT: PORE SIZE EFFECT

I.S. Glaznev, I. Ponomarenko*, S. Kirik*, Yu.I. Aristov (**Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia*)

Int. J. Refrigeration,
34(5) (2011) pp. 1244-1250.

Each specific cycle for adsorptive heat transformation (AHT) requires appropriate adsorbent which ensures the best realization of precisely this cycle. This paper addresses a synthesis of novel composite sorbents “$CaCl_2$ confined to a meso-structured silicate SBA-15” with variable properties which appear to depend on the SBA pore size (8.1 and 11.8 nm). The equilibrium and dynamics of water sorption have been studied under typical conditions of isobaric stages of AHT cycle. Steep sorption isotherms are found, the pressure at which the sharp increase of water sorption is observed being higher in larger pores. This allows fine adjustment of sorbent properties to cycle boundary temperatures: the stronger water bounding by the salt confined to smaller pores results in the appropriate enhancement of the desorption and condensation temperatures. Comparison of the new composites with other adsorbents promising for AHT showed that mono-sized matrices are encouraging for both tailoring step-like sorption isotherms, managing the step position to fit given AHT cycle and fast water sorption.

WATER SORPTION BY THE CALCIUM CHLORIDE/SILICA GEL COMPOSITE: THE ACCELERATING EFFECT OF THE SALT SOLUTION PRESENT IN THE PORES

D.S. Ovoshchnikov, I.S. Glaznev, Yu.I. Aristov

Kinet. Catal.,
52(4) (2011) pp. 620-628.

The kinetics of isothermal water sorption by the $CaCl_2$/silica gel composite initiated by a small stepwise pressure rise over the sample has been investigated at a constant underlying plate temperature of 35°C. The initial portion of the kinetic curves is consistent with Fick's diffusion model: the amount of sorbed water increases in proportion to the square root of the sorption time. This makes it possible to determine the effective diffusivity of water (D_{eff}). At small amounts of sorbed water ($w < 0.19$ g/g), D_{eff} changes slightly. The diffusivity of water in the composite pores (D) calculated for the same conditions is close to the Knudsen diffusivity of water vapor in mesopores. The D_{eff} value grows with an increasing water content of the composite; that is, sorbed water accelerates water transport in the pores. This is likely due to the appearance of an extra diffusion channel, namely, diffusion through the aqueous solution of the salt, whose formation begins on the silica gel surface at $w > 0.1$ g/g. The contribution from this channel increases markedly when the amount of adsorbed water is above 0.25 g/g. This can be explained by the formation of the "connected" phase of the solution in the pores.

LOW TEMPERATURE HEAT CAPACITY OF THE SYSTEM "SILICA GEL–CALCIUM CHLORIDE–WATER"

Yu.I. Aristov, Yu.A. Kovalevskaya*, M.M. Tokarev, I.E. Paukov* (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

J. Therm. Anal. Calorim.,
103(2) (2011) pp. 773-778.

Heat capacity was measured for two composite systems based on silica gel KSK and calcium chloride confined to its pores. One corresponds to an anhydrous state, while another contains water bound with the salt to give the composition of $CaCl_2 \cdot 2.04H_2O$. The measurements were performed in the temperature range of 6–300 K with a vacuum adiabatic calorimeter. The smoothed experimental curves C_p (T) were used for calculating the calorimetric entropy and the enthalpy increment for both studied systems as well as the effective heat capacity associated only with water in the hydrated composite. The heat capacities C_p (298.15 K) of both composites were compared with those calculated as a linear addition of the heat capacities of silica gel and bulk calcium chloride (or its dihydrate) with appropriate weight coefficients.

NOVEL AMMONIA SORBENTS "POROUS MATRIX MODIFIED BY ACTIVE SALT" FOR ADSORPTIVE HEAT TRANSFORMATION: IV. DYNAMICS OF QUASI-ISOBARIC AMMONIA SORPTION AND DESORPTION ON $BaCl_2$/VERMICULITE

J.V. Veselovskaya, M.M. Tokarev

Appl. Therm. Eng.,
31(4) (2011) pp. 566-572.

A novel composite sorbent of ammonia $BaCl_2$/vermiculite has recently been proposed and tested for adsorption cooling. The aim of this paper was a detailed study of its dynamic operation under conditions of isobaric stages of an adsorption chiller cycle. Experiments were performed by a Large Temperature Jump method at the ammonia pressures 5.8, 6.9, 12.2 and 15.8 bar. The ad- and desorption temperatures were fixed, respectively, at 15, 20, 25, 30, 35°C and 65, 70, 80, 90°C. All kinetic curves were described by an exponential function with a single characteristic time τ. The rate constant $k = 1/\tau$ was found to be a linear function of the temperature difference which drives the process, hence, heat transfer between the sorbent layer and the plate heat exchanger determines the process dynamics. The appropriate heat transfer coefficient does not depend on the ammonia pressure and process temperatures and equals 90 $W/(m^2 \cdot K)$. The data obtained were used for analyzing the dynamic performance of adsorption chiller with this composite as a solid sorbent. Appropriate recommendations on optimization of working cycle are made. The analysis showed that the specific cooling power could reach 690–860 W/kg at the cycle duration of 100–300 s.

COMPOSITE SORBENT OF METHANOL “LiCl IN MESOPOROUS SILICA GEL” FOR ADSORPTION COOLING: DYNAMIC OPTIMIZATION

L.G. Gordeeva, Yu.I. Aristov

Energy,
36(2) (2011) pp. 1273-1279.

A novel composite sorbent of methanol “LiCl in mesoporous silica gel” has recently been proposed for AC (adsorption cooling). Its testing in a lab-scale adsorption chiller resulted in the specific cooling power of 210-290 W/kg and the cooling COP of 0.32-0.4. Although these values are rather encouraging, a room for their enhancement still exists. The aim of this paper was a dynamic optimization of the composite performance in AC cycles. Dynamics of methanol sorption on loose grains of the LiCl/silica composites was studied by a Large Temperature Jump method under typical conditions of AC cycle. Effects of number of the sorbent layers, salt content, grain size and cycle boundary temperatures were studied. Physicochemical processes in the three-phase system (salt, solution, vapor) were shown to be quite complex and can strongly affect the dynamics of methanol ad-/desorption. Several obstacles which can retard the sorption were analyzed. Appropriate recommendations on improving the cycle dynamics, which concern optimal conversion degree, salt content and relative durations of ad- and desorption phases, were made.

Nanostructured-Nanocomposite Materials for SOFC Applicatrion

ADVANCED SINTERING TECHNIQUES IN DESIGN OF PLANAR IT SOFC AND SUPPORTED OXYGEN SEPARATION MEMBRANES

V.A. Sadykov, V.V. Usoltsev, Yu.E. Fedorova, N.V. Mezentseva, T.A. Krieger, N.F. Eremeev, M.V. Arapova, A.V. Ishchenko, A.N. Salanov, V.V. Pelipenko, V.S. Muzykantov, A. Ulikhin*, N. Uvarov*, O. Bobrenok, A. Vlasov***, M. Korobeynikov***, A. Bryazgin***, A. Arzhannikov***, P. Kalinin***, O. Smorygo****, M. Thumm** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of Thermal Physics, Novosibirsk, Russia; ***Budker Institute of Nuclear Physics, Novosibirsk, Russia; ****Powder Metallurgy Institute, Minsk, Belarus; *****Karlsruhe Institute of Technology, Karlsruhe, Germany*)

In “*Sintering/Book 1*”, Ed. A. Lakshmanan,
INTECH, Austria, Vienna, 2011, pp. 1-20.

Advanced sintering techniques based upon radiation-thermal sintering by e-beam action and microwave heating allow to provide required density and consolidation of thin functional layers in design of intermediate temperature solid oxide fuel cells and oxygen separation membranes. Due to decrease temperature and duration of sintering as compared with conventional sintering methods, such negative phenomena as variation of functional layers phase composition, their cracking and damage of metallic substrates were prevented. For oxide mixed ionic-electronic conducting composites advanced sintering provides developed interfaces which act as paths for fast oxygen diffusion required for considered applications. As the result, fuel cells and oxygen separation membranes manufactured using advanced sintering techniques demonstrate performance characteristics promising for the practical application.

A novel approach to the design of planar gradient porous supports for the thin-film SOFCs and MIEC membranes is described. The support's thermal expansion is controlled by the creation of a two-component composite metal-ceramic foam structure. Thin MIEC membranes and SOFCs were prepared on the composite supports by the layerwise deposition of composite functional layers including complex fluorites and perovskites. Lab-scale studies demonstrated promising performance of both MIEC membrane and SOFC.

NANOCOMPOSITE CATALYSTS FOR STEAM REFORMING OF METHANE AND BIOFUELS: DESIGN AND PERFORMANCE

V.A. Sadykov, N.V. Mezentseva, G.M. Alikina, R.V. Bunina, V.V. Pelipenko, A.I. Lukashevich, Z.Yu. Vostrikov, V.A. Rogov, T.A. Krieger, A.V. Ishchenko, V.I. Zaikovsky, L.N. Bobrova, J. Ross*, O. Smorygo, A. Smirnova***, B. Rietveld****, F. van Berkel****** (**University of Limerick, Limerick, Ireland; **Powder Metallurgy Institute, Minsk, Belarus; ***Eastern Connecticut State University, USA; ****Energy Research Center of the Netherlands, The Netherlands)*

In *“Nanocomposite Materials, Theory and Applications*”, INTECH, Austria, Vienna, 2011,
pp. 909-946.

Nanocomposite materials developed in this work based upon Ni and doped zirconia electrolyte allow to provide efficient and stable in-cell steam reforming of methane and ethanol required for IT SOFC as well as design of monolithic catalysts of transformation of biofuels into syngas. This is provided by optimization of their composition and preparation procedures ensuring developed interfaces between components activating fuel molecules (Ni, Ni-Pt/Ru alloys) and water molecules (complex oxides with perovskite and fluorite structures). Performance of best compositions supported as porous strongly adhering layers on anode cermets platelets, FeCr alloy gauzes and porous Ni-Al foam substrates was estimated as well and demonstrated to be high and stable to meet target of internal reforming of fuels in the intermediate temperature solid oxide fuel cells. No cracking or detachment of layers after reaction was observed. Analysis of methane reforming kinetics catalyzed by structured catalytic elements with supported nanocomposite layers has been carried out. Performance of catalytic plates in IR mode of ECN cell meets target of design of solid oxide fuel cells with internal reforming of methane by area specific resistance, activity and power density.

PEROVSKITES AND THEIR NANOCOMPOSITES WITH FLUORITE-LIKE OXIDES AS MATERIALS FOR SOLID OXIDE FUEL CELLS CATHODES AND OXYGEN-CONDUCTING MEMBRANES: MOBILITY AND REACTIVITY OF THE SURFACE/BULK OXYGEN AS A KEY FACTOR OF THEIR PERFORMANCE

V.A. Sadykov, S.N. Pavlova, T.S. Kharlamova, V.S. Muzykantov, N.F. Uvarov*, Yu.S. Okhlupin*, A.V. Ishchenko, A.S. Bobin, N.V. Mezentseva, G.M. Alikina, A.I. Lukashevich, T.A. Krieger, T.V. Larina, N.N.Bulgakov, V.M. Tapilin, V.D. Belyaev, E.M. Sadovskaya, A.I. Boronin, V.A. Sobyanin, O.F. Bobrenok*, A.L. Smirnova, O.L. Smorygo***, J.A. Kilner****** (**Institute of Thermophysics, Novosibirsk, Russia; **University of Connecticut, Storrs, USA; ***Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; ***Powder Metallurgy Institute, Belarus; ****Imperial College London, London, UK*)

In “*Perovskites: Structure, Properties and Uses*”,
Ed. M. Borowski, Nova Science Publishers, Inc, 2010,
pp. 67-178.

This paper presents results of research aimed at elucidating factors controlling mobility and reactivity of the surface and bulk oxygen of complex perovskite-like $A_nB_mO_z$ oxides (manganites, ferrites, cobaltites, nickelates of La/Sr) and their nanocomposites with fluorite-like oxides (doped ceria or zirconia) as related to their performance in the intermediate temperature solid oxide fuel cells (IT SOFC) cathodes and oxygen separation membranes. Real/defect structure and surface properties of these materials as a function of both composition, preparation route and sintering temperature were studied by combination of TEM with EDX, XRD, EXAFS, UV-Vis and XPS methods. Lattice oxygen mobility, strength of oxygen species bonding with the surface sites and their reactivity for both dispersed and dense materials were estimated by oxygen isotope exchange, temperature-programmed desorption and reduction by H_2 and CH_4. Coefficients of oxygen diffusion in dense materials were estimated by analysis of dynamics of the oxygen loss monitored by measurements of the weight loss or conductivity relaxations. For analysis of atomic-scale factors controlling oxygen bonding strength and mobility, quantum-chemical approaches including the Density Functional Theory (DFT) in spin-polarized SLDA approximation and semiempirical Interacting Bonds Method were applied.

DESIGN AND CHARACTERIZATION OF LSM/ScCeSZ NANOCOMPOSITE AS MIXED IONIC–ELECTRONIC CONDUCTING MATERIAL FOR FUNCTIONALLY GRADED CATHODES OF SOLID OXIDE FUEL CELLS

V.A. Sadykov, G.M. Alikina, A.I. Lukashevich, V.S. Muzykantov, V.V. Usoltsev, A.I. Boronin, S.V. Koshcheev, T.A. Krieger, A.V. Ishchenko, A. Smirnova*, O. Bobrenok, N.F. Uvarov***** (**University of Connecticut, Storrs, USA; **Institute of Thermophysics, Novosibirsk, Russia; ***Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Solid State Ionics,
192(1) (2011) pp. 540-546.

LSM/ScCeSZ nanocomposite was prepared via ultrasonic dispersion of the mixture of perovskite and fluorite powders in isopropanol in 1:1 ratio with addition of polyvinyl butyral. Studies of the real structure and surface property evolution at sintering under air up to 1100°C revealed some redistribution of elements between the phases without new phase formation. Sizes of both phase domains remain in nanorange even in the dense material, thus providing a developed perovskite–fluorite interface. The surface layer of nanocomposite is enriched by LSM. The oxygen mobility and reactivity estimated by the oxygen isotope exchange and O_2 TPD exceed those for LSM suggesting a positive role of interfaces as fast oxygen migration paths. Button-cell tests with the LSM/ScCeSZ interlayer between LSNF and a thin ScYSZ layer covering Ni/YSZ cermet demonstrated a high and stable performance promising practical application promising for practical application.

DESIGN AND TESTING OF STRUCTURED CATALYSTS FOR INTERNAL REFORMING OF CH_4 IN INTERMEDIATE TEMPERATURE SOLID OXIDE FUEL CELLS (IT SOFC)

A.L. Smirnova*, V.A. Sadykov, N.V. Mezentseva, R.V. Bunina, V.V. Pelipenko, G.M. Alikina, T.A. Krieger, L.N. Bobrova, O.L. Smorygo, F. van Berkel***, B. Rietveld*** (***Eastern Connecticut State University, Willimantic, USA; **Powder Metallurgy Institute, Minsk, Belarus; ***Energy Research Center of the Netherlands, The Netherlands)*

ECS Trans.,
35(1) (2011) pp. 2771-2780.

Procedures for the synthesis of nanocomposite anode materials comprised of Ni-YSZ promoted by doped Ce-Zr-O fluorite-like or La-Pr-Mn-Cr-O perovskite-like oxides and Pt/Ru were elaborated. Their composition, structure, reactivity, and catalytic properties in CH_4 steam reforming were characterized using various techniques, such as SEM, TEM, EDX, TPR, and I-V testing in SOFC conditions. The optimized nanocomposites supported on compressed foam Ni-Al substrates demonstrated high and stable performance at $H_2O:CH_4=1:2$ ratio without coking or sintering. For the SOFC testing, the planar catalytic substrates with the surface area of 5x5 cm^2 have been used. The demonstrated SOFC performance in the internal CH_4 reforming mode was close to the performace obtained with the humidified hydrogen. The achieved power density was up to 300-800 mW/cm^2 at 600-800°C meeting the targets of the area specific resistance, fuel efficiency, and power density.

SYNTHESIS AND CHARACTERIZATION OF DOPED APATITE-TYPE LANTHANUM SILICATES FOR SOFC APPLICATIONS

H. Gasparyan*,*, S. Neophytides**, D. Niakolas**, V. Stathopoulos***,****, T.S. Kharlamova, V.A. Sadykov, O. Van der Biest*****, E. Jothinathan*****, E. Louradour******, J.-P. Joulin******, S. Bebelis*** (**University of Patras, Patras, Greece; **Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece; ***CERECO S.A.-Ceramics and Refractories Technological Development Company, Chalkida, Greece; ****Technological Educational Institute of Chalkida, Psahna, Greece; *****Katholieke Universiteit Leuven, Heverlee, Belgium; ******CTI — Céramiques Techniques et Industrielles SA, Salindres, France*)

Solid State Ionics,
192(1) (2011) pp. 158-162.

A series of iron- and/or aluminium-doped apatite-type lanthanum silicates (ATLS) $La_{9.83}Si_{6-x-y}Al_xFe_yO_{26 \pm \delta}$ (x = 0, 0.25, 0.75, and 1.5, y = 0, 0.25, 0.75, and 1.5) were synthesized using the mechanochemical activation (MA), solid state reaction (SSR), Pechini (Pe) and sol–gel (SG) methods. The total conductivity of the prepared materials was measured under air in the temperature range 600–850°C using 4-probe AC impedance spectroscopy. Its dependence on composition, synthesis method, sintering conditions and powder particle size was investigated. It was found that for electrolytes of the same composition, those prepared via mechanochemical activation exhibited the highest total specific conductivity, which was improved with increasing Al- and decreasing Fe-content. The highest conductivity value at 700°C, equal to 2.04×10^{-2} S cm^{-1}, was observed for the $La_{9.83}Si_5Al_{0.75}Fe_{0.25}O_{26\pm\delta}$ electrolyte. $La_{9.83}Si_{4.5}Fe_{1.5}O_{26\pm\delta}$ electrolyte samples synthesized using the Pechini method exhibited higher conductivity when sintered conventionally than when spark-plasma sintering (SPS) was used.

APATITE TYPE LANTHANUM SILICATE AND COMPOSITE ANODE HALF CELLS

E. Jothinathan*, K. Vanmeensel*, J. Vleugels*, T.S. Kharlamova, V.A. Sadykov, S.N. Pavlova, G. Sourkouni, C. Szepanski**, C. Argirusis**,***, O. Van der Biest*** (**Katholieke Universiteit Leuven, Leuven, Belgium; **Clausthal University of Technology and Energieforschungszentrum, Goslar, Germany; ***National Technical University of Athens, Greece*)

Solid State Ionics,
192(1) (2011) pp. 419-423.

Apatite type rare earth silicates are being extensively studied as electrolyte material for intermediate temperature solid oxide fuel cells (SOFC). In this paper results are presented on synthesis of Al and/or Fe-doped ATLS, the design of compatible anode materials, thermal expansion properties and co-sintering of half-cells from expansion matched materials using the advanced pulsed electric current sintering (PECS) technique. The issues related to the co-sintering of half cells have been addressed successfully by the combined use of nano powders and PECS.

NANOCOMPOSITE CATHODE MATERIALS FOR INTERMEDIATE TEMPERATURE SOLID OXIDE FUEL CELLS

T.S. Kharlamova, S.N. Pavlova, V.A. Sadykov, Yu.N. Bespalko, T.A. Krieger, V.V. Pelipenko, V.D. Belyaev, G.M. Alikina, V.S. Muzykantov, Y. Okhlupin*, N. Uvarov*, A. Smirnova** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **University of Connecticut, Storrs, USA*)

ECS Transactions,
35(1) (2011) pp. 2331-2340.

The present paper is devoted to the optimization of composites (100-z) wt% $La_{1-y}Sr_yFe_{0.7}Ni_{0.3}O_{3-\delta}$ - z wt% $Ce_{0.9}Gd_{0.1}O_{2-\delta}$ (GDC) and study of the effect of Sr doping of perovskite and GDC content in the sample on structural and transport features of the composites. The results on the research of structural and microstructural features of the composits and their transport properties by using XRD, HRTEM, EDX analysis, electrical conductivity measurements, oxygen isotope heteroexchange and conductivity as well as weight relaxation techniques are presented and discussed.

THE EFFECT OF PHASE COMPOSITION ON THE TRANSPORT PROPERTIES OF COMPOSITES $La_{0.8}Sr_{0.2}Fe_{0.7}Ni_{0.3}O_{3-\delta}$ - $Ce_{0.9}Gd_{0.1}O_{1.95}$

Yu.S. Okhlupin*, M.V. Ananyev, N.F. Uvarov*, Yu.N. Bespalko, S.N. Pavlova, V.A. Sadykov** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of High-Temperature Electrochemistry, Yekaterinburg, Russia*)

Russ. J. Electrochem.,
47(6) (2011) pp. 663-670.

Full conductivity, diffusion and oxygen exchange processes in composites $(100-x)La_{0.8}Sr_{0.2}Fe_{0.7}Ni_{0.3}O_{3-\delta} - xCe_{0.9}Gd_{0.1}O_{1.95}$ (x is the volume fraction, $0 \le x \le 71.1\%$) at 700°C over the oxygen partial pressure range from 0.2 to 3×10^{-3} atm are studied by the electrical conductivity relaxation method. The composites' conductivity was shown to decrease monotonically with the increasing of $Ce_{0.9}Gd_{0.1}O_{1.95}$ fraction, while the oxygen chemical diffusion coefficient increased. The oxygen exchange constant is higher for the composites than for the individual phases of $La_{0.8}Sr_{0.2}Fe_{0.7}Ni_{0.3}O_{3-\delta}$ and $Ce_{0.9}Gd_{0.1}O_{1.95}$. Possible reason of the dependence of the parameters D_{chem} and k_{chem} on the temperature, oxygen pressure, and the composite composition is the effect of the interface on the oxygen transfer processes. Most effective oxygen transfer occurs in the composites whose composition approaches $La_{0.8}Sr_{0.2}Fe_{0.7}Ni_{0.3}O_{3-\delta}$ - $Ce_{0.9}Gd_{0.1}O_{1.95}$ ($x = 71\%$).

STUDIES OF OXYGEN TRANSPORT MECHANISM IN ELECTROLYTES BASED ON DOPED LANTHANUM SILICATE WITH APATITE STRUCTURE USING TECHNIQUES OF OXYGEN ISOTOPIC HETEROEXCHANGE AND IMPEDANCE SPECTROSCOPY

V.A. Sadykov, T.S. Kharlamova, N.V. Mezentseva, S.N. Pavlova, E.M. Sadovskaya, V.S. Muzykantov, Yu.N. Bespalko, V.V. Usoltsev, E.G. Zevak, T.A. Krieger, A.V. Ishchenko, N.F. Uvarov*, A.S. Ulikhin*, M.V. Chaikina, C. Argirusis**,***** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Clausthal University of Technology, Clausthal–Zellerfeld, Germany; ***National Technical University of Athens, Athens, Greece*)

Russ. J. Electrochem.,
47(4) (2011) pp. 427-441.

The work presents the results of studying the mechanism of oxygen transport for a new promising class of oxygen-containing electrolytes based on lanthanum silicate with an apatite structure using impedance spectroscopy and isotopic oxygen heteroexchange. At 1000 K, in the case of samples with an optimum composition including codoped Fe and Al, $\sigma \sim 3 \times 10^{-3}$ to 10^{-2} S/cm and D^* reaches $\sim 10^{-8}$ cm^2/s, which is close to the values of YSZ and $Ce_{0.9}Gd_{0.1}O_{2-\delta}$ (GDC). Lower energies of conductivity activation and oxygen diffusion for doped apatites (~0.5–0.8 eV instead of ~1 eV for GDC) and also equivalence as regards exchange of all oxygen atoms within apatite agree with the model, in which oxygen mobility is determined by a nonlinear cooperative migration process of oxygen atoms with fast exchange between interstitial and regular sites.

DESIGN OF MEDIUM–TEMPERATURE SOLID OXIDE FUEL CELLS ON POROUS SUPPORTS OF DEFORMATION STRENGTHENED Ni–Al ALLOY

V.A. Sadykov, V.V. Usoltsev, Yu.E. Fedorova, V.A. Sobyanin, P.V. Kalinin*, A.V. Arzhannikov*, A.Yu. Vlasov, M.V. Korobeinikov**, A.A. Bryazgin**, A.N. Salanov, M.R. Predtechenskii***, O.F. Bobrenok***, A.S. Ulikhin****, N.F. Uvarov****, O.L. Smorygo*****, A.F. Il'yushchenko*****, V.Yu. Ul'yanitskii******, S.B. Zlobin******** (**Novosibirsk State University, Novosibirsk, Russia; **Budker Institute of Nuclear Physics, Novosibirsk, Russia; ***Institute of Thermal Physics, Novosibirsk, Russia; ****Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; *****Institute of Powder Metallurgy, Minsk, Belarus; ******Lavrent'ev Institute of Hydrodynamics, Novosibirsk, Russia*)

Russ. J. Electrochem.,
47(4) (2011) pp. 488-493.

An approach was developed towards design of medium-temperature solid-oxide fuel cells based on a deformation strengthened Ni-Al alloy. Methods of sintering were described that allowed obtaining layers of complex oxides with ionic and mixed conductivity and with regulated porosity in the range of 40–1%. Power density of a fuel cell on a metallic support reaches 500 mW/cm^2 already at 700°C when humid H_2 was used as fuel and air was used as an oxidant. Analysis of fuel cell cross-section after tests showed absence of fractures, flaking, and new phases with low conductivity, which proves good compatibility of all materials used in fuel cell design.

SOLID OXIDE FUEL CELL COMPOSITE CATHODES BASED ON PEROVSKITE AND FLUORITE STRUCTURES

V.A. Sadykov, N.V. Mezentseva, V.V. Usoltsev, E.M. Sadovskaya, A.V. Ishchenko, S.N. Pavlova, Yu.N. Bespalko, T.S. Kharlamova, E.G. Zevak, A.N. Salanov, T.A. Krieger, V.D. Belyaev, O. Bobrenok*, N. Uvarov, Yu. Okhlupin**, O. Smorygo***, A. Smirnova****, P. Singh*****, A. Vlasovh******, M. Korobeynikov******, A. Bryazgin******, P. Kalinin******, A. Arzhannikov******** (**Institute of Thermal Physics, Novosibirsk, Russia; **Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; ***Powder Metallurgy Institute, Minsk, Belarus; ****Eastern Connecticut State University, Willimantic, USA; *****University of Connecticut, Storrs, USA; ******Budker Institute of Nuclear Physics, Novosibirsk, Russia*)

J. Power Sources,
196(17) (2011) pp. 7104-7109.

This work presents the results related to the functionally graded fluorite (F) - perovskite (P) nanocomposite cathodes for IT SOFC. Nanocrystalline fluorites (GDC, ScCeSZ) and perovskites (LSrMn, LSrFNi) were synthesized by Pechini method. Nanocomposites were prepared by the ultrasonic dispersion of F and P powders in isopropanol with addition of polyvinyl butyral. Different techniques for deposition and sintering of functionally graded cathode materials were applied including traditional approaches as well as original methods, such as radiation-thermal sintering under electron beam or microwave radiation. Morphology, microstructure and elemental composition of nanocomposites was characterized by XRD and HRTEM/SEM with EDX. Even for dense composites, the sizes of perovskite and fluorite domains remain in the nanorange providing developed P-F interfaces. Oxygen isotope heteroexchange and conductivity/weight relaxation studies demonstrated that these interfaces provide a path for fast oxygen diffusion. The redistribution of the elements between P and F phases in nanocomposites occurs without formation of insulating zirconate phases. Button-size fuel cells with nanocomposite functionally graded cathodes, thin YSZ layers and anode Ni/YSZ cermet (either bulk or supported on Ni-Al foam substrates) were manufactured. For optimized composition and functionally graded design of P-F nanocomposite cathodes, a stable performance in the intermediate temperature range with maximum power density up to 0.5 W cm^{-2} at 700°C in wet H_2/air feeds was demonstrated.

Photocatalytic and Related Processes

GLOSSARY OF TERMS USED IN PHOTOCATALYSIS AND RADIATION CATALYSIS (IUPAC RECOMMENDATIONS 2011)

S.E. Braslavsky*, A.M. Braun, A.E. Cassano***, A.V. Emeline****, M.I. Litter*****, L. Palmisano******, V.N. Parmon, N. Serpone********* *(*Max Planck Institute for Bioinorganic Chemistry, Mülheim/Ruhr, Germany; **University of Karlsruhe, Karlsruhe, Germany; ***Universidad Nacional del Litoral, Santa Fe, Argentina; ****V.A. Fock Institute of Physics, St. Petersburg, Russia; *****National Atomic Energy Commission, Buenos Aires, Argentina; ******University of Palermo, Palermo, Italy; *******Concordia University, Montreal, Canada and University of Pavia, Pavia, Italy*)

Pure Appl. Chem.,
83(4) (2011) pp. 931-1014.

This glossary of terms covers phenomena considered under the very wide terms photocatalysis and radiation catalysis. A clear distinction is made between phenomena related to either photochemistry and photocatalysis or radiation chemistry and radiation catalysis. The term “radiation” is used here as embracing electromagnetic radiation of all wavelengths, but in general excluding fast-moving particles. Consistent definitions are given of terms in the areas mentioned above, as well as definitions of the most important parameters used for the quantitative description of the phenomena. Terms related to the up-scaling of photocatalytic processes for industrial applications have been included. This Glossary should be used together with the Glossary of terms Used in Photochemistry, 3rd edition, IUPAC Recommendations 2006: (doi:10.1351/pac200779030293) as well as with the IUPAC Compendium of Chemical Terminology, 2nd ed. (the “Gold Book”, 2006–doi:10.1351/goldbook) because many terms used in photocatalysis are defined in these documents.

PHOTOCHEMISTRY OF A 6 '-CYANOSUBSTITUTED SPIRONAPHTHOOXAZINE: PHOTO-INDUCED DECAY OF AN OPEN FORM

M.I. Nikolaeva, V.V. Korolev*, E.A. Pritchina*, E.M. Glebov*, V.F. Plyusnin*, A.V. Metelitsa, N.A. Voloshin**, V.I. Minkin**** (**Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia; **Southern Federal University, Rostov-on-Don, Russia*)

J. Phys. Org. Chem.,
24(9) (2011) pp. 833-842.

Photochemistry of three 6'-cyanosubstituted spironaphthooxazines (SNO) in ethanol matrices at 77 K was studied by means of ultraviolet (UV) and erythrocyte sedimentation rate (ESR) spectroscopy and quantum chemistry. The quantum yield of the open form photolysis is found to be 0.01-0.02, which is high enough for 77 K. For one of the SNO, the formation of a merocyanine form radical was observed. The radicals were formed by an H atom abstraction from the solvent molecule to the light-excited merocyanine isomers. The formation of a merocyanine radical represents a new specific channel of photochemically induced degradation of spirooxazines.

PHOTOCHROMISM OF 6'-CYANOSUBSTITUTED SPIROOXAZINES IN FROZEN ALCOHOL MATRICES

M.I. Nikolaeva, V.V. Korolev*, E.A. Pritchina*, E.M. Glebov*, V.F. Plyusnin*, A.V. Metelitsa, N.A. Voloshin**, V.I. Minkin**** (**Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia; **Institute of Physical and Organic Chemistry, Southern Federal University, Rostov-on-Don, Russia*)

Kinet. Catal.,
52(2) (2011) pp. 202-209.

For three 6'-cyanosubstituted spironaphthooxazines, spectral characteristics of an open form and quantum yields of photoisomerization were determined both at room temperature and in frozen alcohol matrices. Spironaphthooxazines have demonstrated fairly high (0.01–0.02) quantum yields of open form appearance at 77 K. The observed peculiarities of the open form UV spectra were explained by the temperature dependence of the open form isomers distribution. Partial stabilization of the nonequilibrium isomers of an open form in the low-temperature matrices was revealed.

PHOTOINDUCED CATALYTIC SYNTHESIS OF BIOLOGICALLY IMPORTANT METABOLITES FROM FORMALDEHYDE AND AMMONIA UNDER PLAUSIBLE "PREBIOTIC" CONDITIONS

I.V. Delidovich, O.P. Taran, A.N. Simonov, L.G. Matvienko, V.N. Parmon

Adv. Space Res.,
48(3) (2011) pp. 441-449.

The article analyzes new and previously reported data on several catalytic and photochemical processes yielding biologically important molecules. UV-irradiation of formaldehyde aqueous solution yields acetaldehyde, glyoxal, glycolaldehyde and glyceraldehyde, which can serve as precursors of more complex biochemically relevant compounds. Photolysis of aqueous solution of acetaldehyde and ammonium nitrate results in formation of alanine and pyruvic acid. Dehydration of glyceraldehyde catalyzed by zeolite HZSM5-17 yields pyruvaldehyde. Monosaccharides are formed in the course of the phosphate-catalyzed aldol condensation reactions of glycolaldehyde, glyceraldehyde and formaldehyde. The possibility of the direct synthesis of tetroses, keto- and aldo-pentoses from pure formaldehyde due to the combination of the photochemical production of glycolahyde and phosphate-catalyzed carbohydrate chain growth is demonstrated. Erythrulose and 3-pentulose are the main products of such combined synthesis with selectivity up to 10%. Biologically relevant aldotetroses, aldo- and ketopentoses are more resistant to the photochemical destruction owing to the stabilization in hemiacetal cyclic forms. They are formed as products of isomerization of erythrulose and 3-pentulose. The conjugation of the concerned reactions results in a plausible route to the formation of sugars, amino and organic acids from formaldehyde and ammonia under presumed `prebiotic' conditions.

PHOTOCHEMICAL ACTIVITY OF THE ADSORBED AEROSOL, PRODUCED FROM PERICLASE (MgO) CRYSTAL UNDER AMBIENT AIR

V.S. Zakharenko, E.B. Daibova* (**Tomsk State University, Tomsk, Russia*)

Atmos. Oceanic Opt.,
24(6) (2011) pp. 516-520.

The adsorption and photoadsorption properties of aerosol particles, produced by grinding of periclase crystal (MgO) under ambient air, were studied. The composition analysis of adsorption surface layer formed by grinding of crystal is carried out. The kinetics of dark and photo adsorption of oxygen and carbon monoxide including ^{13}CO were considered. The quantum yield quantities and spectral dependencies of photoadsorption were determined. The comparison of photoadsorption properties of samples used in this work and magnesium oxide powders produced by traditional ways was realized.

STRUCTURED CATALYSTS FOR PHOTO-FENTON OXIDATION OF ACETIC ACID

D. Sannino*, V. Vaiano*, P. Ciambelli*, L.A. Isupova (**University of Salerno, Fisciano, Italy*)

Catal. Today,
161(1) (2011) pp. 255-259.

In this work photo-Fenton oxidation of acetic acid, was carried out on perovskites based structured catalysts, in the presence or in the absence of low amounts of Pt. Homogeneous photo-Fenton reaction by ferrioxalate complex has been also performed. The comparison of homogeneous and heterogeneous photo-Fenton oxidation indicates that the use of a heterogeneous structured catalyst greatly improves the total organic carbon (TOC) removal and leads to a more effective use of H_2O_2. The rate of TOC removal during the runtime decreased because of the occurring side H_2O_2 decomposition to O_2 that subtracts the oxidant to the photo-Fenton reaction. Moreover it allows enlarging the pH range of operation without the formation of sludge or significant metal leaching. $LaFeO_3$ and $Pt/LaMnO_3$ resulted the best catalysts for this process in terms of reaction rate.

PHOTO-FENTON OXIDATION OF ACETIC ACID ON SUPPORTED $LaFeO_3$ AND $Pt/LaFeO_3$ PEROVSKITES

D. Sannino*, V. Vaiano*, L.A. Isupova,
P. Ciambelli* (**University of Salerno, Fisciano, Italy*)

Chem. Eng. Trans.,
25(2) (2011) pp. 1013-1018.

Photo-Fenton process uses Fe^{2+} as homogeneous catalyst, hydrogen peroxide and UV light to mineralize organic pollutants by the formation of highly reactive hydroxyl radicals. Several limitations to this process are present, such as the limited operational pH range to avoid oxyhydroxide sludge formation and the catalyst recovery. Heterogeneous photo-Fenton process based on structured catalyst can avoid a subsequent separation stage, overcoming these disadvantages. In this work, the comparison of performances of $LaFeO_3$ and $Pt/LaFeO_3$ perovskites supported on different honeycomb monoliths, made of cordierite or corundum, were studied. Photo-Fenton oxidation of acetic acid showed that $LaFeO_3$ supported on corundum honeycomb was more active than on cordierite monolith. The addition of Pt on catalysts did not help to increase their performance in the studied reaction. Photo-Fenton oxidation tests carried out on catalysts having different content of $LaFeO_3$ evidenced the existence of an optimal loading of active phase.

THE INFLUENCE OF CORONA ELECTRODES THICKNESS ON THE EFFICIENCY OF PLASMACHEMICAL OXIDATION OF ACETONE

M.N. Lyulyukin, A.S. Besov, A.V. Vorontsov

Plasma Chem. Plasma Process.,
31(1) (2011) pp. 23-39.

Current–voltage characteristics (CVC) and acetone vapors oxidation in atmospheric pressure corona discharge (CD) of negative and positive polarity were studied in double wires-to-plate geometry. Negative CD was more stable than positive one towards breakdown and allowed to reach higher current. CVC for negative CD can be well described by model for cylindrical geometry with correction in one coefficient only. The ignition voltage of negative CD obeys Peek's law. The rate of acetone vapors oxidation increased with the increase of corona wire radius in the range of discharge power 15–60 W. The highest oxidation rate was obtained at power 60 W, negative polarity and wire radius 400 lm but the highest energetic efficiency (g/kWh) was obtained at maximum wire radius (400 lm) and minimum power level (15 W). The oxidation rate was directly proportional to the volume of discharge area which grows together with the increase of wire radius.

INFLUENCE OF THE METHOD OF PLATINUM DEPOSITION ON ACTIVITY AND STABILITY OF Pt/TiO_2 PHOTOCATALYSTS IN THE PHOTOCATALYTIC OXIDATION OF DIMETHYL METHYLPHOSPHONATE

E.A. Kozlova, T.P. Lyubina, M.A. Nasalevich,
A.V. Vorontsov, A.V. Miller, V.V. Kaichev,
V.N. Parmon

Catal. Commun.,
12(7) (2011) pp. 597-601.

Gas-phase photocatalytic oxidation of organophosphorous compound dimethyl methylphosphonate was carried out in a flow reactor on platinized TiO_2 Degussa P25. Platinization was performed by soft chemical reduction (SCR) and photodeposition (PD) techniques. Dispersion and chemical state of platinum were studied by X-ray photoelectron spectroscopy (XPS) and high-resolution transmission electron microscopy (HRTEM). It was found that SCR gave mostly metallic platinum, whereas PD gave only Pt^{2+} form. During the oxidation, the state of platinum on a SCR catalyst remained unchanged, which determined its good stability. The catalyst with PD platinum deactivated quite fast due to aggregation of Pt particles. The SCR technique was found to provide better stability and activity.

PARAMETRIC STUDIES OF DIETHYL PHOSPHORAMIDATE PHOTOCATALYTIC DECOMPOSITION OVER TiO_2

B. Sun*, A.V. Vorontsov, P.G. Smirniotis*
(**University of Cincinnati, Cincinnati, USA*)

J. Hazard. Mater.,
186(2-3) (2011) pp. 1147-1153.

The present study is focused on influences of parameters including pH, temperature, TiO_2 catalyst concentration, and reactant concentration on the rate of photocatalytic diethyl phosphoramidate (DEPA) decomposition with Hombikat UV 100 (HK) and Degussa P25 (P25) TiO_2. Total mineralization of DEPA is observed. Two regimes of pH, namely in acid and near-neutral environments were found where maximum total carbon (TC) decomposition was observed. The electrostatic effects on adsorption over the TiO_2 surface explain the above phenomena. The maximum rate is observed for P25 at DEPA concentration 1.3 mM whereas the rate grows continuously with DEPA concentration rise for HK. The temperature dependence of TC decomposition rate in the range of 15–63°C with both HK and P25 follows the Arrhenius equation. The activation energy for total carbon decomposition with HK and P25 are 29.5 ± 1.0 and 24.3 ± 3.1 kJ/mol, respectively. The decomposition rate of DEPA is larger over P25 than over HK. The rate over P25 increases faster than that with HK for each unit of the titania added when the TiO_2 concentration is less than 375 mg/l. The higher light absorption and particles aggregation of P25 are responsible for the decrease of reaction rate the authors observed at catalyst concentration above a certain level. In contrast, the rate over HK increases monotonically with the concentration of the photocatalyst used.

DEVELOPMENT OF MULTISTAGE PHOTOCATALYTIC REACTORS FOR AIR PURIFICATION

D.V. Kozlov, A.V. Vorontsov

Chem. Sustain. Devel.,
19(1) (2011) pp. 67-76.

The basic principles of the performance of catalysts in the processes of profound oxidation of organic compounds present in the air are considered. Within the framework of Langmuir-Hinshelwood model, the authors calculated the kinetic parameters of photooxidation of a number of compounds (rate constants and adsorption constants) and then used them in the development of reactors for air purification. It was demonstrated that in order to increase the rate of photocatalytic oxidation, it is necessary to optimize the geometry of the photocatalytic filter, and to use inorganic air-permeable membranes (foam ceramics and glas cloth) as supports for the photocatalyst. In addition, the efficiency of air purification can be increased due to the use of multistage reactors in which the air to be purified passes consecutive stages of electrostatic filtration, adsorption and photocatalytic purification. An example of implementation of the proposed concept of multistage purification of the air at the industrial enterprise SPA Luch (Novosibirsk) is described.

SIZE EFFECTS IN PHOTOEXCITATION OF TRIPLET STATES OF AMMONIUM TETRAPHENYLBORATE

V.A. Nadolinny*, O.V. Antonova*, E.A. Il'inchik*, M.K. Kovalev, M.S. Melgunov, A.P. Yelisseev, A.A. Ryadun*** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia*)

Phys. Solid State,
53(2) (2011) pp. 284-291.

This paper reports on the results of complex investigations of photoexcited states of ammonium tetraphenylborate, which are characterized by self-sensitized luminescence. It has been established that the excitation by UV light at 77 K leads to the formation of stable triplet states due to the capture of electrons on electron traps. The EPR and luminescence excitation spectra exhibit the formation of a set of triplet states with different distances between electrons and holes. The performed investigations give grounds to affirm that, in bulk samples, cations in the structure of ammonium tetraphenylborate are electron traps. When the size of the ammonium tetraphenylborate sample is changed to 6 and 3 nm, the capture of excited electrons on sorbed oxygen molecules becomes dominant. In this case, the appearance of the spectrum of O_2^- anion radicals has been detected by the EPR method. The proposed interpretation of the observed effects has been confirmed by the thermoluminescence data on the recombination of electron-hole pairs, which correlate with a change in the intensity of the EPR spectra during annealing.

Polymerization Catalysts and Polymer Materials

KINETICS OF ETHYLENE POLYMERIZATION IN THE PRESENCE OF A HOMOGENEOUS CATALYST BASED ON A *bis*(PHENOXYIMINE) COMPLEX OF ZIRCONIUM(IV)

**A.A. Barabanov, N.V. Semikolenova,
M.A. Matsko, L.G. Echevskaya, V.A. Zakharov**

Kinet. Catal.,
52(2) (2011) pp. 217-221.

Changes in the molecular-weight characteristics of the product of ethylene polymerization in the course of reaction in the presence of a homogeneous catalytic system and in the number and reactivity of catalyst active sites were studied. The catalytic system consisted of *bis*[*N*-(3-*tert*-butylsalicylidene)anilinato] zirconium dichloride and methylalumoxane as an activator. This catalytic system exhibited the signs of unsteady-state conditions: the rate of polymerization dramatically decreased as the reaction time increased. At the onset of polymerization (to 5 min), the catalyst was single-site, and it produced low-molecular-weight polyethylene with M_w = (4–10) × 10^3 g/mol. The fraction of active sites at the initial point in time was as high as 11% based on the initial amount of the zirconium complex. The reactivity of these centers was very high (the rate constant of polymer chain growth was 5.4×10^4 l mol^{-1} s^{-1} at 35°C). As the polymerization time increased, the number of active sites decreased and the molecular-weight distribution of polyethylene broadened because of the decay of a portion of initial centers and the formation of new centers that produced high-molecular-weight polyethylene with M_w to 130 × 10^4 g/mol. The propagation rate constant measured at a sufficiently long polymerization time (20 min) was lower than that at the initial point in time; this fact suggests the much lower reactivity of the new active sites.

INFLUENCE OF TRIISOBUTYLALUMINUM ON THE POLYMERIZATION OF ETHYLENE BY SiO_2-SUPPORTED ANSA-ZIRCONOCENE CATALYSTS

V.N. Panchenko, L.G. Echevskaya, V.A. Zakharov, M.A. Matsko

Appl. Catal., A.,
404(1-2) (2011) pp. 47-53.

Catalysts for the polymerization of ethylene, which contain *rac*-$Me_2Si(Ind)_2ZrCl_2$ ($SBIZrCl_2$) bound to methylalumoxane-pretreated SiO_2 supports ($SiO_2/MAO/SBIZrCl_2$), were studied with respect to leaching of zirconocene and MAO into heptane solutions caused by triisobutylaluminum (TIBA). The latter is found to solubilize surface-bound MAO and zirconocene components, such that the Al content in the solid catalysts is reduced by 15–40 wt% and their Zr content by 50–60 wt%. Consequently, ethylene polymerization with such TIBA-containing catalyst systems occurs both on the surface of the solid catalyst and in the solution phase. Polymerization in solution is favored by high MAO contents in the SiO_2 carrier. Polymerization in solution leads to polyethylene (PE) products with lower molecular masses than polymerization on the support surface; this is the main cause of formation of PE with bimodal molecular mass distribution when ethylene is polymerized with $SiO_2/MAO/SBIZrCl_2$ catalysts co-activated by TIBA. It is proposed that the co-activator TIBA interacts with surface-bound MAO to modify MAO in such a manner that it becomes soluble in aliphatic hydrocarbons and capable of solubilizing some active zirconocene component.

ETHYLENE POLYMERIZATION OVER SUPPORTED TITANIUM-MAGNESIUM CATALYSTS: EFFECT OF POLYMERIZATION PARAMETERS ON THE MOLECULAR WEIGHT DISTRIBUTION OF POLYETHYLENE

**M.I. Nikolaeva, T.B. Mikenas, M.A. Matsko,
L.G. Echevskaya, V.A. Zakharov**

J. Appl. Polym. Sci.,
122(5) (2011) pp. 3092-3101.

The data on the effects of polymerization duration, cocatalyst, and monomer concentrations upon ethylene polymerization in the absence of hydrogen, and the effect of an additional chain transfer agent (hydrogen) on the molecular weight (MW), molecular weight distribution (MWD), and content of vinyl terminal groups for polyethylene (PE) produced over the supported titanium-magnesium catalyst (TMC) are obtained. The effects of these parameters on nonuniformity of active sites for different chain transfer reactions are analyzed by deconvolution of the experimental MWD curves into Flory components. It has been shown that the polymer MW grows, the MWD becomes narrower and the content of vinyl terminal groups in PE increases with increasing polymerization duration. It is assumed to occur due to the reduction of the rate of chain transfer with $AlEt_3$ with increasing polymerization duration. The polydispersity of PE is found to rise with increasing $AlEt_3$ concentration and decreasing monomer concentration due to the emergence of additional low molecular weight Flory components. The ratios of the individual rate constants of chain transfer with $AlEt_3$, monomer and hydrogen to the propagation rate constant have been calculated.

SUPPORTED ZIEGLER TYPE CATALYSTS FOR PRODUCTION OF POLYETHYLENE (PE): EFFECT OF THE COMPOSITION OF THE ACTIVE COMPONENT, THE METHODS OF ITS FORMATION, AND THE USE OF MODIFYING AGENTS ON CATALYTIC ACTIVITY AND MOLECULAR STRUCTURE OF PE AND COPOLYMERS OF ETHYLENE WITH α-OLEFINS

T.B. Mikenas, V.A. Zakharov, V.E. Nikitin, L.G. Echevskaya, M.A. Matsko

Catal. Ind.,
3(2) (2011) pp. 122-127.

Summarized results are presented on studying the formation of the active component of supported Ziegler type catalysts, investigation the effect of the composition of these catalysts on the molecular mass characteristics of PE, and seeking new methods for producing catalysts with optimum morphology.

ANALYSIS OF THE MOLECULAR STRUCTURE OF ETHYLENE HEXENE-1 COPOLYMERS PRODUCED OVER HIGHLY ACTIVE SUPPORTED ZIEGLER–NATTA CATALYSTS

M.A. Matsko, L.G. Echevskaya, T.B. Mikenas, M.I. Nikolaeva, M.P. Vanina, V.A. Zakharov

Catal. Ind.,
3(2) (2011) pp. 109-115.

The mechanical and rheological properties of ethylene α-olefin copolymers are governed by a molecular and supramolecular structure that depends on its molecular weight characteristics, comonomer concentration, and the uniformity of branching distributions for polymer chains with different molecular weights (compositional heterogeneity). Using state-of-the-art methods, the authors studied the parameters of molecular weight distribution, molecular structure, and compositional heterogeneity of ethylene hexane-1 copolymers with different compositions, produced over highly active supported Ti–Mg and V–Mg Ziegler–Natta catalysts, and showed the possibility of controlling these parameters to improve the quality of the resulting polymers.

STUDY OF THE COMPOSITIONAL HETEROGENEITY OF ETHYLENE-1-HEXENE COPOLYMERS VIA THERMAL FRACTIONATION WITH THE USE OF DIFFERENTIAL SCANNING CALORIMETRY

M.A. Matsko, M.P. Vanina, L.G. Echevskaya, V.A. Zakharov

Polym. Sci., ser. A,
53(4) (2011) pp. 296-302.

The compositional heterogeneity of ethylene–1-hexene copolymers synthesized with various types of supported catalysts, namely, the titanium–magnesium catalyst $TiCl_4/MgCl_2$ and the zirconocene catalyst $SiO_2(MAO)/Me_2Si(Ind)_2ZrCl_2$, is studied via the method of successive self-nucleation–annealing (SSA) with the use of differential scanning calorimetry. On the basis of the data on the temperatures of individual peaks on SSA curves, the thickness of lamellas composed of macromolecules with a certain degree of short-chain branching is estimated. The copolymer synthesized with the zirconocene catalyst has a narrower range of fusion and does not contain large lamellas composed of molecules with a low degree of short-chain branching. With the use of the broadness index, it is shown that the copolymer synthesized with the zirconocene catalyst has a more uniform distribution of the comonomer than does the copolymer synthesized with the titanium–magnesium catalyst. For the copolymers synthesized with the titanium–magnesium catalyst, the compositional heterogeneity increases with an increase in the content of 1-hexene.

STATE OF TITANIUM IN SUPPORTED TITANIUM-MAGNESIUM CATALYSTS FOR PROPYLENE POLYMERIZATION

N.N. Chumachenko, G.D. Bukatov, S.A. Sergeev, V.A. Zakharov

Kinet. Catal.,
52(2) (2011) pp. 234-241.

The oxidation state of titanium and the coordination state of Ti^{3+} ions in $TiCl_4/D_1/MgCl_2$ (D_1 is a phthalate) supported titanium-magnesium catalysts (TMCs) after the interaction with an

$AlEt_3/D_2$ cocatalyst (D_2 is propyltrimethoxysilane or dicyclopentyldimethoxysilane) were studied by chemical analysis and EPR spectroscopy. Different oxidation state distributions of titanium ions were observed in the activated catalyst and mother liquor: Ti^{3+} and Ti^{2+} ions were predominant in the activated catalyst and mother liquor, respectively. The effects of interaction conditions (reaction temperature and time and Al/Ti and D_2/Ti molar ratios) of TMCs with the cocatalyst on the state of titanium in activated samples were studied. The interaction of TMCs with the cocatalyst decreased the titanium content and caused the appearance of aluminum in the activated sample, which was most clearly pronounced at a temperature of 25°C and occurred within the first 10 min of treatment. An increase in the temperature to 70°C and an increase in the interaction time to 60 min only slightly affected the concentrations of titanium and aluminum. The presence of D_2 as a cocatalyst constituent facilitated the removal of titanium compounds and restricted the adsorption of aluminum compounds on the catalyst surface. The main fraction of titanium consisted of Ti^{3+} ions (62–89%), and the rest was Ti^{4+} ions (22–35%) under mild interaction conditions (25°C; Si/Ti = 25) or Ti^{4+} (0–21%) and Ti^{2+} (9–21%) ions under more severe conditions (50 or 70°C; Si/Ti from 0 to 5). According to EPR-spectroscopic data, at D_2/Ti from 1 to 5, Ti^{3+} ions mainly occurred as associates, whereas they occurred as isolated ions at D_2/Ti = 25. The initial and activated catalysts were similar in activity in the reaction of propylene polymerization, and titanium compounds, which were removed from the catalyst upon interaction with $AlEt_3/D_2$, were inactive in this process.

TITANIUM–MAGNESIUM CATALYSTS FOR PROPYLENE POLYMERIZATION: THE EFFECT OF DONORS

G.D. Bukatov, S.A. Sergeev, V.A. Zakharov, L.G. Echevskaya, M.A. Matsko

Catal. Ind.,
3(2) (2011) pp. 103-108.

The chain transfer reaction with hydrogen at propylene polymerization over Ti–Mg catalysts (TMCs) of composition $TiCl_4/D_1/MgCl_2–AlEt_3/D_2$ is studied in a wide hydrogen concentration range. A two-step mechanism of this reaction is suggested. This mechanism accounts for the fractional order of the reaction with respect to hydrogen concentration. Constants of chain transfer reaction with hydrogen are determined for TMC with different donors: 1,3-diether or dibutyl phthalate as D_1 and tetraethoxysilane or dicyclopentyldimethoxysilane as D_2. In propylene polymerization over the TMCs, the length of the polymer chain is mainly determined by the ratio of the propylene and hydrogen concentrations because the propagation and chain transfer rate constants are comparable. The rate constant of chain transfer with hydrogen at ethylene polymerization is significantly (more than one order of magnitude) less, and higher hydrogen concentrations are required for attaining the same degree of polymerization. The results of this study might be helpful in simulation of industrial polymerization processes and in control of the polymer molar mass.

COPOLYMERIZATION OF TETRAFLUOROETHYLENE WITH PERFLUORO(3,6-DIOXA-4-METHYL-7-OCTENE)SULFONYL FLUORIDE IN A WATER-EMULSION MEDIUM

S.S. Ivanchev, V.S. Likhomanov, O.N. Primachenko, S.Ya. Khaikin, V.G. Barabanov*, A.Yu. Men'shikova, N.N. Shevchenko**** (**Applied Chemistry Russian Scientific Center, St. Petersburg, Russia; **Institute of Macromolecular Compounds, St. Petersburg, Russia*)

Doklady Chem.,
437(1) (2011) pp. 66-68.

In the present work, based on the data on the kinetics of copolymerization of TFE and the sulfo-containing fluorinated monomer FS-141, it was demonstrated for the first time the possibility of realization of safe and efficient water-emulsion technology for producing a Nafion-type copolymer with satisfactory proton-conducting operational properties.

POLYMER HYDROGELS WITH THE MEMORY EFFECT FOR IMMOBILIZATION OF DRUGS

V.N. Pavlyuchenko*, S.S. Ivanchev, O.N. Primachenko, S.Ya. Khaikin, V.F. Danilichev*, V.S. Proshina*, V.A. Trunov, V.T. Lebedev**, Yu.V. Kul'velis**** (**Kirov Academy of Military Medicine, St. Petersburg, Russia; **Petersburg Nuclear Physics Institute, Gatchina, Leningrad oblast, Russia*)

Polym. Sci., ser. A,
53(4) (2011) pp. 323-335.

Hydrogels with the memory effect are synthesized from crosslinked copolymers of 2-hydroxyethyl methacrylate and functional monomers (acrylic acid or dimethylaminoethyl methacrylate) via the method of template synthesis with the use of the drug cephazoline as a matrix. It is shown that the hydrogels show an increased sorption activity against the target drug and a slow rate of drug release from the hydrogel (the memory effect) under certain conditions. In combination with cephazoline, these hydrogels may be regarded as a new prolonged-drug-release system for the treatment of infectious diseases.

SMALL-ANGLE NEUTRON SCATTERING FROM POLYMER HYDROGELS WITH MEMORY EFFECT FOR MEDICINE IMMOBILIZATION

Yu.V. Kulvelis*, V.T. Lebedev*, V.A. Trunov*, V.N. Pavlyuchenko, S.S. Ivanchev, O.N. Primachenko, S.Ya. Khaikin** (**Konstantinov Nuclear Physics Institute, Gatchina, Leningrad oblast, Russia;* ***Kirov Military Medical Academy, St. Petersburg, Russia*)

Cryst. Rep.,
56(7) (2011) pp. 1114-1117.

Hydrogels synthesized based on cross-linked copolymers of 2-hydroxyethyl methacrylate and functional monomers (acrylic acid or dimethylaminoethyl methacrylate), having a memory effect with respect to target medicine (cefazolin), have been investigated by small-angle neutron scattering. The hydrogels are found to have a two-level structural organization: large (up to 100 nm) aggregates filled with network cells (4–7 nm in size). The structural differences in the anionic, cationic, and amphiphilic hydrogels and the relationship between their structure and the ability of hydrogels to absorb moisture are shown. A relationship between the memory effect during cefazolin immobilization and the internal structure of hydrogels, depending on their composition and type of functional groups, is established.

BIOLIGAND CARRIERS BASED ON METHYL METHACRYLATE COPOLYMERS WITH *N*-VINYLFORMAMIDE OR GLYCIDYL METHACRYLATE

A.Yu. Men'shikova*, K.S. Inkin*, T.G. Evseeva*, Yu.O. Skurkis*, B.M. Shabsel's*, N.N. Shevchenko*, S.S. Ivanchev (**Institute of Macromolecular Compounds, St. Petersburg, Russia*)

Colloid J.,
73(1) (2011) pp. 76-82.

Emulsifier-free emulsion copolymerization of methyl methacrylate with N-vinylformamide and glycidyl methacrylate initiated by a cationic or anionic azoinitiator in the presence of dextran is used to produce monodisperse polymer particles with a developed multifunctional surface. As a result, monodisperse particles are obtained with a diameter of 350–660 nm, the surface layer of which contains, in addition to carboxyl groups, amino or epoxy groups. The conditions are determined for the formation of multifunctional hydrophilic particle surface via the hydrolysis of comonomer units and residual groups of initiators. The limiting values of bovine serum albumin chemisorption (2.4 and 1.0 mg/m^2 on the particles of methyl methacrylate copolymers with glycidyl methacrylate or N-vinyl formamide, respectively) indicate that the obtained particles have sufficient sorption capacity to be applied as carriers for immunoreagents.

POLYMER MEMBRANES FOR FUEL CELLS: ACHIEVEMENTS AND PROBLEMS

S.S. Ivanchev, S.V. Myakin

Carbon Nanomaterials in Clean Energy Hydrogen Systems – II, NATO Science for Peace and Security Series C: Environmental Security, Springer,
Eds. S.Yu. Zaginaichenko, D.V. Schur,
V.V. Skorokhod, A. Veziroglu, B. Ibrahimoglu,
2011, V. 2, ch. 21, pp. 245-267.

The current state in the field of synthesis, structural modification and implementation of polymer membranes for fuel cells is analyzed. Synthetic methods, physicochemical characteristics and specific features of their composition, microphase separation and the structure of water ionic channels are considered for different types of proton-conducting materials together with the approaches to enhancement of their technical performances. The main focus is addressed to Nafion and other similar perfluorinated proton conducting polymer membranes as currently leading materials in respect of both R&D progress and commercial implementation in fuel cells of different purpose. The recent advances in submarine and automotive applications of Nafion based fuel cells are discussed.

SPECIFIC FEATURES OF ETHYLENE POLYMERIZATION ON SELF-IMMOBILIZING CATALYTIC SYSTEMS BASED ON TITANIUM *bis*(PHENOXY IMINE) COMPLEXES

N.I. Ivancheva, V.K. Badaev, E.V. Sviridova, D.A. Nikolaev, I.V. Oleinik*, S.S. Ivanchev
(** Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia*)

Russ. J. Appl. Chem.,
84(1) (2011) pp. 118-123.

The kinetics of ethylene polymerization on six methylalumoxane-activated self-immobilizing *bis*(phenoxy imine) complexes of titanium chloride with allyloxy groups in the *m*- and *p*-positions of the N-phenyl ring and with various substituents in the salicylaldehyde fragment was studied. The activity of the complexes in the temperature range 20–60°C and ethylene pressure of 0.4 MPa was evaluated.

EFFECT OF THE BASIC PROCESS PARAMETERS DURING POLYMERIZATION OF TETRAHYDROFURAN WITH PERCHLORIC ACID

A.E. Bal'tser*, V.M. Komarov*, A.G. Bazanov, N.G. Zubritskaya*, N.N. Machalaba** (**Applied Chemistry Russian Center, St. Petersburg, Russia; **Scientific-Research Institute of Synthetic Fibres, Tver, Russia*)

Fiber Chem.,
42(4) (2011) pp. 215-219.

Polymerization of tetrahydrofuran in the presence of the perchloric acid — acetic anhydride catalytic system evolves reversibly in time and is subjected to the strong effect of the temperature, where the yield and molecular weight of the oligomer decrease when the temperature increases. The molecular weight of the oligomer can be regulated by changing the amount of catalyst. It is most sensitive to a change in the amount of perchloric acid, which must be measured very precisely, while finer regulation can be performed by varying the amount of acetic anhydride.

THE INFLUENCE OF ADDITION OF LOW-MOLECULAR RUBBER ON PROPERTIES OF MIXTURES AND RUBBERS. II. MODIFICATION OF COMPOSITIONS BASED ON BUTADIENE-NITRILE RUBBER

D.V. Voronchikhin*, K.A. Dubkov, S.V. Semikolenov, D.P. Ivanov, I.A. Ilyin*
(**Siberian State Technological University, Novosibirsk, Russia*)

Kauchuk & Rezina,
1 (2011) pp. 4-7.

The effect of modifying butadiene-nitrile rubber based polymer compositions with two oligobutadienes and a functional oligomer of new type – unsaturated polyketone (Mn=2200, 17.3 wt% of C=O groups) – on properties of the said composition was studied. The addition of polyketone was shown to improve technological behavior of the rubber mixture and characteristics of the vulcanizate.

ELASTOMER COMPOSITES CONTAINING PRODUCTS OF RUBBER RECLAIMING USING NITROGEN(I) OXIDE

D.V. Voronchikhin*, K.A. Dubkov, I.A. Ilyin*, M.A. Khudoley*, S.V. Semikolenov, D.P. Ivanov
(**Siberian State Technological University, Novosibirsk, Russia*)

Kauchuk & Rezina,
5 (2011) pp. 33-35.

The influence of a regenerate obtained through treatment of rubber crumb with nitrogen suboxide on the properties of elastomer compositions was studied. The application of such a regenerate was shown to improve some parameters of rubber mixtures and vulcanizates.

IMMOBILIZATION OF A RECOMBINANT STRAIN PRODUCING GLUCOSE ISOMERASE INSIDE SiO_2-XEROGEL AND PROPERTIES OF PREPARED BIOCATALYSTS

G.A. Kovalenko, L.V. Perminova, T.V. Chuenko, L.I. Sapunova*, E.A. Shlyakhotko*, A.G. Lobanok* (**Institute of Microbiology, Minsk, Belarus*)

Appl. Biochem. Microbiol.,
47(2) (2011) pp. 151-157.

An original method of immobilization of non-growing microorganism cells inside xerogel of silicium dioxide containing insoluble hydroxyl compounds of cobalt(II) has been developed. A recombinant strain producing glucose isomerase has been constructed on the basis of *Escherichia coli* with the use of a gene of *Arthrobacter nicotianae*. It was revealed that glucose isomerase activity and stability of biocatalysts prepared on the basis of the recombinant *E. coli* strain was 3–5 times greater compared with the biocatalysts prepared with the use of the donor strain *A. nicotianae*. Under conditions of continuous hydrolysis of 3 M fructose at 62–65°C in a fixed bed reactor, time of half-inactivation of the biocatalysts prepared from the recombinant strain and *A. nicotianae* was ～60 and ～25 days, respectively.

Fe-EXCHANGED ZEOLITES AS MATERIALS FOR CATALYTIC WET PEROXIDE OXIDATION. DEGRADATION OF *RODAMINE G* DYE

R. Prihod'ko*, I. Stolyarova*, G. Gündüz, O.P. Taran, S.A. Yashnik, V.N. Parmon**, V. Goncharuk* (**Institute of Colloid and Water Chemistry, Kiev, Ukraine; **Ege University, Chemical Engineering Department, Izmir, Turkey*)

Appl. Catal., B,
104(1-2) (2011) pp. 201-210.

The effect of surface acidity, nature, and dispersion of iron species, controlled by the catalyst preparation techniques and parent zeolite Si/Al ratio, on the catalytic wet peroxide oxidation of *Rodamine G* dye over the Fe-ZSM-5 materials has been studied.

Fe-ZSM-5 and Fe-USY have been prepared using two techniques: improved aqueous ion exchange (IE) and conventional aqueous ion exchange (CE). The former procedure causes some rearrangement of the coordination sphere of four-fold coordinated Al^{3+}, accompanied by formation of a small amount of octahedrally coordinated non-framework aluminium species. In case of Fe-ZSM-5(IE), iron is predominantly present in the form of well-dispersed Fe^{2+} ions, while Fe-ZSM-5(CE) and Fe-USY(CE) contain small aggregated oligonuclear $(FeO)_n$ clusters formed by Fe^{3+}. In both cases, iron species are mainly located inside the zeolite pore system. The contribution of the zeolite is a controlling factor in enhancing the *Rhodamine G* dye degradation activity of the Fe-ZSM-5 catalysts, which is influenced by the specific procedure used for preparation of these materials.

The catalytic wet peroxide oxidation (CWPO) behaviours of the materials prepared *via* the (IE) and (CE) procedures differ due to different nature of the iron species involved. The non-framework Al^{3+} species present in both the Fe-exchanged ZSM-5 and USY zeolites may participate in formation of the active sites responsible for CWPO of *Rhodamine G* dye over these catalysts.

At near ambient temperature (323 K), quasi-neutral pH (4.9), short reaction time (around 150 min), catalyst concentration of $1.0\ g\ L^{-1}$, and H_2O_2 addition rate of $41.2–82.3\ mmol\ h^{-1}$, the (IE)-prepared Fe-ZSM-5 catalyst enables the total degradation of the dye, accompanied by removal of *ca.* 80% of TOC without notable leaching of the Fe ions.

GUAIACOL HYDRODEOXYGENATION IN THE PRESENCE OF Ni-CONTAINING CATALYSTS

M.V. Bykova, O.A. Bulavchenko, D.Yu. Ermakov, M.Yu. Lebedev, V.A. Yakovlev, V.N. Parmon

Catal. Ind.,
3(1) (2011) pp. 15-22.

A series of Ni-containing catalysts supported on different materials has been tested in the hydrodeoxygenation of guaiacol, a compound modeling the products of biomass fast pyrolysis. The reaction has been carried out in an autoclave at 320°C and a hydrogen pressure of 17 MPa. The main guaiacol hydrodeoxygenation products are cyclohexane, 1-methylcyclohexane-1,2-diol, and cyclohexanone (which result from aromatic ring reduction). A guaiacol conversion scheme explaining the formation of the main products is suggested. The highest activity is shown by the Ni-containing catalysts on SiO_2 and SiO_2–ZrO_2 supports prepared by the sol–gel method. According to X-ray diffraction and electron microscopic data, the high activity of these catalysts is due to the high concentration of dispersed nickel as reduced films on the surface of the silicate structures. The catalysts offer promise for refining the biomass fast pyrolysis products (bio-oil) into hydrocarbon fuel.

INVESTIGATION OF DIRECT HYDROCRACKING OF TRIGLYCERIDES OF FATTY ACIDS ON Ni-Cu/CeO_2-ZrO_2 CATALYST

S.A. Selishcheva, D.E. Babushkin, V.A. Yakovlev

Chem. Sustain. Devel.,
19(2) (2011) pp. 187-193.

Catalytic hydrocracking of triglycerides of fatty acids of colza oil resulting in the formation of a mixture of C_{12}-C_{19} alkanes was studied under mild conditions (0.5 MPa H_2, 300-380°C) over Ni-Cu/CeO_2-ZrO_2 catalyst. On the basis of the obtained distributions of hydrocracking products for different contact times and temperatures, a scheme of the stage-by-stage hydrocracking of triglycerides of fatty acids was proposed. It takes into account the formation of intermediate oxygenated products (fatty acids, esters, alcohols, wax).

THE MECHANISM OF INTERACTING BIOLOGICALLY ACTIVE COMPLEXES DEHYDROEPIANDROSTERONE OR TETRAHYDROCORTISOL - APOLIPOPROTEIN A-I WITH DNA AND THEIR ROLE IN ENHANCEMENT OF GENE EXPRESSION AND PROTEIN BIOSYNTHESIS IN HEPATOCYTES

L. Panin*, O. Gimautdinova*, P.A. Kuznetsov*, F.V. Tuzikov (**Research Institute of Biochemistry, Novosibirsk, Russia*)

Curr. Chem. Biol.,
5(5) (2011) pp. 9-16.

Dehydroepiandrosterone (DHEA), dehydroepiandrosterone-sulfate (DHEAS) and tetrahydrocortisol (THC) with apolipoprotein A-I form the biologically active complexes able to interact specifically with eukaryotic DNA. This conjugate is highly cooperative and results in local splitting of DNA. Specific binding sites of steroid-apoA-I complexes are the (GCC/GGC)n sequences. At the sites of splitting, single-stranded regions sensitized to the action of S1-nuclease form. These regions are irregularly distributed over DNA. The formation of single-stranded DNA regions can promote the interaction with RNA-polymerase. Formation of the biologically active THC (DHEA)-apoA-I complexes is related with resident macrophages having 5 α- and 5 β-reductase activity. These complexes greatly enhance the rate of protein biosynthesis in hepatocytes. The cortisol-apoA-I complex does not show such effect. So, the reduced forms of fascicular zone and reticular cortex adrenal zone hormones have synergism of action toward gene expression and protein biosynthesis. The intensification of tissues regeneration during the stress period as a result of given mechanism is discussed.

ECOLOGICAL AND MORPHOLOGICAL FEATURES OF NANO- AND MICROPARTICLES OF MINERALS OF ORAL ROUTES

K.S. Golokhvast*, N.N. Kiselev*, V.V. Chaika*, A.M. Panichev, P.A. Nikiforov*, A.A. Vedyagin, I.V. Mishakov, I.E. Pamirskii***, A.N. Gulkov*** (**Far East State Technical University, Vladivostok, Russia; **Pacific Institute of Geography, Vladivostok, Russia; ***Institute of Geology and Natural Manegement, Blagoveshchensk, Russia*)

Proceed. Samara Sci. Center RAS,
13(1(5)) (2011) pp. 1253-1255.

Results of studies of the effect of zeolites from Vanginsky, Lyulinsky, Kulikovsky and Kholinsky deposits on morphometric parameters of stomach and intestine cells of mouse Mus muscuus are represented. It is shown that Nanoparticles from all 5 fields of zeolites taken in the experiment, at a dosage of 3-5% of body weight and ranging from 100 nm to 1 micron are toxic.

ECOTOXICOLOGY OF NANO- AND MICROPARTICLES

K.S. Golokhvast*, A.M. Panichev, I.V. Mishakov, A.A. Vedyagin, M.S. Melgunov, M.M. Danilova, S.G. Kozlova***, S.P. Gabuda***, N.K. Moroz***, M.S. Melgunov, N.N. Kiselev*, V.V. Chaika*, A.N. Gulkov*** (**Far East State Technical University, Vladivostok, Russia; **Pacific Institute of Geography, Vladivostok, Russia; ***Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Proceed. Samara Sci. Center RAS,
13 (1(5)) (2011) pp. 1256-1259.

Approaches to studying inorganic water insoluble materials toxicity – nano- and microparticles of natural minerals are considered. Possible reasons and mechanism of various biological effects of the last are discussed.

CURRENT APPROACHES TO DEVELOPMENT OF CONTRAST AGENTS FOR MRI DIAGNOSTICS

K.N. Sorokina, A.A. Tulupov*, T.G. Tolstikova, V.Yu. Ussov***** (**International Tomography Center, Novosibirsk, Russia; **Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia; ***Tomsk Institute of Cardiology, Tomsk, Russia*)

Bull. Siberian Med.,
6 (2011) pp. 79-86.

Magnetic resonance imaging (MRI) is primarily used in medical imaging to visualize the structure and function of the body and essential tool for diagnostics of broad range of pathologies. But still in a growing number of cases there are indications to use contrast agent to delineate areas of interest and for more precise diagnosis definition. In a review the properties and clinical applications of most popular paramagnetic contrast agents based on Gd(III), Fe(II) и Mn(II) are discussed. It is also focused on discussion of modern experimental targeted contrast agents (conjugates of antibodies, nanoparticles and dendrimers) and advances of their application for early diagnostics of most common pathologies: cardiovascular, cancer and Alzheimer diseases.

PHYSICOCHEMICAL EXOMETABOLITE PROCESSING FOR CLOSED LIFE SUPPORT SYSTEMS

E.F. Sutormina, S.V. Trifonov*, Yu.A. Kudenko*, Yu.A. Ivanova, L.G. Pinaeva, A.A. Tikhomirov*, L.A. Isupova (**Institute of Biophysics, Krasnoyarsk, Russia*)

Chem. Sustain. Devel.,
19(4) (2011) pp. 413-420.

Composition of gas mixtures formed during the electrochemical (in the presence of H_2O_2) oxidation of the wastes of human vital activities and subsequent decomposition of carbamide remaining in solution after the oxidation of metabolites was studied. The principal possibility of catalytic selective oxidation of ammonia evolved in the decomposition of carbamide to form nitrogen oxides was demonstrated, for the purpose of obtaining the salts of nitric acid that are well assimilated by plants.

Catalysis in Organic Synthesis

NEW METHOD OF DIMETHYL SULFIDE SYNTHESIS

A.V. Mashkina

Russ. J. Org. Chem.,
47(5) (2011) pp. 678-681.

The synthesis of dimethyl sulfide consists in the reaction of dimethyl disulfide with methanol in the presence of solid catalyst, aluminum γ-oxide. The yield of dimethyl sulfide grows with growing temperature, contact time, and content of methanol in the reaction mixture. At 350-400°C, molar ratio methanol-dimethyldisulfide 2.0-2.5, and total conversion of the reagents the yield of dimethyl sulfide reached 95 mol%.

A CATALYTIC PROCESS FOR PREPARATION OF THIOPHENE FROM FURAN AND HYDROGEN SULFIDE

A.V. Mashkina

Russ. J. Appl. Chem.,
84(7) (2011) pp. 1223-1228.

Thiophene formation under various conditions from furan and H_2S in the presence of γ-Al_2O_3, both unpromoted and promoted with transition metal oxides, was examined. The conditions enabling preparation of thiophene in a 95–98 mol% yield were determined.

INVESTIGATION OF THE MECHANISM OF CATALYTIC RECYCLIZATION OF FURAN TO THIOPHENE

A.V. Mashkina

Chem. Heterocycl. Compd.,
9 (2010) pp. 1063-1067.

Investigation of the formation of thiophene from furan and hydrogen sulfide at various catalysts showed that the activity of the catalysts increases with increase in the strength and concentration of Lewis acid centers. It was found by IR spectroscopy that if the degree of coverage of the aluminum oxide surface with hydrogen sulfide is higher than monolayer its dissociative chemisorption does not occur. Mechanism was postulated which assume that the reaction takes place through stage with the formation of a surface intermediate, including coordination of the α-carbon atoms of the furan ring with the Lewis acid center and with the sulfur atom of molecular hydrogen sulfide.

EPOXIDATION OF BUTADIENE WITH HYDROGEN PEROXIDE CATALYZED BY THE SALTS OF PHOSPHOTUNGSTATE ANIONS: RELATION BETWEEN CATALYTIC ACTIVITY AND COMPOSITION OF INTERMEDIATE PEROXO COMPLEXES

L.I. Kuznetsova, N.I. Kuznetsova, R.I. Maksimovskaya, G.I. Aleshina, O.S. Koscheeva*, V.A. Utkin (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*)

Catal. Lett.,
141(10) (2011) pp. 1442-1450.

Epoxidation of 1,3-butadiene has been studied in acetonitrile solutions of aqueous H_2O_2 and tetrabutylammonium or 1-ethyl-3-methylimidazolium salts of phosphotungstate anions: $[(n\text{-}C_4H_9)_4N]_3\{PO_4[WO(O_2)_2]_4\}$, $[(n\text{-}C_4H_9)_4N]_5Na_{0.6}H_{1.4}[PW_{11}O_{39}]$ or $[(C_2H_5)(CH_3)C_3H_3N_2]_5NaH[PW_{11}O_{39}]$.
The selectivity of the 1,3-butadiene to 3,4-epoxy-1-butene (EpB) conversion attains 97% at nearly 100% efficiency of the H_2O_2 consumption. The rate of the EpB formation has been correlated with the solution compositions as found by ^{31}P NMR under the reaction conditions.

Bis[3-(3,5-DIALKYL-4-HYDROXYPHENYL)PROPYL]MONO- AND DISULFIDES AS THE SEVILEN STABILIZERS

A.P. Krysin*, T.B. Khlebnikova (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia*)

Russ. J. Gen. Chem.,
81(6) (2011) pp. 1159-1162.

The effect of the shielding degree of the phenol hydroxy group on the hydrolytic and thermal stability of ethylene-vinyl acetate copolymer (Sevilen) was studied on a series of phenols containing one or two sulfur atoms in the aliphatic chain of the para-substituent. Among the synthesized compounds a group of disulfides was found with a high antioxidant efficiency, which increase the Sevilen hydrolytic stability. The most effective are the 6-tert-butyl-2-methylphenol derivatives.

NEW APPROACH TO THE SYNTHESIS OF *tris*(PERFLUOROALKYL)BORANE ADDUCTS WITH DIALKYLAMINES

N.Yu. Adonin, V.V. Bardin*, U. Florke, H.-J. Fron***** (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia; **Paderborn University, Germany; ***Duisburg-Essen University, Germany*)

Russ. J. Gen. Chem.,
81(3) (2011) pp. 509-516.

A convenient synthetic approach to the adducts $(C_nF_{2n+1})_3BNHR_2$ (n = 2–4, 6; R = Me, Et) was developed, based on the reaction of lithium perfluoroalkyls with dichloro(dialkylamino)boranes at temperatures below –90°C. The target products can be synthesized with preparative yields of 50–90%.

MECHANISTIC INSIGHTS INTO OXIDATION OF 2-METHYL-1-NAPHTHOL WITH DIOXYGEN: AUTOXIDATION OR A SPIN-FORBIDDEN REACTION?

O.A. Kholdeeva, I.D. Ivanchikova, O.V. Zalomaeva, A.B. Sorokin*, I.Y. Skobelev, E.P. Talsi (**Institut de Recherches sur la Catalyse, Villeurbanne Cedex, France*)

J. Phys. Chem. B,
115(42) (2011) pp. 11971–11983.

Oxidation of 2-methyl-1-naphthol (MNL) with molecular oxygen proceeds efficiently under mild reaction conditions (3 atm O_2, 60–80°C) in the absence of any catalyst or sensitizer and produces 2-methyl-1,4-naphthoquinone (MNQ, menadione, or vitamin K_3) with selectivity up to 80% in nonpolar solvents. ^1H NMR and $^1H,^1H$-COSY studies revealed the formation of 2-methyl-4-hydroperoxynaphthalene-1(*4*H)-one (HP) during the reaction course. Several mechanistic hypotheses, including conventional radical autoxidation, electron transfer mechanisms, photooxygenation, and thermal intersystem crossing (ISC), have been evaluated using spectroscopic, mass-spectrometric, spin-trapping, $^{18}O_2$ labeling, kinetic, and computational techniques. Several facts collectively implicate that ISC contributes significantly into MNL oxidation with O_2 at elevated pressure: (i) the reaction rate is unaffected by light; (ii) C–C-coupling dimers are practically absent; (iii) the reaction is first order in both MNL and O_2; (iv) the observed activation parameters ($\Delta H^{\ddagger}$ = 8.1 kcal mol^{-1} and $\Delta S^{\ddagger}$ = −50 eu) are similar to those found for the spin-forbidden oxidation of helianthrene with $^3O_2$ (Seip, M.; Brauer, H.-D.

*J. Am. Chem. Soc.***1992**, *114*, 4486); and (v) the external heavy atom effect (2-fold increase of the reaction rate in iodobenzene) points to spin inversion in the rate-limiting step.

SYNTHESIS OF A NEW OPTICALLY PURE CHIRAL DIAMINE FROM LEVOPIMARIC ACID

V.N. Konev, T.B. Khlebnikova, Z.P. Pai

Chem. Sustain. Devel.,
19(2) (2011) pp. 165-168.

Synthesis of a new chiral optically pure diamine of diterpene series was carried out on the basis of the components of available natural renewable raw material. The resulting tricyclic *trans*-1,2-diamine and its derivatives can be used as the ligands in metal complex catalysts of asymmetrical reactions.

MEERWEIN–PONNDORF–VERLEY REDUCTION OF ALDEHYDES FORMED *in situ* FROM α- AND β-PINENE EPOXIDES IN A SUPERCRITICAL FLUID IN THE PRESENCE OF ALUMINA

V. Il`ina*, S.Yu. Kurbakova*, K.P. Volcho*, N.F. Salakhutdinov*, V.I. Anikeev (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia*)

J. Saudi Chem. Soc.,
15(4) (2011) pp. 313-317.

The use of a system consisting of flow-type reactor, supercritical fluid containing isopropanol/CO_2 and alumina as a catalyst allows the one-pot isomerization of α- and β-pinene epoxides into campholenic aldehyde and myrtanal and Meerwein–Ponndorf–Verley reduction of these aldehydes to the corresponding alcohols.

REARRANGEMENTS OF VERBENOL EPOXIDE IN SUPERCRITICAL FLUIDS

K.P. Volcho*, I.V. Il`ina*, N.F. Salakhutdinov*, V.I. Anikeev (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk,* Russia)

ARKIVOC,
8 (2011) pp. 134-140.

Transformations of verbenol epoxide in a supercritical mixture of CO_2, isopropyl alcohol, and water were studied. The main identified products were similar to those obtained in the presence of Montmorillonite clays, but with much shorter contact times and without an acid catalyst. The reactivity of verbenol epoxide in supercritical media differs dramatically from the behavior of this epoxide in the presence of Lewis acid $ZnBr_2$. In contrast to studies of α-pinene epoxide transformations, the presence of water caused no essential changes in product distribution. The presence of triethylamine suppressed the rearrangements; obviously the reaction has cationic character.

STEP CHANGES AND DEACTIVATION BEHAVIOR IN THE CONTINUOUS DECARBOXYLATION OF STEARIC ACID

A.Th. Madsen*,, B. Rozmyszowicz**, I.L. Simakova, T. Kilpiö**, A.-R. Leino***, K. Kordás***, K. Eränen**, P. Mäki-Arvela**, D.Yu. Murzin**** (**Technical University of Denmark, Lyngby, Denmark; **Abo Akademi University, Turku, Finland; ***University of Oulu, Oulu, Finland*)

Ind. Eng. Chem. Res.,
50(19) (2011) pp. 11049–11058.

Deoxygenation of dilute and concentrated stearic acid over 2% Pd/C beads was performed in a continuous reactor at 300°C and 20 bar pressure of Ar or 5% H_2/Ar. Stable operation was obtained in 5% H_2 atmosphere, with 95% conversion of 10 mol % dilute stearic acid in dodecane and 12% conversion of pure stearic acid. Deactivation took place in H_2-deficient gas atmosphere, probably as a result of the formation of unsaturated products and coking in the pore system. Transient experiments with step changes were performed: 1 h was required for the step change to be visible in liquid sampling, whereas steady states were achieved after a total of 2.5–3 h. Postreaction analysis of the spent catalyst revealed that a deactivation profile was formed downward over the catalyst bed.

THE CHEMISTRY OF 2,3-DIHYDROISOXAZOLE DERIVATIVES

N.V. Chukanov, V.A. Reznikov* (**Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia*)

Russ. Chem. Bull.,
60(3) (2011) pp. 379-399.

Methods for the synthesis and transformations of 2,3-dihydroisoxazole derivatives are reviewed. Data on reduction and oxidation reactions and intramolecular rearrangements are generalized; their mechanisms are discussed.

Mathematical Simulation, Calculating Models

EVALUATION OF GOLD ON ALUMINA CATALYST DEACTIVATION DYNAMICS DURING α-PINENE ISOMERIZATION

Yu.S. Solkina, S.I. Reshetnikov, M. Estrada*, A.V. Simakov, D.Yu. Murzin***, I.L. Simakova** (**Posgrado de Fisica de Materiales de CICESE-UNAM, Ensenada, B.C., Mexico; **Universidad Nacional Autonoma de Mexico, Ensenada, B.C., Mexico; ***Abo Akademi University, PCC, Turku/Abo, Finland*)

Chem. Eng. J.,
176-177 (2011) pp. 42-48.

Synthesis of camphene is an important step in an industrial process for camphor production from α-pinene. Compared to conventional way of α-pinene to camphene transformation over acid-hydrated TiO_2, gold on alumina catalyst was found to provide α-pinene isomerization conversion up to 99.9% and selectivity 60–80% making this catalyst very promising from an industrial viewpoint. However, deactivation of gold catalyst might be a serious obstacle for real industrial implementation. According to TPO and UV–vis-mass *in situ* it was shown that deactivation is caused by adsorption of hydrocarbons on the gold species. The dynamics of catalyst deactivation during α-pinene isomerization was presented based on a so-called "separable" deactivation model assumption. Effects of isomerization temperature, initial α-pinene concentration and gas atmosphere on catalyst deactivation with time-on-stream were investigated experimentally and correlated with the proposed deactivation function. The results showed that the α-pinene concentration was the major factor governing the deactivation of $Au/\gamma\text{-}Al_2O_3$ catalyst under substrate-feeding conditions. When the α-pinene concentration was controlled at a relatively low level such as 0.4 vol.%, especially in hydrogen atmosphere, the total deactivation rate was negligible. An equation of the reaction rate taking into account the catalyst deactivation was suggested making prediction of deactivation behavior in α-pinene conversion at different initial concentrations.

INFLUENCE OF CLUSTER SIZE DISTRIBUTION ON CLUSTER SIZE DEPENDENT CATALYTIC KINETICS

D.Yu. Murzin*, I.L. Simakova (**Åbo Akademi University, Turku, Finland*)

Catal. Lett.,
141(7) (2011) pp. 982-986.

A theoretical analysis of the influence of particle size distribution on observed TOF dependence on cluster size is presented for a two step catalytic cycle. Such mechanism can display different TOF behavior including maxima. In the later case simulations demonstrated broadening of TOF curves compared to an idealized case of very narrow PSD. However, for more often observed cases with smooth TOF increase or decrease with cluster size increase incorporation of particle size distribution in kinetic analysis is not required at least for often experimentally observed particle size distributions.

THERMODYNAMIC ANALYSIS OF THE CLUSTER SIZE EVOLUTION IN CATALYST PREPARATION BY DEPOSITION–PRECIPITATION

D.Yu. Murzin*, O.A. Simakova, I.L. Simakova, V.N. Parmon (**Åbo Akademi University, Turku, Finland*)

React. Kinet. Mech. Catal.,
104(2) (2011) pp. 259-266.

Several gold catalysts supported on various inorganic supports with different point zero charge (*pzc*) were prepared by deposition–precipitation with urea (DPU). A thermodynamic model accounting for cluster evolution was advanced. The key element in the model is the dependence of the interfacial energy on the relative approach to *pzc* during DP. Experimental data were compared with the model, showing a possibility to utilize the theoretical approach to predict the cluster size.

MODELING AND CALCULATION OF THE PROCESS OF RAPID EXPANSION OF SUPERCRITICAL FLUID YIELDING NANOPARTICLES

V.I. Anikeev, D.A. Stepanov, An. Yermakova

Theor. Found. Chem. Eng.,
45(2) (2011) pp. 141-155.

A mathematical model is proposed and the calculation is carried out for the process of rapid expansion of the supercritical fluid containing a dissolved solid compound via a capillary into a volume with specified temperature and pressure. The analysis of sensitivity of the model toward the process parameters makes it possible to choose the most important parameters for producing nanoparticles with preset properties and dimensions. The calculations demonstrate that all the parameters of the expansion process under study have a particular effect on the size of the particles being formed.

PHASE AND CHEMICAL EQUILIBRIA IN THE TRANSESTERIFICATION REACTION OF VEGETABLE OILS WITH SUPERCRITICAL LOWER ALCOHOLS

V.I. Anikeev, D.A. Stepanov, An. Yermakova

Russ. J. Phys. Chem. A,
85(8) (2011) pp. 1336-1346.

Calculations of thermodynamic data are performed for fatty acid triglycerides, free fatty acids, and fatty acid methyl esters, participants of the transesterification reaction of vegetable oils that occurs in methanol. Using the obtained thermodynamic parameters, the phase diagrams for the reaction mixture are constructed, and the chemical equilibria of the esterification reaction of free fatty acids and the transesterification reaction of fatty acid triglycerides attained upon treatment with supercritical methanol are determined. Relying on the analysis of the obtained equilibria for the esterification reaction of fatty acids and the transesterification reaction of triglycerides attained upon treatment with lower alcohols, the authors select the optimum conditions for performing the reaction in practice.

CALCULATING THE THERMODYNAMIC CHARACTERISTICS OF THE STEPWISE TRANSESTERIFICATION OF SIMPLE TRIGLYCERIDES

V.I. Anikeev, D.A. Stepanov, An. Yermakova

Russ. J. Phys. Chem. A,
85(12) (2011) pp. 2082-2087.

Thermodynamic data for mono- and diglycerides of palmitic, oleic, and linoleic fatty acids participating in the stepwise transesterification reaction of the corresponding simple triglycerides in methanol are calculated. The obtained thermodynamic parameters allow to calculate the chemical equilibrium and the equilibrium composition of the products of the stepwise transesterification reaction of fatty acid triglycerides with supercritical methanol.

CALCULATIONS OF PHASE EQUILIBRIA FOR MIXTURES OF TRIGLYCERIDES, FATTY ACIDS, AND THEIR ESTERS IN LOWER ALCOHOLS

D.A. Stepanov, An. Yermakova, V.I. Anikeev

Russ. J. Phys. Chem. A,
85(1) (2011) pp. 21-25.

The objects of study were mixtures containing triglycerides and lower alcohols and also the products of the transesterification of triglycerides, glycerol and fatty acid esters. The Redlich-Kwong-Soave equation of state was used as a thermodynamic model for the phase state of the selected mixtures over wide temperature, pressure, and composition ranges. Group methods were applied to determine the critical parameters of pure substances and their acentric factors. The parameters obtained were used to calculate the phase diagrams and critical parameters of mixtures containing triglycerides and lower alcohols and the products of the transesterification of triglycerides, glycerol and fatty acid esters, at various alcohol/oil ratios. The conditions of triglyceride transesterification in various lower alcohols providing the supercritical state of reaction mixtures were selected.

REACTION REVERSIBILITY IN α-PINENE THERMAL ISOMERIZATION: IMPROVING THE KINETIC MODEL

A.M. Chibiryaev*, An. Yermakova, I.V. Kozhevnikov (**Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia*)

Russ. J. Phys. Chem. A, 85(8) (2011) pp. 1347-1357.

Revision of the experimental data on α-pinene thermal isomerization attained in supercritical ethanol allowed to expand the reaction scheme, which includes now six main products and eleven reversible reactions. The equilibrium constants of every reaction (K_{Tj} and $K\Phi_j$) were calculated to allow for reversibility of reactions. The thermochemical data of the pure compounds required to calculate constants K_{Tj} and $K\Phi_j$ (standard enthalpy and entropy of formation $\Delta_f H$ (298.15 K), $\Delta_f S$ (298.15 K), heat capacity $C_p(T)$, critical parameters T_{cr} and p_{cr}, boiling point T_b, and the acentric factor ω) were preliminary estimated using the empirical Joback and Benson methods. A kinetic model based on the new expanded scheme of reversible reactions was successfully identified and its kinetic parameters k_j (600 K) and E_j were determined. Detailed examination of the new kinetic model allowed us to refine the generally accepted mechanism of α-pinene thermal isomerization and to distinguish additional features of the multistep process.

ACTIVATION PARAMETERS OF SUPERCRITICAL AND GAS-PHASE β-PINENE THERMAL ISOMERIZATION

A.M. Chibiryaev*, An. Yermakova, I.V. Kozhevnikov (**Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia*)

Russ. J. Phys. Chem. A, 85(9) (2011) pp. 1505-1515.

New data on enthalpy and entropy contributions to the energy barrier of β-pinene thermal isomerization were obtained. The rate of β-pinene conversion is higher in supercritical EtOH (P = 120 atm) than in the gas phase ($P \leq 1$ atm, without solvent, or for inert carrier gas N_2) at equal temperatures. The highest activation energy E_Σ of total β-pinene conversion is also observed in reactions in the supercritical (sc) condition. Activation parameters $\Delta H_\Sigma^\#$, $\Delta S_\Sigma^\#$, and $\Delta G_\Sigma^\#$ depend strongly on the reaction pressure. Thus, at $P \leq 1$ atm (gas-phase reaction) the values of $\Delta S_\Sigma^\#$ are negative, while at sc conditions at P = 120 atm is positive. The linear dependences $\ln k_{\Sigma 0} - E_\Sigma$ and $\Delta S_\Sigma^\# - \Delta S_\Sigma^\#$ indicate an isokinetic relation (IKR) and enthalpy-entropy compensation effect (EEC). The isokinetic temperature was calculated ($T_{iso} = 605.5 \pm 22.7$ K). It was shown that elevation of temperature reduces the value of $\Delta G_\Sigma^\#(T)$ upon sc thermolysis only, whereas in all gas-phase reactions $\Delta G_\Sigma^\#(T)$ increases. At equal reaction temperatures, the greatest values of $K_{eq}^\#(T)$ proved to be typical for thermolysis in sc-EtOH. It was hypothesized that the rate of total β-pinene conversion increases dramatically due to a considerable shift in equilibrium toward higher concentrations of activated complex $y_{TS}^\#$. A detailed analysis of activation parameters shows that the IKR and EEC coincide, evidence of a common mechanism of β-pinene conversion observed under different reaction conditions, including thermolysis in sc-EtOH.

MATHEMATICAL MODELING OF β-PICOLINE OXIDATION TO NICOTINIC ACID IN MULTITUBULAR REACTOR: EFFECT OF THE GAS RECYCLE

E.V. Ovchinnikova, N.V. Vernikovskaya, T.V. Andrushkevich, V.A. Chumachenko

Chem. Eng. J., 176-177 (2011) pp. 114-123.

Mathematical modeling of nicotinic acid synthesis process by means of β-picoline air oxidation in multitubular reactor was carried out. Factors that impact the process efficiency were studied. Special attention was focused on the role of recycling. The analysis was based on a two-dimensional quasi-homogeneous mathematical model of a tubular reactor and proprietary kinetic model of β-picoline oxidation over V_2O_5–TiO_2 catalyst.

MATHEMATICAL MODELING OF THE PROPANE DEHYDROGENATION PROCESS IN THE CATALYTIC MEMBRANE REACTOR

E.V. Shelepova, A.A. Vedyagin, I.V. Mishakov, A.S. Noskov

Chem. Eng. J., 176-177 (2011) pp. 151-157.

The two-dimensional non-isothermal stationary mathematical model of the catalytic membrane reactor for the process of propane dehydrogenation has been developed. The made calculations have shown the higher efficiency of the membrane reactor in comparison with the tubular one which is achieved due to removal of hydrogen from reactionary zone through the membrane to shift the reaction equilibrium towards formation of products. The use of membrane was found to cause the propane conversion increase from 41% to 67%. The highest value of propane conversion (X = 96%) was reached in case of additional oxidation of the removed hydrogen (conjugated dehydrogenation). The maximum value of propylene selectivity S = 98% can be as well reached in case of conjugated dehydrogenation in the membrane reactor at the reaction temperature of 500°C. The oxidation of hydrogen in conjugated dehydrogenation process gives the increase of propylene yield from 65% (the tubular reactor) to 95%. The maximum propylene yield corresponds to T = 525°C. It was also established that the gas space velocity in both internal and external parts of the membrane reactor is to be the one of the most important factors defining efficiency of the conjugated dehydrogenation process.

EFFECT OF CATALYTIC COMBUSTION OF HYDROGEN ON THE DEHYDROGENATION PROCESSES IN A MEMBRANE REACTOR.
I. MATHEMATICAL MODEL OF THE PROCESS

E.V. Shelepova, A.A. Vedyagin, A.S. Noskov

Combust. Explos. Shock Waves,
47(5) (2011) pp. 499-507.

Mathematical modeling of a catalytic membrane reactor was performed for thermodynamically coupled processes using as an example the endothermic dehydrogenation of propane and the exothermic combustion (oxidation) of hydrogen. Benefits of using the membrane reactor to increase the yield of target products by shifting equilibrium was demonstrated theoretically. The effect of hydrogen combustion on the main characteristics of the endothermic dehydrogenation process was studied. The hydrogen combustion reaction makes it possible to further increase the conversion of propane and compensate for the energy consumption in the endothermic dehydrogenation process.

VARIATIONAL PRINCIPLES IN IRREVERSIBLE THERMODYNAMICS WITH APPLICATION TO COMBUSTION WAVES

A.P. Gerasev

J. Non-Equilib. Thermodyn.,
36(1) (2011) pp. 55-73.

The thermodynamics of physicochemical processes in a reacting distributed kinetic system are considered, and the entropy balance equation for traveling waves of laminar combustion is derived for arbitrary Lewis number. Qualitative and numerical analysis of a dynamic system with a three-dimensional phase space and of the local and complete entropy production in the system were performed. It is shown that the complete entropy production in the system is a functional of the traveling wave solution of the problem, possessing extreme properties, whose minimum corresponds to the only physically meaningful traveling wave solution. The procedure of "cut-off" (zeroing) of the reaction rate is justified by methods of non-equilibrium thermodynamics. A variational formulation of the problem is presented for calculation of a steady laminar combustion wave.

SIMULATION OF CATALYTIC PROCESSES IN A FIXED BED WITH THE USE OF MICROWAVE RADIATION FOR PERFORMING AN ENDOTHERMIC REACTION

A.P. Gerasev

Kinet. Catal.,
52(6) (2011) pp. 907-913.

A quasi-homogeneous model of a catalytic fixed-bed reactor, in which an endothermic chemical reaction occurs with the use of microwave radiation energy, was proposed and numerically analyzed. The versions of the arrangement of a radiation source at the reactor inlet and outlet and also the versions of microwave radiation energy conversion into heat by a catalyst and an initial gaseous reagent were considered. The effects of model parameters on the dynamic behavior of the system were studied, and a qualitative structural difference between the resulting steady-state conditions was demonstrated. The phenomenon of endothermic chemical reaction autowave propagation was discovered, and the regularities of this propagation were studied.

DISTRIBUTION OF CATALYTIC, FILTRATIONAL AND HYBRID AUTOWAVES IN THE HETEROGENEOUS ENVIRONMENT

A.P. Gerasev

Chem. Ind. Today,
1 (2011) pp. 6-12.

Mathematical modeling of autowave heterogeneous processes with chemical reactions in a gas phase and on the catalyst is carried out. Values of factors of interphase heat– and masstransfer and heat conductivity of a solid phase were defined on current values of parameters of system. Qualitative distinction of structure of three kinds of autowaves is shown: filtrational burning of gases in a mode of low speeds, with catalytic reaction and hybrid autowaves with simultaneously going reactions in a gas phase and on the catalyst. Numerical modelling of the system on the basic technological indicators of autowave process is performed.

KINETICS STUDY OF THE PERCHLOROETHYLENE HYDROFLUORINATION INTO PENTAFLUOROETHANE (FREON 125) OVER CHROMIUM-BASED CATALYST

S.I. Reshetnikov, A.A. Zirka, R.V. Petrov, E.A. Ivanov

Chem. Eng. J.,
176-177 (2011) pp. 22-25.

The gas-phase hydrofluorination of perchloroethylene (PCE) into pentafluoroethane (non ozonedepleting Freon 125) at T = 330–390°C and P = 0.4 MPa in the presence of a chromium–magnesium catalyst has been studied. A hydrofluorination scheme including main product and by-products formation routes is deduced from the observed dependences of particular products selectivity. The kinetic model of the PCE hydrofluorination has been developed. The rate parameters and the activation energy of the reactions were determined. The model satisfactorily describes the experimental data in the temperature range 330–390°C.

EFFECT OF THE MOBILITY OF OXYGEN IN PEROVSKITE CATALYST ON THE DYNAMICS OF OXIDATIVE COUPLING OF METHANE

S.I. Reshetnikov, Yu.I. Pyatnitskii*, L.Yu. Dolgikh* (**L.V. Pisarzhevskii Institute of Physical Chemistry, Kyiv, Ukraine*)

Theor. Exp. Chem.,
47(1) (2011) pp. 49-54.

The effect of the diffusion of oxygen from the volume of the catalyst to its surface on the dynamics of the oxidative coupling of methane was assessed on the basis of a mathematical model of the reaction of methane with the oxidized surface of $KNaSrCoO_{3-x}$ perovskite. It was shown that the possible values of the diffusion coefficient lie in the range of 10^{-18}-10^{-16} cm^2/s characteristic of the diffusion of oxygen in oxide catalysts.

THE STABILITY OF AN ISOTHERMAL GASEOUS SPHERE WITH GRAVITATION

V.N. Snytnikov, O.A. Stadnichenko

Astron. Rep.,
55(3) (2011) pp. 214-223.

A dispersion relation has been obtained for waves propagating in an inhomogeneous gas with viscosity and gravity in the direction of the density gradient. It has been shown that a stationary distribution of isothermal gas is unstable under gravitational-convective perturbations. It is suggested that the initial- and boundary-value problems of the non-stationary dynamics of an isothermal gas with gravity but without viscosity are incorrect and require regularization, for example, by adding viscosity. The presence of viscosity does not prevent the development of the Jeans long-wave instability. Numerical experiments based on a fully three-dimensional, non-stationary numerical code have demonstrated the development of a collapse inside an isothermal cloud.

EFFECT OF WATER ON OXIDATIVE SCISSION OF 1-BUTENE TO ACETIC ACID OVER V_2O_5-TiO_2 CATALYST. TRANSIENT ISOTOPIC AND KINETIC STUDY

W. Suprun*, E.M. Sadovskaya, Ch. Rüdinger, H.-J. Eberle**, M. Lutecki*, H. Papp***
(**Universität Leipzig, Leipzig, Germany; **Wacker Chemie AG, Consortium für Elektrochemische Industrie GmbH, München, Germany*)

Appl. Catal. A,
391(1-2) (2011) pp. 125-136.

The role of water in the oxidation of 1-butene to AcOH over VO_x-TiO_2 was investigated using spectroscopic and transient isotopic exchange methods. It was shown that the influence of water strongly depended on the temperature of reaction. In particular, DRIFTS and NH_3-TPD studies confirmed the temperature influence on the acidity and the amount of adsorbed water. XPS investigations suggested that not only oxygen from vanadia, but also from the lattice of titania was involved in the oxygen transfer during the reaction. Formation of oxidation products proceeded over two types of active vanadium oxide centers, i.e., VOH and VO. Hydrated vanadium species exhibited high selectivity towards AcOH formation. On the other hand, VO centers favored total oxidation. Kinetic model was developed for an unambiguous interpretation of the experimental results. Modelled reaction constants of the formation of AcOH over VOH centers were ca. 3.5 times higher than over VO centers. At the same time, the reaction rate constant of total oxidation in the presence of water was ca. 3.2 times lower than in dry flow. Estimated values suggested that in the presence of water the number of VOH centers was substantially lower than VO sites; however their contribution to the rate of AcOH formation was much higher.

INVESTIGATION OF MASS TRANSFER ON GLASS FABRIC CATALYST DURING CO OXIDATION REACTION

O.V. Chub, A.S. Noskov, L.G. Simonova

Chem. Ind. Today,
5 (2011) pp. 19-24.

The mass transfer during CO oxidation reaction has been investigated using Pd-containing catalyst prepared on the basis of glass fabrics of various weaves. The mathematical model of experimental reactor is formulated. The results are shown in the form of criterial dependency $Sh = A\ Re_n\ Sc^{1/3}$, mass transfer coefficients and equation parameters have been determined.

ON A LIMIT EQUATIONS AND ATTRACTION FOR NONAUTONOMOUS SYSTEMS WITH DELAY

I.A. Finogenko*, N.A. Chumakova (**Institute for System Dynamics and Control Theory, Irkutsk, Russia*)

Tambov University Reports. Ser.: Nat. Techn. Sci.,
16(5) (2011) pp. 1247-1253.

For nonautonomous functional-differential equations property of quasiinvariance for limiting sets and analogue of the La-Salle principle of invariancy by use of Lyapunov functional with constant sign derivative is established.

COMPUTATIONAL FLUID DYNAMICS IN THE DESIGN OF CATALYTIC REACTORS

O.P. Klenov, A.S. Noskov

Catal. Ind.,
3(4) (2011) pp. 331-349.

Computational fluid dynamics is becoming an important tool in the study of chemical engineering processes and apparatuses (in particular, the share of works with the application of this method is nearly 6% of the total number of all chemical engineering works issued by Elsevier Science Publishers in 2010). The possibilities of computational fluid dynamics are demonstrated using examples from three different chemical engineering fields: developing a method for loading a tubular reactor for the steam conversion of natural gas, studying heat transfer in a reactor for the hydrogenation of vegetable oils upon the replacement of a catalyst, and investigating the transitional processes in an automobile neutralizer. The results from computational fluid dynamics are verified by comparing them with experimental data in developing a method for loading a tubular reactor, using the problem of decelerating a catalyst particle with a flow of air as an example. The obtained data are compared with classical measurement data on the aerodynamic drag of a ball and a cylinder and represent the further development of works on the flow around particles of complex shape. In this work, the results from inspecting a reactor for the hydrogenation of oils with allowance for the possible heating and uniform distribution of a flow before its entering the catalyst bed are presented. It is shown that the construction of the reactor does not ensure homogeneity of the reaction flow at the desired level and requires modification of heating elements. The efficiency of computational fluid dynamics for investigating fast processes with a chemical reaction is exemplified by studying the transitional processes in an catalytic automobile neutralizer (the effect of flow dynamics and heat transfer on the thermal regime in a honeycomb catalyst particle is very difficult to study by experimental methods). The application of computational fluid dynamics allows us to reduce considerably the time and cost of developing and optimizing the designs of efficient catalytic fixed-, fluidized-, or moving-bed reactors (particularly multiphase stirred (slurry) reactors), along with mixers, adsorbers, bubblers, and other chemical engineering apparatuses with moving media.

SOLID DISPERSION IN THE SLURRY REACTOR WITH MULTIPLE IMPELLERS

O.P. Klenov, A.S. Noskov

Chem. Eng. J.,
176-177 (2011) pp. 75-82.

A whole series of significant catalytic processes are carried out in a slurry reactor with multiple impellers. The selective hydrogenation of sunflower seed oil is the characteristic example of such a process. The liquid phase is the main medium into stirred tank and an investigation of a fluid dynamics of one just as transient regime of solid distribution in liquid volume could be helpful to practical application.

In the present work, CFD simulations have been carried out to study solid distribution in liquid–solid stirred tank using Mixture multifluid approach along with standard $k–\varepsilon$ turbulence model. A multiple frame of reference (MFR) and Sliding Mesh Model have been used to model the multiple impellers and tank region. The effects of specific density of fine-dispersed solid phase and place of injection of solid have been investigated for “steady-state” and time-depended cases.

MODELING DESIGN AND ANALYSIS OF MULTI-LAYER SOLID OXIDE FUEL CELLS

R. Hasanov*, A. Smirnova, A. Gulgazli*, M. Kazimov*, A. Volkov*, V. Quliyeva*, O. Vasylyev***, V.A. Sadykov** (**Azerbaijan State Oil Academy, Baku, Azerbaijan; **Eastern Connecticut State University, Willimantic, USA; ***Institute for Problems of Materials Science, Kiev, Ukraine*)

Int. J. Hydrogen Energy,
36(2) (2011) pp. 1671-1682.

The thermo-mechanical analytical model proposed for different solid oxide fuel cell (SOFC) designs addresses the deformation behavior and mechanical stability of SOFCs at various thermal stresses, specifically the creep resistance and the long-term endurance beyond the elastic limit.

The model considers the deformation of multi-layer SOFC in the temperature range of 600–800°C and presents the combination of the correlated parameters for SOFC performance evaluation, stability and long-term endurance under realistic operating conditions and temperature gradients. The numerical analysis of the thermo-mechanical properties of the SOFC materials is presented in terms of mechanical behavior at failure conditions and the influence of rheological and structural properties on SOFC long-term endurance. The SOFC thermal behavior, creep parameters of the SOFC materials and long-term stability are analyzed in terms of stresses, deformations and displacements.

In terms of broader impact, the algorithms for Maurice-Levi and Voltaire theorems and their validity for non-elastic, e.g. viscous-elastic, viscous-plastic, and elastic-plastic deformations were confirmed. This result allowed to apply the stress condition of non-elastic body to the stress condition of the elastic body which is relevant to the SOFC operation at elevated temperatures.

ETHYLENE GLYCOL OXIDATION OVER SUPPORTED CATALYST IN TUBULAR REACTOR

M.A. Salaev*, A.A. Krejker*, O.V. Magaev*, V.S. Malkov*, A.S. Knyazev*, E.S. Borisova, V.M. Khanaev, O.V. Vodyankina*, L.N. Kurina* (**Tomsk State University, Tomsk, Russia*)

Chem. Eng. J., 172(1) (2011) pp. 399-409.

Macrokinetics for chemical transformation of ethylene glycol into glyoxal (including side-reactions) as well as 2D heterogeneous mathematical model were suggested. Numerical results obtained using this model were compared with the experimental data obtained at lab-scale and pilot reactor, and showed good correlation. It was shown that due to catalyst activity change it is possible to manage the process selectivity with respect to glyoxal in diffusion mode. The optimal value of catalyst activity providing the highest process selectivity can be found.

SIMULATION OF HETEROGENEOUS CATALYTIC REACTION BY ASYNCHRONOUS CELLULAR AUTOMATA ON MULTICOMPUTER

A.E. Sharifulina*, V.I. Elokhin (**Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russia*)

Lecture Notes Comput. Sci., 6873 (2011) pp. 204-209.

In the paper parallel implementation of ACA simulating dynamics of carbon monoxide oxidation over the Pd(100) is presented. Parallel implementation of ACA is based on its approximation by block-synchronous CA. To estimate approximation accuracy comparative analysis of statistical characteristics and bifurcation diagrams, obtained by ACA and BCSA simulation, is performed. Results of parallel implementation of BSCA algorithm and estimations of its efficiency are presented.

Fuel Chemistry and Technology

DEACTIVATION AND OXIDATIVE REGENERATION OF MODERN CATALYSTS FOR DEEP HYDROPURIFICATION OF DIESEL FUEL: OXIDATIVE REGENERATION OF IC-GO-1 CATALYST

S.V. Budukva, O.V. Klimov, G.S. Litvak, Yu.A. Chesalov, I.P. Prosvirin, T.V. Larina, A.S. Noskov

Russ. J. Appl. Chem., 84(1) (2011) pp. 95-102.

Oxidative regeneration of a deactivated IC-GO-1 catalyst was studied in removal of carbonaceous deposits and sulfur from the catalyst composition. Elemental analysis data, texture characteristics, and catalytic activities of fresh and regenerated samples were compared. Raman spectroscopy, X-ray phase analysis, electronic diffuse reflectance spectroscopy, and X-ray photoelectron spectroscopy were used to examine the structure of cobalt and molybdenum compounds entering into the composition of the catalysts.

HYDROCRACKING OF VACUUM GAS OIL IN THE PRESENCE OF SUPPORTED NICKEL–TUNGSTEN CATALYSTS

A.S. Ivanova, E.V. Korneeva, G.A. Bukhtiyarova, A.L. Nuzhdin, A.A. Budneva, I.P. Prosvirin, V.I. Zaikovsky, A.S. Noskov

Kinet. Catal., 52(3) (2011) pp. 446-458.

The supports containing 70% Al_2O_3 and 30% β zeolite (AZ-1 and AZ-2), which differed in mixing procedures, and the Ni-W/AZ-1 and Ni-W/AZ-2 catalysts were characterized using an adsorption technique, high-resolution electron microscopy, IR spectroscopy, and X-ray photoelectron spectroscopy and tested in the hydrocracking reaction of vacuum gas oil (VGO). It was found that the supports differed in texture characteristics and surface Lewis acidity at the same composition and similar concentrations of Brønsted acid sites. The formation of Ni-W-S sulfide species on the surfaces of both of the supports occurred in different manners: multilayer Ni-W-S sulfide species were formed on AZ-1 ($S_{sp} = 220$ m^2/g), whereas single-layer species were mainly formed on AZ-2 ($S_{sp} = 380$ m^2/g). It was found that catalysts containing multilayer Ni-W-S sulfide species, which were characterized by a higher degree of sulfidation, provided a higher yield of diesel fuel upon the hydrocracking of VGO, whereas catalysts containing single-layer Ni-W-S sulfide species were more active in the reactions of VGO hydrodesulfurization and hydrodenitration.

CATALYTIC DEOXYGENATION OF TALL OIL FATTY ACIDS OVER A PALLADIUM-MESOPOROUS CARBON CATALYST: A NEW SOURCE OF BIOFUELS

P. Mäki-Arvela*, B. Rozmysłowicz, S. Lestari***, O.A. Simakova, K. Eränen*, T. Salmi*, D.Yu. Murzin*** (**Åbo Akademi University, Turku, Finland; **Poznan University of Technology, Poznan, Poland; ***University of Queensland, Brisbane, Queensland, Australia*)

Energy Fuels,
25(7) (2011) pp. 2815-2825.

Catalytic deoxygenation of tall oil fatty acids (TOFAs) was investigated over 1 wt% Pd/C Sibunit, which is a synthetic mesoporous carbon. The reactions were performed in a semi-batch reactor using dodecane as a solvent under 17 bar of total pressure. The main studied parameters were the reaction temperature, initial concentration of TOFA, effect of the reaction atmosphere, and metal loading. The temperature and initial concentration ranges were 300-350°C and 0.15-0.6 mol/L, respectively. The total conversion of fatty acids increased, as expected, with increasing temperatures and decreasing initial TOFA concentrations. The main liquid-phase products were *n*-heptadecane and *n*-heptadecene. In addition to the desired linear C_{17} hydrocarbons, also aromatic C_{17} compounds, such as undecylbenzene, were formed. The best conditions for the formation of the desired C_{17} hydrocarbons were lower initial concentrations of TOFA, 300-325°C, and the presence of hydrogen. An increase of the metal loading (4 wt%) led to an increase of the selectivity to linear C_{17} hydrocarbons.

CATALYTIC DEOXYGENATION OF C18 FATTY ACIDS OVER MESOPOROUS Pd/C CATALYST FOR SYNTHESIS OF BIOFUELS

I.L. Simakova, B. Rozmysłowicz*, O.A. Simakova, P. Mäki-Arvela*, A. Simakov, D.Yu. Murzin*** (**Abo Akademi University, Turku, Finland; **Centro de Nanociencias y Nanotecnología, UNAM, Ensenada, BC, México*)

Top. Catal.,
54(8-9) (2011) pp. 460-466.

Deoxygenation was systematically investigated using either stearic, oleic or linoleic acids as a feedstock at 300°C under 1 vol% hydrogen in argon over a mesoporous Pd/C (Sibunit) catalyst producing one less carbon containing, diesel-like hydrocarbons. The results revealed that catalyst activity and selectivity increased with less unsaturated feedstock. The main products in the case of stearic acid were desired C17 hydrocarbons, whereas the amounts of C17 aromatic compounds increased in case of oleic and linoleic acids. Catalyst deactivation was relatively prominent in linoleic acid deoxygenation giving only 3% conversion of fatty acids in 330 min. The deactivation originated from the formation of C17 aromatic compounds and fatty acid dimers, which was confirmed by size exclusion chromatographic analysis. The latter compounds were formed via Diels-Alder reaction.

CATALYSIS IN BIOMASS PROCESSING

D.Yu. Murzin*, I.L. Simakova (**Åbo Akademi University, Turku, Finland)*

Catal. Ind.,
3(3) (2011) pp. 218-249.

Biomass has in recent years been considered as a raw material for the production of fuels and chemicals. This work discusses the reasons for the increased interest in mainly lignocellulosic biomass. Gasification, pyrolysis, and depolymerization by hydrolysis are analyzed as key biomass technology. The authors also discuss which of the sugars obtained via depolymerization by hydrolysis can be processed into fuel or key intermediates of the chemical industry. Lignocellulosic biomass contains such extractants as fatty acids and terpenes, and the authors therefore describe the catalytic reactions of these substances for the synthesis of fuels and chemicals. Some typical reactions of biomass processing (oxidation, hydrogenation, cracking, etc.) are conceptually close to the process widely known in the refining and chemical industries. There are, however, other considerations due to, e.g., the large number of functional (hydroxyl and other) groups, and the processing of biomass components therefore requires dehydration, aldol condensation, ketonization, decarboxylation, etc. The authors cover the fundamentals of the approaches to selecting catalysts for these reactions.

METHANE CONVERSION TO VALUABLE CHEMICALS OVER NANOSTRUCTURED Mo/ZSM-5 CATALYSTS

Z.R. Ismagilov, E.V. Matus, M.A. Kerzhentsev, L.T. Tsykoza, I.Z. Ismagilov, K.D. Dosumov*, A.G. Mustafin** (**Sokol'skii Institute of Organic Catalysis and Electrochemistry, Almaty, Republic of Kazakhstan; **Bashkir State University, Ufa, Russia*)

Pet. Chem.,
51(3) (2011) pp. 174-186.

Results of the ongoing study of nonoxidative methane dehydroaromatization (DHA) over Mo/ZSM-5 catalysts have been analyzed. The effects of the composition, preparation procedure, pretreatment, and the CH_4 DHA reaction conditions on the physicochemical and catalytic properties of Mo/ZSM-5 catalysts have been discussed. The data on Mo-containing active sites, the methane DHA reaction mechanism, and the nature of carbonaceous deposits have been considered. The principal causes of the deactivation of Mo/ZSM-5 catalysts and means of their regeneration have been revealed. Approaches to the improvement of the methane DHA process and trends of its further development have been detailed.

OXIDATIVE DESULFURIZATION OF HYDROCARBON FUELS

Z.R. Ismagilov, S.A. Yashnik, M.A. Kerzhentsev, V.N. Parmon, A. Bourane*, F.M. Al-Shahrani*, A.A. Hajji*, O.R. Koseoglu* (**Saudi Aramco, Research and Development Center, Dhahran, Kingdom of Saudi Arabia*)

Catal. Rev. - Sci. Eng.,
53(3) 2011) pp. 199-255.

New requirements for very low sulfur content (10 ppm) in liquid motor fuels demand novel approaches for ultra-deep desulfurization. For production of near-zero-sulfur diesel and low-sulfur fuel oil, removal of refractory sulfur compounds, like 4,6-dimethyldibenzothiophene and other alkyl-substituted thiophene derivatives, is necessary. Elimination of these compounds by hydrodesulfurization (HDS) requires high hydrogen consumption, high pressure equipment, and new catalysts. Various oxidative desulfurization processes, including recent advances in this field for diesel fuels, and the drawbacks of this technology in comparison with HDS are examined and discussed. It is shown that the oxidation of sulfur compounds to sulfones with hydrogen peroxide allows for production of diesel fuels with a sulfur content of 10 ppmw or lower at atmospheric pressure and room temperature. The gas phase oxidative desulfurization of sulfur compounds with air or oxygen is feasible at atmospheric pressure and higher temperatures: 90–300°C and offers better economic solutions and incentives.

CARBON DIOXIDE REFORMING OF METHANE OVER Co-Ni CATALYSTS

G.B. Aldashukurova*, A.V. Mironenko*, Z.A. Mansurov*, N.V. Shikina, S.A. Yashnik, Z.R. Ismagilov (**Institute for Problems of Combustion*, *Almaty, Kazakhstan*)

Chem. Eng. Trans.,
25 (2011) pp. 63-68.

Low-percentage catalysts for dry reforming of methane (DRM) with Ni and Co deposited on a glass fiber support by the “solution combustion” (SC) method have been developed. Particle size and state of the active component were studied by XRD, TPR, TEM, SEM and AFM. The active component was shown to be dispersed in the near-surface layer of support as nanoparticles of size 10–20 nm, which have a Co_3O_4 or $(Co,Ni)Co_2O_4$ spinel structure depending on the catalyst composition. Spinel structure of the active component is resistant to carbonization and provides high catalytic activity toward DRM.

HETEROGENEOUS CATALYSTS FOR THE TRANSFORMATION OF FATTY ACID TRIGLYCERIDES AND THEIR DERIVATIVES TO FUEL HYDROCARBONS

V.A. Yakovlev, S.A. Khromova, V.I. Bukhtiyarov

Russ. Chem. Rev.,
80(10) (2011) pp. 911-925.

The results of studies devoted to the catalysts for transformation of fatty acid triglycerides and their derivatives to fuel hydrocarbons are presented and described systematically. Various approaches to the use of heterogeneous catalysts for the production of biofuel from these raw materials are considered. *The bibliography includes 134 references.*

PYROLYSIS OF RAPIDLY GROWING GRASS BIOMASS UNDER ISOTHERMAL CONDITIONS

S.G. Zavarukhin, I.A. Streltsov, V.A. Yakovlev

Kinet. Catal.,
52(4) (2011) pp. 499-505.

The pyrolysis of rapidly growing grass biomass in an inert atmosphere was studied by thermogravimetric analysis using sorghum as an example. Pyrolysis was performed under isothermal conditions at temperatures from 250 to 400°C. To describe the reaction kinetics, a single-component model including six first-order reactions was proposed. A special feature of this model is the occurrence of a step of the formation of an intermediate carbonaceous substance from the volatile products of biomass decomposition

PRODUCTION OF BIODIESEL FORM RAPESEED OIL USING HETEROGENEOUS Ba-Al CATALYST IN THREE-PHASE REACTOR

S.G. Zavarukhin, M.Yu. Lebedev, A.N. Simonov, L.G. Matvienko, A.S. Ivanova, V.N. Parmon, V.G. Sister*, O.V. Sherstyuk, M.V. Bukhtiyarova, V.A. Yakovlev (**Moscow State University of* Ecological Engineering)

Chem. Ind. Today,
10 (2011) pp. 14-22.

The production of biodiesel by transesterification of rapeseed oil using methanol and heterogeneous Ba-Al catalyst was studied in three-phase reactor. Simplified kinetic model of transesterification process was proposed and the catalyst volume was calculated for the industrial reactor with the performance 2250 kg/hour of oil with oil conversion 95 %.

POROUS NICKEL BASED CATALYSTS FOR PARTIAL OXIDATION OF METHANE TO SYNTHESIS GAS

V.A. Kirillov, Z.A. Fedorova, M.M. Danilova, V.I. Zaikovsky, N.A. Kuzin, V.A. Kuzmin, T.A. Krieger, V.D. Meshcheryakov

Appl. Catal., A,
401(1-2) (2011) pp. 170-175.

The phase composition and texture of nickel catalysts supported on ribbon porous nickel with a magnesium oxide underlayer were investigated by X-ray diffraction, low-temperature nitrogen adsorption, and electron microscopy combined with energy dispersive X-ray microanalysis. The MgO underlayer was obtained by impregnation the porous nickel with a $Mg(NO_3)_2$ solution followed by calcination at 550°C; nickel was supported additionally by impregnation with a $Ni(NO_3)_2$ solution followed by calcination at 450°C. In the supported reduced nickel catalysts (800–900°C, H_2) the phases of Ni and a solid solution of NiO in MgO were observed; a considerable part of nickel crystallites was epitaxially bound with MgO. The partial oxidation of methane to synthesis gas (800°C, $O_2/C = 0.65$, GHSV = 127 L/g h) over porous nickel based catalysts was studied. The activity of initial nickel support decreased considerably during the partial oxidation of methane; the value of methane conversion decreased slightly after 100 h of testing on the supported nickel catalysts.

Chemical Engineering

EFFECT OF INTERNAL DIFFUSION ON PREFERENTIAL CO OXIDATION IN A HYDROGEN-RICH MIXTURE ON A COPPER-CERIUM OXIDE CATALYST IN A MICROCHANNEL REACTOR

D.I. Potemkin, P.V. Snytnikov, V.D. Belyaev, V.A. Sobyanin

Kinet. Catal.,
52(1) (2011) pp. 139-144.

The effect of internal diffusion on preferential CO oxidation in a hydrogen-rich mixture on a copper-cerium catalyst in a microchannel reactor was estimated. It was found that the internal effectiveness factor $\eta_{CO} > 0.8$ was reached at a catalytic coating thickness of ~30 μm.

PREFERENTIAL CO OXIDATION OVER Cu/CeO_{2-x} CATALYST: INTERNAL MASS TRANSPORT LIMITATION

D.I. Potemkin, P.V. Snytnikov, V.D. Belyaev, V.A. Sobyanin

Chem. Eng. J.,
176-177 (2011) pp. 165-171.

The effect of internal mass transport limitation on the preferential CO oxidation in hydrogen-rich mixture over copper-cerium oxide catalyst in a form of pellets and washcoat in microchannel reactor is estimated. Internal effectiveness factor $\eta_{CO} > 0.8$ in the optimum interval of reaction temperature (170–230°C) is reached if the pellet diameter and washcoat thickness do not exceed 100 and 20 μm, respectively.

Compared to conventional packed-bed reactor with catalyst pellets, microchannel catalytic washcoated reactor is more appropriate for practical use.

TECHNIQUE FOR COMPLETE OXIDATION OF ORGANIC COMPOUNDS IN SUPERCRITICAL WATER

V.I. Anikeev, An. Yermakova

Russ. J. Appl. Chem.,
84(1) (2011) pp. 88-94.

Results are presented of tests of a pilot stationary installation for supercritical water oxidation of organic compounds, first created in Russia. A high oxidation efficiency of nitro compounds formed as waste in manufacture of explosives is demonstrated.

APPLICATION OF SYNTHESIS GAS AS A FUEL ADDITIVE ONBOARD THE VEHICLE: STATE OF THE ART AND PROSPECTS

V.N. Parmon, V.A. Kirillov, V.A. Sobyanin, V.A. Burtsev*, V.K. Emel'yanov, N.A. Kuzin, V.V. Kireenkov, Yu.I. Amosov**
(**OOO Gasomotor-R, Rybinsk, Yaroslavl oblast, Russia; **International Science and Technology Center, Moscow, Russia*)

Theor. Found. Chem. Eng.,
45(2) (2011) pp. 127-140.

A method for the production of a hydrogen-rich gas on board a vehicle was suggested and driving- and bench-tested for application in studies on energy-efficient internal combustion engines with minimum CO, CO_2, CH, and NO_x emissions. The generated gas is further added to the main fuel fed to the engine. Catalysts for hydrocarbon fuel conversion to syngas were developed. A compact on-board syngas generator mounted under the motor hood and a generator control system adapted to the engine control system were designed. It was shown experimentally that the suggested solution allows a reduction of 13–40% in the fuel rate depending on the operating mode under the urban cycle conditions and considerably decreases the release of CO, CO_2, and NO_x. Prospects for the applications of this technology for creating ecologically clean engines were assessed.

CATALYSTS FOR THE CONVERSION OF HYDROCARBON AND SYNTHETIC FUELS FOR ONBOARD SYNGAS GENERATORS

V.A. Kirillov, N.A. Kuzin, Yu.I. Amosov, V.V. Kireenkov, V.A. Sobyanin

Catal. Ind.,
3(2) (2011) pp. 176-182.

The use of syngas derived on board a vehicle as a supplement to the main fuel fed to engines ensures engine operation using dilute fuel mixtures. This leads to a decrease in emission toxicity and an increase in the fuel efficiency of the engine. The preparation of new types of efficient catalysts for the conversion of hydrocarbon and synthetic fuels for onboard syngas generators requires the use of new approaches to the design of catalysts not only as catalytically active material, but also as a structural component of a chemical reactor. The authors prepared and tested a set of catalysts for the conversion of hydrocarbons, i.e., natural gas, diesel and biodiesel fuels, biofuels, and alcohols (ethanol, methanol) to syngas. Primary supports for the catalysts were metals grids and porous tapes; secondary supports were oxides of aluminum and magnesium deposited on or sintered to a primary support. The catalysts exhibited high thermal stability and mechanical strength, and were characterized by the conformity of the coefficients of thermal expansion of the support material and the catalytically active bed. The catalysts can be used as structural components of reactors and as a basis for the preparation of monolithic blocks and planar components of radial and planar reactors. The developed catalysts were subjected to laboratory and bench tests and examined as components of onboard generators of vehicles.

USE OF Pd MEMBRANES IN CATALYTIC REACTORS FOR STEAM METHANE REFORMING FOR PURE HYDROGEN PRODUCTION

A.B. Shigarov, V.D. Meshcheryakov, V.A. Kirillov

Theor. Found. Chem. Eng.,
45(5) (2011) pp. 595-609.

This review analyzes publications on experimental studies and mathematical modeling in the field of development of a catalytic reformer (mainly, steam methane conversion) with a fixed catalytic bed. The specific feature of such a reformer is its integration with a Pd membrane for the purpose of producing high-purity hydrogen to power a low-temperature fuel cell battery.

DESIGN, SCALE-OUT, AND OPERATION OF A PREFERENTIAL CO METHANATION REACTOR WITH A NICKEL–CERIA CATALYST

M.M. Zyryanova, P.V. Snytnikov, Yu.I. Amosov, V.A. Kuzmin, V.A. Kirillov, V.A. Sobyanin

Chem. Eng. J.,
176-177 (2011) pp. 106-113.

Preferential CO methanation in a reformate gas was investigated over 10 wt% Ni/CeO_2 pelleted catalyst in the fixed-bed reactor. It provided the reduction of the CO concentration in the reformate gas to less than 10 ppm over wide temperature interval (250–300°C), while keeping hydrogen consumption relatively low.

The design, scale-out, and operation of a preferential CO methanation reactor with integrated heatexchanger were reported. The nickel–ceria catalyst was deposited onto metal gauzes, assembled into catalytic blocks. Direct contact of the catalyst with metal support provided high heat conductivity of the assembly and feasible temperature control upon variation of operation regimes. Nickel–ceria catalyst showed high activity and selectivity for the reaction of CO methanation in the presence of CO_2 excess. The preferential CO methanation reactor allowed the decrease of CO concentration to less than 20 ppm in realistic reformate generated by fuel processor via the reaction of methane steam reforming followed by CO water gas shift reaction.

SORPTION PROPERTIES OF LITHIUM CARBONATE DOPED CaO AND ITS PERFORMANCE IN SORPTION ENHANCED METHANE REFORMING

V.S. Derevshchikov, A.I. Lysikov, A.G. Okunev

Chem. Eng. Sci.,
66(13) (2011) pp. 3030-3038.

In-house prepared lithium carbonate doped CaO was tested for its CO_2 sorption properties and suitability as a CO_2 sorbent for sorption-enhanced reforming of methane. The new material demonstrated CO_2 capacity at the temperatures above the equilibrium for CaO recarbonation reaction. However, the capacity was unstable and decreased during carbonation–regeneration cycles. After sufficiently large number of cycles Li dopant escaped from the sorbent and its sorption behavior resembled to that of CaO. The main route of escape is, probably, a crossover of liquid Li_2CO_3 onto crucible in TG experiments and onto catalyst in SER tests. Sorption enhanced methane reforming at 2 bar pressure, 750°C and H_2O to CH_4 ratio of 4 using novel sorbent yielded as high as 99.8 vol% pure hydrogen during the first cycle. In subsequent cycles the hydrogen purity drastically decreased as a result of severe catalyst poisoning by Li.

HIGH TEMPERATURE CaO/Y_2O_3 CARBON DIOXIDE ABSORBENT WITH ENHANCED STABILITY FOR SORPTION-ENHANCED REFORMING APPLICATIONS

V.S. Derevshchikov, A.I. Lysikov, A.G. Okunev

Ind. Eng. Chem. Res.,
50(22) (2011) pp 12741-12749.

To improve the stability of high temperature CO_2 absorbent for sorption enhanced reforming applications yttria supported CaO were synthesized using two methods: calcination of mixed salt precursors and wet impregnation of yttria support. According to XRD data, CaO does not interact with the yttria matrix. However, introduction of CaO drastically changes the morphology of primary yttria particles. Increase in CaO concentration results in gradual plugging of the smaller pores and sintering of yttria support. The CO_2 absorption uptake in recarbonation-decomposition cycles increases with increase in CaO content and reach 9.6 wt% at CaO content of 19.9 wt%. CaO recarbonation extent varies from 49 to 77%. CaO/Y_2O_3 absorbents are extremely stable under overheating and maintain their capacity in long series of decomposition-recarbonation cycles even after calcination at 1350°C. The novel material resists moisture and retains its strength during storage in the air. According to tests, CaO/Y_2O_3 can be considered as a promising CO_2 absorbent for fixed bed sorption enhanced hydrocarbons reforming.

EFFECT EXERTED BY TEXTURE OF CALCINED CALCIUM OXIDE ON ITS SORPTION CAPACITY IN THE CO_2 SORPTION-REGENERATION CYCLES

A.G. Okunev, A.I. Lysikov

Russ. J. Appl. Chem.,
84(2) (2011) pp. 173-178.

The dynamic capacity of a set of sorbents prepared by calcination of different precursors was studied in multiple CO_2 sorption-regeneration cycles.

The effect exerted by type of a precursor and calcination temperature on the steady state value of the dynamic capacity attained after several tens of cycles was determined. A model was suggested for estimate of the sorption capacity of CaO sintered above the Tammann temperature from data on the mercury porosimetry.

PROMISING CHEMICAL ADSORPTION CYCLIC PROCESSES FOR CO_2 ISOLATION FROM SMOKE FUMES

A.G. Okunev, A.I. Lysikov

Chem. Sustain. Devel.,
19(1) (2011) pp. 105-112.

Promising cyclic processes of hydrocarbon combustion distinguished by the type of the chemisorbent used are considered. In the carbonate cycle, solid high-temperature regenerable chemisorbent for CO_2 is used to isolate carbon dioxide. In the oxygen cycle, a solid chemisorbent of oxygen is used; it gets recovered when in contact with fuel and gets oxidized when in contact with the air. A common feature of these processes includes solid-phase reactions of binding and release of the products or reagents at different stages of the process. Requirements to chemisorbents for cyclic processes are determined. Various factors affecting the efficiency of their use are considered, literature data on the efficiency of the proposed cycles of CO_2 concentrating are reported.

PROTON CONDUCTING HYDROCARBON MEMBRANES: PERFORMANCE EVALUATION FOR ROOM TEMPERATURE DIRECT METHANOL FUEL CELLS

I.M. Krivobokov, E.N. Gribov, A.G. Okunev

Electrochim. Acta,
56(5) (2011) pp. 2420-2427.

The methanol permeability, proton conductivity, water uptake and power densities of direct methanol fuel cells (DMFCs) at room temperature are reported for sulfonated hydrocarbon (sHC) and perfluorinated (PFSA) membranes from Fumatech®, and compared to Nafion® membranes. The sHC membranes exhibit lower proton conductivity (25–40 mS cm^{-1} vs. ~95–40 mS cm^{-1} for Nafion®) as well as lower methanol permeability ($1.8–3.9 \times 10^{-7}$ cm^2 s^{-1} vs. $2.4-3.4 \times 10^{-6}$ cm^2 s^{-1} for Nafion®). Water uptake was similar for all membranes (18–25 wt%), except for the PFSA membrane (14 wt%). Methanol uptake varied from 67 wt% for Nafion® to 17 wt% for PFSA. The power density of Nafion® in DMFCs at room temperature decreases with membrane thickness from 26 mW cm^{-2} for Nafion® 117 to 12.5 mW cm^{-2} for Nafion® 112. The maximum power density of the Fumatech® membranes ranges from 4 to 13 mW cm^{-1}. Conventional transport parameters such as membrane selectivity fail to predict membrane performance in DMFCs. Reliable and easily interpretable results are obtained when the power density is plotted as a function of the transport factor (TF), which is the product of proton concentration in the swollen membrane and the methanol flux. At low TF values, cell performance is limited by low proton conductivity, whereas at high TF values it decreases due to methanol crossover. The highest maximum power density corresponds to intermediate values of TF.

PYROLYSIS OF LIQUID HEXADECANE WITH SELECTIVE MICROWAVE HEATING OF THE CATALYST

E.I. Udalov, V.A. Bolotov, Yu.Yu. Tanashev, Yu.D. Chernousov*, V.N. Parmon (**Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*)

Theor. Exp. Chem.,
46(6) (2011) pp. 384-392.

The pyrolysis of liquid *n*-hexadecane was studied on various catalysts with selective microwave (MW) heating of a catalyst possessing much greater microwave absorption capacity than the long-chain hydrocarbon studied. This method permits rapid heating of the catalyst to temperatures much higher than 400°C, leading to reflux of the liquid substrate, movement of the catalyst granules within the substrate, and chemical transformations (cracking) of hexadecane. High pyrolysis selectivity relative to α-olefins was found on various catalysts such as magnetic microspheres (coal combustion ash), Al_2O_3/Al, and Pd/KTP (glass fiber). This behavior may be attributed to tempering of the primary products in the bulk of the liquid reagent. Furthermore, MW pyrolysis on magnetic microspheres was found to be accompanied by formation of rather thick carbon microfibers with diameter 300-500 nm.

ANALYSIS OF THE DEACTIVATION OF CLAUS ALUMINA CATALYST DURING ITS INDUSTRIAL EXPLOITATION

P.N. Kalinkin, O.N. Kovalenko, O.I. Platonov*
(**Gipronickel Institute, LTD, St. Petersburg, Russia*)

Catal. Ind.,
3(2) (2011) pp. 183-188.

Change in the activity of AO-NKZ-2 (AO-MK-2) alumina catalyst in the Claus reaction and transformations of carbonyl sulfide during operation over four years in the Claus reactor at the Magnitogorsk Metallurgical Combine's coke-oven gas purification shop were studied at an average temperature of 245–260°C and a volume velocity of ~2000 h^{-1}. The rate constants of the Claus reactions and COS transformation were determined, and the changes in the active surface area of the catalyst were investigated. Fundamental discrepancies in the rate and deactivation mechanism of the Claus catalysts were revealed with respect to the reactions of the conversion of hydrogen sulfide and carbonyl sulfide.

SELECTION OF MODIFYING ADDITIVES FOR IMPROVING THE STEAM TOLERANCE OF METHANE AFTERBURNING PALLADIUM CATALYSTS

**M.A. Mashkovtsev*, A.K. Khudorozhkov,
I.E. Beck, A.V. Porsin, I.P. Prosvirin,
V.N. Rychkov*, V.I. Bukhtiyarov** (**Ural Federal University, Yekaterinburg, Russia*).

Catal. Ind.,
3(4) (2011) pp. 350-357.

In this work, the authors discuss the problem of the afterburning of methane from the exhaust gases of automobile engines fueled by natural gas. In exhaust neutralizers, the PdO/Al_2O_3 catalyst, the main drawback of which is the reduction of its activity under the action of steam that always present in exhaust gases, is commonly used. To improve the tolerance to steam, a series of PdO-Me_xO_y /Al_2O_3 binary catalysts (*Me* is Co, Cu, Fe, Ni, Mn, or Sn) was prepared and studied. Comparative tests under conditions modeling the methane afterburning process in automobile neutralizers show that Pd catalysts promoted with nickel, cobalt, and tin oxides are more resistant to the inhibiting action of steam. The high crystallinity of supported PdO and its uniform distribution over the surface of modified Al_2O_3 are indicated as criteria for the stability of catalysts in the presence of steam. Optimization of the concentration of promotors and the preparation method used for their introduction allows the deactivation of Pd catalysts under the action of steam to be almost completely eliminated.

CATALYTIC TECHNOLOGIES BASED ON APPLICATION OF GLASS-FIBER CATALYSTS

A.N. Zagoruiko, B.S. Bal'zhinimaev

Chem. Ind. Today,
2 (2011) pp. 2-11.

Engineering questions of catalytic technologies based on application of new generation of catalysts on glass-fiber carriers are discussed.

MICROCHANNEL CATALYTIC SYSTEMS FOR THE INTENSIFICATION OF HYDROGEN PRODUCTION FROM CARBON-CONTAINING FEEDSTOCKS

L.L. Makarshin, V.N. Parmon

Catal. Ind.,
4(1) (2012) pp. 27-38.

In the early 1990's, the progress in modern microelectronic technologies gave an impetus to studies of specific behavior of microchannel systems in various physicochemical processes. The microchannel systems were shown, with heat exchangers, mixers and microchannel reactors (microreactors) as examples, to intensify all the processes in the microchannels. In the present review paper, principal criteria, that make possible to classify a flow system as the microchannel one, are discussed. Three main catalytic processes – steam conversion, partial oxidation and autothermal conversion of light hydrocarbons and alcohols into hydrogen-containing gas – are considered and analyzed. It is shown with methane and methanol as examples that the process of hydrogen generation is enhanced indeed in the microreactor. In steam conversion of methanol catalyzed by Zn/TiO_2 at 450°C, the specific hydrogen productivity per catalyst weight was as high as 78,6 L/(h·g_{cat}), the outlet quantity of carbon monoxide being no more than 1 mol.%. In partial oxidation of methane over catalyst $La_{0,2}Zr_{0,4}Ce_{0,4}$/LaNiPt (0,48 g) in a microreactor at 700°C, the specific hydrogen productivity was 521 L/(h·gcat) per catalyst weight and 42 L/(h·cm^3) per reaction zone volume. When so, the thermal capacity (heat generated at hydrogen combustion) is 117 kW for the microreactor with 1,0 dm^3 reaction volume that is comparable to the power of the gasoline engine of a modern vehicle. Hydrogen production from bioethanol, gasoline and diesel fuel also seems promising. Inspection of relevant literature in the field demonstrated that these fuels can compete successfully with methanol and methane, even though the catalytic conversion proceeds at temperatures 650°C or higher. Results obtained in developing fuel cell – catalytic generators of hydrogen-containing gas with a low content of carbon monoxide (less than 20 ppm) – are reported in the last Section. Integrated microchannel systems are shown to be the most promising fuel cells.

CATALYTIC PARTIAL OXIDATION OF METHANE IN MICROCHANNEL REACTORS WITH CO-CURRENT AND COUNTERCURRENT REAGENT FLOWS: AN EXPERIMENTAL COMPARISON

L.L. Makarshin, D.V. Andreev,
A.G. Gribovskii, V.N. Parmon

Chem. Eng. J.,
178(15) (2011) pp. 276-281.

Microchannel catalytic reactors have repeatedly proved their high efficiency in the process of partial oxidation of methane (POM) as compared to traditional fixed-bed catalytic reactors. However, a serious problem of the microchannel reactor operation at this process appears to be high thermal power evolved on the narrow front edge of the microchannel (MC) plates. As a result, the front edge of the plates may undergo thermal corrosion and destruction during the POM process. The way out is to develop microchannel plates, which design would provide a countercurrent reagents flow inside the reactors. A comparison of the operation of microchannel reactors using co-current and countercurrent reagent flows shows substantial advantages of the latter. At high and prolong heating load, a microchannel reactor with the countercurrent reagent flow (MCR-Z) outperforms a reactor with the co-current reagent flow (MCR-P) both in the methane conversion and carbon monoxide selectivity. This is associated with the lower temperature of the front edge of the microchannel plate as well as the lower inner temperature gradient in the MCR-Z in comparison to the MCR-P. Thus, the countercurrent flow scheme allows solving some serious problems of corrosion and destruction of the microchannel plate front edge at high heat loads during the POM process.

USING CATALYSTS BASED ON MOLYBDENUM AND TUNGSTEN CARBIDES IN THE WATER-GAS SHIFT REACTION

G.L. Semin, A.R. Dubrovsky*, P.V. Snytnikov,
S.A. Kuznetsov*, V.A. Sobyanin (**Tananaev*
Institute of Chemistry and Technology
of Rare Elements and Mineral Raw Materials,
Murmansk Region, Apatity, Russia)

Catal. Ind.,
4(1) (2012) pp. 59-66.

The review presents data on the main areas of application of molybdenum and tungsten carbides as catalysts for several industrially important reactions and the basic solutions for the synthesis of catalysts. Some of these methods can be considered as the initial phase of technology development of industrial catalysts based on molybdenum and tungsten carbides. The greatest prospect as a catalyst in the CO conversion by water vapor have a composition based on Mo_2C.

ECOLOGICAL AND ENERGY ASPECTS OF THE PROPANE DEHYDROGENATION PROCESS REALIZED IN THE MEMBRANE REACTOR

E.V. Shelepova, A.A. Vedyagin

Alternative Energy Ecol.,
2 (2011) pp. 98-101.

The both energy and ecological aspects of propylene production in the membrane reactor were analyzed. An approach considering the simultaneous occurrence of the thermodynamically conjugated reactions in the membrane reactor has been suggested and theoretically realized. Such method allows one to reduce the contribution of side reactions due to shifting the equilibrium of the propane dehydrogenation reaction towards formation of propylene. The effect of hydrogen oxidation in the membrane reactor upon the propane conversion has been studied. It was shown that the heat of hydrogen oxidation reaction allows one to minimize energy operating costs for the process of propane dehydrogenation.

KINETICS OF PHENOL HYDROGENATION OVER Pd-CONTAINING HYPERCROSSLINKED POLYSTYRENE

E.M. Sulman*, A.A. Ivanov, V.S. Chernyavskii, M.G. Sulman*, A.I. Bykov*, A.I. Sidorov*, V.Yu. Doluda*, V.G. Matveeva*, L.M. Bronstein, B.D. Stein**, A.S. Kharitonov**
(**Tver Technical University, Tver, Russia; **Indiana University, Bloomington, IN, USA*)

Chem. Eng. J.,
176-177 (2011) pp. 33-41.

Hypercrosslinked polystyrene (HPS) has been used as a support for preparation of the palladium-based catalyst, Pd/HPS, for gas phase hydrogenation of phenol to cyclohexanone. At the phenol conversion 99%, the catalyst provides selectivity for ketone not lower than 95 mol%. The Pd/HPS catalyst showed high stability, retaining its catalytic performance at least for 20 days. Kinetics was used to compare Pd/HPS with the commercial Pd/Al_2O_3 catalyst. The catalytic efficiency was assessed using the derived dimensionless kinetic equation without a ‘time’ parameter. Three major reaction routes with their rate parameters and activation energies were revealed. From kinetic parameters, the maximum possible yield of cyclohexanone in the temperature range of 120–180°C was determined. The important feature of the Pd/HPS catalyst is that selectivity is independent of the temperature at a certain phenol conversion. At elevated temperatures (160–180°C), the selectivity is at least 2–3% higher as compared to the commercial catalyst Pd/Al_2O_3, which makes Pd/HPS largely promising for industrial applications.

DEHYDROGENATION OF PROPANE–ISOBUTANE MIXTURE IN A FLUIDIZED BED REACTOR OVER Cr_2O_3/Al_2O_3 CATALYST: EXPERIMENTAL STUDIES AND MATHEMATICAL MODELLING

N.V. Vernikovskaya, I.G. Savin*, V.N. Kashkin, N.A. Pakhomov, An. Yermakova, V.V. Molchanov, E.I. Nemykina, O.A. Parahin**
(**JSC “Tobolsk-Neftehim”, Tobolsk, Russia; **JSC “NPK Sintez”, Barnaul, Russia*)

Chem. Eng. J.,
176-177 (2011) pp. 158-164.

An influence of propane addition to the inlet feed on the performance of industrial fluid bed reactor for isobutane dehydrogenation was experimentally and numerically studied. Experiments on dehydrogenation of propane–isobutane mixture in a pilot fluidized and in a lab fixed bed reactors were performed over Cr_2O_3/Al_2O_3 industrial catalyst. Adding C_3H_8 to the reactor inlet was found to increase experimental conversion of C_3–C_4 mixture and the total process selectivity to olefins. Results of the mathematical modelling of the industrial-scale fluidized bed reactor show some benefits of C_3H_8 addition. Selectivity to i-C_4H_8 was found to be high enough and grows slightly from 86 to 89% on increasing inlet C_3H_8 fraction from 0 to 60 wt%. Inlet concentrations of C_3H_8 up to 20 wt% lead to the apparent selectivity to C_3H_6 exceeding 100%. Coke yield rises slowly allowing safe industrial fluid bed reactor operation.

CATALYTIC DEHYDRATION OF BIOETHANOL TO ETHYLENE: PILOT-SCALE STUDIES AND PROCESS SIMULATION

A.P. Kagyrmanova, V.A. Chumachenko, V.N. Korotkikh, V.N. Kashkin, A.S. Noskov

Chem. Eng. J.,
176-177 (2011) pp. 188-194.

Process of bioethanol dehydration to ethylene over alumina-based catalyst in tubular fixed bed reactor was studied both experimentally and numerically. Kinetic studies were carried out to determine the reaction network, to estimate the parameters of the kinetic model and to find the optimal conditions that provide the maximal ethylene yield in the reaction of bioethanol dehydration. Pilot scale studies and process simulation were carried out to determine the optimal technological regimes in a single catalyst tube as an element of a multi-tubular reactor. The optimal characteristics and process parameters of industrial tubular fixed bed reactor for ethylene production from bioethanol at capacity of 60,000 TPA have been determined.

INFLUENCE OF ADDITIVES IN THE BATCH ON BENZOPYRENE EMISSION DURING THE PRODUCTION OF ANODIC CARBON AND GRAPHITE

Ch.N. Barnakov*, A.P. Kozlov*, V.I. Malysheva*, Z.R. Ismagilov, V.F. Anufrienko, V.N. Parmon
(**Institute of Coal-Chemistry and Material Science, Kemerovo, Russia*)

Coke Chem.,
54(7) (2011) pp. 241-243.

The influence of various additives to the initial batch on benzopyrene emissions is investigated, both in the production of self-sintering anodes and in the formation of green anodes for graphite production. Benzopyrene is bound in the presence of transition-metal compounds at 600–1000°C.

A CAPILLARY GAS CHROMATOGRAPHIC COLUMN WITH A POROUS LAYER BASED ON THE DIVINYLBENZENE-VINYLIMIDAZOLE COPOLYMER

O.A. Nikolaeva, Yu.V. Patrushev, V.N. Sidelnikov

Russ. J. Phys. Chem. A,
85(9) (2011) pp. 1647-1651.

Capillary columns with a new sorbent based on the divinylbenzene-vinylimidazole organic copolymer are proposed. The properties of the prepared columns are discussed. It is demonstrated that columns based on the divinylbenzene-vinylimidazole polymer with different selectivities can be prepared by varying the relative amount of vinylimidazole in the initial polymerization mixture. The examples of separation of light hydrocarbons, permanent gases, and oxygen-containing compounds are given.

LIQUID-PHASE DECHLORINATION OF TOXIC TECHNOGENIC PRODUCTS USING NANO-DISPERSED PALLADIUM CATALYSTS BASED ON SIBUNIT

A.V. Mekhaev*, M.G. Pervova*, O.P. Taran, I.L. Simakova, V.N. Parmon, M.A. Samorukova*, V.P. Boyarskii, T.E. Zhesko**, V.I. Saloutin*, Yu.G. Yaltuk*** (**Postovsky Institute of Organic Synthesis Yekaterinburg, Russia; **St.-Petersburg State University, St. Petersburg, Russia)*

Chem. Sustain. Devel.,
19(2) (2011) pp. 179-186.

Liquid-phase catalytic reductive dechlorination of toxic technogenic products using catalysts M/Sibunit (M = Ni, Pt, Pd) was investigated. It was shown that the highest activity is exhibited by catalysts based on palladium.

ADSORPTION-CATALYTIC NEUTRALIZATION OF EXHAUST GASES OF DIESEL ENGINES

I.V. Mishakov, A.A. Vedyagin, A.M. Volodin, M.S. Myakisheva

Chem. Sustain. Devel.,
19(1) (2011) pp. 97-104.

The basic aspects of environmental protection from hazardous gaseous impurities present in the exhaust gases of diesel engines are considered. Approaches used for the development of fundamental investigation of adsorbents and catalysts for after-burning CO and hydrocarbons are outlined. Results of the investigation of adsorption capacity of zeolites BEA- and Y-types with respect to heavy hydrocarbons (decane and toluene) obtained with the help of the gravimetric microanalyzer TEOM are presented. It is shown that both zeolites possess comparable capacities with respect to toluene, while the presence of mesopores in BEA-zeolite determines its substantially larger adsorption capcsity with respect to decane. For Pd/Al_2O_3 catalysts as example, the effect of the nature of precursor of active component and treatment conditions on the activity of the catalysts in the oxidation of CO is considered. It is demonstrated that in the case of the mass fraction of deposited chloride components up to 0.25-0.5 % atomically dispersed forms of palladium are formed; they are responsible for the high activity of palladium catalysts.

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SCIENTIFIC PUBLICATIONS

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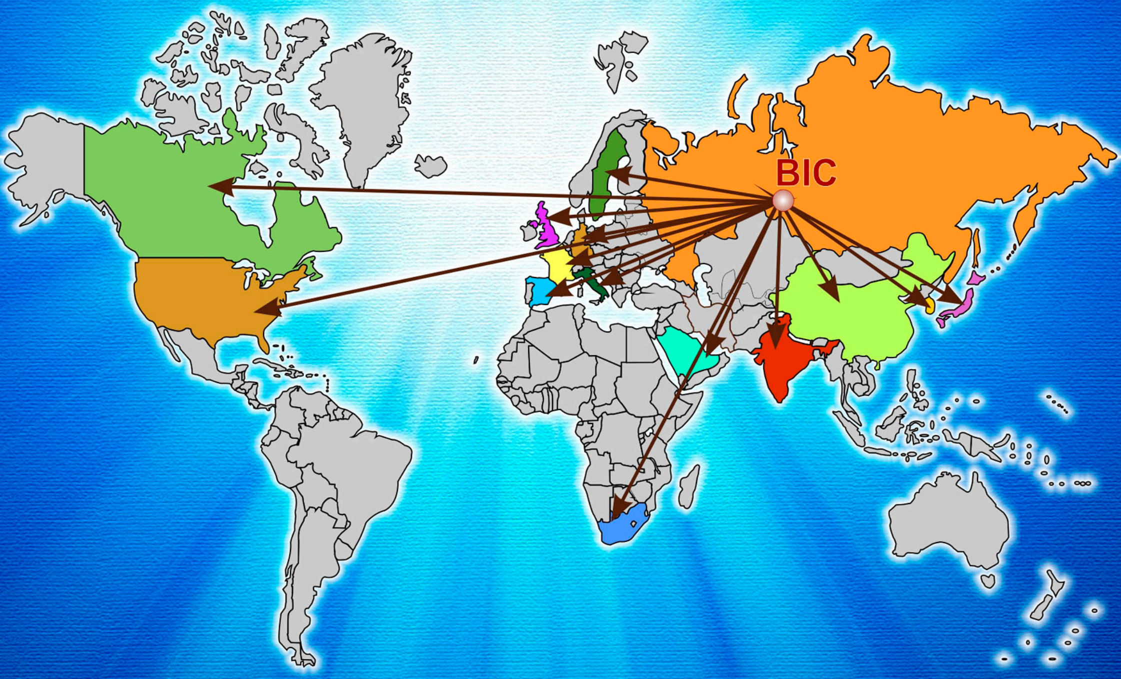

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