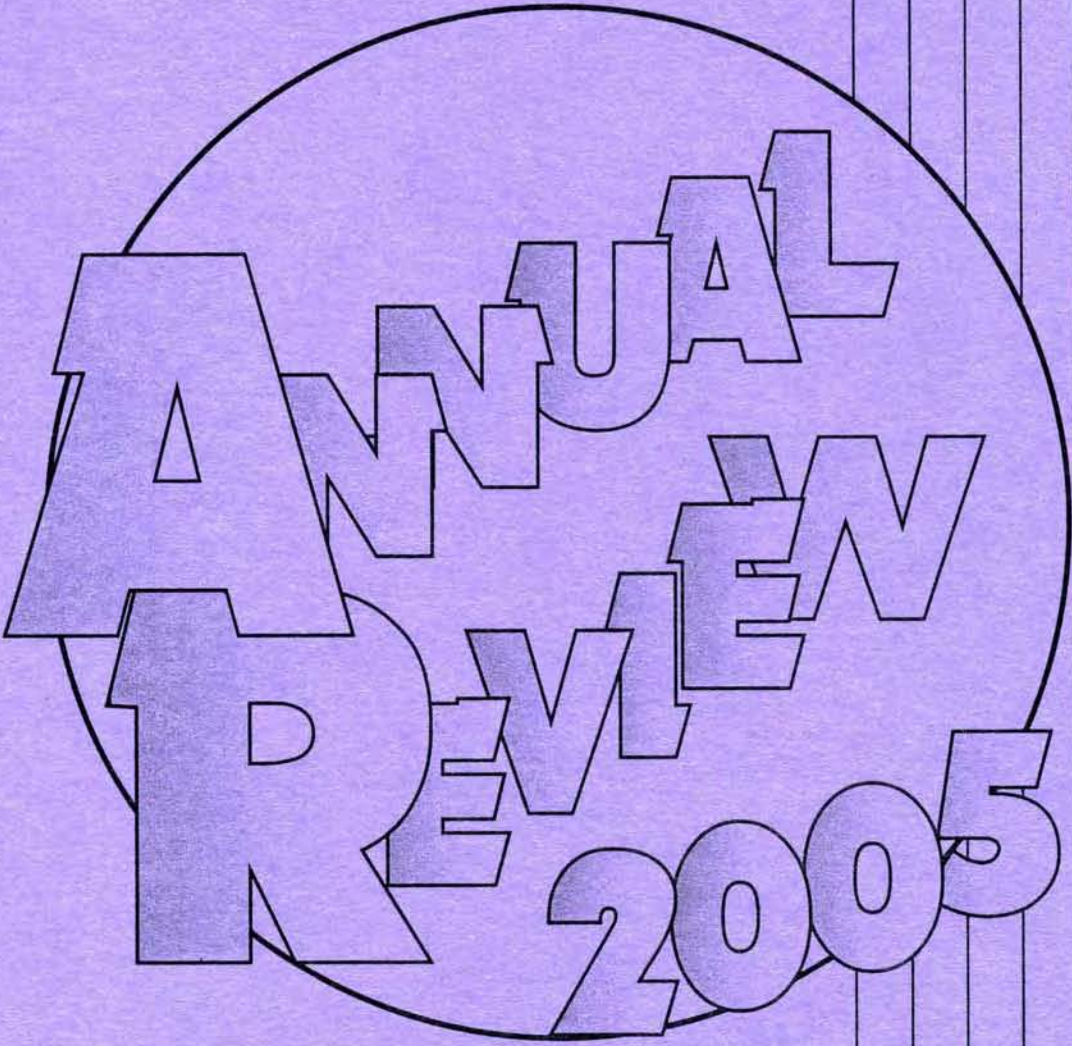
BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES



ANNUAL REVIEW 2005

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ANNUAL REVIEW
of Activities in Fundamental Areas
2004

BORESKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

CONTENT

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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 2004 and reflects now more than the ten-year experience of the Institute in publishing such reviews.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and NIS, but also in many western and oriental countries. Since 1960's it remains the largest Russian chemical research institution in the Asian part of Russia and has numerous 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 real applied problems, including the development of commercial catalysts and catalytic technologies.

The current features of BIC reflect Russia entering into the market economy. BIC belongs to the Siberian Branch of the Russian Academy of Sciences (SB RAS). However, according to new realities of Russia, a lot deal of activity of BIC is now 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 even higher as before. Fortunately, the Institute gained in research in catalysis fundamentals, thus continuing the old traditions originated from the beginning of the Institute due to a very powerful 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.

The year 2004 was very important for the life of BIC in many aspects. First of all, BIC participated very actively in a largest innovation project of new Russia in the field of application of catalysis in large scale oil refinery. All the technical targets of that project, sponsored by the Russian Ministry of Industry and Energetics, have been fulfilled: Russia was offered two excellent industrial catalysts and one principally new industrial chemical technology. Also, BIC started working actively in development of efficient mobile systems for the production of hydrogen for modern fuel cells, and succeeded in this work, which was supported by one of the largest Russian manufacturing company "Norilsk Nickel".

Thus, reestablishing strategic collaboration with the Russian industries is, undoubtedly, a new and very important feature of the scientific activity of the Boreskov Institute, as well as of many academic institutes of RAS.

Since 1998, the Institute has operated in the status of the Key Russian institution and federal coordinator in the field of catalysis and catalytic technologies, i.e. in the very high federal status, the same as the Institute had in the former USSR.

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, which was called the United Institute of Catalysis (UIC). According to the UIC bylaw, the director of the Boreskov Institute of Catalysis is simultaneously the general director of the UIC. In 2004 there were some rearrangements in the UIC structure, since the Omsk Division of the BIC has separated from BIC as an Institute of Hydrocarbons Processing (IHP), and the Volgograd Scientific center has joined the BIC as its Volgograd Division. Thus, now UIC consists of two large R&D entities: BIC and IHP. The facilities of the UIC include three powerful semi-industrial plants capable of providing manufacturing of 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. Indeed, current management of the Institute realises all the existing problems 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.

Hope, this issue of the Annual Review of the Boreskov Institute of Catalysis is exhibiting many sides of the current 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 or are inviting to visit the Institute’s website.

Valentin N. Parmon

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

The Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences (BIC) still remains the largest specialized institute working in the field of catalysis not only at the territory of Asian part of Russia, but in the world too. It is the only institution in the country fully specialized on the problems of catalysis and encompasses all its aspects from fundamental and theoretical to industrial mastering of new catalysts.

The Institute was founded in 1958. 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 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 (up to 1000 people in staff) 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) includes the Boreskov Institute of Catalysis, St. Petersburg Division, Moscow Department, Volgograd Scientific-Engineering Center, BIC Europe BV (The Netherlands) and the Institute of Hydrocarbons Processing in Omsk.

CONTENT

STRUCTURE OF THE INSTITUTE

The Institute of Catalysis with its St. Petersburg Division currently has 900 employees including researchers and their co-workers, of these 1 Members of the RAS, 2 Corresponding Members of the RAS, about 60 Professors, about 200 have a Ph.D. degree, more than 60 Ph.D. students, personnel of Service, Managing, Engineering and Pilot Departments to support and promote R&D activities. The Institute presents the unique society of qualified specialists in broad spectra of catalysts problems, able to solve any questions related to phenomena of catalysis, from theoretical problems like quantum-chemical calculations up to designing of industrial catalysts and processes.

The structure of the Institute incorporates 6 Scientific-Research Departments, Department of Applied Catalysis, Center for Catalyst Characterization and Testing, and Information Center. The structure of the Institute includes also scientific-supportive units, manufacturing facilities, administration and services.

The Center for Catalyst Characterization and Testing has a bank of catalyst samples, supports and adsorbents, a set of State Standard Samples to calibrate and certify instruments for measurements of specific surface areas of various dispersed and porous materials.

The main directions of its activity are:

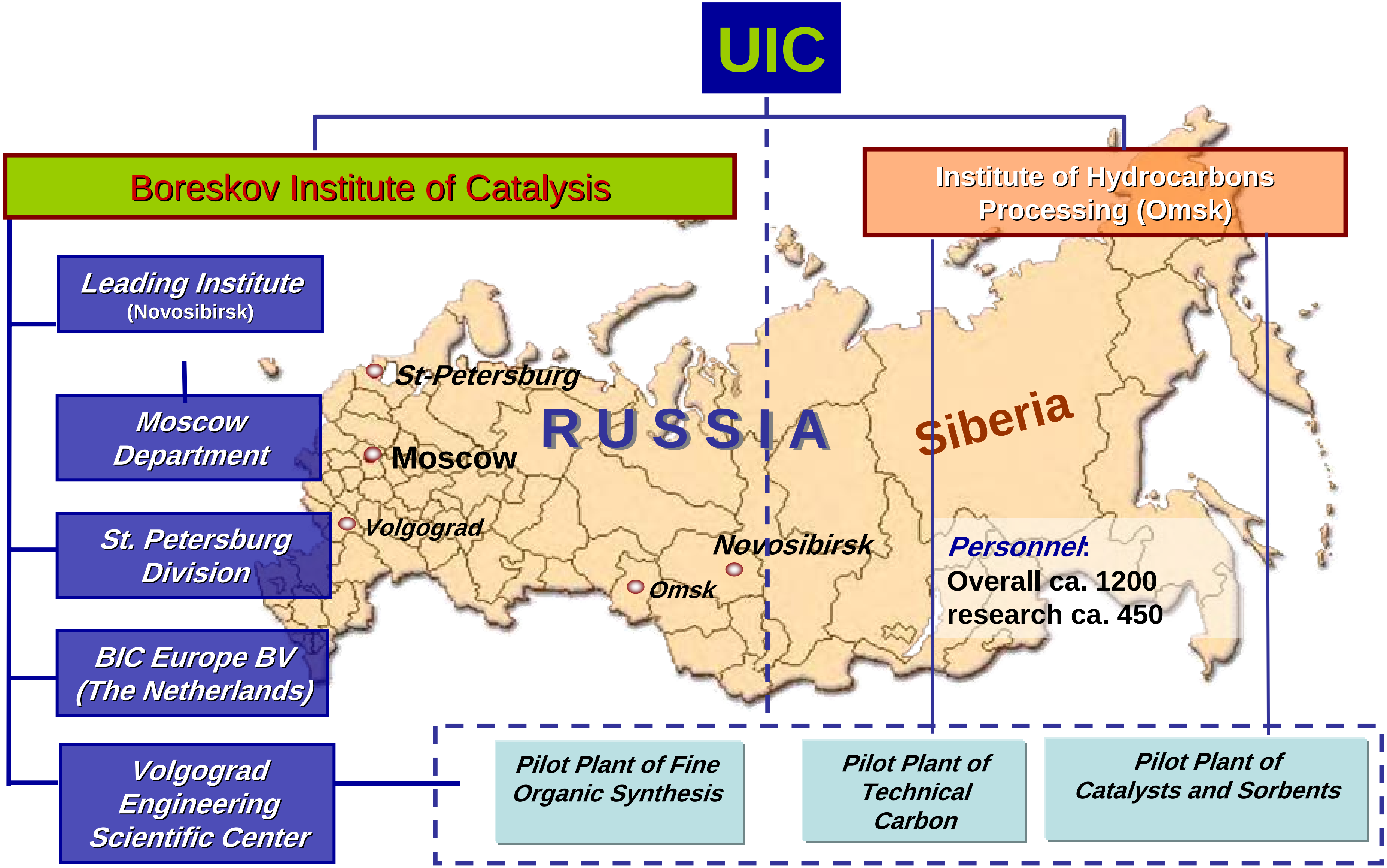
- Complex investigation and characterization of the catalysts by a set of modern physicochemical methods.
- Joint scientific projects with foreign firms and organizations on studying certain catalytic processes and catalysts for the purpose of their improvement.
- Development of modern standard experimental methods and equipment for catalyst studies and tests. Design of catalysts and materials with certificated properties.

In its work Center bases on high potential of the Institute, its fundamental and applied studies in all fields of catalysis, its outdated instrumentation and methods for catalytic systems studying.

The Information Center of the Institute comprises the Library of Scientific Literature and the Group of mathematical and program support. It has developed the information system 'Catalysis', which includes the updated data bases, such as the bibliography and the actual state of the art, related to research and applied works in the field of catalysts, commercial catalysis and catalytic processes developed in foreign countries and countries of the former USSR. The Centre can connect with remote databases through Internet and offers information on clients request.

Department of Applied Catalysis with a complex bench of adoption and testing of processes and catalysts provides commercialization of new developments in shortest time.

UNITED INSTITUTE OF CATALYSIS (UIC)
(Founded in 1997)



UIC

Boreskov Institute of Catalysis

- *Leading Institute* (Novosibirsk)
- *Moscow Department*
- *St. Petersburg Division*
- *BIC Europe BV (The Netherlands)*
- *Volgograd Engineering Scientific Center*

Institute of Hydrocarbons Processing (Omsk)

- *Pilot Plant of Fine Organic Synthesis*
- *Pilot Plant of Technical Carbon*
- *Pilot Plant of Catalysts and Sorbents*

***Personnel*:**
Overall ca. 1200
research ca. 450

STRUCTURE OF THE INSTITUTE

Directorate:
V.A. Sobyanin, R.A. Buyanov, V.N. Parmon,
A.S. Noskov, B.I. Ermakov, O.N. Martyanov,
S.P. Kildyashev, S.E. Glaznev, B.S. Bal'zhinimaev,
I.A. Kamolkin, V.I. Bukhtiyarov

DIRECTOR

Directorate

Scientific Council

Research Departments

☑ 

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
Head: Prof. Dimitrii I. Kochubey

☑ 

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

☑ 

DEPARTMENT OF HETEROGENEOUS CATALYSIS
Head: Prof. Vladimir A. Sobyanin

☑ 

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS
Center for Catalyst Characterization and Testing
Head: Prof. Bair S. Bal'zhinimaev

☑ 

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

☑ 

SCIENTIFIC PRODUCTION DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC SYNTHESIS
Head: Prof. Zinaida P. Pai

DEPARTMENT OF APPLIED CATALYSIS
Head: Dr. Il'ya A. Zolotarskii

☑ 

INFORMATION CENTER
Head: Dr. Andrey O. Kuzmin

Scientific-Supportive Units

Manufacturing Facilities

Administration and Services

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

Head of the Department Prof. Dimitrii I. Kochubey

☑

Surface Science Laboratory

Head: Prof. Valerii I. Bukhtiyarov

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

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: Prof. Vladimir B. Fenelonov

Group of Synthesis of Surface Compounds

Head: Dr. Vladimir L. Kuznetsov

Group of Low Temperature Catalysis by Metals

Head: Prof. Vladimir V. Gorodetskii

Group of Solid-State NMR Spectroscopy

Head: Prof. Olga B. Lapina

Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion

Head: Prof. Alexander G. Stepanov

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES

Head of the Department Acad. Valentin N. Parmon

☑ 

Laboratory of Catalytic Methods of Solar Energy Conversion

Head: Acad. Valentin N. Parmon

Laboratory of Energy Accumulating Materials

Head: Prof. Yurii I. Aristov

Laboratory of Catalytic Processes for Desulfurization

Acting Head: Dr. Olga N. Kovalenko

Laboratory of Adsorption

Head: Dr. Oleg N. Martyanov

Laboratory of Sulfide Catalysts

Head: Prof. Anatolii N. Startsev

Group of Metal Complex Catalysis

Head: Prof. Nina I. Kuznetsova

Group for Stereoselective Catalysis

Head: Dr. Oxana A. Kholdeeva

Group of Photocatalysis on Semiconductors

Head: Dr. Alexandr V. Vorontsov

Group of Aerosol Catalysis

Head: Dr. Valerii N. Snytnikov

Group of Catalytic Reduction of Organic Compounds
Head: Prof. Valentina I. Simagina

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

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

Group of Metallorganic Catalysts
Head: Prof. Alexandr S. Lisitsyn

Group of Biocatalysis
Head: Dr. Galina A. Kovalenko

Group of High-Energy Processes
Head: Gennadii I. Anisiforov

Group of Electrocatalysis and Fuel Cells
Head: Dr. Elena R. Savinova

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

DEPARTMENT OF HETEROGENEOUS CATALYSIS

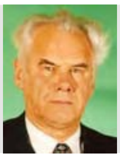
Head of the Department Prof. Vladimir A. Sobyanin

☑

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

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

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



Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov

Laboratory of Oxidative Catalysis over Zeolites
Head: Prof. Gennadii I. Panov

Laboratory of Heterogeneous Selective Oxidation
Head: Prof. Tamara V. Andrushkevich

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

Group of Heterogeneous Catalysts on the Basis of Noble Metals
Head: Prof. Anatolii V. Romanenko

Group of Selective Oxidation over Metal Oxides
Head: Dr. Vladimir I. Sobolev

Group of Reactions of Oxidation on Metals

Head: Prof. Aleksandr V. Khasin

Group of Synthesis of Nanodispersed Materials

Head: Prof. Oleg P. Krivoruchko

Laboratory of Aerosol Nucleation

Head: Prof. Mikhail P. Anisimov

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS

Head of the Department Prof. Bair S. Bal'zhinimaev

☐

Center for Catalysts Characterization and Testing

Head: Prof. Bair S. Bal'zhinimaev

Laboratory of Zeolites and Acid Base Catalysis

Head: Prof. Eugenii A. Paukshtis

Laboratory of Catalysts Activity Testing

Head: Dr. Nikolai N. Bobrov

Group of Catalytic Conversion of Sulfur-Containing Compounds

Head: Prof. Anna V. Mashkina

Department of Applied Catalysis

Head: Il'ya A. Zolotarskii

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 Industrial Catalytic Processes

Head: Il'ya A. Zolotarskii

Laboratory of Catalytic Polymerization

Head: Prof. Vladimir A. Zakharov

Laboratory of Catalytic Hydrocarbon Conversion

Head: Prof. Gennadii V. Echevsky

Laboratory of Multiphase Processes Modeling

Head: Prof. Valerii A. Kirillov

Laboratory of Catalytic Conversion of Carbon Oxides

Head: Dr. Aleksandr A. Khassin

Laboratory of Dynamics of Catalytic Processes

Head: Dr. Andrey N. Zagoruiko

Laboratory of Catalytic Conversion of Solid Fuels and Wastes

Head: Dr. Aleksandr D. Simonov

Group of Catalytic Technologies for Carbon Materials Synthesis,

Head: Dr. Vadim A. Yakovlev

Group of Kinetics of Catalytic Processes

Head: Dr. Sergei I. Reshetnikov

Group of Mathematical Methods for Catalytic and Adsorption Processes Modeling

Head: Dr. Natalia A. Chumakova

SCIENTIFIC PRODUCTION DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC SYNTHESIS

Head of the Department Prof. Zinaida P. Pai

Laboratory of Catalytic Liquid-Phase Synthesis of Organic Compounds

Head: Prof. Zinaida P. Pai

Group of Catalysts and Processes Based on Heteropoly Acids

Head: Prof. Klavdii I. Matveev

ST. PETERSBURG DIVISION
OF THE BORESKOV INSTITUTE OF CATALYSIS

Director and Scientific Manager
Prof. Sergey S. Ivanchev

Vice-Director Dr. Valery P. Tulmankov

Laboratory of Micellar Catalysis, Emulsion Polymerization and Processes for Obtaining Polymeric Composites
Head: Prof. Valery N. Pavlyuchenko

Laboratory of Novel Catalytic Systems for Olefin Polymerization and Copolymerization
Head: Prof. Sergey S. Ivanchev

SCHOOLS OF THE BORESKOV INSTITUTE OF CATALYSIS

The Boreskov Institute of Catalysis has numerous and deep traditions and continues intensive fundamental and applied investigations. It possesses an actively and fruitfully working school of specialists in catalysis.

Many works by the school of **Acad. Georgii K. Boreskov** in the field of deep and partial oxidation processes are well known in our country and far from its frontiers.

The principal importance has the concept of chemical nature of phenomenon the decisive role in which belongs to the intermediate chemical interaction between the reagents and catalysts. The fundamentals of the theory of heterogeneous oxidative catalysis are:

— The key importance of the energy of reagent bonding to the catalyst for the rate and rote of oxidation reactions;

— The influence of cation nearest environment on catalytic properties;

— A viewpoint on reaction medium and catalyst as an indivisible system;

— An idea of stepwise and concerted mechanisms of redox reactions.

Under the guidance of **Prof. Mikhail G. Slin'ko** in 60-70th years a school raised famous not only in Russia, but abroad as well.

M.G. Slin'ko developed a method of mathematical modeling of catalytic reactors and processes, based on hierarchical principle. This method was developed for multi-phase processes and reactors with fixed and fluidized beds.

Design of real industrial catalysts with optimum strength, pore structure; providing their reproducibility on a large scale are the necessary elements of all aspects in the field of applied catalysis. **Prof. Vera A. Dzis'ko** contributed significantly to the development of methods of preparation and studying the regularities of oxide catalysts formation.

The revealed correlation of preparation conditions and physico-chemical properties of oxide systems allowed to formulate the criteria to control phase composition, surface area, stability, and acid-base properties, that appeared to be the basis for creation of a number of industrial catalysts and carriers.

At the end of the 60s big progress was in the field of homogeneous catalysis and catalysis by transition metal complexes. Of essential importance in this field not only for our country were the works by **Prof. Yurii I. Yermakov**.

Yu.I. Yermakov formulated the conception of the surface metal-organic compounds as active sites precursors for the supported catalysts. It served as a basis for the new approach in catalysis – application of principles used in homogeneous catalysis to study fundamental problems of heterogeneous catalysis. Methods for purposeful synthesis of supported catalysts of desired composition and dispersity have been developed.

In the 1977-1978 a big team of chemical physicists of the younger generation headed by **Acad. Kirill I. Zamaraev** came from Moscow. The flow of these specialists significantly enlivened the atomic-molecular studies of catalytic reaction mechanisms and catalytic properties of heterogeneous catalysis by physicochemical methods.

CONTENT

The school by K.I. Zamaraev contributed much to:

— Development of theory of electron tunneling in condensed media;

— Coordination chemistry of metal-complexes solutions;

— Step-wise description of homogeneous catalytic reactions;

— The works in photochemistry, photocatalysis and solar-to-chemical energy conversion.

The main principle of these works is the complex application of modern physico-chemical technique to mechanistic studies of heterogeneous and homogeneous reactions, studies of the structure and the active sites at the molecular level, search of new nontraditional directions in catalysis.

The teams headed by Prof. Roman A. Buyanov, Prof. Vladimir A. Likholobov, Acad. Valentin N. Parmon, Prof. Georgii M. Zhidomirov won the competitive Program “Leading Scientific Schools” supported by RFBR.

Prof. Roman A. Buyanov developed the home school of fundamentals for catalyst preparation and technology**.**

The main research areas covered are:

— Design and application of new methods to increase solid phases activity at catalysts preparation and to control their activity and selectivity;

— Study of catalysts deactivation and carbon-mineral compositions formation;

— Development of the theory of non-branched radical chain reactions in the absence of oxygen (pyrolysis);

— Design of industrial catalysts.

The works by school of **Prof. Vladimir A. Likholobov** initiated development of methodological and fundamental approaches to the synthesis of effective homogeneous and heterogeneous catalysts for organic synthesis.

The main conceptions of this school are:

— Molecular design of catalytic compositions on all hierarchical levels;

— “Assembly” of active centers of metal complex catalysts;

— Synthesis of porous supports with desired texture and surface properties.

The works of school by **Acad**. **Valentin N. Parmon** relate to:

— Design and study of novel and nontraditional catalytic processes, first of all, photocatalytic and thermochemical methods for the direct conversion of solar energy and ionizing radiation energy;

— Development of an original approaches to description of catalytic processes by methods of nonequilibrium thermodynamics;

— Study of a possible impact of photocatalysis over the troposphere aerosols on the global chemistry of the Earth atmosphere.

The school of **Prof. Georgii M. Zhidomirov** develops the quantum-chemical direction in theoretical spectroscopy and molecular theory of catalysis:

The methodological basis for molecular (cluster) modeling of catalytic systems is formulated, the cluster approximation is widely used to calculation of electronic structure and reactivity of active sites on zeolites and oxide catalysts.

R&D ACTIVITY OF THE INSTITUTE

Fundamental catalysis

- Determination of general physico-chemical regularities of catalysis
- Development of scientific basis for molecular design of substances and materials
- Development of the theoretic basis for realization of catalytic processes.

Applied catalysis

- Design of highly efficient catalysts of new generation for the production of key chemicals and oil processing
- Design of catalytic compositions and technologies for innovative application areas
- Development of innovative catalysts and catalytic technologies manufacturing complex chemicals and polymers with preconceivable properties
- Design of sorbents, catalysts and technologies for detoxication of hazardous technogenous wastes.

Strategic R&D Priorities

Fundamental Studies

1. *In situ* methods for studies of catalyst states and mechanisms of catalytic reactions of practical importance
2. Methods and algorithms for prediction of catalytic action
3. Methods and facilities for rapid selection and testing of catalysts
4. Theoretical methods of quantum chemistry and computational gas- and hydrodynamics

Research Studies

1. Selective oxidation of light paraffins C1-C4 by molecular oxygen into organic products
2. Gas-phase epoxidation of propylene by molecular oxygen
3. Processes based on catalytic membranes and microreactors

New catalytic technologies owned by BIC

- A family of new unsteady-state technologies in catalysis:
  — «Reverse-process»
  — Partial oxidation over unsteady-state catalysts
- A family of technologies based on combustion in a fluidized catalyst bed «Catalytic Heat Generators»

- Processing of oil, natural gas, and coal
- Large-scale inorganic synthesis
- Catalytic technologies for carbon-carbonaceous composites production
- Catalytic technologies for energy production

Catalytic Processes from Molecular Level to Industrial Plants

2004 Post-treatment of tail gases of Claus process, Russia

2003 BIMF process - production of high-quality motor fuels, Russia

2002 Selective water sorbents, Russia

2001 Reforming catalysts, Russia

BCS , Estonia, 2001

2000 New technology of loading the reactors with catalysts, Russia

1999 Catalyst for hydropurification of terephthalic acid

Developed in cooperation with Samsung Chemicals, Korea, 2000

1998 One-step technology for production of nicotinic acid, Russia

Degussa, Germany, 2000

1997 Non-platinum catalyst for production of nitric acid, Russia

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

Jointly designed with SOLUTIA, USA, 1996

1995 Catalyst for FCC (oil cracking), Russia

1993 Carbonaceous material SIBUNIT, Russia

Sibunit for phosgene synthesis, DuPont, 1994, USA

1992 ZEOFORMING process for synthesis of gasoline, Russia

Lurgi, Germany, 1994

1988 Catalysts for polypropylene polymerization, USSR

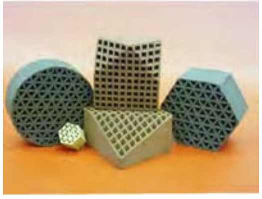
DSM, the Netherlands, 1995

1982 REVERS-Process, USSR

Monsanto Enviro-Chem. Systems, USA, 1992

1978 Vanadium catalysts for sulfuric acid production, USSR

1958



- Catalytic technologies for environmental protection
- Production of food, medicines, and biopreparations
- Purification of hydrocarbon-containing gases from H_2S *via* its partial oxidation to sulfur

- Processing of sulfur-containing organics
- Partial oxidation of organics with bounded oxygen
- Zeolite-based processes (zeoforming, condensation, nitration
- Catalytic partial oxidation of aromatics under unsteady-state conditions
- Oxidation of methanol in an adiabatic catalyst bed to produce formaldehyde
- Direct oxidation of methanol to formic acid
- Direct gas-phase oxidation of β-picoline to nicotinic acid
- SOZh technology (the Claus process in aqueous solutions to remove sulfur compounds)
- Catalytic combustion using honeycomb and mat catalysts
- Synthesis of vitamins C, K and E
- Synthesis of aromatic amines and other fine organics
- HPA-based technologies
- «Chemical Heat Accumulators»

New industrial catalysts by BIC

- Catalysts for inorganic synthesis
- Catalysts for organic and fine synthesis
- Catalysts for olefin polymerization
- Catalysts for oil processing
- High silica zeolites
- Catalysts for treatment of gaseous and liquid wastes of industries, energetics, transport, etc.
- Catalysts for treatment of technological gases.

New catalyst supports by BIC

- A systematic set of alumina supports prepared through a single technology
- Catalyst supports of very high mechanical strength for fluidized and moving catalyst beds
- Mechanically strong carbon supports with adjustable porous structure
- Ceramic and carbon monoliths
- Mechanically strong supports for immobilization of enzymes
- Aerogels.

CONTENT

INSTRUMENT FACILITIES

The Institute engages the leading position in the world in the improvement and design of new physicochemical methods for catalyst study. 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.

Analytical (composition of catalysts and catalytic reaction products)

Bulk composition

Atomic emission spectrometry
Atomic absorption spectroscopy
X-Ray fluorescence analysis of macro- and microprobes

Phase analysis

X-Ray diffraction, including *in situ* diffraction
Differential dissolution
Thermally programmed reduction, oxidation, desorption
X-Ray diffusion scattering
EXAFS spectroscopy (for amorphous materials)

Morphology

Transmission electron microscopy
High resolution transmission electron microscopy (HRTEM)
Scanning electron microscopy
Scanning tunneling microscopy
X-Ray small-angle scattering

Surface

X-Ray photoelectron spectroscopy (XPS)
Secondary ion mass-spectrometry (SIMS)
Determination of the surface acidity using IR spectroscopy of probe molecules

Molecular composition of individual compounds and their mixtures

Gas, gas-liquid and liquid chromatography on packed, capillary and polycapillary columns
Superrapid chromatography
Mass-spectrometry

Adsorptive (specific surface area, pore structure, adsorption heat)

Porosimetry
Calorimetry

Kinetic

- Gradientless and integral differential reactors
- Fast relaxation technique
- Stop flow technique
- Radiochemical and isotopic methods
- Mass-spectrometric detection of free radicals.

Spectral methods

- NMR spectroscopy on different nuclei, including high-temperature and *in situ*
- ESR spectroscopy, including *in situ*
- FMR spectroscopy, including *in situ*
- VUV electron spectroscopy
- UV-VIS electron spectroscopy
- Vibrational spectroscopies (IR, including *in situ,* and RAMAN)
- HREELS
- LEED
- X-Ray and NMR tomography

CONTENT

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

Brazil	1	Germany	31	Poland	4
Canada	2	Hungary	2	Saudi Arabia	4
China	13	Israel	3	Serbia	3
Cyprus	1	Italy	10	Spain	1
Czechia	8	Mexico	1	Switzerland	10
Denmark	1	Netherlands	11	Thailand	1
Finland	2	Northern Ireland	1	UK	5
France	38	Japan	3	USA	15

Visits of foreign specialists to the Boreskov Institute of Catalysis

Canada	1	Israel	2	Sought Korea	2
China	12	India	2	Switzerland	1
Denmark	1	Japan	14	Syria	2
France	7	Netherlands	3	UK	8
Germany	4	Saudi Arabia	1	USA	19

CONTENT

SCIENTIFIC COOPERATION WITHIN THE FRAMEWORK OF CONTRACTS AND AGREEMENTS WITH NATIONAL SCIENTIFIC CENTERS OF FOREIGN COUNTRIES

ITALY

The cooperation in the frame of the agreement between Russian Academy of Sciences (RAS) and National Council on the Scientific Research of Italy:

- **Istituto di Trasformazione e Accumulazione d'Energia**, Messina – **BIC**, Novosibirsk, *"Catalysis for Solving the Energy Problem"*. Coordinators: **Prof. Yu. Aristov** (*BIC*) and **G. Restucchia** (*Istituto di Trasformazione e Accumulazione d'Energia*).
- **Istituto di Ricerhe sulla Combustione**, Napoli - **BIC**, Novosibirsk, *"Study of Combined Process of Catalytic Combustion and Olefins Production from Natural Gas at Ultrashort Contact Times"*. Coordinators: **Prof. Z. Ismagilov** (*BIC*) and **Prof. G. Russo** (*Istituto di Ricerhe sulla Combustione*).

FRANCE

According to the agreement between RAS and CNRS BIC collaborates with:

- **Institute de Recherches sur la Catalyse**, Villeurbanne in the frame of the Russian-French European associated Laboratory on Catalysis which 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*
- *Clean Catalytic Oxidation Reactions for Fine Chemistry*
- *Dynamics of Protons and Confined Species in Solids*

Coordinators: **Prof. B. Bal'zhinimaev** (*BIC*) and **Dr. P. Gallezot** (*IRC*).

- **Université Pierre et Marie Curie**, Paris, **Université des Sciences et Technologies de Lille** on the Project *"Development of Novel Method of Quadrupole Nuclei to Study Vanadium Systems"*. Coordinators: **Prof. O. Lapina** (*BIC*) and **Prof. J. Fraissard** (*Université Pierre et Marie Curie*).

INDIA

In the frame of Indo-Russian Integrated Long Term Programme of cooperation in science and technology (ILTP) BIC collaborates with

- **Indian Institute of Chemical Technology**, Hyderabad, on the Project *"Study and Development of Heterogeneous Photocatalytic Removal of Hazardous Compounds from Air and Water"*. Coordinators: **Dr. A. Vorontsov** (*BIC*) and **Dr. M. Sabramaniam** (*Indian Institute of Chemical Technology*)
- **National Chemical Laboratory**, Pune on the Project *"Design of Bifunctional Supported Non-Iron Catalysts for Low Temperature Ammonia Synthesis"*. Coordinators: **Prof. V. Likholobov** (*UIC*), **Dr. B. Moroz** (*BIC*) and **Dr. S.B. Halligudi** (*National Chemical Laboratory*).

POLAND

In the frame of RAS-PAS agreement **BIC** cooperates with the **Institute of Chemical Technology**, Glivitse on the Project *"Synthesis and Utilization of Hyperporous Solids"*. Coordinators: **Prof. Yurii I. Aristov** (*BIC*) and **Prof. A.B. Jarzębski** (*Institute of Chemical Technology*).

GERMANY

The cooperation in the frame of the agreement between RAS and German Scientific Research Society (GSRS) with

- **Munich Technical University**, Munich on the Project *"Study of Macrokinetics in Direct Methanol Fuel Cells with Given Layer Structure". Coordinators:* **Dr. P. Simonov** (*BIC*) and **Prof. U. Stimming** (*Munich Technical University*)
- **Fritz-Haber-Institut der Max-Planck-Gesellschaft**, Berlin on the Projects
- *"Study of the Catalysts for Partial Oxidation"*. Coordinators: **Prof. V. Bukhtiyarov** (*BIC*) and **Prof. R. Schlögel** (*Fritz-Haber-Institut der MPG*)
- *"Development of in situ Methods for Study of Solid Surfaces"*. Coordinators: **Prof. V. Bukhtiyarov** (*BIC*) and **Dr. H.-J. Freund** (*Fritz-Haber-Institut der MPG*)
- **Institute for Mineralogy, Crystallography and Material Science at Leipzig University** on the Project *"Novel Nanomaterials of Complex Sulphides in PdS-Bi_2S_3 and $CuPdBiS_3$-Bi_2S_3 Systems"*. Coordinators: **Prof. S. Tsybulya** (*BIC*) and **Prof. Dr. K. Bente** (*Leipzig University*).

COOPERATION WITH FOREIGN ORGANIZATION IN THE FRAMEWORK OF BILATERAL AGREEMENT

SPAIN

The cooperation with research institutions of Spain:

- **Institute of Computational Chemistry**, Girona - *"Development and Applications of New Theoretical Approach to Investigation of the Electronic Structure and Spectra of Fullerene-Like Systems*". Coordinators: **Prof. B. Plakhutin** (*BIC*), **Prof. R. Carbo-Dorca** (*Institute of Computational Chemistry*)
- **Sevilla Institute of Material Sciences** - "*Nanoparticles on the Base of Mixed Oxides of the Transition Metals. Catalytic and Photocatalytic Activity in the Ecological Processes, Oxides for Microelectronics"*. Coordinators: **Prof. D. Kochubey** (*BIC*), **Dr. J. Navio** (*Sevilla Institute of Material Sciences*)
- **Institute of Catalysis and Petrochemistry**, Madrid - *"Fundamental and Technical Aspects of in-situ Spectroscopy of Oxide Catalysts"*. Coordinators: **Prof. O. Lapina** (*BIC*), **Dr. M. Banares** (*Institute of Catalysis and Petrochemistry*).

CONTENT

COOPERATION IN THE FRAME OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

I. Advanced Highly Ordered Thermostable Nanoscale Silicates, their Derivatives and Composite Materials

Project Coordinator:

Dr. A. Gedeon, Pierre and Marie Curie University, Paris, France

Participants:

Dr. R. Dinnerbier, Max-Plank Institute for Solid State Research, Stuttgart, Germany
Prof. V. Fenelonov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. S. Kirik, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia.

II. Nanocrystalline Dense Oxide Materials as High Mixed Conductivity Membranes for Efficient Methane Conversion into Syngas by the Oxygen of Air; Fundamentals of Synthesis by Advanced Methods and Factors Determining their Performance

Project Coordinator:

Dr. S. Neophytides, Institute of Chemical Engineering & High Temperature Processes-FORTH, Patras, Greece

Participants:

Dr. V. Zyryanov, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia
Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. L. Ivashkevich, Research Institute for Physical and Chemical Problems, Belarus State University, Minsk, Belarus
Prof. J.M. Criado, Sevilla Institute of Material Sciences, University of Sevilla–Consejo Superior de Investigaciones Cientnficas (C.S.I.C.), Sevilla, Spain.

III. Study of Solar Assisted Adsorption Cooling Unit Using New Adsorbed Materials

Participants:

Istituto di Tecnologie Avanzate per L'energia, CNR-ITAE, Italy
Aachen University of Technology, RWTH-Aachen, Germany
Boreskov Institute of Catalysis, Novosibirsk, Russia **(Prof. Yu. Aristov**)
Institute for High Temperatures, Moscow, Russia
Moscow Lomonosov State University, Moscow, Russia
Institute of Engineering Thermophysics, Kiev, Ukraine.

IV. Transformation of Gas Condensates into Gasoline: Elucidation of the Mechanism and Catalytic Design

Project Coordinator:

Prof. F. Fajula, Ecole Nationale Superieure de Chemie de Monpellier, France

Participants:

Prof. I. Ivanova, Moscow Lomonosov State University, Moscow, Russia
Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. E. Derouane, Universidade to Algarve Faculdade de Ciencias e Technologia, Faro, Portugal
Dr. Ya. Khimyak, University of Liverpool, Liverpool, UK.

NATO PROGRAMME: SCIENCE FOR PEACE

I. Novel Photocatalysts and Processes for Degradation of Chemical Warfare Agents

NATO Country Project Director:

Prof. P. Smirniotis, University of Cincinnaty, Cincinnaty, USA

Partner Country Project Director:

Dr. A. Vorontsov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

II. Mixed Conducting Membranes for Partial Oxidation of Natural Gas to Synthesis Gas

NATO Country Project Director:

Prof. J. Frade, Department of Ceramics and Glass Engineering, University of Aveiro, Aveiro, Portugal

Partner Country Project Director:

Dr. V. Kharton, Institute of Physicochemical Problems, Belarus State University, Minsk, Belarus

Project Co-Directors:

Dr. J. Irvine, School of Chemistry, University of St. Andreas, Scotland, UK
Dr. T. Norby, Centre for Material Science, University of Oslo, Oslo, Norway
Dr. J. Jurado, Institute of Ceramics and Glass, Madrid, Spain
Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Kozhevnikov, Institute of Solid State Chemistry, Ekaterinburg, Russia
Dr. L. Boginsky, Institute for Personal Development and Staff Retraining in New Areas of Techniques, Technologies and Economics of the Belarus Ministry of Education, Minsk, Belarus.

CRDF

I. Polyoxometalate - Fabric Catalysts for the Purification of Polluted Air in Human Environments

Project Coordinators:

Dr. O. Kholdeeva, Boreskov Institute of Catalysis, Novosibirsk, Russia

Dr. C. Hill, Emory University, Atlanta, USA.

II. Catalysis by *in-situ* Generated Oxidants

Project Coordinators:

Prof. V. Bukhtiyarov, Boreskov Institute of Catalysis, Novosibirsk, Russia

Dr. W. Goodman, Texas A&M University, Texas, USA.

INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)

I. Development of Ecological Pure Technology for Effective and Safely Treatment and Destruction of Organic and Inorganic Materials and Hazardous Wastes in Supercritical Water

Project Manager:

Prof. V. Anikeev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

II. Development of a Compact Low Emission Wall-Mounted Catalytic Water Boiler of 5-25 kW Power Based on the Two Stage Oxidation of Natural Gas

Project Manager:

Prof. V. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

III. Development of Compact and Economic Apparatus of Gas Conditioning for Proton Exchange Membrane Fuel Cells

Project Manager:

Prof. T. Yurieva, Boreskov Institute of Catalysis, Novosibirsk, Russia.

IV. Development of Galvanochemical Technology of Liquid Radioactive Waste Treatment with Following Immobilization of Radionuclides in Alumosilicate Glass Ceramics and Glasses

Project Manager:

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

V. Development of a Compact Unit for Steam Natural Gas Reforming Conjugated by Heat with Oxidation of Waste Anode Gas of Fuel Cells

Project Manager:

Prof. V. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

VI. Nanocomposite Catalyst

Project Manager:

Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

VII. Small Capacity Fuel Cells

Project Manager:

Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia.

NWO–RFBR

I. Characterization and Catalytic Activity of Multivalent Cation Species Occluded in High Silica Zeolites

Project Coordinators:

Prof. R.A. van Santen, Eindhoven Technical University, Eindhoven, The Netherlands
Prof. G. Zhidomirov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

II. Experimental and Theoretical Studies of Non-Linear Phenomena in Catalytic Oxidation of NH_3 and Reduction of N_2O over Platinum Metal Surfaces

Project Coordinators:

Prof. B. Nieuwenhuys, Leiden University, Leiden, The Netherlands
Prof. V. Gorodetskii, Boreskov Institute of Catalysis, Novosibirsk, Russia.

III. Nanosized Au Clusters as Novel Catalysts for Low-Temperature CO Oxidation and Selective Oxidation of Light Hydrocarbons

Project Coordinators:

Prof. B. Nieuwenhuys, Leiden University, Leiden, The Netherlands
Prof. V. Bukhtiyarov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

IV. Mechanism of the Active Surface Formation in Cu/ZnO Catalysts Characterized by SPM, EXAFS, Neutron Scattering, DFT Cluster and Surface Modelling

Project Coordinators:

Prof. A. Bliek, University of Amsterdam, Amsterdam, The Netherlands
Prof. T. Yurieva, Boreskov Institute of Catalysis, Novosibirsk, Russia.

V. Microstructured Catalytic Reactors for Oxidation of Unsymmetrical Dimethylhydrazine

Project Coordinators:

Prof. J. Schouten, University of Amsterdam, Amsterdam, The Netherlands
Dr. S. Khairulin, Boreskov Institute of Catalysis, Novosibirsk, Russia.

VI. Development of Oxygen-Permeable Membranes for the Conversion of Methane to Syngas

Project Coordinators:

Prof. H. Bouwmeester, University of Twente, Enschede, The Netherlands
Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia.

VII. Catalytic Partial Oxidation of Methane. Novel Approaches to the Catalysts Design and Process Study

Project Coordinators:

Prof. J.A. Mouljin, Delft Technological University, Delft, The Netherlands

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia

CONFERENCE AND EXHIBITION ACTIVITIES

Participation in exhibitions, discussion of commercial prospects of the displayed innovations illustrates the research and social activities of an institution and promotes an increase in its rating, and expanding of the potential market for new technologies and materials. Besides, the level and consumer properties of the scientific achievements may be evaluated in more realistic manner.

In 2004, the most important BIC's achievements in the area of applied Catalysis were presented at the Exhibitions:

- ***Strategy of Sustainable Development for Metropolis***, 27-29 January, Novosibirsk, Russia
- ***IV Moscow International Salon of Innovations and Investments***, February 25-28, Moscow, Russia. **Diploma** and **Golden Medals** for "BMF – One-Stage Process for Motor Fuels and Liquefied Gas Production" and Photocatalytic Air Cleaner "AIRLIFE".
- ***IV Interregional Exhibition-Fair "North-Russia–2004"*** for North Infrastructure Development and ***International Industrial Exhibition "Siberia: Export-Import"***, 30 March-2 April, Novosibirsk, Russia
- ***The 5th International Forum and Exhibition "High Technologies of XXI Century HT'2004"***, April 19-23, Moscow, Russia
- ***2004 China (Shenyang) International Construction Technology Exhibition***, May 13-15, Shenyang, China
- ***Advanced Russian Technologies***, May 28-June 1, Bangkok, Thailand
- ***13th Commercial-Economic Fair***, June15-19, Kharbin, China
- ***2004 China International Patent Fair***, August 18-21, Dalian, Northeast China
- ***"Science of Siberia"***, October 26-29, Novosibirsk, Russia
- ***Days of Business and Cultural Cooperation "Novosibirsk – Minsk", Exhibition "Novosibirsk 2004"***, November 22-26, Minsk, Belarus.

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 scientists from NIS, but foreign participants as well.

THE 3rd RUSSIA–CHINA SEMINAR ON CATALYSIS
April 17-19, Novosibirsk, Russia

Seminar Organizers

- Boreskov Institute of Catalysis, Russian Academy of Sciences, Russia
- Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China
- Chinese Academy of Science
- Scientific Council on Catalysis of Russian Academy of Sciences
- Russian Catalytic Society
- Chinese Catalytic Society

The scientific program of the Seminar comprised 27 Oral Presentations and 26 Posters in the following topics:

- Natural Gas Conversion
- Biomass Conversion
- Energy Related Catalysis

Chinese scientists presented the following lectures:

Xinhe Bao (*Dalian Institute of Chemical Physics, Dalian, China*) – *"Research and Development of Natural Gas Conversion in Dalian Institute of Chemical Physics"*

Xuebin Liu, **Wenzhao Li**, Hengyong Xu, Yanxin Chen and Qingjie Ge (*Dalian Institute of Chemical Physics, Dalian, China*) – *"Homogeneous and Heterogeneous Contributions to Light Alkenes Production from the Catalytic Oxidative Cracking of Hexane"*

Baocai Zhang, Xiaolan Tang, Yong Li, Yide Xu, **Wenjie Shen** (*Dalian Institute of Chemical Physics, Dalian, China*) **-** *"Bio-Ethanol Steam Reforming over Ceria-Supported Ni and Ir Catalysts"*

Yushui Bi, **Gongxuan Lu** (*Lanzhou Institute of Chemical Physics, Lanzhou, China*) – *"Investigation of CO Oxidation over Pd/NaZSM-5 Supported Catalyst Modified by Fe"*

Ying Sun[a,b], Min Yang[a], Wei Wang[b], **Chenglin Sun[a]** ([a]*Dalian Institute of Chemical Physics, Dalian, China;* [b]*Dalian Railway Institute, Dalian, China*) – *"Cu-Zn-Al Mixed Oxide Catalysts Prepared via Hydrotalcite-Like Precursors for Wet Air Oxidation of Phenol"*

Haihui Wang, You Cong, **Weishen Yang** (*Dalian Institute of Chemical Physics, Dalian, China*) – *"Partial Oxidation of Methane (POM) to Syngas in Tubular* $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ *Membrane Reactor"*

Shudong Wang, Liwei Pan (*Dalian Institute of Chemical Physics, Dalian, China*) – *"Study on a Compact Plate-Fin Steam Reformer for Fuel Cell System"*

Zhengang Sun, **Zhongmin Liu**, Lei Xu, Yue Yang, Yanli He (*Dalian Institute of Chemical Physics, Dalian, China*) – *"Hydrothermal Synthesis and Characterization of Two Organically Templated Trivalent Metal-Containing Zirconium Phosphates"*

The Seminar was very productive, and all the participants took an active part in discussing. It was held in an amiable atmosphere of co-operation and mutual understanding and demonstrated that the participants are ready to engage in bilateral and multilateral cooperation.

MEMORIAL SEMINAR “PHYSICAL METHODS FOR CATALYTIC INVESTIGATIONS ON MOLECULAR LEVEL”,

dedicated to 65th Anniversary of Academician Kirill I. Zamaraev

May 21, Boreskov Institute of Catalysis, Novosibirsk, Russia

This day marks 65th anniversary of the birthday of Academician Kirill I. Zamaraev, the Director of the Institute of Catalysis since 1984 up to 1995.

Professor Zamaraev is known for his mechanistic studies on catalysis at the molecular-atomic scale, and in particular for in situ characterization by the use of radiospectroscopic methods. He has discovered and kinetically characterized numerous electron tunneling reactions over large distances. He was one of the pioneers of modern multinuclear solid state NMR in studies of the structure and active sites on catalyst surfaces and of intermediates of catalytic reactions in solution and on solid surfaces. He was among the first to study catalytic reactions in the gas phase by ion cyclotron resonance (ICR). His works in photocatalysis and design of catalytic converters of solar energy utilization, as well as on the role of photocatalytic phenomena in the global chemistry of atmosphere became a contribution to the XXI century science and technology.

Academician Valentin Parmon opened the Memorial Seminar with the lecture “*Kirill Zamaraev: Life Devoted to Science and Catalysis*”.

The scientific part of the Seminar program began with the lecture by **Sir John Meurig Thomas** (*The Royal Institution of Great Britain*) “*New Nanoporous and Nanoparticle Catalysts*”.

Four lectures were given by the followers of K. Zamaraev:

N.M. Bazhin (*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*) – *"Methane Emission to the Atmosphere"*

E.A. Duban, K.P. Bryliakov, **E.P. Talsi** (*Boreskov Institute of Catalysis, Novosibirsk, Russia*) – *"Structure and Reactivity of Hydroperoxo (LFe(OOH)) and Alkylperoxo (LFe(OOR)) Complexes of Fe, Key Intermediates of the Partial Hydrocarbon Oxidation"*

B.N. Plakhutin (*Boreskov Institute of Catalysis, Novosibirsk, Russia*) – *"High-Spin Molecular Structures with Icosahedral Symmetry: Unique Features of the States' Energy Spectrum"*

PhD student, scholar of the Zamaraev International Charitable Scientific Foundation **A.N. Usoltseva** (*Boreskov Institute of Catalysis, Novosibirsk, Russia*) – *"Thermodynamic Analysis of Carbon Nucleation on Metal Surfaces for Carbon Nanotubes Synthesis"*

Diplomas of the winners of the competition of postgraduate grants of the Zamaraev International Charitable Scientific Foundation were delivered after the vocal concert.

Dr. G.I. Skubnevskaya, Academician Y.N. Molin (*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*), **Academician G.V. Sakovich** (*Institute of the Problems of the Chemical-Energetic Technologies, Biysk, Russia*), **Academician A.E. Kontorovich** (*Institute of Geology of Oil and Gas, Novosibirsk, Russia*) and **Dr. L.A. Zamaraeva** shared their memoirs and personal moments with Kirill Zamaraev.

INTERNATIONAL OLEFIN POLYMERIZATION CONFERENCE "MOSPOL-2004"

June 22-25, Moscow

The Conference was organized by Semenov Institute of Chemical Physics (Moscow) and Boreskov Institute of Catalysis (Novosibirsk).

Catalytic polymerization of olefins is an area of the great scientific and technological interests. Ziegler-Natta catalysts, discovered 50 years ago, and many new catalysts remain the subject for continuous intensive R&D activities worldwide. As a result, the traditional catalysts have been improved greatly and new highly efficient catalysts have been developed over past few decades. These advances formed the basis for the development of novel technologies and production of polymers with the controlled structure and improved properties.

For the last 10 years the International Conferences on catalytic olefin polymerization have become traditional, since they provide and excellent opportunity to discuss the latest results, advances and prospects in this field.

"MOSPOL-2004" brought together the scientists involved in synthesis and characterization of catalysts, studies of catalytic activation, polymerization kinetics, structure and properties of polymers. 250 scientists including 130 foreign specialists took part in the Conference.

Conference was devoted to the following topics in the area of catalysis for polyolefins:

- Metallocene catalysts
- Postmetallocene catalysts
- Late transition metal catalysts
- Ziegler-Natta and other traditional catalysts
- Polymerization processes and engineering

All these topics include the various aspects:

- New catalyst composition, catalyst formation, activation and characterization
- Polymerization kinetics and polymer characterization
- Process technology and commercial developments
- Computer chemistry.

The participants presented 12 Invited Lectures, 50 Oral Presentations and 90 Posters.

V RUSSIAN CONFERENCE "SCIENTIFIC FUNDAMENTALS OF CATALYSTS PREPARATION AND TECHNOLOGY" and IV RUSSIAN CONFERENCE "PROBLEMS OF CATALYSTS DEACTIVATION"

September 6-9, Omsk, Russia

The event was organized by

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Hydrocarbons Processing, Omsk, Russia
- Ministry of Education and Science of Russian Federation

- Scientific Council on Catalysis
- Government of Omsk Region
- Omsk Scientific Center
- Russian Foundation for Basic Research
- Association of Enterprises, Institutions and Organizations of Petrochemical Complex of Omsk Region.

180 scientists and engineers took part in the Conferences.

Scientific program of the Conference comprised 15 Plenary Lectures, 63 Oral Presentations and 23 Posters presented by 11 research institutes, 12 universities and 13 industrial enterprises.

In the Plenary Lecture *"Modern Trends in Development of Traditional and Design of New Methods of Catalyst Preparation"* by **N.A. Pakhomov** and **R.A. Buyanov** (Boreskov Institute of Catalysis, Novosibirsk) on the specific examples it was shown that dew to new ideas and modern technique so called traditional methods of catalyst preparation do not exhaust their possibilities. Some more lectures also were devoted to the improvement of traditional methods of catalyst and support preparation and studying.

Non-traditional methods of catalyst synthesis at various stages of their development were presented in a number of lectures.

Plenary Lectures *"Catalysts Based on Carbon Materials: Technological Aspects and Tendencies"* (**V.A. Likholobov**, Institute of Hydrocarbons Processing, Omsk) and *"Novel Catalysts Metal-Filamentous Carbon: From Fundamental Studies to Technology"* (**V.V. Molchanov, V.V. Chesnokov, R.A. Buyanov**, Boreskov Institute of Catalysis, Novosibirsk) attracted big interest. They considered the opportunities for design of principally new generation of catalysts for the processes of olefin oligomerization and selective hydrocarbon hydrogenation.

The lecture by **V.K. Duplyakin** (Institute of Hydrocarbons Processing, Omsk) *"Approaches to Design of New Catalyst Generation for Petroleum Refining and their Production"* gave the comprehensive analysis of modern state and prospects of development of petroleum refining complex of the country based on creation of novel, more effective catalysts.

The materials focused on metal complex catalysis in organic and metalorganic synthesis were presented at a special section.

Round Table on the subject *"Problems of National Market of Catalysts"* was organized in the framework of the Conference and appeared to be quite representative. The managers and key specialists of the enterprises of petroleum chemistry and oil processing industries participated in the event.

SEMINAR, DEVOTED TO 90th ANNIVERSARY OF PROFESSOR MIKHAIL G. SLINKO

October 1, Boreskov Institute of Catalysis, Novosibirsk, Russia

September, 2004 was the 90th anniversary of the birth and 70th anniversary of scientific and public-pedagogical activities of well-known scientist in the field of physical chemistry and chemical technology, the Lenin and the USSR and UkrSSR State Prize-winner, Corresponding Member of the RAS, Professor Mikhail G. Slinko.

Mikhail G. Slinko laid the foundation of a new scientific direction of chemical technology - mathematical modeling of chemical processes and catalytic reactors, which nowadays serves as a theoretical bases for solution of many technological problems, appeared upon engineering and development of chemical production. He created a world-famed school. More than 30 high-performance reactors of high capacity for production of main chemical products such as ammonia, sulfur acid, formaldehyde and others were applied in industry under his guidance.

Professor **Aleksandr S. Noskov** gave an opening address at the Seminar.

Young scientists of the Boreskov Institute of Catalysis presented the following lectures:

V.N. Kashkin, A.S. Noskov, I.A. Zolotarskii, E.M. Slavinskaya, S.A. Pokrovskaya, V.N. Bibin, V.V. Mokrinskii, V.N. Korotkikh, I.A. Polukhina – *"Innovative High-Capacity Technology for Nitrogen Oxide Production"*

T.L. Pavlova, N.V. Vernikovskaya, N.A. Chumakova, G.S. Litvak, A.S. Noskov – *"Mathematical Modeling of Catalytic Soot Filters"*

E.A. Lashina, N.A. Chumakova, G.A. Chumakov* (**Sobolev Institute of Mathematics, Novosibirsk*) – *"Solution – Canards and Chaotic Dynamics in Kinetic Model of Heterogeneous Catalytic Reaction of Hydrogen Oxidation"*

E.V. Ovchinnikova, T.V. Andrushkevich, E.M. Alkaeva, G.A. Zenkovets, V.D. Mescheryakov, V.N. Korotkikh – *"Nicotinic Acid Production by β-Picoline Oxidation"*

The presentation of the monograph by M. Slinko *"Bases and Principles of Mathematical Modeling of Catalytic Processes"* also took place.

VII CONFERENCE “ANALYTICAL CHEMISTRY IN SIBERIA AND FAR EAST-2004”

October 11-16, Novosibirsk, Russia

The Conference was held in the Congress Center of the Sanatorium “*Sosnovka*” situated 15 minutes drive from Akademgorodok, in the picturesque pine forest on the coast of the Ob’ Sea.

Conference Organizers:
Russian Academy of Sciences
Scientific Council on Analytical Chemistry RAS
Boreskov Institute of Catalysis SB RAS

Conference Sponsors:
Shimadzu Europe
Interlab Inc.
INTERTECH Corporation
JSC “VMK Optoelectronics”
PerkinElmer International C.V.

Presentations were generally concentrated on the most recent advances in the following areas:

- Fundamentals of the Methods of Chemical Analysis
- Metrology and Standardization of Analysis Principles
- Methods of Analytical Chemistry (Chromatographic, Electrochemical, Spectrum and Mass-Spectrum, etc)
- Analysis of Major Inorganic, Organic, Biological, Medical, Pharmaceutical, Environmental Objects

400 specialists from 36 cities and 5 countries participated in the Conference.

The Conference program comprised 19 Plenary Lectures, 14 Presentation Reports on modern developments of leading instrument-making firms, 70 Oral Presentations and 300 Posters. The exhibition of analytical and measuring instruments was organized in the framework of Conference. 22 analytic companies took part in the exhibition. The Conference was finished by the Round Table "Analytics in Medicine and Pharmacy", which appeared to be of great interest for participants.

I CONFERENCE "CHEMISTRY FOR MOTOR VEHICLES"

October 27-29, Novosibirsk, Russia

The scientific program of the Conference comprised 8 Plenary Lectures, 30 Oral Presentations and 4 Reports on the following topics:

- Ecology of Vehicle
- Chemistry of Combustive-Lubricating Materials
- Auto Cosmetics (Protective Covering, Paints, Polyroles, Additives)
- Chemistry of Roadway Covering.

Two Plenary Lectures were given by the specialists of Boreskov Institute of Catalysis:

Z.R. Ismagilov - "*Ecology of Motor Transport. Achievements and Prospects*"

V.A. Sadykov, V.A. Matyshak*, A.Ya. Rozovskii**, V.V. Lunin***, J. Ross**** (**Semenov Institute of Chemical Physics, **Topchiev Institute of Petrochemical Synthesis, ***Moscow Lomonosov State University, Moscow, Russia; ****University of Limeric, Limeric, Ireland*) - *"Removal of Nitrogen Oxides from Diesel Exhausts: Problems and Prospects of Their Decision"*

Total number of participants was about 60.
The Round-Table discussion on the subject "*Alternative Motors and Fuels of Future*" in the framework of the Conference was very interesting.

SEMINAR "FUNDAMENTAL SCIENCE FOR THE DEVELOPMENT OF THE CHEMICAL AND CHEMICO-PHARMACEUTICAL INDUSTRIES"

November 16-19, Perm, Russia

9 Plenary Lectures, 27 Oral Presentations and 22 Communications on fundamental and applied aspects of low capacity chemical and biochemical processes were included in the Seminar program. The Round Table *"Promotion of the Results of Fundamental Studies to Practical Developments"* and Seminar of Young Scientists "*Chemistry for Medicine"* were arranged in the frames of Seminar.

INTERNATIONAL SEMINAR "PROMOTING THE MOBILITY AND CAREER DEVELOPMENT OF RESEARCHERS BETWEEN THE RUSSIAN FEDERATION AND THE EUROPEAN UNION"

23 November, Novosibirsk, Russia

The International Seminar "Promoting the Mobility and Career Development of Researchers Between the Russian Federation and the European Union" took place in the Small hall of the House of Scientists of Novosibirsk Scientific Center on November 23, 2004. It brought together 180 participants. The Seminar was part of the joint project in organizing workshops for discussing the problems of the career development of researchers. It joined in the series of the workshops in Moscow, St. Petersburg, Novosibirsk, Tomsk. The organizers of the Seminars – the Representatives of the European Commission in Russia and State University-Higher School of Economics. Boreskov Institute of Catalysis of the Siberian Branch of Russian Academy of Scientists was responsible for the organization of the Seminar in Novosibirsk.

The delegation of European Union headed by the Ambassador, **Mr. Marc Franco**, presented the European programs on promoting the mobility of the researchers in the field of education and science between European Union and Russian Federation. Mr. Marc Franco opened the Seminar. He told about the efforts of the Euro-Union to enlarge and increase the strength of scientific cooperation of the researchers working in different countries. The Deputy Head of Administration of the Novosibirsk region **Mr. Gennadii Sapozhnikov** noted in his greeting word that the problems of the scientific career of young people, establishment of connections with colleagues from other countries have always been in the focus of the attention of the academic society of Novosibirsk. The general meeting of Novosibirsk Scientific Center just recently raised the questions of the integration of academic institutions and educational organizations of Novosibirsk and their participation in organizing of an innovation net. He reminded that the Siberian Branch of RAS had good traditions in establishment of international contacts, implementation of joint programs and projects. He underlined that the current Seminar was a very important step on the way of the development of academic mobility under the conditions of economy globalization.

Academician Valentin Parmon, Director of the Boreskov Institute of Catalysis, also took part in the Seminar opening. He stated that inspite of the fact that Siberia is not a part of the Europe, it has represented Russia on many forums and has very strong relations with European states. In his presentation "*The Experience of the Boreskov Institute of Catalysis SB RAS in the Field of S&T Cooperation with the Countries of Euro Union*" he told the participants that the researchers of the Institute have a very fruitful cooperation with the countries of Euro Union. He stated that chemical investigations in the institute are directed to the decision of wide spectrum of problems – from studying the mechanisms of elemental chemical reactions to design of new materials and progressive technologies. To be in progress, the scientists of the Institute tend to broadening of international scientific cooperation and widely use traditional forms: organization and participation in international conferences, exchanging research fellows, visiting scientific centers. The Institute has even stored a broad experience of long-term bilateral scientific collaboration with organizations of the EU Countries, International scientific collaboration of BIC, supported by the West European Grants. The private company B.I.C. Europe BV was established in The Netherlands to assist in transferring BIC developments to the West Europe industries. Valentin Parmon noted a current problem in the visa arrangement for the scientific collaborations. In general, Siberian scientists, especially young researchers, support the idea of mobility and intensive scientific change between countries. **Mr. Raffaele Liberali**, Director for "The Human Factor, Mobility and Marie Curie activities" of European Commission took part in the procedure of the Seminar opening, and then he prolonged his presentation. He told about "*EC Perspectives in International Mobility*". EC has very ambitious plans – to build a "knowledge society" by 2010, to increase the volume of the capital investment to the science. It is necessary to develop a qualified scientific stuff. The budget of the next 7fp of the Marie Curie program will be doubled. Now it is 10% of the general program budget. The main principle of the program is "Bottom-up", which means that participation in the program does not depend on the field of the scientific investigation and the age of the participants. The main criterion is the quality of the scientific investigations and projects.

Mr Liberali regretted that only 2-3 western researchers have applied for the work in Russian laboratories. He was very disappointed with this fact. The problem is not the shortage of knowledge in Russia, or climate particulates, but the shortage of information about possibilities of Russian scientific centers. One of the main problems is the lack of co-ordinated, one-stop information sources. Mr Liberali said: "It is a very important thing - the establishment of an Internet portal (European Mobility Portal) to provide mobile researchers with up-to-date legal, administrative and cultural information. We also want to see the representatives of third (non-EU) countries working in Europe". This is a new tendency – all programs are open for the International cooperation. The main idea is long-term cooperation, but not brain drain. To avoid it, the scheme of reintegration is proposed. It provides the granting the researcher during 1 year in his native country after 1-year work in the host country. Third country researchers face cumbersome problems with visa, residence permit and work permit requirements. Immigration restrictions often make it impossible for non-EU nationals to take up residence in the host country for more than short stays. These bureaucratic problems should be solved. The aim of the mobility program is establishment of the nonfragmentative liberal market of research labor. Mobility is the instrument of the career development of researchers. Circulation of researchers, participation in European mobility programs looks very promising.

This topic was continued in the presentation of **Mr. Georges Bingen**, Head of Unit for "Strategy and policy", Directorate for "The Human Factor, Mobility and activities" of European Commission. He emphasized the positive tendency of increasing the expenses on science and geographical expanding of Marie Curie program activities because of including the third (non-EU) countries in its circles. Mr. Bingen also talked about the problem of brain drain. He noted that in spite of the seriousness of this problem, it has some positive moments – the drained scientists keep contacts with their colleagues at home, promoting the increase and improvement of the International cooperation. Nevertheless, the circulation of the researchers is the main principle of the mobility. United European standards and certification should be developed.

The contribution "*The Marie Curie Actions for the Training, Mobility and Career Development of Researchers*" was presented by **Ms. Anna Pikalova**, Manager of Mobility National Contact Point for Russia, State University – Higher School of Economics. She described in details the trends of the Marie Curie program for participation of RF researchers, the regulations and demands.

Ms. Svetlana Knyazeva (Regional INTAS Representative) presented the contribution "*INTAS Mobility and Research Partnerships*". She described INTAS programs emphasizing their connection with mobility between new independent countries and the countries of European Union.

The contribution "*FFG Activities Regarding the Mobility of Researchers*" was presented by **Mr. M. Robert Schwertner**, Austrian Research Promotion Agency (FFG). He told about the activity of the Austrian Research Promotion Agency and made the accents on cooperation with the researchers from Russia. He described the concrete possibilities of mobility development for Russian researchers in Austria, search of the partners.

Mr. R. Sobotta, Head of the German Academic Exchange Agency (DAAD) – Information-Center Novosibirsk, told about *DAAD programs and long-term grants*, academic change, fruitful work between Germany and Russia.

Some questions concerning the details of the proposed programs, financial point, possibilities of the participation in the programs, expert estimation were asked during the discussion leaded by **Professor Valerii Bukhtiyarov**, Deputy Director of the Boreskov Institute of Catalysis SB RAS.

Conclusion remarks summarized all presented information and confirmed the importance of the Seminar topic. There is a raw of the European programs on students and researchers mobility – TEMPUS, ERASMUS MUNDUS, 6FP including the Marie Curie program. The mentioned programs should be oriented not on brain drain, but on research circulation between different countries. The meeting was very important for the change of information in order to find new effective ways of the cooperation. The political problems of cooperation, establishment of the united space of Europe and Russia in the field of economy, safety, science and technology, education will be discussed at EC-Russia Summit in November.

Mr. Bingen highly estimated the level and practice use of the presented information. Full view of financial and organizing abilities was given not only from EU side, but from the side of public organizations and funds. Mr. Bingen has a hope that the Seminar will stimulate new steps in establishment of stable contacts and cooperation in all fields of science and education.

The lively discussion was continued after the Seminar, during the Fourchette. Young researchers, well-known scientists, teachers demonstrated a big interest to the European programs, desire to participate in their work, support of the ideas of the scientific mobility.

Scientific Social Life

- *Celebration of Academic Science*

The year 2004 there were two anniversaries on the Day of Science, February, 8: the 280th anniversary from the date of the founding of the Russian Academy of Sciences as well as the 60th one of the founding of the West-Siberian Branch of the USSR Academy of Sciences which has initiate the Academic Science in Siberia. The holiday of Science was broadly celebrated in all the scientific centers and Academic institutes of the Siberian Branch of the RAS.

- Professors of the California University, member of the National Academy of Engineering and American Association for the Advancement of Science, Alexis T. Bell is known for many years in Novosibirsk and is called by right “big friend of Russian chemists”. At the Annual General Meeting of the SB RAS he was handed with Diploma of Honorary Doctor of the SB RAS.

Alexis T. Bell visited the Institute of Catalysis for the first time in 1974 in the frames of Russian-American collaboration. Since 1987 he almost annually visited the Institute. He is sponsor and initiator of establishing Kirill Zamaraev Fund for Support of Travel for Students and Scholars from Russia and FSU Countries to assist students and scholars working in the field of catalysis in Russia and FSU countries, who plan to attend a technical meeting within the U.S.

This year Alexis T. Bell presented excellent lectures at the Annual General Meeting of the SB RAS and at the Institute of Catalysis. He also has a talk with Prof. Gennadii I. Panov and Dr. Aleksandr A. Khassin.

- Museum of SB RAS in Akademgorodok began a series of presentations. The aim of these presentations is to show the formation and development of the research institutes. Exposition of Boreskov Institute of Catalysis presented interesting materials.

July, 12-13. Delegation of Chinese Academy of Sciences headed by the CAS President Lu Yongxiang visited Akademgorodok. Contracting parties expressed their interest in strengthening their cooperation and making further contribution to science and technology cooperation between the two countries and discussed the opportunity of creation Chinese-Russian Scientific-Technical Center. The delegation visited the Boreskov Institute of Catalysis, Budker Institute of Nuclear Physics, Institute of Theoretic and Applied Mathematics and Novosibirsk State University.

- Prize-winners of the Program "Prominent Scientists. Candidates (equivalent to Ph.D) and Doctors of Sciences" in 2004-2005:

Konstantin P. Bryliakov
Alexandr V. Vorontsov
Mikhail V. Luzgin
Aleksandr A. Khassin

- On **August, 4, 1997 Zamaraev International Charitable Scientific Foundation** has been 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 «Altai», 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.

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 means is spent on Zamaraev post-graduate scholarships, prizes and grants. Foundation plans to support the 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 2004 **M. Simonova** has got the post-graduate scholarship; **Yu. Larichev, M. Grushetskaya, I. Glaznev, A. Barabanov, N. Maksimchuk, N. Mezentseva, A. Stadnichenko** and **I. Mazov** – incentive post-graduate scholarships. **Yu. Pak** and **P. Pyryaev** have got the Scholarships.

- 15 Ph.D. students and scientific employees of the Institute form the personnel of the **Council of Scientific Youth.** The main principle of the Council is submission of the interests of the youth in the Institute. It includes 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 directions of activity connected with the improving of a position of the young employees 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 Institute (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.

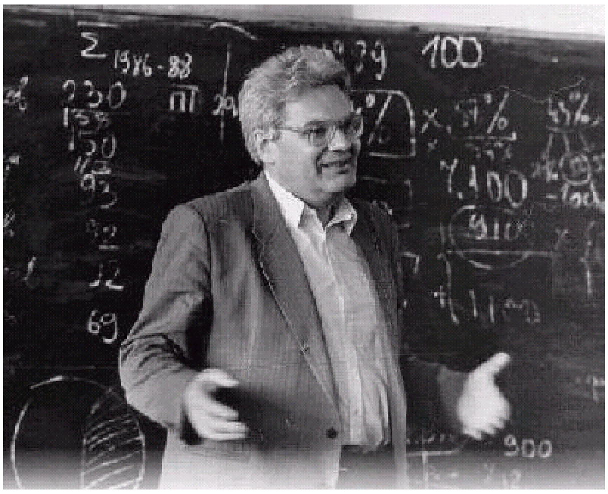
Of particular interest among the exhibit is the personal book collection of Georgii Konstantinovich including more than 1000 scientific volumes and 15 sets of Russian and foreign scientific journals. There are especially memorable copies with dedicatory inscriptions by the authors and the rarities published 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 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.

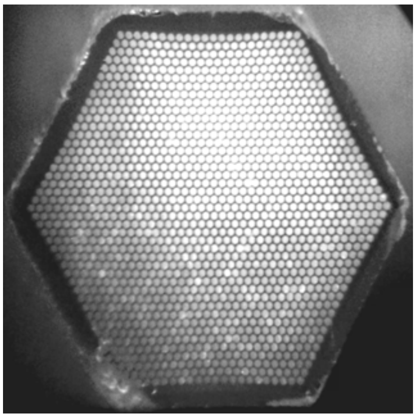
IMPORTANT RESULTS OF THE R&D ACTIVITY

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

It is developed a new approach to expand the unrestricted determinant (of Hartree–Fock and Kohn–Sham type) in the basis of restricted determinants composed by a α-spin paired orbitals (POs). The active POs (which are related to natural orbitals having fractional occupancies) are responsible for the spin contamination associated with unrestricted wave functions. Although above mentioned restricted basis determinants are not the spin eigenfunctions they describe all possible distinct electron configurations with k pairs of spatially separated α and β spins over closed and half-closed shells which are the same for all configurations. The developed approach allows one to consider any unrestricted solution as a weighted sum of ionic (no active pairs) and covalent resonance structures. In its turn spin contamination can be considered as an indicator of covalent bonding in the system treated by means of the unrestricted method. The spin contamination of the unrestricted determinant in the basis of POs becomes determined only by $2k$ active POs composing subspace of functions with S_z=0.

This approach was realized in U2R program, which uses the results of Gaussian-98 program.

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

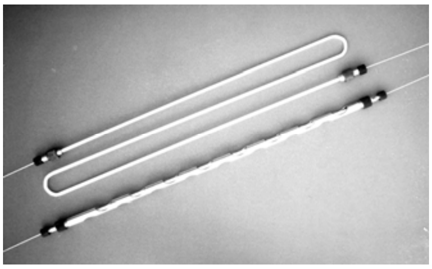


Number of capillars 1375,
capillary diameter – 40 microns

The process of analytic GC separation can be considerably accelerated using multicapillary columns (MCC).

The currently used commercial multicapillary columns have been prepared with stationary liquid phases and, therefore, can only be used for gas-liquid chromatography. At the same time there exist analytic problems that require the gas adsorption chromatography technique for successful separation. A typical example of such a problem is separation of fixed gases or C1–C3 hydrocarbons.

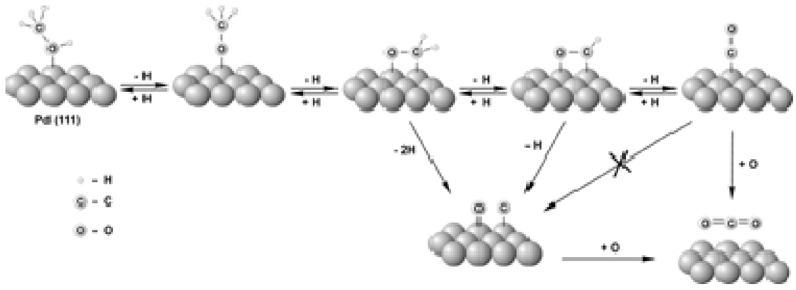
An innovative technology has been developed for preparation of express multicapillary columns which allow the gas adsorption chromatography to be applied for separation of gases. With the columns, mixtures of light C1–C4 hydrocarbons can be analytically separated for the times of 5 to 15 sec at the efficiency up to 12000 theoretical plates per meter. Chromatographic properties of the columns have been characterized. The columns are promising for creation of unique on-line methods of high-speed analysis and control of stages of real industrial processes.



Surface Science Laboratory

Head: Prof. Valerii I. Bukhtiyarov

In cooperation with the Fritz Haber Institute (Berlin, Germany), XPS and Sum Frequency Generation studies of the decomposition and oxidation of methanol, adsorption and hydrogenation of CO on the (111) face of the Pd single crystal were carried out *in situ* (i.e. under the reaction conditions) to understand more about the nature of interaction between methanol and palladium. Palladium is of particular interest because it is a promising catalyst for hydrogenation of CO to methanol and for partial oxidation of methanol to H_2 and CO_2. Mass spectrometry and gas chromatography were used to characterize the catalytic activity. *In situ* experiments at elevated pressure (0.1 mbar) demonstrated that the methanol decomposition follows two pathways even at room temperature: apart from the dehydrogenation of methanol to CO and hydrogen, which also occurs in vacuum ($P < 10^{-3}$ mbar), dissociation of methanol with the deposition of carbon on the palladium surface is observed. Latter pathway is shown to proceed via the cleavage of the C–O bond in intermediates (CH_2O, CHO), which are also intermediates of the methanol dehydrogenation. The rate of the carbon formation increases with an increase in temperature and pressure that results eventually in the complete deactivation of the catalyst. The thermal and chemical stabilities of the carbon deposits are very high. Even in an excess of oxygen, a sharp decrease in the equilibrium carbon concentration is observed on the palladium surface but at temperatures above 450 K. In oxygen-deficient conditions at low temperatures, the pathway of partial methanol oxidation to CO_2 and H_2 may occur through formation of XPS- and SFG-detected formates on the palladium surface.



Laboratory of Investigation of the Mechanisms of Catalytic Reactions

Head: Prof. Eugenii P. Talsi

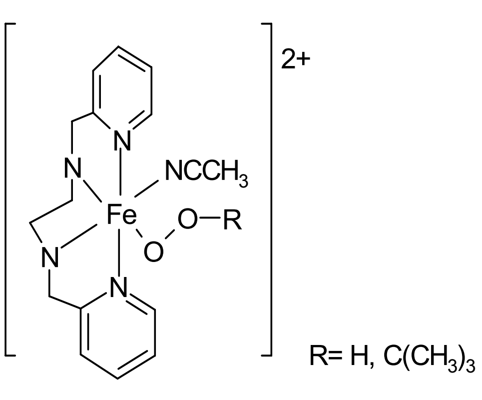
I. Cr^{III}(salen) catalyzed asymmetric epoxidations: Insight into the catalytic cycle

Chromium-salen complexes are well-known catalysts of asymmetric alkene epoxidations. However, mechanism of their catalytic action is not entirely clear. In our work, intermediates of chromium-salen catalyzed alkene epoxidations were studied *in situ* by EPR, ^1H and ^2H NMR, UV-vis/NIR spectroscopy (where chromium-salens were (S,S)-(+)-*N,N'*-bis(3,5-di-*tert*-butylsalicylidene)-1,2-cyclohexanediamino chromium(III) chloride (**1**) and racemic *N,N'*-bis(3,4,5,6-tetra-deuterosalicylidene)-1,2-cyclohexanediamino chromium(III) chloride (**2**).

High-valence chromium complexes, intermediates of epoxidation reactions, were detected and characterized by EPR and NMR. They are the mononuclear oxochromium(V) intermediate (**A**) responsible for epoxidation $Cr^{V}O(salen)L$ (where L = Cl^{-} or solvent molecule) and an inactive chromium-salen binuclear complex (**B**) which acts as a reservoir of the active species. The latter complex demonstrates an EPR signal characteristic of oxochromium(V)-salen species an ^{1}H NMR spectra typical for chromium(III)-salen complexes, and it is identified as mixed-valence binuclear $L_1(salen)Cr^{III}OCr^{V}(salen)L_2$ (L_1, L_2 = Cl^{-} or solvent molecules).

II. Characterization of low-spin ferric hydroperoxo complexes with N, N'-dimethyl-N,N'-bis(2-pyridylmethyl)-1,2-diaminoethane (BPMEN)

The catalytic system $[Fe^{II}(BPMEN)(CH_3CN)_2](ClO_4)_2$ (**1**)/H_2O_2 in CH_3CN (BPMEN = N,N'-dimethyl-N,N'-bis(2-pyridylmethyl)-1,2-diaminoethane) (Scheme 1) is a very rare example of nonheme iron catalyst/H_2O_2 combination capable of selective olefin epoxidation, and the first example of an MMO model system that is useful for preparative oxidation chemistry. It is assumed that mononuclear hydroperoxo species $[Fe^{III}(BPMEN)(OOH)L](ClO_4)_2$, where L = CH_3CN or H_2O are active species (or their closest precursors) of this catalytic system. However, until now there were no data on characterization of hydroperoxo intermediates in BPMEN based systems. Using EPR and $^{1,2}H$ NMR spectroscopy, peroxidic intermediates and other ferric species formed via interaction of $[Fe^{II}(BPMEN)(CH_3CN)_2](ClO_4)_2$ (**1**) with H_2O_2 in 2:1 CH_2Cl_2/CH_3CN mixture were characterized for the first time. It was shown that in the catalytic system **1**/H_2O_2 in 2:1 CH_2Cl_2/CH_3CN mixture at 20°C, the major part of iron exists in the form of μ-oxo binuclear ferric species **2** with proposed structure $[(OH)(BPMEN)Fe^{III}\text{-O-}Fe^{III}(BPMEN)(H_2O](ClO_4)_3$. At the early stage of the reaction between **1** and H_2O_2 in 2:1 CH_2Cl_2/CH_3CN mixture at –70 to –60°C, very unstable low-spin hydroperoxo complexes $[Fe^{III}(BPMEN)(OOH)CH_3CN](ClO_4)_2$ (**3**-CH_3CN) and $[Fe^{III}(BPMEN)(OOH)H_2O](ClO_4)_2$ (**3**-H_2O) were identified for the first time. These EPR active mononuclear hydroperoxo intermediates exist in detectable amount only at the early stage of interaction of **1** with H_2O_2 at low temperature, and then they irreversibly convert into EPR silent binuclear species. The attempts to restore them by addition of fresh portions of oxidant into the reaction mixture were unsuccessful. Thus the actual precursors of the active species of the catalytic system **1**/H_2O_2 responsible for selective oxidation of organic substrates could be EPR silent binuclear μ-oxo ferric complexes containing OOH-moiety $[(BPMEN)(HOO)Fe^{III}\text{-O-}Fe^{III}(BPMEN)(H_2O)](ClO_4)_3$.



Scheme 1

III. The active intermediates of ethylene polymerization over 2,6-bis(imino)pyridyl iron complex activated with aluminum trialkyls and methylaluminoxane

The intermediates of olefin polymerization over homogeneous catalysts based on bis(imino)pyridine iron(II) chloride ($LFeCl_2$, L=2,6-bis[(1-2,6-dimethylphenylimino)ethyl] pyridine) with different activators (trimethyl-, triisobutyl-, trioctylaluminum and MAO) have been studied by ^{1}H and ^{2}H NMR. In conditions approaching to real polymerization, neutral species of the type $[LFe(II)Cl(\mu\text{-}R)_2AlR_2]$ or $[LFe(II)R(\mu\text{-}R)_2AlR_2]$ dominate in the reaction solution in $LFeCl_2+AlR_3$ systems, whereas in $LFeCl_2$/MAO system, ion pairs $[LFe(II)(\mu\text{-}Me)(\mu\text{-}Cl)AlMe_2]^+[Me\text{-}MAO]^-$ (at Al/Fe<200) and $[LFe(II)(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$ (at Al/Fe > 500) are the predominant species.

Laboratory of Catalyst Texture Studies
Head: Prof. Vladimir B. Fenelonov

- A mesoporous mesophase catalyst IC-47-1 was developed on the basis of the silicate mesophase SBA-3 with the titanium implantation to the structure of the mesophase walls. The catalyst is active and stable in the reactions of selective oxidation of organic compounds with aqueous H_2O_2 at the temperature ranging from 20 to 90°C.

- Structurally ordered mesoporous carbon materials were developed, in which the surface area is 300 to 600 m^2/g and the pore size is controlled between 3 and 7 nm. The materials are synthesized through replication of the silicate mesophase SBA-15 with carbon produced by thermal decomposition of hydrocarbons at 600 to 800°C.

The materials are unique in textural characteristics (a large surface area at a comparatively large in size calibrated mesopores); they are promising catalysts and catalyst supports.

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

The kinetics of the conversion of ^{13}C-labeled *n*-butane adsorbed on sulfated zirconia (SZ) was monitored by *in situ* ^{13}C MAS NMR spectroscopy. Rate constants of *n*-butane to isobutane isomerization and of the ^{13}C-isotope scrambling from the primary to the secondary carbon atoms in *n*-butane were determined. The monomolecular scrambling of the ^{13}C-label in adsorbed *n*-butane has activation energy of 17±3 kcal mol^{-1} and occurs faster than the bimolecular process of *n*-butane isomerization which has an activation energy of 15.1±0.2 kcal mol^{-1}. The transfer of the selective ^{13}C-label from the primary to the secondary carbon atom in the adsorbed *n*-butane seems to consist of two reaction steps: (i) a hydride abstraction by SZ leading to the formation of *sec*-butyl cations and (ii) a label scrambling in the *sec*-butyl cations. This two-step process with the formation of *sec*-butyl cations as intermediate increases the apparent activation energy for the ^{13}C-label scrambling, which is almost twice as large compared with the activation energy for carbon scrambling of *sec*-butyl cations in a superacidic solution.

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

- X-ray photoelectron spectroscopy was used for identification of the conditions for penetration of oxygen atoms into upper layers of palladium metal to form a layer of "subsurface" oxygen or surface palladium oxide. The increasing reactivity of oxygen atoms $^{18}O_{ads}$ upon co-adsorption of $^{18}O_{ads} + CO_{ads} + NO_{ads}$ on Pd(111) and Pd(110) planes was discovered using the isotopic label TPR method. In the reaction with CO, atomic oxygen species O_{ads} were found much more reactive than "subsurface" oxygen atoms O_{sub}. The self-organization processes of the reaction CO + O_2 on Pd(110) under self-oscillation conditions were simulated in terms of the Monte-Carlo method. The modes of alternating the adsorption coverages in the form of mobile waves were revealed with the most intensive formation of CO_2 molecules within the narrow front of the waves. A considerable influence of the "subsurface" oxygen species on the self-oscillation kinetics was established. The angular dependence of formation of N_2, N_2O, $N^{18}O$, $C^{16}O^{16}O$ and $C^{16}O^{18}O$ products in the steady state of reaction $CO+NO^{18}+O_2$/Pd(110) was studied by the molecular beam technique. It was established that CO_2 molecules escape along the normal to the surface, while N_2, $N^{18}O$ and N_2O molecules at an angle of 30° to the surface. A model was suggested implying that the reaction between CO and oxygen atoms occurs on active sites between metal atom rows, and nitrogen atoms are recombined at lateral sides of the rows.
- The semi-empirical calculations in terms of interacting bonds method allowed an alternative model of nonlinear kinetic phenomena in the reaction NO + H_2 on platinum metal surfaces to be suggested.
- In DAPS spectra acquired after adsorption of oxygen on the Pt(100) single crystal surface, peaks were first identified along with the expected satellites of conjugated electron excitation O2p; the peaks were assigned to the threshold excitation of platinum bulk plasmons.

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

Using TPD and XPS techniques and method of mathematical modeling it is established that the surface reconstruction in Pd(poly) crystallites is accounted for by formation of oxide-like species on the (100) face due to lateral interactions in the saturated adsorption layer at $\theta \geq 0.5$. The reconstruction of the Pd(110) surface is caused by interaction of the atomic Pd adsorbate with the molecular O_2 adsorbtive followed by gradual penetration of the oxygen atoms to surface palladium layers.

The reaction pathway of CO oxidation over Pd(110) is established to depend on the processes of formation-destruction of reconstructive chain species at low pressures ($\leq 10^{-2}$ Pa) and on diffusion of oxygen from the subsurface metal layer to the surface at high pressures ($\geq 10^{-2}$ Pa).

(Group of Electron Microscopy headed by Dr. Alexey N. Salanov)

Group of Synthesis of Surface Compounds
Head: Dr. Vladimir L. Kuznetsov

- Theoretical analysis of the influence of reaction conditions and catalyst compositions on the carbon deposition on the surface of metal catalysts was pursued. The studies were based on the assumption that the carbon nucleation on the metal surface has a crucial impact on the type of carbon deposits. This approach was used to develop a multicomponent catalyst FeCo/CaO for synthesis of carbon nanotubes from acetylene. The product is carbon multiwall nanotubes (MNT) with a narrow tube diameter distribution (10–20 nm). The nanotube yield is more than 100 g MNT/g metal.

- The same approach was used to develop methods for fabrication of coatings that contain carbon nanotubes implanted to a semiconductor surface. Mono- (Ni) and bimetal (Ni/Mn, Ni/Mo, Ni/Cu) systems with the metal layers of different thickness (50–150 Å) were prepared on Si(100) surface by lithography and electron beam spraying of the metals. The obtained catalytic systems were characterized in synthesis of carbon nanotubes through catalytic decomposition of CH_4 and CH_4/H_2 mixtures (at different H_2 contents) at the temperature varied from 700 to 1100 °C. Atomic force microscopic studies allowed a considerable influence of the catalyst composition on the type of the carbon deposit to be established.

- X-ray and photoemission spectroscopies were used to study the process of nanodiamond (ND) transformation into nano-sp^2/sp^3 composites and onion-like structured carbon (OLC) in vacuum at 1200–2140 K. The results obtained indicate the possibility of the controlled generation of defects in the OLC-based nanocarbon materials with the purpose of creating materials with controlled electron properties.

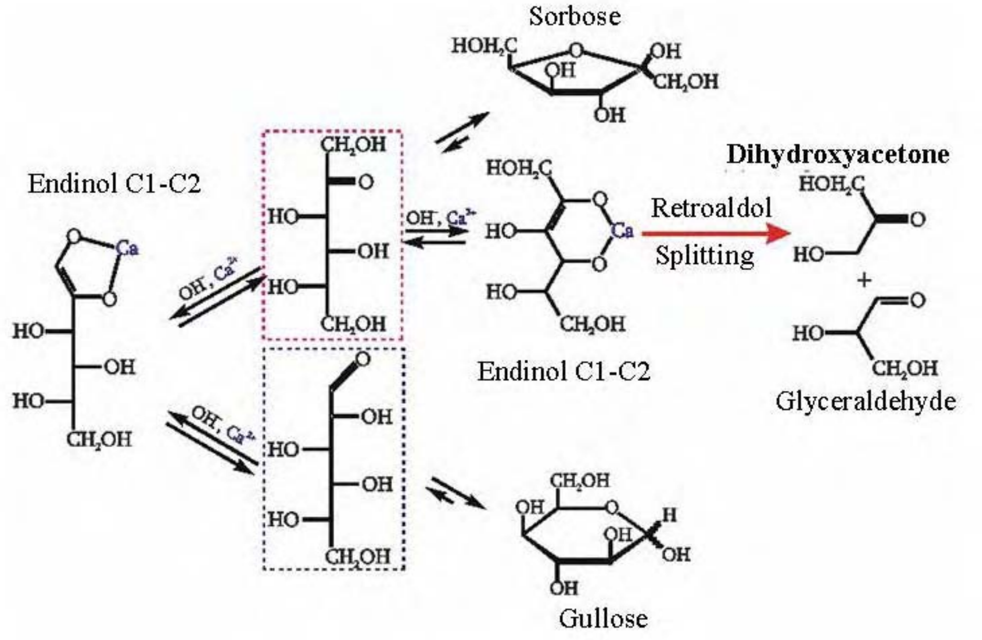
A model of OLC formation from ND was suggested to explain the formation of inner defects in fullerene-like structures in terms of different graphitization rates of different diamond crystallographic faces.

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

- The key idea underlying the studies concerns the origin of “natural selection” on the prebiotic Earth. According to the current hypothesis, the selection existed already at the chemical stage of evolution of biosphere among autocatalytic reactions. An example of the reactions is the Butlerov “formose” reaction to produce, for example, ribose as the monosaccharide. Ribose is a constituent of the most important molecules in the chemical pre-history of life – RNA, DNA, ATP.

The mechanism of the autocatalytic Butlerov “formose” reaction, which is one of the most important reactions of the chemical pre-history of life, is systematically studied in terms of homogeneous catalysis by Ca^{2+} cations. In the reaction, higher sugars are synthesized by condensation from simplest molecules of formaldehyde. Among the sugars is ribose, one of the key components of RNA and DNA molecules, carriers of biological information. It is discovered that higher sugars can behave as initiators of the Butlerov reaction depending on their specific structure and potentiality to decompose into lower C_2- and C_3-hydrocarbons, which are established to be most effective initiators of the synthesis of sugars from formaldehyde. At stationary external conditions, the formaldehyde condensation gives practically identical products even though the initiators are different in nature; the product composition is accounted for by pairwise coupling of lower C_2- and C_3-hydrocarbons (Fig.). Ribose is one of the reaction products. Experimental studies show that UV radiation can initiate the Butlerov reaction through photochemical synthesis of first molecules of either glycol aldehyde or glycerin aldehyde in the initially pure formaldehyde solution. Contrary to the commonly accepted opinion, the higher sugars are shown to form via condensation of lower hydrocarbons but not via successive addition of formaldehyde molecules.

Hence, the possibility of initiation of the natural selection in chemical processes at the early stages of Earth evolution is demonstrated with this rather simple system.



- The dark and photoinduced adsorption of Freons 12 (CF_2Cl_2), 22 (CHF_2Cl) and 134a (CF_3CH_2F) on the samples of calcium carbonate prepared by various methods is studied. Spectral dependencies of the quantum efficiency of Freons photosorption are studied. Analysis of the gas phase composition upon $CaCO_3$ surface irradiation with UV or full spectrum light from mercury lamp in vacuum, Freon or mixture of Freon and nitrogen oxides is carried out.

It is suggested that highly dispersed samples of calcium carbonate obtained from the minerals of calcite and aragonite must possess higher photosorption activity than the industrial calcium carbonate.

- It has been developed:

– The method of production of sub-micron channels on the aluminum and stainless steel plates;

– The method of anchoring of a catalyst sample in the plate channels;

– A plate-type micro-reactor with spiral channels (PSC-2);

– A micro-reactor supplied with a bulk porous current-conductive catalyst bed (BPCC-1);

Testing of the model micro-reactor PSC-2 supplied with the SNM-1 catalyst (0.6 g) showed that: (1) the hydrogen output in the reaction of steam methanol reforming per weight of the catalyst sample in the PSC-2 micro-reactor is four-times higher than in the conventional reactor with a fixed catalyst bed, which confirms effective application of the catalyst grain in the micro-catalytic system; (2) the output of hydrogen is 33 ml/min at the contact time of 12000 h^{-1} and the methanol conversion of 100%. This output is only three-times lower than that exhibited by the foreign analogue (team of L. Kiwi-Minsker from Federal Institute of Technology, Lausanne (EPFL)).

- A technology is developed for generation and stabilization of steady vortex gas-liquid and fluidized (gas – dispersed solid) layers in the vortex chamber of a multiphase centrifugal vortex reactor to provide an ordered quasicrystalline dense structure of the layers and uniform jet-type streamline around each particles. Large Reynolds numbers and high gas capacity is characteristic of the layers. The structure and basic parameters of the generated vortex layers have been studied. The technology is promising for designing principally new chemical reactors that feature smaller dimensions and lower metals consumption at a higher efficiency. Model multiphase vortex reactors have been designed and assembled for a number of chemical multiphase processes.

Group of Biocatalysis

Head: Dr. Galina A. Kovalenko

High-stable biocatalysts are developed for the heterogeneous process of starch saccharification to treacle and glucose syrup. The biocatalysts are prepared by immobilization of glucoamylase on granular carbon and carbon-mineral supports with different surface morphologies of catalytic filamentous carbon (CFC), pyrolytic or graphite-like layers. The adsorbability of the carbonaceous supports coated by CFC and pyrolytic carbon is the highest with respect to glucoamylase. Also the stability and enzymatic activity of the heterogeneous biocatalysts based on these supports are very high. From the experimental data, the supports under study are arranged in the following order to obtain higher stable and more active biocatalyst: CFC-coated claydite < CFC-coated glass foam ≈ sapropel < pyrocarbon-coated η-, γ-alumina ≈ bulky CFC < Sibunit. Non-carbonized supports or supports coated by graphite-like carbon layer, are inappropriate for enzymes immobilization.

A vortex immersed reactor for heterogeneous biocatalytical process of starch saccharification to treacle is designed and tested in lab-scale setup. The operation conditions are optimized to provide the highest conversion rate and productivity of the process.

Laboratory of Energy Accumulating Materials
Head: Prof. Yurii I. Aristov

1. The different types of the intermetallic hydrides with varied atomic relation of Zr:Fe (2,6:1, 1:1, 1:2) and hydrogen content H/Me (~1,5; ~0,6; ~0,1) have been synthesized. By means of hydrothermal oxidation of the mixtures with aluminum powder a composites, containing intermetallic powders as well as simple oxides of iron and zirconium encapsulated in Al_2O_3/Al matrix have been prepared. Both not capsulated intermetallic powders, simple Al_2O_3/Al matrixes and a model $MeO_x/Al_2O_3/Al$ composites as comparing systems have been also synthesized.

2. The phase content, textural, mechanical and chemical properties of the composites on the various stages of the synthesis and for different content of the composites have been studied. For the first time, a strong positive effect of the Al_2O_3/Al matrix has been found. This effect reveals large enhancement in the long hydrocarbons (C5+) output of the capsulated intermetallides. Non-monotone character of the output per mass and selectivity with the increase of the iron content was discovered. The crushing strength of the granulated composites with the capsulated intermetallides was found to be less then for encapsulated oxides. Chemical and mechanical properties were compared with the structural and textural ones.

3. Variation of synthesis conditions of composites "a salt inside porous matrix", namely, a shift of ion-exchange equilibrium and calcination temperature, allows desirable modification of their sorption properties, in particular, a transition between mono- and divariant equilibrium and water sorption capacity.

4. Kinetics of water sorption on loose grains of composite sorbent “$CaCl_2$ confined to mesoporous silica (SWS-1L)” was measured at T = 33-69°C and $P(H_2O)$ = 8–70 mbar over water uptake range 0–0.47 g/g for various particle sizes R_p (between 0.355 and 1.4 mm). The measurements were performed in a constant pressure unit based on a CAHN microbalance under isothermal external conditions. The results obtained evidence an enhancement of the sorption rate and apparent diffusion constant with the decrease in the particle size (approximately as R_p^{-2} at $R_p > 0.71$ mm). Contribution of thermal effects was found for water sorption on smaller SWS particles (0.355-0.425 mm), which decreases the sorption rate. The apparent water diffusivity was found to depend on the local slope of the SWS water sorption isotherm. The pore diffusivity of water in the temperature range 33-69°C was calculated from experimental data $D_e = (0.12\pm0.06)\cdot10^{-6}$ m^2/s that is approximately 20 times lower than the Knudsen pore diffusivity estimated for pores of silica KSK.

Group of Photocatalysis on Semiconductors
Head: Dr. Alexandr V. Vorontsov

Group of photocatalysis carries out research on advanced oxidation technologies for environment purification. Such processes include photocatalytic oxidation in liquid and gas phases as well as liquid phase oxidation over heterogeneous Fenton catalysts. Various gaseous and condensed substances are utilized as substrates for oxidation – CO, acetone, ethanol, acetaldehyde, ammonia, phenol, organophosphorous, organosulfur compounds, dimethylhydrazine, etc. Recently developed novel modified photocatalysts and Fenton catalysts possess advanced activities towards complete oxidation of air and water impurities and serve as the basis for creation of water and purification instruments. Research is on the way to develop inorganic catalyst supports that have high stability and vast area for contacting with reagents and light quanta. Of special interest is to fix liquid purification catalysts over supports. Such heterogenized photocatalysts and Fenton reagents allow catalyst-free reactor effluents without costs of filtration. Kinetic studies that are intensively carried out in the group provide for conditions to conduct oxidation processes at the best rates and lowest catalyst deactivation. Insight into reaction mechanisms is provided by quantum chemical calculations of interaction of substrates with catalysts as well as reagents transformation thermodynamics. Thus, it has been demonstrated that dissociative adsorption of dimethylmethylphosphonate over anatase facets (100) and (001) is possible only over hydroxylated surface and cannot proceed over pure surface.

Laboratory of Adsorption
Head: Dr. Oleg N. Martyanov

Experimental approaches and methods for analysis of ferromagnetic (superparamagnetic) resonance (FMR) spectra were developed to be used for characterization of heterogeneous catalysts based on magnetic compounds. Early stages of the formation of ferromagnetic nanoparticles via thermolysis of lamellar binary hydroxides with incorporated EDTA-complexes of Ni, Co and Cu were studied for the first time. Particles of different sizes and shapes were shown to form in the process depending on the chemical composition and structure of the precursor compound. For example, the treatment of FMR spectra of nickel nanoparticles obtained by decomposition of the precursor at different temperatures revealed that the formation of the ferromagnetic phase starts at T~340°C. As the temperature rises above T~400°C, the FMR line is broadened and the shape of the absorption line is distorted that indicates the particles enlargement due to coagulation. However, at high temperatures the FMR line intensity increases much faster with the rise of temperature of the spectrum recording than in the case of bulky nickel; this fact is an evidence of the small size of the nickel particles. The superparamagnetic resonance spectra were analyzed to define qualitatively the metal size distribution with the maximum at around 4–5 nm. The data obtained agree well with the related XRD and EM data.

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

- There are studied the influence of different substitutes on the catalytic properties of derivatives of cobalt phthalocyanine in the reaction of the liquid-phase oxidation of H_2S. The catalytic properties of following compounds: $CoPc(4\text{-}Br)_4(5\text{-}SO_3H)_4$, $CoPc(SO_3H)_2$,

$CoPc(4\text{-}Cl)_4(5\text{-}SO_3H)_4$, $CoPc(4\text{-}COOH)_4(5\text{-}Br)_4$, $CoPc(4\text{-}t\text{-}Bu)_4(5/6\text{-}SO_3H)_4$ are studied. Except $CoPc(4\text{-}t\text{-}Bu)_4(5/6\text{-}SO_3H)_4$, all these catalysts are active in the reaction of the liquid-phase oxidation of H_2S in the weak alkaline solutions. The greatest catalytic activity has $CoPc(4\text{-}COOH)_4(5\text{-}Br)_4$.

- A method was developed for synthesis of a strong, thermostable and highly active Mn-Al oxide catalyst for high-pressure combustion of low-calorific methane/air mixtures. The process can be used for utilization of waste gases to generate power. At the flow rate up to 75000 h^{-1} and pressure of 5 bar, the catalyst is ignited at 400°C and remains active after operation at 950°C. The active component of the catalyst consists of 30–40 nm particles of tetragonal spinel $\beta\text{-}Mn_3O_4$; the particles are assembled into blocks with monomodal pore size distribution (~ 10 nm), which are strongly bound to the $\alpha\text{-}Al_2O_3$ support.

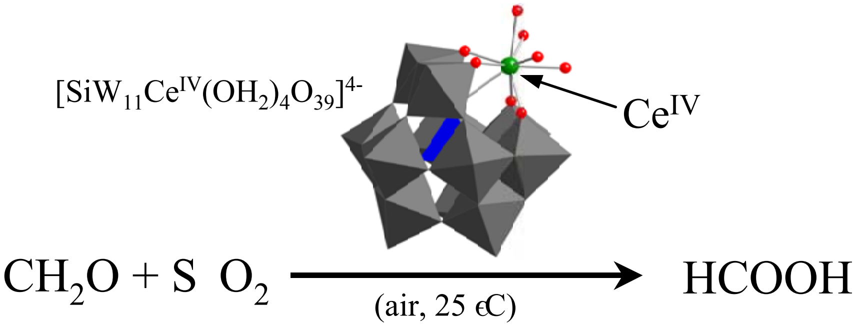
Thermodynamic data on the efficiency of combustion of low-calorific gases in gas-turbine plants were used to develop optimal flowsheet for utilization of waste gases in order to provide the maximal efficiency of the plant and mild conditions of the catalyst operation: comparatively low temperatures and a small temperature interval between the inlet and outlet of the catalyst bed.

- Kinetics of oxidation of H_2S with oxygen over V_2O_5 catalyst was studied under isothermal conditions at temperatures below sulfur dew point. ESCA, EPR and NMR techniques were used to characterize the vanadium state in supported catalysts containing 2 to 20 wt % of V_2O_5. It was established that a part of V^{5+} is reduced to V^{4+} in the course of the reaction. The reduction degree depends on the reaction parameters (temperature, gas mixture composition) and on the degree of association of the supported V_2O_5 particles. The particles, in which the vanadium-oxygen polyhedrons are least associated and strongly bound to the support, are reduced first. The high catalytic activity of the 2–5% V_2O_5 supported on Al_2O_3 or TiO_2 is accounted for by the mononuclear sites V^{5+} in tetrahedral (Al_2O_3) or strongly disordered octahedral (TiO_2) oxygen environment, which are bound directly to the base sites of the support.

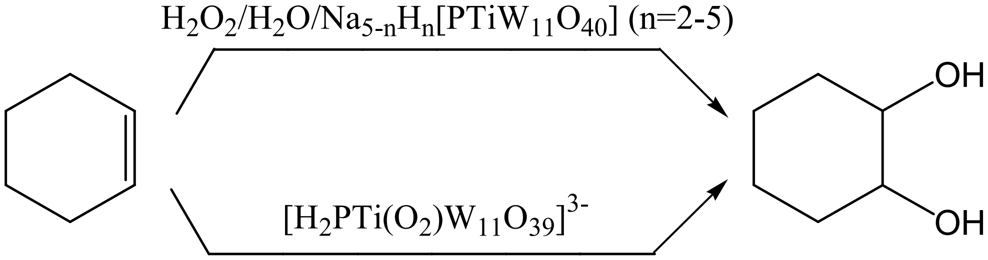
Group for Stereoselective Catalysis
Head: Dr. Oxana A. Kholdeeva

The joint FSU (Boreskov Institute) and US (Emory University) team with funding from their CGP award (RC1-2371-NO_02) discovered and developed the most effective catalysts to date for the aerobic (air-based) oxidation of formaldehyde (as well as other toxic aldehydes) under ambient conditions. The catalysts are polyoxometalates or “POMs” containing redox-active d-block (Co(II)) or f-block (Ce(IV)) centers in surface sites. A number of results of both fundamental and applied value were achieved. These results include discovery of new POM types, the roles of POM structure and composition on catalytic activity (O_2 oxidation of formaldehyde, and by extension many other possible target toxics) and development of effective methods to attach the POM catalysts to useful solid supports without the loss of POM catalytic activity.

The polyoxometalate $NaH_3[SiW_{11}Ce^{IV}O_{39}]$ (**$NaH_3$1**) was identified from a targeted library of 50 POMs to be a selective and effective catalyst for the aerobic oxidation of formaldehyde to formic acid under very mild (including ambient) conditions. ^{183}W NMR, UV-Vis, cyclic voltammetry, and potentiometric titration establish the catalyst is a monomer of C_s symmetry, **1**, in solution, while X-ray crystallography and IR establish it to be a dimer, **1_2**, of C_i symmetry in the solid-state.



2. In the framework of the RFBR grant 04-03-32113 “Polyoxometalates as molecular models for studying active catalytic sites and mechanisms of oxidation catalysis”, a new polyoxometalate catalyst, $Na_{5-n}H_nPTiW_{11}O_{40}$ (n = 2-5), has been found for efficient oxidation of cyclohexene to *trans*-cyclohexane-1,2-diol by aqueous H_2O_2. The ^{31}P and ^{183}W NMR studies revealed that the diprotonated peroxotitanium species $[H_2PTi(O_2)W_{11}O_{39}]^{3-}$ is an active species responsible for cyclohexene oxidation via heterolytic oxygen atom transfer mechanism.



Group of Metallorganic Catalysts
Head: Prof. Alexandr S. Lisitsyn

The Sibunit-based Pd/C, Ru/C and Pt/C catalysts are shown to be promising for synthesis of unsaturated aldehydes through direct oxidation of the respective alcohols with molecular oxygen (the simplest and ecologically sound method for production of these products). The platinum catalysts provide the quantitative yield of allyl aldehyde derivatives; in the performance, it is competitive to the known intentionally promoted catalysts, while being much more active than the known homogeneous catalysts.

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

- Systematic studies of potentialities of laser induced luminescence for characterization of supports and catalysts are continued. Threshold values of the laser irradiation power at the wavelength of 193 nm are determined for main regimes of its interaction with α-alumina. When the power density on the target increases in the range of 0.001 to 100 MW/cm^2, the one-photon regime of interaction of the irradiation with the substance is shown to transform to the one-photon regime at $Q \approx 0.1$ MW/cm^2, then to sublimation at $Q \approx 5$ MW/cm^2 and to ionization of the sublimated products at $Q \approx 15$ MW/cm^2. The efficiency of the substance removal is determined at the power density $Q \approx 100$ MW/cm^2.

In gas-dynamic reactors for laser-controlled chemical reactions, synthesis of ethylene from methane is established to occur at $CH_4/C_2H_4 \sim 4$ in a narrow range of parameters (consumption of fed ethylene–natural gas mixture, irradiation power), otherwise ethylene is converted to propylene. According to gas-dynamic calculations, olefins are synthesized from methane in the high-temperature zone out of the nozzle in the gas mixing zone.

- Computational experiments based on the fundamental conservation laws demonstrated that gas-dust bunches – planet nuclei – can emerge in circumstellar disks upon evolution of gravitational instability. Characteristics of the instability were determined for the gas-dust media in self-gravitation disks and central field disks. In the absence of coagulation and chemical processes, the estimated hydrogen and helium pressures in the bunches are of the order of hundreds and thousands atmospheres. Algorithms were suggested for calculation of dissipative processes, coagulation and chemical reactions using supercomputer codes in order to determine temperature and the other conditions of planet formation.

Laser vapor deposition of meteorite matters and Earth rocks was used to synthesize nanomaterials. The catalytic activity of these materials in chemical reactions with simple carbon compounds is studied to understand putative conditions of planet formation.

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

An original method is proposed for implementation of the process of hydrogen sulfide decomposition into sulfur and hydrogen. The method implies that the catalyst capable of decomposing hydrogen sulfide at room temperature is immersed in a liquid solvent bed. When so, the limiting stage – recombination (oligomerizarion) of molecular sulfur into cyclooctasulfur – is accelerated that results in a considerable increase, by an order of magnitude or even more, in the reaction turnover number per cycle.

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

1. Oxidation of benzene, toluene and phenol with the mixture of oxygen and hydrogen activated on Pt/SiO_2 has been studied in a solution containing dissolved heteropoly compounds. In the presence of redox active $H_4PMo_{11}VO_{40}$ heteropoly acid or tetrabutylammonium salts $TBA_4PMo_{11}VO_{40}$ and $TBA_4HPW_{11}Fe(OH)O_{39}$ oxidation results in hydroxylation of the benzene ring to form phenol and hydroquinones from benzene and phenol, and is accompanied by oxygenation of methyl group in the case of toluene. Reactivity of the substrates has been determined to grow in order of benzene < toluene < phenol. The comparative reactivity of substrates, composition of products and some other observations indicated essentially the same mechanism of oxygen transfer in oxidation by the O_2/H_2 gases and hydrogen peroxide. In both cases heteropoly compound bonded hydroxy radicals are suggested to be responsible for oxidation.

2. The compositions based on platinum, rhodium or iridium and molybdophosphoric heteropoly acid, $(M_nCl_mO_xH_y)\cdot(H_3PMo_{12}O_{40})$, $n \approx 1$, have been prepared. Stabilized with heteropoly acid (HPA), hydroxoparticles of platinum(II), rhodium(III) or iridium(III), can be partly or completely reduced to zerovalent metal; the interaction with reduced HPA being retained. These species are active in the gas phase benzene oxidation with O_2/H_2 mixture. Isolated under conditions of bicomponent catalyst preparation for the reaction, the species can be considered as an active form of a catalyst.

Laboratory of Aerosol Nucleation
Head: Prof. Mikhail P. Anisimov

- A computer algorithm for nucleation rate surface design is developed. An obvious advantage of the computer semi-empirical design of nucleation rate surfaces is the ability to construct this surface over the full interval of nucleation parameters that are unavailable for any experiments. Examples of conditions that are difficult to achieve include very low temperatures, high-pressures and/or very high-temperature medium (such as stars) etc. It is assumed that the current algorithm can be further developed for the semi-empirical design of nucleation rate surfaces for one- and two-component systems.

- Some general requirements for nucleation experiments associated with any phase transformation of the first order are formulated. Measurement of the single-channel nucleation rate plays the key role in comparison of the experimental data on nucleation rate and one-channel nucleation theory. Interpretation of multi-channel nucleation in the approximation of one channel nucleation produce the unsolvable problem of theory and experiment consistency.

- The current generalization of the Ostwald rule for the formation of phases is proved on the basis of common results on nucleation. The present consideration uses the qualitative prove on the base of several plausible assumptions.

- Treatment of multiple nucleation rate surfaces in the one surface approximation can be mentioned as one of the reasons of the nucleation theory inconsistence and experimental results on nucleation. Unfortunately the most experimental data (possible from two or more nucleation rate surfaces) are interpreted in one-surface approximation of Classical Nucleation Theory. The experimental detection of nucleation rate from individual nucleation rate surface is available only in the resent time. The present research illustrates several examples of nucleation rate surface topologies which are designed over diagrams of phase equilibria. It can be shown the continuum of nucleation rare surfaces for binary system.

- The considerable body of the available for the current time of the nucleation rate data have been studied. It was estimated the critical embryo sizes for several series of components (mostly organic chemicals) and *correlate* ions for vapor nucleating critical embryo parameters with the nucleation conditions, dielectric constants and surface tension for the bulk liquids have been found.

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

- Bimetallic Pt-Co containing catalysts supported on Sibunit and γ-Al_2O_3 for preferential CO oxidation in hydrogen rich gas mixtures were prepared by impregnation of supports with water solution of Pt and Co compounds ($[Co(NH_3)_5NO_2]Cl_2$ and $K_2[Pt(NO_2)_4]$). A high performance of these catalysts in the reaction of preferential CO oxidation has been demonstrated.

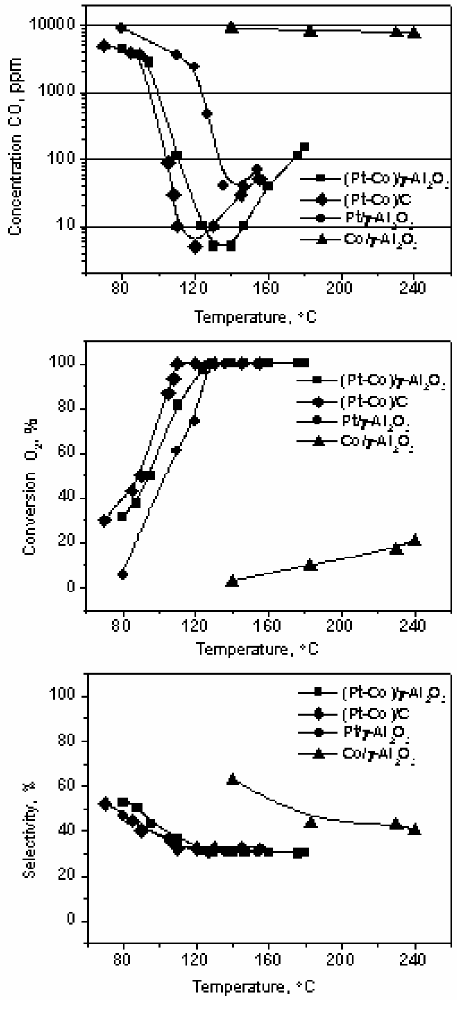


Fig. Dependence of outlet CO concentration, O_2 conversion and selectivity on temperature during CO oxidation in the presence of H_2 over catalysts 2 vol.% Pt/γ-Al_2O_3, 2 vol.% (Pt-Co)/γ-Al_2O_3 and 2 vol.% Co/γ-Al_2O_3. Input gas mixture: 1 vol.% CO, 1.5 vol.% O_2, 65 vol.% H_2, 10 vol.% H_2O, 0 vol.% CO_2. Gas flow rate is 8000 liters per hours.

- In the frames of studying the mechanism of reactions of selective oxidation over Ib group metals the focus was on the following studies:

1. XPS technique was used to develop a method for cleaning polycrystalline fibers of electrolytic silver that is applied to steam oxidation of ethylene glycol to glyoxal.

2. The interaction between oxygen and the reaction medium ethylene/oxygen was studied on the surface of a highly defect bulky electrolytic oxygen.

3. The catalytic activity of phosphorus promoted silver catalyst was studied in the process of partial oxidation of ethyleneglycol. XPS technique was used to show that the oxygen states are considerably different on the surfaces of non-promoted and phosphorus-containing silver.

4. XPS and thermodesorption techniques were used to show a diversity of oxygen species on the surface of bulky gold. Conditions of the species formation were studied, as well as their thermostability and reactivity.

- Experimental studies were aimed at catalytic decomposition of simple hydrocarbons – methane and ethylene – on (111) face of a platinum single crystal. XPS, UPS and AES spectra were acquired *in situ* during interaction of methane and ethylene with the Pt(111) surface at varied temperatures, exposures and hydrocarbon pressures. The data obtained were used to suppose about the role of C– and C–C fragments in the formation of nanocarbon structures of plane (graphite-like) and curved (fullerene-, nanotube-like) types.

- XPS technique was used to characterize nitrogen- and fluorine-containing nanotubes synthesized by different methods. Spectra of core levels of carbon, oxygen, nitrogen and fluorine are obtained. The spectra are used to compare with the spectra recorded during formation and oxidation of carbon nanostructures on the Pt(111) surface.

- It was shown that $Rh/Cs_xH_{3-x}PW_{12}O_{40}$ ($1.5 \le x \le 2$) - the best catalysts for halide-free DME carbonylation are bifunctional catalysts: 1) activation of C-O bond in DME molecule and formation of metal-alkyl bond occurs in the presence of the strong Bronsted acid sites, and 2) these acid sites act in conjunction with Rh carbonyl complexes, which are responsible for CO insertion and acetates formation

$$CH_3\text{-}O\text{-}CH_3 + CO \rightarrow CH_3\text{-}CO\text{-}O\text{-}CH_3$$

The strong Bronsted acid sites with strength PA = 1120 kJ mol^{-1} and density ~120 μmol g^{-1} were determined by monitoring the pyridine adsorption. The rhodium carbonyls: $Rh(CO)_2^+$, $Rh_2(CO)_3$ and $Rh_6(CO)_{16}$ were registered on the surface of the *in situ* reduced $Rh/Cs_2HPW_{12}O_{40}$ catalyst upon admission of CO.

(Group of Bifunctional Heterogeneous Catalysis headed by Dr. Galina G. Volkova

Laboratory of Heterogeneous Selective Oxidation

Head: Prof. Tamara V. Andrushkevich

1. Conditions of phase formation are studied in MoVTe and MoVNbTe oxide systems. Formation of the following phases is observed in the both systems: orthorhombic (M1) and hexagonal (M2) vanadium-molybdenum-tellurium phases of variable compositions and monoclinic molybdenum-tellurium phase $TeMo_5O_{16}$. Tellurium is the key structure-building

element of these phases. The relative content of the phases in the samples is determined by conditions of the precursor synthesis and conditions of the subsequent redox treatment. The said phases are considerably different in their catalytic behavior in the reactions of oxidation and oxidative ammonolysis of propane. The orthorhombic vanadium-molybdenum-tellurium phase M1 is most active to the selective transformation of propane, the activity being increased remarkable on addition of niobium. The conditions of formation of the M1 phase in three- and four-component catalysts are identified.

2. In the V-Mo-Nb oxide catalysts ($V_{0.3}Mo_1Nb_x$, where x = 0.048, 0.15, 0.22, 0.27), a ReO_3-like structured ternary V-Mo-Nb compound of a variable composition ($V_xMo_1Nb_y$, where x = 0.2÷0.25, y = 0.23÷0.35) is established to be the active component. In the compound, Mo is in the oxidation state 6+ in oxygen octahedrons with identical Mo–O bonds, and V in the states of 5+ (predominant) and 4+. Two configurations, square pyramid and trigonal pyramid, are identified for V^{5+}, while Nb^{5+}, similar to Mo^{6+}, is in the octahedral surrounding. Specific features of the formation of the active component are studied in the processes of thermal treatment in various media.

3. A vanadium-titanium catalyst, which is highly selective to formation of nicotinic acid, was used to study dependencies of partial reaction rates at 270, 285 and 300°C and selectivities for the reaction products on the conversion of β-picoline. A consecutive-parallel reaction pathway with almost constant contributions of the both routes was established for formation of nicotinic acid. A saturation curve was found to describe the rate of the formation of nicotinic acid as a function of β-picoline concentrations at the initial concentration ranging from 0.5 to 2.0 %. A similar curve was characteristic of the dependence on the oxygen content in the concentration range of 10–20 mol %. For the industrial process, the minimal permissible ratio of oxygen and β-picoline concentrations was established to be $C_O/C_{\beta p}$ = 18–20 in the reaction mixture to provide the reaction kinetics and the catalyst stability.

Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov

- The composition and method for synthesis of an emulsifier for preparation of aqueous bitumen emulsions to be used in road construction, as well as the formula of aqueous bitumen emulsions based on the new emulsifier are developed. A technology for the emulsifier production (of annual capacity 10 and 250 t) is suggested. The emulsifier is synthesized from an inexpensive abundant feedstock: polyethylenepolyamines and plant oils (spent, off-test and tall oils). The emulsifier production does not need sophisticated facilities or high energy consumption. At the same time, the involvement of spent oils contributes to resolving the problem of utilization of technogenic wastes.

Among the advantages are:

- Low cost of the emulsifier;
- Utilization of inexpensive abundant feedstock including technogenic wastes;
- Simple synthetic procedure;
- Low energy consumption;
- No harmful liquid and gaseous wastes;
- Higher adhesion of the bitumen to crushed limestone in comparison to that of the currently used materials.

Experimental samples of the emulsifier have been successfully tested. The product is covered by a Russian Patent.

➢ The mechanochemical activation has been established to affect considerably the selectivity of vanadium oxide and zinc oxide with respect to oxidation of formaldehyde and transformations of isopropyl alcohol, respectively. In both cases, the reaction selectivity is most influenced by aprotonic acid sites formed during the mechanochemical activation.

A high efficiency of catalytic hydrogenation of a number of aromatic nitrogen compounds was demonstrated under conditions of mechanochemical activation at high hydrogen pressures. A variation of temperature from ambient to 100°C is shown to have no remarkable effect on the rate of mechanochemical synthesis of magnesium intermetallide hydrides at a high hydrogen pressure.

➢ The process of catalytic decomposition of hydrocarbons and the formation of graphite nanofibers proceeding via the carbide cycle mechanism on the Ni/Al_2O_3 catalysts can be controlled by varying the initial carbon source (hydrocarbons or chlorine hydrocarbon derivatives) and adding some metals such as Cu, Pd, Zn, Sn to yield alloyed particles Ni-M in the $Ni\text{-}M/Al_2O_3$ catalyst. It was established that the surface of the Ni-M alloyed particles (being in contact with the gas phase) is enriched with the second component M. As carbon nanofibers grow from hydrocarbons, the Ni-M alloyed particles are in the non-equilibrium dynamic state. As a result, solubility of the modifying metal exceeds the equilibrium solubility, the alloyed particles undergo in some cases phase transitions providing formation of solid solutions, intermetallides or mixed carbides.

Laboratory of Oxidative Catalysis over Zeolites

Head: Prof. Gennadii I. Panov

➢ The kinetics and mechanism of non-catalytic liquid phase oxidation of 1- and 2-butene by nitrous oxide (N_2O) in the temperature range 180-240°C have been studied. It was shown that in both cases the oxidation leads to the formation of carbonyl compounds with total selectivity of 74% for 1-butene, and more then 90% for 2-butene. The selectivity of 2-butene oxidation to methylethylketone comprises 84%. Regularities in the oxidation of terminal and nonterminal alkenes C_2-C_8 by nitrous oxide were analyzed in respect to their reactivity and contribution of different reaction routs.

➢ Transition states and mechanism of oxygen transfer from nitrous oxide to 1-butene and 2-butene molecules have been analyzed by quantum-chemical methods. It was shown that the reaction proceeds via the 1,3-dipolar cycloaddition of nitrous oxide to C=C bond of alkenes leading to the formation of carbonyl compounds.

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

1. By using a polymerized complex precursor (Pechini) method, procedures for synthesis of fluorite-like solid solutions based upon CeO_2-ZrO_2 system doped with up to 30% of La cations have been developed. The structural and surface properties of these systems were characterized by using a complex of physico-chemical methods including TEM, X-ray diffraction, SAXS, EXAFS, WAXS, UV-Vis, Raman, SIMS. By using temperature-programmed desorption of oxygen, oxygen isotope exchange and temperature-programmed reduction by H_2 and CH_4 mobility and reactivity of the surface and lattice oxygen was estimated. Effect of surface dopants (Pt, Pt+Ni) on the mobility and reactivity of the surface and lattice oxygen as well as selectivity of methane transformation into syngas in steady-state and dynamic processes of selective oxidation, steam and dry reforming has been studied. These systems were shown to be efficient and stable catalysts of methane transformation into syngas at short contact times.

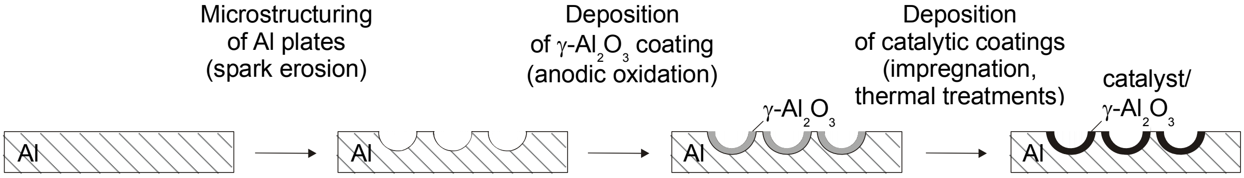
2. For nanocrystalline perovskites systems based upon doped lanthanum ferrite or lanthanum manganite as well as more complex multicomponent perovskite-like systems such as ferrite-cobaltite solutions, procedures for their synthesis via mechanical activation route and polymerized precursors (Pechini) route were elaborated. Their real structure and surface properties have been characterized and the surface/lattice oxygen mobility and reactivity have been studied. The most active surface centers stabilizing weakly bound reactive oxygen forms were shown to be associated both with the point defects (cation and anion vacancies) and extended defects (stacking faults, intergrain/domain boundaries, dislocations etc).

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

Design of catalysts and microstructured catalytic reactor for oxidation of liquid rocket fuel unsymmetrical dimethylhydrazine

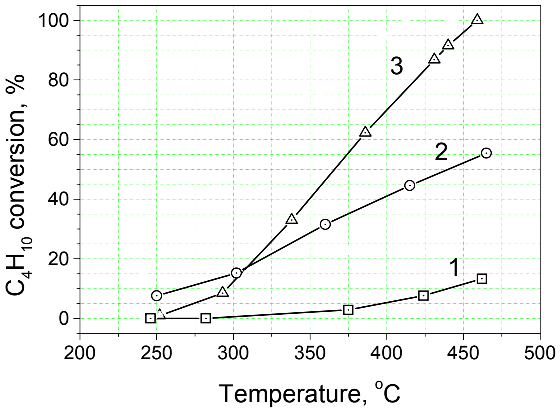
A microreactor for oxidation of unsymmetrical dimethylhydrazine (UDMH) has been designed. This microreactor is intended for the study of intrinsic kinetics of the total catalytic oxidation of a very toxic liquid rocket fuel UDMH for finding optimum and safe methods for disposal of UDMH and purification of tail gases containing UDMH vapor.

The microreactor will be assembled from 78 manufactured individual plates with a length of 40 mm, width 27 mm and thickness 416 μm made from AlMgSiCu1 alloy (97% Al). In each plate, 45 semi-cylindrical microchannels of 400 μm in diameter with the distance in between of 150 μm are machined. This is followed by anodic oxidation of aluminum in oxalic acid solution to make a uniform 25 μm thick $\gamma\text{–}Al_2O_3$ coating, which is further used as a support for catalytic coatings. The plates will be combined in pairs to form 1755 cylindrical channels in the microreactor.



Catalyst Development. For oxidation of UDMH copper chromite catalyst was selected because of its high activity in reactions of deep oxidation. The synthesis of copper chromite catalysts was performed by impregnation of the alumina coating with an aqueous solution of copper dichromate followed by drying and calcination. As confirmed by XRD, XPS and ESDR, the selected method provides formation of Cu-Cr spinel already at 450°C, which is still far below the melting point of the AlMgSiCu1 alloy. Series of experiments with different concentration of copper dichromate in the solution, duration and number of impregnations were carried out to find the procedure for obtaining most active catalytic coatings. X-ray microprobe analysis showed that the preparation methods provide uniform catalyst distribution along the plates.

The catalytic activity of the plates was characterized by butane conversion in oxidation by air, which was chosen as a model reaction. The catalyst containing 2.8 wt.% of copper chromate (related to the mass of alumina layer) demonstrated the highest activity superior to that of granulated catalysts with 20 wt.% loading of the active component.



Conversion in butane oxidation on a supported $CuCr_2O_4$ catalyst as a function of temperature. Butane concentration: 2000 ppm, GHSV: 120000 h^{-1}
(1): Al_2O_3/Al support;
(2): 20 wt.% $CuCr_2O_4/Al_2O_3$ pellets,
(3): 2.8 wt.% $CuCr_2O_4/Al_2O_3/Al$ coatings

For uniform distribution of velocities over the cross section of a microstructured reactor an original design of a flow diffuser has been developed. The diffusor includes a three dimensional screen with two sections that have a number of thick bars with a thickness equal or exceeding the spacing between them. The parameters of the screen were optimized by using the CFD code Fluent to get a flow non-uniformity across the microchannels as low as 0.2%.

This research was performed in cooperation with Eindhoven University of Technology, Holland.

Process for utilization of solid rocket propellant charges

An environmentally friendly and effective process for utilization of composite solid rocket propellant (SRP) charges with recovery of main propellant components has been developed as an alternative to conventional environment-polluting propellant destruction by burning. The technology is intended for application in processing of full-scale solid propellant charges in order to dispose of the strategic missiles discarded due to technical reasons and also subject to dismantlement according to the START-2 treaty.

The technology is based on SRP preliminary fragmentation by jet cutting, followed by the treatment of SRP lumps by a special composition – disrupting mixture (DM) containing organic solvent and additives accelerating the rupture of the cross-linked polymer binder of the propellant, with subsequent recovery of commercial products: octogen, ammonium perchlorate and aluminum compounds.

The process of SRP charge fragmentation by high-pressure toluene jets was worked out and adjusted. Kinetic studies of chemical destruction of propellants were conducted. The composition of the reaction products was studied by NMR, IR spectroscopy, UV-VIS spectroscopy, GC/MS, etc. Basing on these studies a general tentative mechanism of the process was proposed. The stages of charge fragmentation, SRP chemical destruction, separation of SRP components, regeneration of the disrupting mixtures, catalytic treatment of off-gases and catalytic combustion of organic waste residues were tested and optimized in bench-scale installations.

Based on the conducted studies Technical Requirement for the design of an experimental-industrial plant for processing of the full-scale third stage SRP charges with masses up to 3.5 tons, and the block diagram and main requirements for scaling the process to charges with masses up to 50 tons were developed.

This work was performed under ISTC project # 1632 with participation of following Russian Institutions: Boreskov Institute of Catalysis (Head Institution), Federal Research and Production Center “Altai” (Biysk), State Rocket Center “Makeyev Design Bureau” (Miass), Institute of Chemical Kinetics and Combustion (Novosibirsk) and a foreign collaborator: Lawrence Livermore National Laboratory, Livermore, USA.

Laboratory of Catalytic Conversion of Carbon Oxides

Head: Dr. Aleksandr A. Khassin

1. The studies on the structure of the $Cu_{0.08}Zn_{0.92}O$ methanol synthesis catalyst

The studies on the structure of the $Cu_{0.08}Zn_{0.92}O$ methanol synthesis catalyst were continued.

Cu K EXAFS studies of the structure of Cu-Zn oxide catalyst were performed for the as prepared samples, those after activation by hydrogen (CuZn-R) and further reoxidation (CuZn-RO). The RDA experimental curves are displayed in Fig. 1.

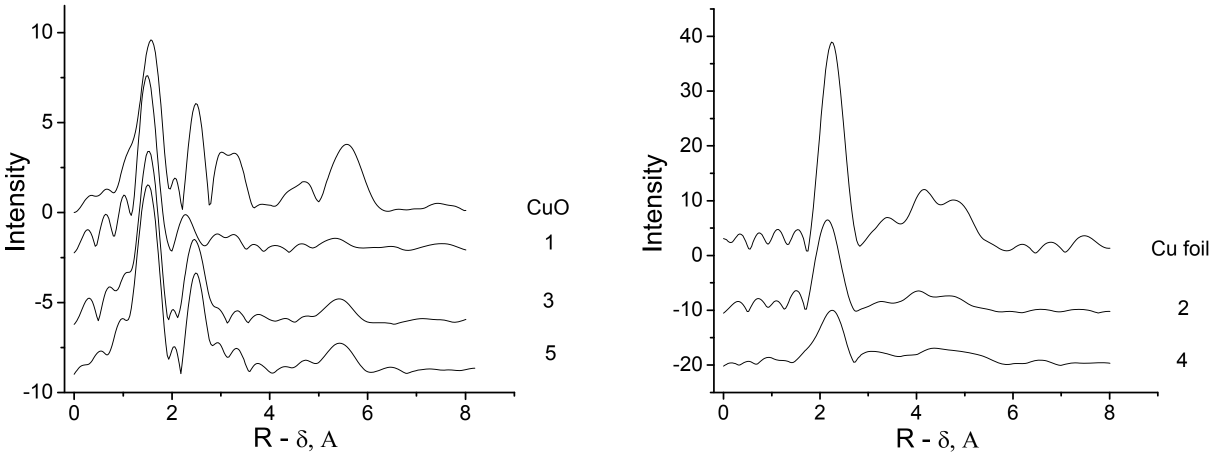


Fig. 1 Module of Fourier transformation EXAFS data for Cu K edge for CuZn oxide (1), reduced sample CuZn-R (2), reoxidized sample CuZn-RO (3), re-reduced sample CuZn-ROR (4) and re-re-oxidized sample CuZn-RORO (5), as well as of CuO and Cu foil.

During the primary formation of the $Cu_{0/08}Zn_{0/92}O$ sample copper cations are present as Cu^{2+} cations in the distorted octahedral surrounding, they form ultra-small clusters comprising no more than 4 copper atoms. Copper cations are localized in the extended stacking faults of the ZnO lattice. Basing on the EXAFS data, one cane supposedly describe these copper sites as the product of introducing the $Cu(OH)_2$ molecules to the extended stacking faults of anion-modified zinc oxide (Fig. 2).

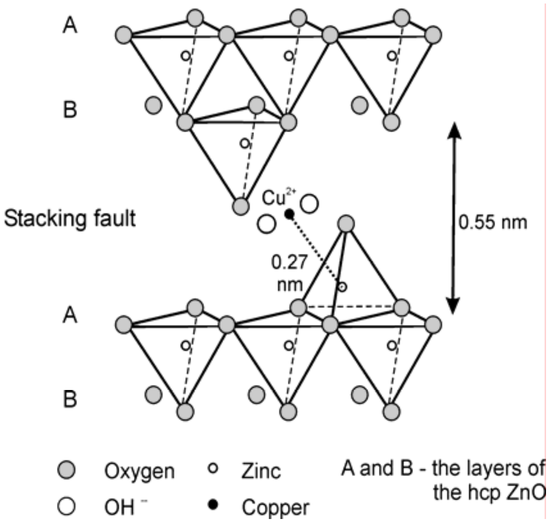


Fig. 2 The schematic presentation of the copper cation localization in the ZnO stacking fault.

The process of the samples reduction leads to the Cu^0 state. Stabilization of Cu^{+1} cations is not observed in the hydrogen medium. The EXAFS data on Cu-Cu coordination numbers allow supposing that Cu^0 atoms form the dispersed particles of the characteristic size close to 1.2-1.6 nm and probably of a disordered structure. Comparative analysis of EXAFS and HR-TEM data shows the stabilization of flat metallic copper particles over the surface of zinc oxide, with their thickness being ca. 3-4 lattice parameters (1.2-1.6 nm) and diameter being 2-3 nm and more.

During the reoxidation, copper atoms go into the Cu^{2+} state, don't form the CuO phase, but return back to the extended stacking faults of ZnO as the clusters of flat-square coordinated copper cations. The clusters far exceed those of the initial state $Cu_{0.08}Zn_{0.92}O$ in size, they are ordered and have the tape-like geometry.

2. Characterization of the nickel amesite (Ni-Mg-Al-Si) system: The structure of the active component after the catalyst reduction and after the methane decomposition

Electron micrographs of the sample Ni-Mg amesite after consequent calcination in argon at 925 K and reduction in H_2 at 925 K are given in Fig. 3. The sample represents itself the metallic Ni particles distributed over the surface of the phylloalumosilicate sheets. The TEM data confirm our earlier conclusion that the phylloaluminosilicate structure is preserved during the calcination and reduction. The size of the Ni^0 particles seems to be distributed between 4 and 8 nm, which is slightly less than follows from the XRD and hydrogen thermodesorption studies. The high resolution microscopy (see the right frame in Fig. 3) shows, that the well crystallized Ni^0 particles (B) are covered by a rather thick layer (*ca.* 2 nm) of amorphous oxide (A), while the phylloaluminosilicate support is well crystallized (C). The interatomic distances (*ca.* 0.20 nm for the particle B and *ca.* 0.45 nm for the support C) are in a good agreement with the data on Ni^0 ([111] fcc planes) and chlorite-vermiculite structures (JCPDS file 34-0163, planes [020] and [110] of the triclinic structure). We failed to observe the atomic order in the oxide layer (B) for any of the similar oxide shells as well as for the particle in Fig. 3.

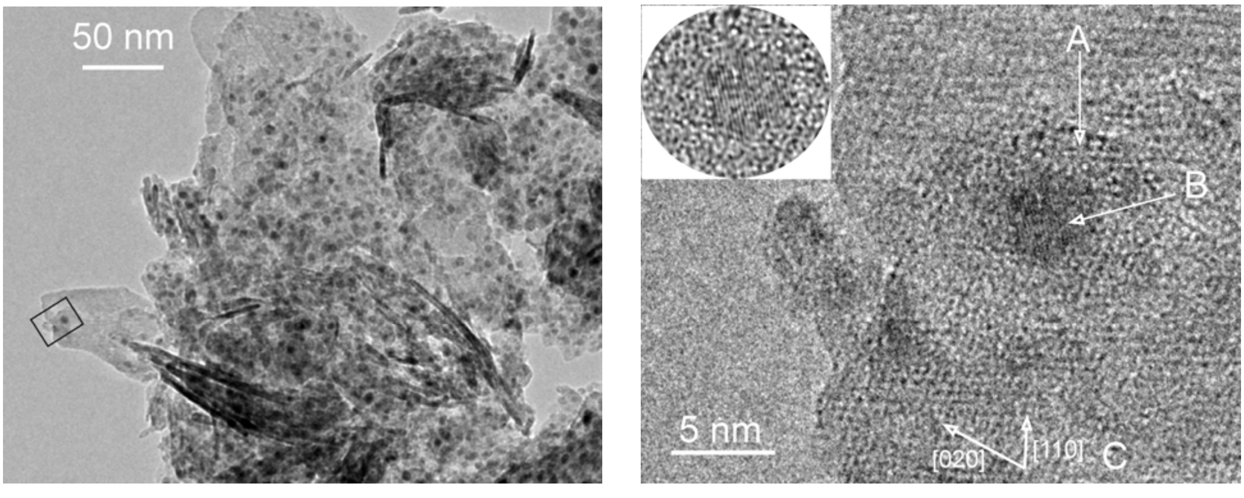


Fig. 3 Electron micrographs of the sample NAS2 after the consecutive calcination in Ar at 925 K and reduction in hydrogen at 925 K. The incut to the left micrograph shows the Fourier-filtered image of the particle B.

These TEM data agree with our earlier data on the Ni-Mg amesite system by XPS and oxygen adsorption from N_2O, that the thick oxide layer covers the metallic nickel particles. The thickness of the oxide layer is ca. 2 nm, as it follows from both XPS and TEM studies. From these data it comes apparent that the reduced NAS samples can’t be expected to adsorb oxygen, since the surface of these samples is already saturated with oxygen. The important question here is the nature of the oxide layer. This layer is amorphous and it is evident, that it cannot be “pure” NiO_x film, since the reduction temperature was high enough (925 K) to expect the reduction of any NiO_x film. Therefore one can suppose the presence of ad-cations Si^{4+} (and, probably, Al^{3+}) in the amorphous oxide layer.

Meantime NAS samples, despite they don’t contain a “free” metallic surface, have an ability to chemisorb reversibly hydrogen. The “metal core-oxide shell” particles are also active in the steam methane reforming and CO hydrogenation processes.

On the other hand, the Ni-amesite catalysts were earlier found almost inactive in the carbon formation reactions by methane decomposition. The electron micrographs of the carburized sample of the Ni-Mg amesite show that the “metal core - oxide shell” particles are not active in the process of carbon formation (no coking, no graphite-like nanofibers or other graphite-like phases).

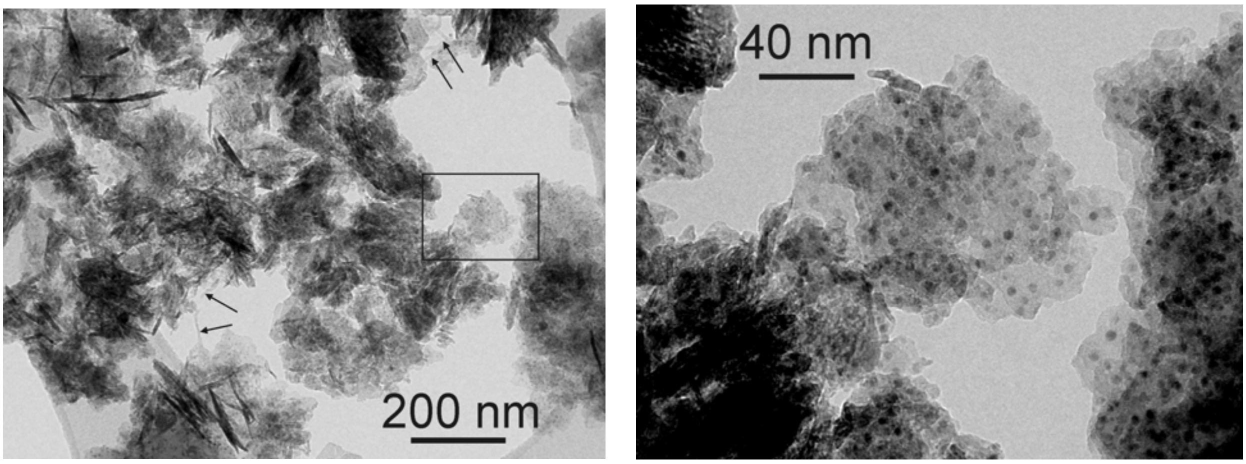


Fig. 4 Electron micrographs of the sample NAS2 after the methane decomposition at 790 K.

Therefore, the “metal core - oxide shell” nickel particles are active in the steam methane reforming and resistant to coking. The Ni-Mg amesite system could be interesting for the industrial application.

Group of Heterogeneous Catalysts on the Basis of Noble Metals

Head: Prof. Anatolii V. Romanenko

- Dispersion of Pt/C catalysts prepared through adsorption of H_2PtCl_6 on carbon support followed by reduction with H_2 shows volcano-shaped dependence on metal loading in the range from 0.1 to 10% wt for microporous active carbons, but it remains rather high and nearly unchanged in the case of mesoporous carbons of the Sibunit family. Other factors being the same, metal dispersion drops with increasing size of grains of these supports. The effects are due to multiplicity of states of the adsorbed metal precursors, which weight ratio changes by definite manner with their total content on the support surface and the adsorption conditions as well.

- Mass activity and specific activity of PtRu/Sibunit anode catalysts operating in a DMFC was found to change dramatically with S_{BET} of the Sibunit support, increasing with the decrease of the latter. Comparison of the metal surface area measured by gas phase CO chemisorption and electrochemical CO stripping indicates close to 100% utilisation of nanoparticle surfaces for catalysts supported on low (22–72 m^2/g) surface area carbons, which drops to 20% with increase in S_{BET} to 415 m^2/g.

10%PtRu/Sibunit (72 m^2/g) catalyst shows mass specific activity exceeding that of commercial 20%PtRu/Vulcan XC-72 (E-TEK) by nearly a factor of 3.

- The original procedure for the synthesis CFC, bulky modified by the atoms of nitrogen (N-containing CFC, N-CFC), is developed. Approach is used, being consisted in the decomposition on the high percentage $NiCu/Al_2O_3$ catalyst of the hydrocarbon raw material of the composition: CH_4/H_2 + N-containing additive (C_5H_5N, Py). CH_4/H_2 composition can vary in the limits, %% by vol.: 0-80 CH_4, 0-90 H_2. Optimum temperature range is 550-750°C with the total pressure of reaction mixture 1 atm. Obtained N-CFC are of the mesoporous structure with the specific surface area $S_{BET} \leq 360$ m^2/g, with the total pores volume $V_\Sigma \leq 0{,}54$ cm^3/g and with the mean pores diameter from 5 to 20 nm depending on the selected parameters of synthesis. The merits of procedure are: 1) sufficiently high catalyst activity in the synthesis N-CFC (75 g of carbon / g of metal with the decomposition of the mixture H_2/Py (10 mol. %); 2) reproducibility of results (CFC output, the parameters of porous structure, the morphology of fibers and the chemical composition of the samples, C_xN) since the parameters of process are determined, with which the pyridine is decomposed predominantly catalytically, and the influence of side non-catalytic reactions is brought to the minimum possible; 3) the possibility of the goal-directed synthesis N-CFC with the specific arrangement of properties (textural parameters, the chemical composition C_xN ($x \geq 20$) and relationship of the N-containing groups).

The series of N-CFCs for synthesis of the Pt- containing catalysts are prepared.

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

Hydrogenolysis of dimethyl sulfide was studied in the presence of cobalt sulfide catalysts. The process features depending on the catalyst composition and reaction temperature were identified. The process conditions were determined for the predominant formation of methanethiol.

Center for Catalyst Characterization and Testing
Head: Prof. Bair S. Bal'zhinimaev

Statistical lattice model of the CO oxidation reaction over Pd(110) was studied. A hysteresis was discovered in the oscillation behavior of the reaction: two oscillation modes can exist at identical parameter values. A variety of the surface spatiotemporal structures were revealed: these were cellular and turbulent patterns, spiral, ring and banded waves of oxygen.

A mathematical model is formulated for CO oxidation over polycrystalline iridium; the model involves the formation of the subsurface oxygen-modified iridium surface with the adsorptive and catalytic properties differing from those of the initial surface. Numerical analysis of the system demonstrates the possible existence of five stationary states and limit cycles (self-oscillations) in the physically achievable range of parameters.

The reaction of CO oxidation that proceeds in oscillation mode on supported palladium particles is simulated.

Laboratory of Catalyst Activity Testing

Head: Dr. Nikolai N. Bobrov

At 2004 year the development of BI-GASfow devices for the preparation of gaseous mixtures with given compositions and flow rates has been ended in the laboratory. These devices characteristics and the results of testing permit one to recommend them for certification. The BI-GASflow devices can be effectively used for the calibration of different gas analyzers and chromatographs as well as for the catalytic installations set up and other devices.

Laboratory of Catalytic Polymerization

Head: Prof. Vladimir A. Zakharov

Development of a new modification of the supported titanium-magnesium catalyst for synthesis of the fiber-forming ultrahigh molecular polyethylene (UHMPE) to be used in production of high-tenacity fibers

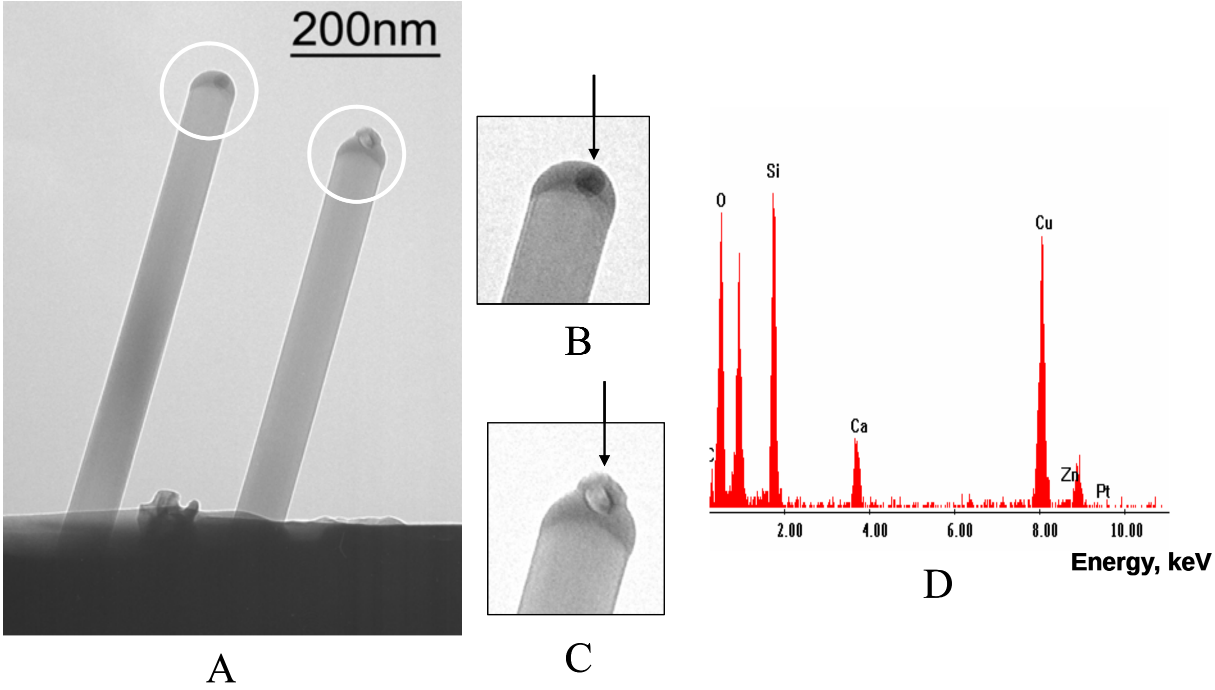
UHMPE can be applied, for example, for production of high-tenacity fibers to be used in protection means (body armors, helmets, bullet-proof sheets), as well as in ropes, nets, shroud lines. Recent studies have demonstrated that the manufacturing of high-tenacity yarns requires special sorts of UHPME with different type molecular and supramolecular structures than those in the currently used ones.

The influence of the preparation conditions and composition of ICT-8-20 type supported catalysts on the molecular and supramolecular structure of polyethylene was studied to develop a new modification of the catalyst (ICT-8-20-B) for synthesis of the high-tenacity fiber-forming UHMPE. After the technology was adapted and an experimental batch of the catalyst prepared, the catalyst was employed at the Tomskneftekhim Co. to produce a pilot batch of UHMPE. The polymer was tested in the spinning process to produce fibers with improved strength properties (maximal ratio of stable stretching was 53, fiber tenacity 300 cN/tack).

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

The formation of nanofibers on a high-temperature woven fiberglass

The formation of nanofibers (50 nm diameter and 1000 nm length) from $Si(Ca)O_2$ was observed on the treatment of a high-temperature woven fiberglass bearing calcium oxide and platinum in the flowing reaction mixture. Platinum was shown fixed in two ways: in the metal state as the particles of ca. 5 nm in size on the fiber tips under the $Ca_xSi_yO_2$ layer and in the oxidized state on the surface of $Ca_xSi_yO_2$.



Silica fibers with foreign inclusions in the tips
Pt catalyzes the fiber growth and is brought away from the glass fiber surface;
A – circles indicate tip regions for microanalysis
B – Pt metal inclusion in the tip
C – oxidized Pt
D – EDX spectrum indicating the presence of a $Ca_xSi_yO_2$ compound in the tip

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

✱ Theoretical and experimental studies of methods for loading in tube reactors in petrochemical processes

Theoretical and experimental basis was developed for unique methods of loading into tube reactors.

Main types of particle packing achieved in the tube reactors during loading were identified, and algorithms were suggested to model each packing type. The loading procedure was shown to effect the parameters of the layer formed in the tube; the effect was studied at the tube to particle diameter ratio of 5 to 10. NMR-tomographic technique was used for experimental studies of the porosity distribution in the fixed bed.

Mathematical models were developed for exo- and endothermic catalytic reactions in a tube of the tube reactor to take into account radial profiles of layer porosities formed during loading. The following catalytic process parameters were calculated: temperature distribution through the bed, feedstock conversions and yields of the target products for the specific loading procedures. The Table illustrates the influence of different loading procedures on the yield parameters in oxidation of methanol to formaldehyde over oxide catalysts.

Loading procedure	Conversion of methanol, X, %	Yield of formaldehyde, Y, %
Successive packing of particles to the sites with minimal potential energy	97.48	90.92
Particle packing started from the reactor wall	99.87	92.92
Tetrahedral (maximally dense) particle packing	99.91	72.79

A prototype facility for catalyst loading into tube reactors was designed, assembled and tested. Technical data were prepared for creation of a loading facility to load simultaneously into tubes (up to 36 in number) of tube reactors.

- **Studies of catalytic activity of perovskite-structured catalysts for neutralization of automotive exhausts**

The behavior of complex noble metal promoted oxide systems with the perovskite structures was studied in the reactions of complete oxidation of hydrocarbons and reduction of nitrogen oxides. Basic features of the reactions were determined for the catalytic systems of $A^{III}B^{III}O_3$ type {$A_{1-x}M_x(Mn,Co,Fe,Ni)_{1-y}P_yO_{3-\delta}$, $A_{1-x}M_x(Fe,Co)_{1-z-y}Bi_zP_yO_3$ (A = La, Ce, Pr; M = Sr, Ba; P = Pd, Rh or Pd-Rh)} and $A^{II}B^{IV}O_3$ {$ATi(Zr,Sn)_{1-x-y}M_xP_yO_3$ (A = Ca, Sr, Ba; M = Fe, Co, Ni; P = Pd, Rh or Pd-Rh)}:

I. Among fresh $A^{III}B^{III}O_3$ samples, Sr-containing catalysts are most active.
II. Among $A^{III}B^{III}O_3$ samples, La-Ba-containing catalysts are most thermostable.
III. Among fresh $A^{II}B^{IV}O_3$ samples, Ti-containing catalysts are most active.
IV. Among $A^{II}B^{IV}O_3$ samples, Ca-Zr-containing catalysts are most thermostable.

Laboratory of Unsteady-State Catalytic Methods for Gas Purification

Head: Prof. Aleksandr S. Noskov

Group of Mathematical Methods for Catalytic and Adsorption Process Modelling

Head: Dr. Natalia A. Chumakova

Parametrical analysis was applied to the process of utilization of methane/air mixtures in a catalytic reactor with reversal gas flow. The basic parameters of autowave regimes were shown to coincide when obtained by the two-phase model of unsteady-state processes in a granular bed and by the asymptotic model of heat front.

Group of Mathematical Methods for Catalytic and Adsorption Processes Modeling

Head: Dr. Natalia A. Chumakova

The dynamic system was shown to alter from the regular mode to chaos (strange attractor) following the Feigenbaum scenario, i.e. through a cascade of bifurcations of period doubling on changing one of the control parameters.

The phenomenon of chaotic dynamics in the kinetic model of self-oscillating heterogeneous catalytic reaction with fast, moderate and slow variables was studied with the interaction of hydrogen and oxygen over metal catalysts as an example. Numerical analysis demonstrated the existence of a strange attractor with a transversal homoclinic trajectory in the system; the fractal dimension of the attractor was estimated.

Analysis of the global integration error revealed a high parametric sensitivity of the solutions to the initial data on the strange attractor; the sensibility was discovered during Poincare mapping in the neighborhood of the attractor. Such a sensible behavior of the system is accounted for, in particular, by the existence of Canards solutions and homoclinic orbits in the one-parameter family of two-dimensional subsystems with the fast and moderate variables.

Laboratory of Industrial Catalytic Processes

Head: Il'ya A. Zolotarskii

The focus was on the scientific basis for catalytic processes in reactors with fixed catalyst beds, honeycomb monolith catalysts, fluidized or turbulent catalyst beds:

1. For a large-scale turbulent fluidized bed reactor, the hydrodynamics was studied, experimental dependencies of the bed expansion and of gas residence time in the bed on the operation conditions in the model of 0.7 m diameter were obtained.
2. Optimal technological regimes were found using a pilot fluidized catalyst bed setup to provide maximal selectivity and yield of nitrous oxide in the reaction of selective ammonia oxidation.
3. Perforated wall honeycomb monoliths were used to study the flow turbulization in the channels. The wall holes were shown to behave as a factor of flow destabilization and mass transfer intensification. Critical (loss of gas dynamic stability) size of the hole, as well as its

position with respect to the exposed edge of the channel was determined for the operation regime of a UKL-7 reactor; dependencies of such parameters as the flow fluctuation and channel pressure drop on the hole size and position were obtained.

4. Variational principles of non-equilibrium thermodynamics were applied to autowave processes in catalytic reactors: Entropy balance equations were derived and analyzed in terms of the two-phase model of processes in a fixed catalyst bed during a reversible reaction; the variational problem of autowave propagation was formulated based on the principle of minimizing the full entropy production in the system.

Group of Catalytic Technologies for Carbon Materials Synthesis

Head: Dr. Vadim A. Yakovlev

Highly effective catalytic action of multi-walled carbon nanotubes in the process of selective oxidation of hydrogen sulfide into sulfur by molecular oxygen is found. New carbon catalyst consists of granules formed by densely interlaced carbon nanotubes. High selectivity of the catalyst is observed for temperatures up to 320^0C under conditions with air excess coefficient of 1-2. This catalyst can be used widely for hydrogen sulfide removal from gases.

Laboratory of Catalytic Conversion of Solid Fuels and Wastes

Head: Dr. Aleksandr D. Simonov

Technical data on a pilot fluidized catalyst bed facility for drying a zirconium concentrate was prepared for the Tara Mining and Industrial Co. (capacity 8 t of wet concentrate per hour).

Bench test of combustion of natural gas in a fluidized bed of catalyst IC-12-73 was performed at the stoichiometric natural gas – air ratio (α = 1.03-1.05). The natural gas is shown to transform completely to CO_2 and H_2O at 700–750 °C, nitrogen oxides being in amount no more than 3–5 ppm. Hence, it was for the first time demonstrated experimentally that natural gas, along with liquid and solid fuels, can be effectively combusted in catalytic heaters.

A technical project was developed for a steam generator of 0.5 MW capacity, where natural gas is combusted in the fluidized bed of a catalyst-sand mixture. The generator efficiency is 0.7 t/h at 40 atm and 400°C.

Laboratory of Dynamics of Catalytic Processes

Head: Dr. Andrey N. Zagoruiko

- Development of pilot plant for oxidative destruction of chloro-organic wastes with capacity of 5 kg of wastes per hour for Caustik Company (Volgograd, Russia) was performed including development, lab testing and production of pilot batch of efficient catalyst as well as basic engineering and flow-sheeting of the pilot plant.

Mathematical modelling and basic engineering was performed for the process of catalytic neutralization of diesel exhausts on the base of glass-fiber catalysts, resulting in preparation of design data for catalytic neutralizer for diesel electricity generators of Moscow Metropoliten.

- An effective iron oxide catalyst ICT-27-42 was developed. The catalyst is equal to the best analogues in the selectivity to oxidation of H_2S but much superior to them in the operation stability and lifetime. Unlike the analogues, the catalyst is free of chromium and other toxic compounds. The large-scale technology for the catalyst production was developed and implemented in industry.

Development of the technology of oxidation of hydrogen sulfide was based on theoretical studies and mathematical modeling. Technical data were prepared for designing a facility for post-treatment of tail gases.

Advantages of the developed process are:

- A lower capital cost of the setup in comparison with all the known processes for post-treatment of tail gases of Claus plants; low operation expenses;
- An increase in the sulfur extraction ratio in Claus plants from 90–92% up to 99%; a considerable decrease in the amount of sulfur compounds wasted to the atmosphere;
- A high process stability, easy control;
- An inexpensive commercial catalyst with long lifetime.

The process was used for construction of an industrial unit for post-treatment of tail gases from Claus plants at the Omsk Refinery; the unit efficiency is up to 10^4 m^3/h of gas. Implementation of the unit allowed the total ratio of sulfur extraction to be increased from 90–92 to 97–99% at the Omsk Refinery. From preliminary data, the unit operation will allow the amount of H_2S wastes to be decreased by 2000 t annually.

Laboratory of Catalytic Liquid-Phase Synthesis of Organic Compounds

Head: Prof. Zinaida P. Pai

As a result of the investigations carried out within the framework of the theme *"Development of the methods of preparation of peroxopolyoxometallate complexes - catalysts of the oxidative transformations of linear and cyclic unsaturated hydrocarbons"* it was shown for the first time that the anion contained in the quaternary ammonium salt exert influence on the formation of the structure of the tetra(diperoxotungsten)phosphate(-3) complex ion.

Group of Catalysts and Processes Based on Heteropoly Acids
Head: Prof. Klavdii I. Matveev

I. In the frames of the work "*Elaboration and plant development of technology of methylethylketone (MEK) synthesis via oxidation of an industrial mixture of n-butenes by the non-chloride catalyst (Pd + HPA) on the basis of pilot plant with capacity of 300 kg MEK per day at the Public Corporation "Synthesis-Engineering" (Dzerzhinsk, Nizhniy Novgorod region)*" listed below stages were executed.

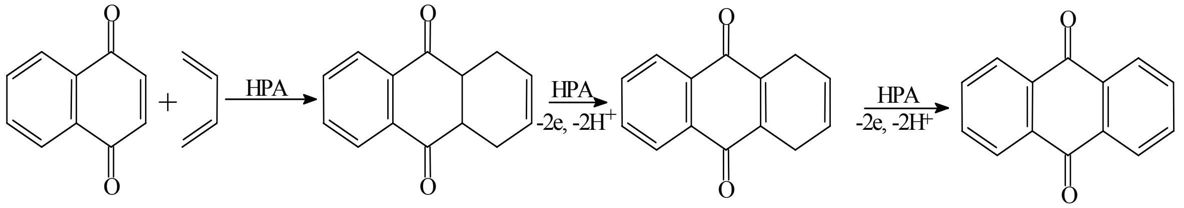
1) Researches of corrosion of constructional steels in the presence of the liquid catalyst, and a choice of steels for the equipment and armature of pilot plant.

2) Correction of composition of the catalyst and the guidance to its preparation on the Catalytic factory in view of influence of steel corrosion products on composition and properties of the catalyst. Patenting of the catalyst (Pd + HPA-x').

3) Development of specifications for the stabilizer of palladium Pc_x.
4) Development of methods of analytical control of pilot plant work.
5) Development of a starting condition and the start-up of pilot plant.

II. There are also important results in the work by the scientific project "*Selective catalytic oxidation of aromatic compounds of benzene, naphthalene, anthracene series to corresponding para-quinones with dioxygen in the presence of Mo-V-phosphoric HPAs*". Fundamentals of a new perspective method of 9,10-antraquinone (AQ) synthesis and its di- and tetrahydro derivatives (DHA, THA) are developed. These compounds are the most effective and ecological catalysts of wood delignification to the cellulose which is a raw material for series of large-capacity manufactures (of paper, artificial fibres, films, and various technical wares from cellulose).

The method of synthesis of these compounds is based on a lot of consecutive reactions, which proceed simultaneously (in one technological operation) in a single reactor. 1,4-Naphthoquinone (NQ) and 1,3-butadiene can be a raw material for manufacture of AQ and its derivatives.



NO THO DHQ AQ

The found method of synthesis of AQ, DHA and THA shows that Mo-V-phosphoric HPAs are the selective bifunctional catalysts of acidic and oxidative reactions that are perspective for processes both fine and basic organic synthesis (MEK, item I).

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

1. The main factors determining the formation of active catalysts of hydrogenation and isomerization of monoterpene compounds have been revealed. Laboratory regulations for preparation of Pt, Pd, Rh, Ru, Ir-catalysts of monoterpene hydrogenation and Na/C - catalysts of monoterpene isomerization have been worked out. A pilot batch of catalysts has been prepared and tested.
2. Kinetic peculiarities and mechanism of following reactions is investigated:
   - regio- and stereoisomerization of olefines
   - pinane isomerization to camfane
   - α-pinene isomerization to β-pinene
   - isomerization of geraniol to nerol
   - 3-carene isomerization to 2-carene

The effects of carbon support and sodium content in Na/C catalyst on products distribution for isomerization of hexene-1 to hexene-2 and isomerization of butene-1 to butene-2 have been studied. It was found that increase of size of transport pores of carbon support from 20 up to 200 nanometers as well as increase of sodium content from 2 up to 20 mass % accelerate the rate of initial olefin conversion to a product that is olefin with more substituted double bond. The mechanism of structural pinane isomerization which includes cis-(trans) pinane transformation in camphane, menthane and tetraalkylcyclohexane by three parallel routes is offered. The kinetic equation and the mechanism of cis-(trans) pinane isomerization including steps of dehydrogenation and hydrogenation of adsorbed species over Pd are proposed.

The kinetics of liquid-phase β-pinene isomerization to α-pinene over Pd/C, Pt/C, Rh/C, Ru/C, Ir/C was studied. Values of rate constants were found, Gibbs energy of reaction and equilibrium distribution of pinene isomers were calculated. It was found that base catalyst Na/C was very active for 3-carene isomerization to 2-carene in interval of temperatures from 130 to 170^{o}C. The optimal conditions are found when yield of 2-carene is more than 50%.

3. The scheme of oxyphellandrene synthesis (semiproduct for menthol) by acid verbenol isomerization is suggested. Kinetics of verbenol conversion by two parallel routes are investigated and optimum conditions of oxyphellandrene formation are found.

St. Petersburg Division of the Boreskov Institute of Catalysis
Head: Prof. Sergey S. Ivanchev

Development of a new generation of postmetallocene catalyst systems and improvement of the process for obtaining polyethylene with their application

1. A new series of highly efficient and thermally stable bis(imino)pyridine-$FeCl_2$ and bis(imine)acenaphthene-$NiBr_2$ complexes is synthesized and studied in ethylene polymerizations. Their application in combination with methylaluminoxane (MAO) as a cocatalyst afforded a wide range of polyethylenes with various structure (from linear to short

chain branched polymers obtained without a comonomer), molecular weights (from high molecular polymers to waxes), molecular weight distribution (from broad to narrow).

2. A possibility for the application of quantum-chemical calculations using a density functional theory method to predict an effective functioning temperature range for the novel nitrogen carcass based catalyst complexes without a polymerization experiment is shown for the first time.

A possibility for combined application of mixtures of Fe- and Ni-based catalysts of this kind in one reactor is experimentally confirmed and shown to effectively produce polyethylenes with different MWs and branching degrees at quite high rates.

3. A method for supporting these Fe- and Ni-based catalysts is developed and shown to provide highly efficient heterogeneous catalyst systems affording polymerization activities and obtained polymer structures close to those achieved using similar homogeneous catalysts and retaining all the advantages intrinsic to supported catalyst systems, i.e. thermal stability at elevated temperatures, almost constant polymerization rate during a long process time, no polymer sticking onto the reactor walls.

4. Research works on the synthesis of Ti and Zr complexes with phenoxy-imine ligands as polymerization catalysts are started. 10 novel phenoxy-imino-Ti complexes are synthesized and studied in ethylene polymerization in the presence of MAO. The ligand structure is shown to be a crucial factor controlling the activity of the obtained phenoxy-imine catalysts. The presence of substituents in the aryl ring in the ortho-position adjacent to nitrogen leads to a significant drop of the catalyst activity, especially provided para-substituents are also present.

5. Bis[N-(3-tert-butyl-5-methylsalicylidene)anilinato]$TiCl_2$ and bis[N-(3,5-di-tert-butylsalicylidene)anilinato]$TiCl_2$ are found to provide “living” ethylene polymerization and ethylene – hexene-1 copolymerization.

Polyethylenes obtained using phenoxy-imine catalysts are featured with high T_m (142°C), very high MW, linear structure and absence of short chain branching confirmed by their high crystallinity.

RESEARCH ACTIVITY

Quantum-Chemical Studies

A QUANTUM CHEMICAL STUDY OF THE MOLECULAR STRUCTURE OF ACTIVE CENTERS AND GROWTH IN ETHYLENE POLYMERIZATION IN THE CATALYTIC SYSTEM $LFeCl_2/AlMe_3$ (L = 2,6-BIS-IMINOPYRIDYL)

I.I. Zakharov, V.A. Zakharov

Kinet. Catal., 45(4) (2004) pp. 508-518.

Density functional theory with hybrid exchange-correlation functional B3P86 is used to calculate the molecular structures of neutral Fe(II) complexes formed in the $LFeCl_2/AlMe_3$ system (L=tridentate bis(imine)pyridyl ligand). A simplified model of the $LFeCl_2$ complex is used in calculations, where L is replaced by three NH_3 ligands. Parameters of geometric and electronic structures of the complexes $(NH_3)_3FeMe(\mu\text{-}Me)AlMe_3$ (**I**) and $(NH_3)_3FeMe(\mu\text{-}Me)_2AlMe_2$ (**IIA** and **IIB**), which are the structures where the Fe–Me and Fe-μ-Me groups are in one or two perpendicular planes, respectively, were determined. Complexes **II**, which were earlier identified using ^1H NMR spectroscopy, are more stable than complex **I**. Complex **IIB** is strongly polarized (the distances *r*(Fe-μ-Me) and *r*(Al-μ-Me) are 3.70 and 2.08 Å, respectively) and coordinatively unsaturated due to the transfer of the methyl group from $(NH_3)_3FeMe_2$ onto $AlMe_3$. It has significant electron density deficit in the coordination sphere of the transition metal $[(NH_3)_3FeMe]^Q$ (Q = +0.80 e). The energetic profile of the reaction of ethylene addition to the Fe–Me bond for the complexes $(NH_3)_3FeMe_2$, **IIA** and **IIB**, was calculated. It was shown that, compared to $(NH_3)_3FeMe_2$, a drastic decrease in the activation energy of ethylene addition is observed in the case of **IIB** (from 135 to 66 kJ/mol). The reason for the more efficient activation of the complexes $LFeMe_2$ by a weak Lewis acid ($AlMe_3$) and for the increased reactivity of the metal-alkyl bond in complex **IIB** compared to the zirconocene complex Cp_2ZrMe_2 is discussed.

A DFT QUANTUM-CHEMICAL STUDY OF THE STRUCTURE OF PRECURSORS AND ACTIVE SITES OF CATALYST BASED ON 2,6-BIS(IMINO)PYRIDYL Fe(II) COMPLEXES

I.I. Zakharov, V.A. Zakharov

Macromol. Theory Simul., 13(7) (2004) pp. 583-591.

A DFT method has been applied for quantum-chemical calculations of the molecular structure of charge-neutral complex $LFeMe(\mu Me)_2AlMe_2$ which is formed in system $LFeMe_2$+$AlMe_3$ (L=2,6-bis(imino)pyridyl). Calculations suggested the formation of highly polarized complex $LFeMe(\mu Me)_2AlMe_2$ (**II**) in system $LFeMe_2$+$AlMe_3$, characterized by *r*(Fe—μMe) = 3.70 Å and *r*(Al—μMe) = 2.08 Å and deficient electron density on fragment $[LFeMe]^Q$ (Q = +0.80 e). Polarization of the complex progresses with the bounding of two $AlMe_3$ molecules (complex $LFeMe(\mu Me)_2AlMe_2$ $2AlMe_3$ (**III**)) and with replacement of $AlMe_3$ by $MeAlCl_2$ (complex $LFeMe(\mu Me)_2AlCl_2$ (**IV**)). The activation energy of ethylene insertion into the FeMe bond of these complexes has been calculated. It was found that the heat of π-complex formation increases with increasing of polarization extent in the order **II** < **III** < **IV**. Activation energy of the insertion of coordinated ethylene into Fe-Me bond decreases in the same order: **II** > **III** > **IV**.

QUANTUM–CHEMICAL CALCULATIONS OF THE EFFECT OF CYCLOALIPHATIC GROUPS IN α-DIIMINE AND BIS(IMINO)PYRIDINE ETHYLENE POLYMERIZATION PRECATALYSTS ON THEIR STABILITIES WITH RESPECT TO DEACTIVATION REACTIONS

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Polymer, 45 (2004) pp. 6453-6459.

For the first time, it is attempted to interpret an experimentally found enhancing effect of cycloaliphatic substituents in aromatic rings of Ni^{II}– and Pd^{II}-α-diimine and Fe^{II}–bis(imino)pyridine ethylene polymerization precatalysts on their catalytic activities at elevated temperatures (60-80°C), using quantum chemical Density Functional Theory calculations of relative stabilities of the complexes with respect to different deactivation processes, including thermal decomposition and one-electron reduction. It was shown that the effect correlates with the calculated higher thermal stabilities of cycloalkyl-substituted Fe^{II}-, Ni^{II}- and Pd^{II}-complexes as compared to the corresponding alkyl-substituted ones. Ni^{II}- and Pd^{II}-α-diimine complexes with cycloalkyl substituents are shown to be more stable than their alkyl-substituted analogues with respect to both thermal decomposition and one-electron reduction. The averaged difference of the thermal decomposition energies between the complexes with cycloaliphatic substituents on one side and aliphatic ones on the other side is ~2.3 kcal/mol, corresponding to ~30 times lower equilibrium constant of the thermal decomposition reaction for the cycloalkyl-containing complexes. For the Fe^{II}- and Pd^{II}-complexes, the thermal stability correlates with the calculated overlap population of the metal-nitrogen bonds. It was shown that the structure of *o*-substituents (cycloalkyls vs. alkyls) in the phenyl rings of the ligands does not affect the reaction energies for the transformation reactions of the precatalysts into their corresponding active cationic forms.

COPPER HYDROXIDE CATALYSTS FOR SELECTIVE OXIDATION: QUANTUM CHEMICAL STUDY OF ACTIVE SITES

A.S. Kosheleva, I.V. Yudanov, G.M. Zhidomirov, V.N. Parmon

React. Kinet. Catal. Lett.,
82(2) (2004) pp. 347-354.

The Cluster models of the copper hydroxide structure were constructed to investigate the oxidation of organic substrates containing unsaturated C-C bonds in the $Cu(OH)_2/[Ncy]_2[Ocy]_2$ catalytic system. The B3LYP density functional calculations of the activation barriers for ethylene epoxidation by the mono- and binuclear Cu^{II} hydroperoxo complexes corroborated the possibility of non-radical oxygen transfer from the terminal CuOOH hydroperoxo group. The activation barriers presented are relatively high compared to the barriers in the range of 12-15 kcal/mol calculated at the same computational level for Ti^{IV} hydroperoxo intermediates and Re^{VII} bisperoxo complexes.

DENSITY FUNCTIONAL STUDY OF Pd NANOPARTICLES WITH SUBSURFACE IMPURITIES OF LIGHT ELEMENT ATOMS

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(**Technische Universität Munchen, Germany*)

Phys. Chem. Chem. Phys.,
6(1) (2004) pp. 116-123.

Atomic H, C, N and O at the surface and in the subsurface region of Pd nanoparticles were studied theoretically using an all-electron scalar relativistic density functional approach. Nanosize metal clusters are modelled by the three-dimensional crystallites Pd_{79} and Pd_{116} chosen as octahedral fragments of bulk Pd; these clusters expose (111) and (001) facets. Adsorbed atoms were located at the three-fold hollow sites in the centre of (111) facets. Migration of the atoms from the surface of the cluster Pd_{79} to the octahedral subsurface (*oss*) site below was considered. Migration of C from the surface hollow site to the *oss* position was found to be almost isoenergetic; migration of H is somewhat endothermic (by 0.5 eV). For N and O, a lager endothermicity was calculated. Both H and C species exhibit moderate activation barriers for the diffusion to the *oss* site. C and O atoms in the tetrahedral subsurface (*tss*) position of the cluster Pd_{116} were also studied. For both species, this location is energetically disfavoured, although the endothermic effect of O atom migration to the *tss* position is ~0.5 eV smaller than to the *oss* site. Subsurface C impurities were calculated to reduce the adsorption energy of CO molecules at Pd clusters.

DFT CLUSTER MODELING OF MOLECULAR AND DISSOCIATIVE HYDROGEN ADSORPTION ON Zn^{2+} IONS WITH DISTANT PLACING OF ALUMINUM IN THE FRAMEWORK OF HIGH-SILICA ZEOLITES

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Catal. Lett., 90(3-4) (2003) pp. 137-142.

The problem of various cationic positions in zeolites with high Si/Al ratio in the framework is discussed. The statistical distribution of Al in the lattice of pentasils makes probable appearance of the structures with distant placing of two Al atoms. Cations, localized at such sites, should be very strong Lewis acids that are highly active in different chemical reactions. An example of such site is considered for two Zn^{2+} ions stabilized in the zeolite fragment represented by two adjacent 5-membered rings sharing the common edge. DFT calculations of molecular and dissociative hydrogen adsorption by such sites are in agreement with experimental results. Adsorption of dihydrogen by zinc ion at such sites results in unusually large low frequency shift of H-H stretching vibrations indicating essential activation of adsorbed H_2 molecule. The calculated path of heterolytic dissociative adsorption of dihydrogen and of the proton migration to the distantly placed basic oxygen of such acid-base pair are in agreement with the previously published DRIFT experimental data.

MODELS OF FINELY DISPERSED MgO AND V_2O_5 ON SILICA. THEORETICAL ANALYSIS OF OPTICAL PROPERTIES BY TD DFT METHOD

V.I. Avdeev, G.M. Zhidomirov

Res. Chem. Intermed., 30(1) (2004) pp. 41-64.

Calculations of the optical properties of vanadium (V) complexes $VOCl_3$, $[VOCl_4]^{1-}$, $[VOCl_5]^{2-}$, and $[VO_4]^{3-}$ ion have been performed in the frames of the density functional theory (DFT). Full spectrum of excited states in the region of 25000-60000 cm^{-1} has been analyzed by the time-dependent DFT method (TDDFT). Spectroscopy of structure defects – low-coordinated (LC) oxygen ions, and surface point defects – F^+ and F sites in MgO has been studied in the cluster approximation. The charge transfer spectra and frequencies of normal vibrations for a number of active site models of finely dispersed oxides MgO and V_2O_5 on silica have been calculated. Comparison of obtained results with experimental electronic diffuse reflectance spectra and fundamental frequencies confirms a hypothesis about the structure of active centers of finely dispersed oxide V_2O_5 on silica as monomeric forms, ($O=V-O_n$).

MOLECULAR MECHANISM OF ETHYLENE EPOXIDATION ON SILVER: STATE OF THE PROBLEM AND THEORETICAL APPROACHES

G.M. Zhidomirov, V.I. Avdeev, A.I. Boronin

In *"Computer Material Science"*,
Eds. C.R.A. Catlow, E. Kotomin,
NATO Sci. Ser. III,
IOS Press, Amsterdam, Vol. 187, 2003, pp. 334-358.

A new concept of the oxygen species epoxidizing ethylene on silver is presented. The epoxidizing oxygen is formed on the defects of the partially oxidized metal silver surface. Oxygen saturates the bulk of silver at high temperature (T>500 K) and pressure of the reaction medium, and the whole subsurface layer becomes highly defective. A cluster model of the defect structure surface AS_V, including a silver atom vacancy and the subsurface oxygen atoms is considered.

Calculations were performed in the framework of DFT approach. It was shown that the subsurface oxygen atoms tend towards self-association and formation of quasi-molecular oxygen structures inside of the vacancy space. Adsorption of the oxygen atom on site AS_V also provides stabilization of the surface quasi-molecular ("ozonide") form, $AS_V + O \rightarrow AS_d\text{-}O$.

The experimental XPS, UPS, IR, and Raman spectroscopy providing evidence in favor of stabilization of the quasi-molecular oxygen forms on the reactive silver surface is discussed. A theoretical interpretation of the experimental data is based on the proposed model of associative oxygen forms.

QUANTUM-CHEMICAL STUDY OF C_nF_{2n+2} CONFORMERS. STRUCTURE AND IR SPECTRA

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J. Struct. Chem., 45(4) (2004) pp. 599-609.

Quantum-chemical calculations of the geometrical structure and vibrational spectra of C_nF_{2n+2} oligomers (n = 5–8) in the chain and branched conformations are reported. The lengthening of the chain of C_nF_{2n+2} does not substantially affect the geometrical parameters of the oligomers. In all cases under study, the most optimal structure of the molecule is a zigzag chain with bond lengths R(C-C) = 1.53–1.54 Å and R(C-F) = 1.36–1.34 Å; the chain is rolled into a helix, which makes an angle of 17° with the plane. The IR spectra are sensitive to the structural deficiency of oligomers C_nF_{2n+2} associated with the lateral trifluoromethyl groups formed in the chain; the spectra can be used for revealing defects of this type in the structure of polytetrafluoroethylene (PTFE). The possibility of defects associated with the lateral CF_3 groups in the structure of PTFE and its low-temperature modifications is explained based on the calculated total energies of C_nF_{2n+2}.

STRUCTURE OF MODIFIED POLYTETRAFLUOROETHYLENE ACCORDING TO DFT CALCULATIONS AND ^{19}F NMR SPECTROSCOPY

V.M. Buznik, S.P. Gabuda*, S.G. Kozlova*, A.K. Tsvetnikov** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institute of Chemistry, Vladivostok, Russia*)

J. Struct. Chem., 44(6) (2003) pp. 1152-1155.

The molecular structure of *n*-C_7F_{16} and the ^{19}F nuclear magnetic screening tensors are calculated by density functional theory (DFT) methods. The results of calculations are compared with ^{19}F NMR data, and it is shown that fine polytetrafluoroethylene (PTFE) contains the terminal CF_3 groups in its structure.

MODELING THE GAS-PHASE REDUCTION OF NITROBENZENE TO NITROSOBENZENE BY IRON MONOXIDE: A DENSITY FUNCTIONAL THEORY STUDY

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J. Phys. Chem. A, 108(22) (2004) pp. 4878-4886.

The gas-phase selective reduction of nitrobenzene (NB) to nitrosobenzene (NSB) by iron monoxide has been for the first time studied by means of density functional theory (DFT) using both the hybrid and pure exchange-correlation functionals. As shown at both DFT levels, when interacting with NB, the iron center donates an electron into the nitro group to form the NB^- anion radical strongly coupled by FeO^+. This electron-transfer characteristic of the NB^--FeO^+ intermediate reveals itself in the S^2 operator expectation value that exceeds its eigenvalue of S(S+1) by almost 1.0. Further reaction steps necessary to obtain nitrosobenzene from this intermediate are discussed. One of the possible steps based on the abstraction of oxygen from the nitro group by a ferrous center is considered in detail. This reaction appears to be favorable at the pure DFT level, whereas the hybrid theory predicts small endothermicity for the process.

POSSIBLE MOLECULAR STRUCTURE OF PROMOTED LEWIS ACIDITY SITES IN ZnZSM-5

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Int. J. Quant. Chem., 100(4) 2004) pp. 489-494.

It is suggested that the abnormal methane IR frequency shift observed in ZnZSM-5 zeolites is caused by adsorptive interaction of CH_4 with particularly strong Zn^{2+} Lewis sites. Various molecular structures of zinc ion species in high-silica zeolites are discussed and it is concluded that increased Lewis acidity of a sites is associated with their decreased structural stability. It is shown that Zn^{2+} in zeolite cationic position with distantly placed Al ions can produce observed shift of vibrational frequencies for adsorbed methane molecule.

COMPUTATIONAL STUDY OF BENZENE TO PHENOL OXIDATION CATALYZED BY N_2O ON IRON EXCHANGED FERRIERITE

N.A. Kachurovskaya*, G.M. Zhidomirov, R.A. van Santen* (**Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands*)

J. Phys. Chem. B, 108(19) (2004) pp. 5944-5950.

An Fe(II) ion at an α-cation exchange position of ferrierite, $(Fe)_\alpha$ was taken as a model for the active site in nitrous oxide decomposition and in the selective oxidation of phenol with nitrous oxide. The oxygen deposited by decomposition of N_2O is commonly referred to as α-oxygen, $(O)_\alpha$. Comparison with the results of cluster model calculations was performed for reaction of benzene to phenol oxidation. Periodic calculations predict the same reaction path for benzene oxidation like cluster model study. Differences in the adsorption modes for both types of calculations were analyzed and discussed.

COMPARATIVE ENERGIES OF Zn(II) CATION LOCALIZATION AS A FUNCTION OF THE DISTANCE BETWEEN TWO FORMING CATION POSITION ALUMINIUM IONS IN HIGH-SILICA ZEOLITES

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R.A. van Santen* (**Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands*)

Res. Chem. Intermed., 30(1) (2004) 99-103.

Periodical calculations of Zn(II) metal cation stabilization in cationic positions with distantly placed aluminium ions has been performed for high-silica ferrierite. It was found that decrease of the stabilization energy at large distances between Al ions (more than 10 Å) is about of 2 eV in comparison with nearest possible position of two Al ions in the zeolite lattice and weekly depended on following increase of the Al---Al distance. Main changes in stabilization energy occurred within 3 Å interval of these distances. Only for the localizations of both Al ions in one zeolite ring zinc cationic form is more stable than hydrogen form.

CLOSED AND OPEN-SHELL ATOMIC OXYGEN ON SILVER: TWO DISTINCT PATTERNS OF THE O1S BINDING ENERGY AND X-RAY ABSORPTION O *K*-EDGE SPECTRA AS REVEALED BY DENSITY FUNCTIONAL THEORY

S.Ph. Ruzankin, I.L. Zilberberg, G.M. Zhidomirov

Res. Chem. Intermed., 30(1) (2004) pp. 75–85.

The electronic structure of atomic oxygen adsorbed species is studied by means of the density functional theory in the context of the ethylene epoxidation on the silver surface. The adsorbed oxygen species are modeled by the Ag_2O molecule either in its closed ($^1A_1$) or open-shell states ($^3B_1$ and $^1B_1$). In both open-shell states the 1s level appears to be lower than that in $^1A_1$ by about 2 eV. This is apparently a sequence of the separation of electron pair, occupying the π^*-type highest occupied molecular orbital (HOMO), decreasing the electron density at the oxygen center. Such variation of the O1s level for closed and open-shell Ag_2O states seems to explain the X-ray photoelectron spectroscopy (XPS) data concerning two distinct atomic oxygen species on silver surface having the O_{1s} binding energy of about 528 and 530 eV, called nucleophilic and electrophilic oxygen, respectively. The X-ray absorption O *K*-edge spectra (XANES) calculated for two types of the Ag_2O states by means of multiple-scattered-Xα-based approach appears to be in a qualitative agreement with those experimentally recorded for nucleophilic and electrophilic oxygen.

EXPANSION OF THE UNRESTRICTED DETERMINANT IN THE BASIS OF PAIRED ORBITALS

I.L. Zilberberg, S.Ph. Ruzankin

Chem. Phys. Lett., 394(1-3) (2004) pp. 165-170.

An analysis of spin mixture contained in the unrestricted determinant using Löwdin–Amos-Hall paired orbitals (POs) is developed. The space of POs is divided into subspaces of completely, partially and non-overlapping orbitals. Spin contamination is shown to be associated with the ‘active’ space of 2*k* partially overlapping POs with *k* being in practice fairly small number. In the basis of POs the unrestricted determinant is expanded in a linear combination of restricted determinants describing ‘basis’ configurations contained 0,1, . . . , *k* pairs of spatially separated α and β spins.

UNRESTRICTED DENSITY FUNCTIONAL THEORY OF THE BONDING BETWEEN NO RADICAL AND FERROUS ION

I.L. Zilberberg, S.Ph. Ruzankin, S.E. Malykhin, G.M. Zhidomirov

Chem. Phys. Lett., 394(4-6) (2004) pp. 392–396.

Bonding between NO and the Fe(II) center to form so-called $FeNO^7$ unit has been studied using simplistic $Fe(NO)(OH)_2$ system within the unrestricted density functional theory using hybrid and pure exchange-correlation functionals. To analyze in details the obtained unrestricted solution for ground state with $S_z = 3/2$ corresponding Kohn–Sham determinant is expanded in the basis of Löwdin–Amos–Hall paired orbitals. This expansion allowed to assign the electron structure of $FeNO^7$ unit as a mixture of charge-transfer configurations $Fe^+ \cdots NO^+$ and $Fe^{3+} \cdots NO^-$, and the covalent configuration $Fe^{2+} = NO^0$.

A COMPARATIVE, TWO-DIMENSIONAL ^{14}N ESEEM CHARACTERIZATION OF REDUCED [2Fe-2S] CLUSTERS IN HYPERTHERMOPHILIC ARCHAEAL HIGH- AND LOW-POTENTIAL RIESKE-TYPE PROTEINS

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J. Biol. Inorg. Chem., 9(6) **(**2004) pp. 753-767.

It is reported here the comparative orientation-selected ESEEM and HYSCORE studies of the reduced clusters from two hyperthermophilic Rieske-type proteins; a high-potential, archaeal Rieske protein called sulredoxin (SDX) from Sulfolobus tokodaii with weak homology to the cytochrome bc-associated Rieske proteins, and a low-potential, archaeal homolog of an oxygenase-associated Rieske-type ferredoxin (ARF) from Sulfolobus solfataricus. ^{14}N ESEEM and HYSCORE spectra of SDX and ARF show well-defined variations, which are primarily determined by changes of quadrupole couplings (up to 50% depending on the selected orientation) of the two coordinated nitrogens. These are due to variations in coordination geometry of the histidine imidazole ligands rather than to variations of hyperfine couplings of these nitrogens, which do not exceed 8–10%. The measured quadrupole couplings and their differences in the two proteins are consistent with those calculated using the reported crystal structures of high- and low-potential Rieske proteins. These results suggest that exploration of quadrupole tensors might provide a more accurate method for characterization of the histidine coordination in different proteins and mutants than hyperfine tensors, and might have potential applications in a wider range of biological systems.

THE INFLUENCE OF TEMPERATURE AND PRESSURE ON HYDROGEN ATOM TRANSFER IN TUNNEL SOLID-PHASE REACTIONS

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Chem. Phys., 23(6) (2004) pp. 56-68.

Dependencies of the rate constant of a solid-phase tunnel reaction on temperature and pressure are considered. The T-dependence is determined by intermolecular and mild intramolecular vibrations in the reactants that cause oscillations in the permeability of the potential barrier for the tunneling atom. The influence of the external pressure is accounted for by a static decrease in the width and height of the potential barrier. The role of various promoting vibrations and T- and P-dependencies in the “acridine-fluorene” system are estimated using quantum chemical calculations of parameters of the reaction system. Anomalous values of $\langle S^2 \rangle$ are discovered before and after annihilation of the first trace constituent of the UHF function in the “acridine-fluorene” system.

Monte-Carlo Simulation to Study Physicochemical Processes

CATALYTIC PROCESSES OVER SUPPORTED NANOPARTICLES: SIMULATION

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In “*Dekker Encyclopedia of Nanoscience and Nanotechnology”*,
Eds. J.A. Schwarz, C.I. Contescu, K. Putyera,
Marsel Dekker, Inc., New York, 2004, pp. 621-632.

In heterogeneous catalysis, adsorption and reaction processes usually occur on supported metal nanoparticles. To study such processes experimentally, a vast variety of surface-science techniques came into the use in the last decades of the 20th century. Along with the appearance of high-precision techniques for surface characterisation, considerable progress in manufacturing of model catalysts with well-defined properties like particle size, shape and separation has been achieved. Despite this progress, the cognitive potential of the experimental studies in this field is still limited because the measurements are usually indirect and the information derived demands quantitative processing and interpretation. This can be done only with the use of mathematical models. Successful interpretation of the results requires constructing mathematical models providing accurate description of systems under consideration. Application of the conventional mean-field models is often limited here due to the peculiarities of the reaction performance on the nm scale, including the inherent heterogeneity of metal crystallites as well as spontaneous and adsorbate-induced changes of the shape and degree of dispersion of supported catalysts. Under such circumstances, the use of stochastic simulations based, e.g., on the Monte Carlo technique, is almost inevitable. This entry is focused on theoretical studies (simulation) of the catalytic reaction kinetics on the active supported nanoparticles. The goal of this contribution is to describe the main achievements of the corresponding theoretical works.

PERIODIC PERTURBATION OF THE KINETICS OF HETEROGENEOUS CATALYTIC REACTIONS

V.P. Zhdanov

Surf. Sci. Rep., 55(1) (2004) pp. 1-48.

Periodic forcing of reaction kinetics via, e.g., variation of reactant pressure(s), temperature or flow reversal is one of the useful tools employed in basic and applied studies of heterogeneous catalytic processes. In the case of conventional (stable) kinetics, this strategy is used to clarify the mechanisms of reactions and obtain data on reaction rate constants or to improve the reaction performance, e.g., to increase reaction rate and/or selectivity with respect to desired products. In experiments, that are focused on oscillatory catalytic reactions, periodic perturbations are employed to stabilize period-1 oscillations. This is easily achieved if the external and internal frequencies are equal. In a more general context, periodic perturbation of chemical reactions, that exhibit period-1 oscillations, may result in complex reaction behaviour, including period doubling and irregular kinetics provided that the external and internal frequencies do not coincide. In this review are considered both the relevant data available in the literature and the results of systematic calculations for a few generic models.

SIMULATION OF THE GROWTH AND DIFFERENTIATION OF STEM CELLS ON A HETEROGENEOUS SCAFFOLD

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden)*

Phys. Chem. Chem. Phys.,
6(17) (2004) pp. 4347-4350.

Monte Carlo simulations illustrating that scaffolds with specially designed heterogeneities can be used as a tool for governing the growth and differentiation of stem cells are presented. This tool is predicted to be efficient provided that the size of the heterogeneities exceeds (but not appreciably) the cellular size and the rate of cell diffusion is relatively fast compared to that of cell division.

FROM A PLURIPOTENT STEM CELL TO AN ENSEMBLE OF DIFFERENTIATED CELLS: ELEMENTS OF THEORETICAL TISSUE ENGINEERING

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Phys. Chem. Chem. Phys.,
6(1) (2004) pp. 138-143.

Monte Carlo lattice simulations are presented illustrating how the growth of stem and differentiated cells on a uniform surface can be governed (guided differentiation) by tuning long-range cell-cell communication. Due to spatial constraints on cell division, the growth rate is shown to strongly depend on the interplay of cellular division, diffusion, and signaling. With decreasing diffusion rate, the kinetics become slower. To increase the selectivity of the growth with respect to "desirable" cells, one can use induced messenger-mediated generation of these cells by stem cells. The simplest schemes based on this idea may, however, result in appreciable slowdown of the growth. A more optimal strategy may be simultaneous promotion of generation of desirable cells and stem cells.

ROLE OF THE FIELD FLUCTUATIONS IN ELECTROCHEMICAL REACTIONS

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Appl. Surf. Sci., 219(3-4) (2003) pp. 256-263.

Rate constants of electrochemical reactions, accompanying by electron transfer via the electrolyte-metal interface, exponentially depend on the electrode potential. Monte Carlo simulations are presented illustrating the effect of fluctuations of the potential near the reactants on the rate of such reactions. The two models employed are based on the phenomenological Frumkin theory and aimed, respectively, at conventional electrolytes and polymer electrolytes widely used in fuel cells. In both cases, the role of spatio-temporal fluctuations is found to be minor if the dielectric constant in the double layer is large, similar or equal to 80 (as in the bulk water). If the double-layer dielectric constant is smaller, e.g. similar or equal to 30 as it often takes place in conventional and polymer electrolytes, the fluctuations result in appreciable increase of the apparent reaction rate constant. This effect is especially important (of a factor of 15) for polymer electrolytes. In the latter case, the reaction rate is actually controlled by the fluctuations. Implications of these findings for basic and applied electrochemistry are briefly discussed.

TOWARDS THE UNDERSTANDING OF THE SPECIFICS OF REACTIONS IN POLYMER ELECTROLYTE FUEL CELLS

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Surf. Sci., 554(2-3) (2004) pp. 103-108.

In low-temperature hydrogen-oxygen polymer-electrolyte fuel cells, catalytic reactions usually occur on nm-sized Pt particles located on the walls of a porous carbon support. The electrolyte is usually a hydrated polymer (e.g., NAF-ION), which consists of hydrophobic chains and hydrophilic subchains and contain appreciable amount of water (up to about 40%). The heterogeneity of the electrolyte has the same length scale (about 10 nm) as the size of catalyst particles. To elucidate some specific aspects of reactions occurring under these conditions, Monte Carlo lattice simulations are presented illustrating probable distributions of polymer and water near Pt particles. In the case of cathodic processes, the Pt surface is predicted to be free of polymer, the double layer near Pt to be uniform, and the role of polymer in the surface electrochemistry to be minor. During anodic processes, the polymer chains seem to directly participate in formation of the double layer near Pt, the field distribution in the double layer is far from uniform, and accordingly the role of polymer in surface electrochemistry is appreciable.

INFLUENCE OF ELECTROLYTE ON ELECTRON DIFFUSION IN MESOPOROUS NANOCRYSTALLINE TiO_2

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

J. Phys.: Condens. Matter,
16(15) (2004) pp. 2625-2629.

Experimental studies show that the rate of electron diffusion in mesoporous nanocrystalline TiO_2 may depend on the electrolyte concentration. In the available literature, this effect is attributed to ambipolar diffusion. The arguments and a kinetic model are presented indicating that it might instead be connected with different arrangements of cations near the traps occupied by an electron before and after tunnelling. With a reasonable choice of the ratio of the kinetic parameters, in agreement with experiment, the model predicts that the electron diffusion coefficient at high electrolyte concentrations may be about five times higher than at low concentrations.

ONE OF THE SCENARIOS OF ELECTROCHEMICAL OXIDATION OF CO ON SINGLE-CRYSTAL Pt SURFACES

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Surf. Sci., 545(1-2) (2003) 109-121.

Monte Carlo simulations are presented illustrating that the transient potential-step kinetics of CO oxidation on single-crystal Pt surfaces are fairly sensitive to adsorbate-adsorbate lateral interactions. Specifically, it is shown that with realistic values of these interactions (similar or equal to 1 kcal/mol) the reaction kinetics may be accompanied by CO segregation provided that surface CO diffusion is fast. In addition, it is demonstrated that the CO-island formation may be one of the reasons of extinction in CO oxidation. Implications of these findings for interpretation of experimental data are discussed.

THE EFFECT OF OXIDE FORMATION ON BISTABILITY IN CO OXIDATION ON Pt

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J. Catal., 220(2) (2003) pp. 478-485.

Kinetics of CO oxidation on Pt is bistable both under UHV conditions and at atmospheric pressure. In the former case, the bistability can be explained by using the established reaction scheme, including reversible CO adsorption, dissociative O_2 adsorption, and reaction between adsorbed CO and O. Also at higher pressures, this model accounts well for the low-reactive (CO-dominated) regime. However, in the high-reactive (oxygen-rich) regime, the kinetics may be influenced by surface oxide formation at the higher pressures. The present Monte Carlo simulations illustrate what may happen when oxide formation and removal occur with participation of gas-phase O_2 and CO molecules, respectively. Specifically, it is shown that these relatively slow steps may control the reaction rate in the high-reactive state. In this case, the hysteresis loop is found to be qualitatively similar to that predicted by the conventional reaction scheme, but the CO_2 formation rate in this state is appreciably lower. These predictions are in qualitative agreement with the results of recent STM studies of CO oxidation on Pt(110) at atmospheric pressure.

COMMENT ON “HYSTERESIS PHENOMENA IN CO CATALYTIC OXIDATION SYSTEM IN THE PRESENCE OF INHOMOGENEITIES OF THE CATALYST SURFACE”

V.P. Zhdanov

Phys. Rev. E, 68 (2003) 068101 (2 pp).

Scrutinizing the Monte Carlo algorithm, used by D.-Y. Hua and Y.-Q. Ma [Phys. Rev. E, 66, 066103 (2002)] in order to simulate the effect of defect sites on bistable kinetics of CO oxidation on single-crystal surfaces, it is shown that in their study (i) the rules for describing CO adsorption, desorption, and surface diffusion contradict the detailed balance principle and (ii) the ratio of the rates of CO diffusion and reaction between adsorbed CO and O species is opposite compared to that observed in reality.

KINETIC OSCILLATIONS ON nm-SIZED CATALYST PARTICLES: NO REDUCTION BY CO ON Pt

V.P. Zhdanov

Catal. Lett., 93(3-4) (2004) pp. 135-138.

Monte Carlo simulations of kinetic oscillations in the NO-CO reaction occurring due to the interplay of catalytic steps including autocatalytic NO dissociation are presented. The lattice size is varied from 100x100 to 10x10 in order to mimic nm-sized catalyst particles. More or less regular oscillations are found for the sizes down to 15x15. In combination with similar results obtained earlier for two other models describing CO oxidation accompanied by oxide formation and surface restructuring, this finding forms one of first firm quantitative ingredients of the theory of oscillatory kinetics on supported catalysts.

COMMENT ON “MODELLING PATTERN FORMATION IN CO+O_2 REACTION ON Pt(100)”

V.P. Zhdanov

Chem. Phys. Lett., 390(1-3) (2004) pp. 301-304.

I.M. Irurzun. R.B. Hoyle, M.R.E. Proctor and D.A. King [Chem. Phys. Lett., 377 (2003) 269] have recently proposed a novel coarse-grained approach to describing the transport of adsorbed CO molecules along the quasi-hexagonal and (1 x 1) patches during kinetic oscillations in CO oxidation on the Pt(100) surface. Analysis indicates that this approach cannot be used as a robust tool for analysing the pattern formation in oscillatory catalytic reactions, because it contradicts the basic principles of general theory of mass transport.

PERTURBATION OF PERIOD-2 OSCILLATIONS IN CATALYTIC REACTIONS ACCOMPANIED BY SURFACE RESTRUCTURING

V.P. Zhdanov

Phys. Rev. E, 68 (2003) 056212 (6 pp.).

Monte Carlo simulations illustrating the effect of periodic forcing on period-2 oscillations related to the interplay of catalytic reaction and surface restructuring are presented. The oscillations are found to be fairly stable if the external frequency equals the main internal frequency. In contrast, perturbations with other frequencies may easily change the type of oscillation. In particular, perturbations with double frequency convert period-2 oscillations into period-1 oscillations with the imposed frequency.

BIFURCATION IN A GENERIC MODEL OF INTRACELLULAR VIRAL KINETICS

V.P. Zhdanov

J. Phys. A: Math. Gen., 37(5) (2004) L63-L66.

The key steps of intracellular virion reproduction include viral genome replication, mRNA synthesis and degradation, protein synthesis and degradation, capsid assembly and virion release from a cell. The analysis, incorporating these steps (with no deterioration of the cell machinery), indicates that asymptotically depending on the values of the model parameters the viral kinetics either reach a steady state or are out of control due to an exponential growth of the virion population. In the latter case, the cell is expected to rapidly die or the virion growth should be limited by other steps.

KINETICS OF PROTEIN AGGREGATION WITH FORMATION OF UNREACTIVE INTERMEDIATES

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Langmuir, 20(7) (2004) pp. 2543-2545.

Irreversible protein aggregation resulting in formation and deposition of insoluble fibrils or amorphous precipitates is usually assumed to occur via sequential attachment of monomers to soluble intermediates. This scheme is complemented by slow conversion of the intermediates to a relatively stable form so that they do not react with monomers but can be trapped by precipitates. For reasonable values of parameters, our model predicts that the aggregation kinetics order may be between 2.0 and 2.5. In particular, the model can be used to explain the reaction order, 2.17 +/- 0.09, observed for aggregation of recombinant human granulocyte colony stimulating factor.

PROPAGATION OF INFECTION AND THE PREY-PREDATOR INTERPLAY

V.P. Zhdanov

J. Theor. Biol., 225(4) (2003) pp. 489-492.

The article contains Monte Carlo simulations illustrating propagation of infection and the prey-predator interplay.

NANOMETER-SIZED ANTENNA FOR ENHANCEMENT OF ABSORPTION OF LIGHT BY DYE MOLECULES

V.P. Zhdanov, B. Kasemo* (**Chalmers University of Technology, Göteborg, Sweden*)

Appl. Phys. Lett., 84(10) (2004) pp. 1748-1749.

One of the ways to increase the absorbance of dye molecules is to optimize the property of their environment. In particular, a dye molecule can be surrounded by a few other molecules absorbing at lower frequencies. Analysis indicates that the amplification factor of such nanometer-sized antennas may be up to about 200.

Physicochemical Methods to Study Active Sites, Mechanism and Reaction Kinetics

PROPYLENE OXIDATION BY PALLADIUM NITRO AND NITRATO COMPLEXES: *IN SITU* NMR AND IR STUDIES

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J. Organometal. Chem., 689(18) (2004) pp. 2880-2887.

The mechanism of the propylene oxidation by $Pd(NO_n)Cl_{2-m}(CH_3CN)_2$ complexes ($n = 2, 3; m = 0, 1, 2$) in chloroform solutions has been studied by ^{1}H NMR and IR spectroscopy. The main reaction products are acetone and 2-nitropropylene, with their ratio depending on the equilibrium existing in the reaction solutions between palladium complexes containing NO_n ligands bonded to a palladium atom via either an oxygen or a nitrogen atom. Reactivities of the oxygen bonded nitrato and nitrito complexes are significantly higher than that of the nitrogen bonded nitro complex. Various new organopalladium intermediates have been observed and monitored *in situ*. A reversible insertion of the coordinated propylene into the Pd–O or Pd–N bonds results in nitrato-, nitrito- and nitropalladation intermediates, which then decompose via a β-hydrogen elimination. Two isomers of the nitritopalladation intermediate have been detected, i.e., a palladium metallacycle and an open ring complex, with the latter being much more reactive towards the β-hydrogen elimination than the former. The decomposition of the nitrato- and nitritopalladation intermediates results in the organometallic precursor of acetone, i.e., an acetonylpalladium complex, and then in acetone itself. On the other hand, the nitropalladation intermediate originates 2-nitropropylene. In the presence of dioxygen, which re-oxidizes the nitrosyl groups, the acetone formation becomes a catalytic reaction with respect to both palladium and nitrogen.

CO DISSOCIATION AND CO HYDROGENATION ON SMOOTH AND ION-BOMBARDED Pd(111): SFG AND XPS SPECTROSCOPY AT MBAR PRESSURES

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Appl. Surf. Sci., 235(1-2) (2004) pp. 26-31.

The CO dissociation probability on transition metals is often invoked to explain the product distribution (selectivity) of catalytic CO hydrogenation. Along these lines, CO adsorption and dissociation on smooth and ion-bombarded Pd(111) at pressures up to 1 mbar were investigated using vibrational sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS). Under high pressure, CO adsorbate structures were observed that were identical to high-coverage structures in UHV. On ion-bombarded surfaces an additional species was detected which was attributed to CO bridge bonded to defect (low-coordinated) sites. On both surfaces, no indications of CO dissociation were found even after hours of 0.1 mbar CO exposure. However, exposing CO/H_2 mixtures to ion-bombarded Pd(111) produced carbonaceous deposits suggesting CH_xO species as precursors for C---O bond cleavage and that the formation of CH_xO is facilitated by surface defects. The relevance of the observations for CO hydrogenation on Pd catalysts is discussed.

C–O BOND SCISSION ON “DEFECT-RICH AND PERFECT” Pd(111)?

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Surf. Sci., 566-568(Part 2) (2004) pp. 1024-1029.

To investigate the influence of surface defects on CO adsorption and dissociation, well-annealed and "defect-rich" Pd(111) were examined by sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS) within the pressure range 10^{-6}–1 mbar. Ar^+ ion sputtering was employed to produce surface defects which exhibited vibrational and photoemission characteristics different from the regular adsorption sites on Pd(111). Even under high-pressure, SFG and XPS indicated that no CO dissociation occurred on both surfaces at 300–400 K. By contrast, C–O bond scission was observed during methanol decomposition producing carbonaceous deposits beside CO and H_2. A possible relationship between the adsorption geometry and C–O bond scission is discussed.

METHANOL DEHYDROGENATION AND FORMATION OF CARBONACEOUS OVERLAYERS ON Pd(111) STUDIED BY HIGH-PRESSURE SFG AND XPS SPECTROSCOPY

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J. Phys. Chem. B, 108(34) (2004) pp. 12955-12961.

Methanol decomposition on Pd(111) at 300 and 400 K was studied *in situ* from 5×10^{-7} to 0.1 mbar by combining vibrational sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS). Two competing decomposition pathways, i.e., dehydrogenation of CH_3OH to CO and H_2 and methanolic C-O bond scission, were observed by monitoring the time-dependent evolution of CO/CH_xO and of carbonaceous deposits CH_x (x=0-3) via their vibrational and photoemission characteristics. Quantification of carbon-containing species was performed by XPS, while the preferred binding site of CH_x was determined by SFG using CO as probe molecule for postreaction adsorption. In contrast to previous reports, Pd(111) was found to be quite active for methanolic C-O bond scission. The CH_x formation rate strongly increased with pressure and temperature, leading to immediate catalyst deactivation at 0.1 mbar and 400 K. The combined SFG/XPS data suggest that the carbonaceous residues are highly dehydrogenated, such as CH or carbon atoms bonded to hollow sites. Complete dehydrogenation of CH_x species and partial dissolution of atomic carbon in the Pd bulk most likely occurred even at 300 K. On the other hand, the CH_x species was found to be unexpectedly thermally stable (up to ~600 K), until carbon dissolution and formation of carbon clusters take place. Regeneration with oxygen above 400 K was able to remove CH_x deposits and to partially restore the initial adsorption properties. Corresponding experiments with CO did not produce any carbon signals, indicating that the cleavage of the C-O bond must occur via CH_xO intermediates (and not within CO). Methanol decomposition at pressures up to 15 mbar and temperatures up to 550 K, followed by gas chromatography, did not produce measurable decomposition products, due to fast carbon poisoning under catalytic reaction conditions.

METHANOL OXIDATION ON A COPPER CATALYST INVESTIGATED USING *IN SITU* X-RAY PHOTOELECTRON SPECTROSCOPY

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J. Phys. Chem. B, 108(38) (2004) pp. 14340-14347.

The surface and near-surface regions of an active catalyst and the adjacent gas-phase reactants were investigated simultaneously under reaction conditions using *in situ* X-ray photoelectron spectroscopy (XPS). This investigation of methanol oxidation on a copper catalyst showed that there was a linear correlation between the catalytic activity of the sample and the presence of a subsurface oxygen species that can only be observed *in situ*. The concentration profile of the subsurface oxygen species within the first few nanometers below the surface was determined using photon-energy-dependent depth-profiling. The chemical composition of the surface and the near-surface regions varied strongly with the oxygen-to-methanol ratio in the reactant stream. The experiments show that the pure metal is not an active catalyst for the methanol oxidation reaction, but that a certain amount of oxygen has to be present in the subsurface region to activate the catalytic reaction. Oxide formation was found to be detrimental to formaldehyde production. Our results demonstrate also that for an understanding of heterogeneous catalysts a characterization of the surface alone may not be sufficient, and that subsurface characterization is essential.

CO ADSORPTION ON Au(110)-(1 x 2): AN IRAS INVESTIGATION

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J. Phys. Chem. B, 107(46) (2003) pp. 12668-12671.

IRAS studies of CO adsorption on the Au(110)-(1×2) surface were performed as a function of CO pressure and sample temperature. It was found that with increasing coverage, the CO IRAS absorption shifts red from 2118 to 2108 cm^{-1}. Clausius-Clapeyron data analysis yielded a heat of CO adsorption ($-H_{ads}$) of 10.9 kcal/mol at low coverages and 7.8 kcal/mol at coverages greater than 19%.

APPLICATION OF NMR MICROIMAGING TO STUDY MASS TRANSFER AND CHEMICAL REACTIONS

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Catal. Ind., Special issue (2004) pp. 60-67.

A possibility of application of NMR-Microimaging to study a wide class of mass-transfer processes in model reactors, granular layers, and porous granules, including that under the conditions of a catalytic reaction, has been demonstrated and systematically investigated. Direct visualization of liquid and gas flows in the channels of different geometry was carried out. Distribution of molecules on rates of movement in a layer were obtained for the processes of filtration of liquids, gases, and solid particles in granular layers and the coefficients of longitudinal and transverse dispersion were measured. Multiphase catalytic processes proceeding in an isolated grain of the catalyst were investigated by NMR-imaging on the examples of reactions of hydrogen peroxide decomposition and α-methylstyrene hydrogenation.

FUNCTIONAL IMAGING AND NMR SPECTROSCOPY OF AN OPERATING GAS-LIQUID-SOLID CATALYTIC REACTOR

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Appl. Catal. A, 267(1-2) (2004) pp. 143-148.

This work reports the first application of nuclear magnetic resonance (NMR) imaging to study the behaviour of a gas–liquid–solid model catalytic reactor operating at elevated temperatures. Two techniques from the magnetic resonance imaging (MRI) toolkit, namely functional MRI and NMR spectroscopic imaging, have been employed to perform a dynamic *in situ* study of α-methylstyrene catalytic hydrogenation on a single catalyst pellet or in a granular bed. Owing to reaction exothermicity, a reciprocating motion of the liquid front within the pellet accompanied by pellet temperature oscillations has been observed even when the external conditions were kept unchanged. Spatially resolved information on the reactant to product conversion within the catalyst bed has been obtained for a steady-state regime. The results represent a first direct MRI visualisation of the mutual influence of mass and heat transport processes and a chemical reaction in an operating reactor and demonstrate that NMR imaging and spectroscopy techniques can be used successfully to study the development of critical phenomena in operating multiphase reactors. It is suggested that further development of the applications of the MRI toolkit in chemical and process engineering and catalysis hold significant promise for the development of safe and efficient technologies based on a detailed understanding of the interplay of various processes in an operating gas–liquid–solid reactor.

THE STUDY OF NITRIC OXIDE ADSORPTION AND THE MECHANISM OF SURFACE “EXPLOSIONS” IN THE REACTION OF CO+NO ON Pt(100) AND Pd(110) SINGLE CRYSTAL SURFACES

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Kinet. Catal., 45(4) (2004) pp. 598-606.

High resolution electron energy loss spectroscopy (HREELS), temperature-programmed desorption (TPD) and temperature-programmed reaction (TPR) were used to study NO adsorption and the reactivity of CO_{ads} and NO_{ads} molecules on Pd(110) and Pt(100) single crystal surfaces. Compared to the Pt(100)-(1×1) surface, the unreconstructed Pt(100)-hex surface is chemically inert toward NO dissociation into N_{ads} and O_{ads} atoms. When a mixed adsorbed CO_{ads} + NO_{ads} layer is heated, a so-called surface “explosion” is observed when the reaction products (N_2, CO_2, and N_2O) synchronously desorb in the form of sharp peaks with a half-width of 720 K. The shape specificity of TPR spectra suggests that the “vacancy” mechanism consists of the autocatalytic character of the reaction initiated by the formation an initial concentration of active sites due to partial desorption of molecules from the CO_{ads}+NO_{ads} layer upon heating to high temperatures. Kinetic experiments carried out on the Pd(110) surface at a constant reaction pressure and a linear increase in the temperature confirm the explosive mechanism of the reaction NO+CO.

AN ION CYCLOTRON RESONANCE STUDY OF THE REACTIVITY OF THE Tc^+ AND Tc_2^+ IONS WITH HYDROCARBONS IN THE GAS PHASE

V.B. Goncharov

Russ. J. Phys. Chem., 78(6) (2004) pp. 882-887.

The reactivity of the Tc^+ and binuclear cluster Tc_2^+ ions toward alkanes, cycloalkanes, and alkenes was studied by ion cyclotron resonance. Unlike its lighter unreactive analogue Mn^+, the Tc^+ ion can activate hydrocarbon C–H bonds and form π complexes with olefins. The cluster Tc_2^+ ion does not react with alkanes but has a higher reactivity toward alkenes compared with the Tc^+ ion. Similar and different features of the mechanisms of C–H bond activation by Tc^+ and Tc_2^+ are discussed. The upper [$D_o(Tc^+–CH_2)$ <111 and $D_o(Tc_2^+–CH_2)$<111 kcal/mol] and lower [($D_o(Tc^+–C_2H_4) > 32.7$, $D_o(Tc^+–C_2H_2) > 76.4$, $D_o(Tc^+–C_3H_6) < 70.5$; $D_o(Tc^+–C_3H_4) > 69.2$, $D_o(Tc^+–C_4H_6) > 58.5$, $D_o(Tc^+–C_5H_6) > 67$, $D_o(Tc^+–C_6H_6) > 59.7$, $D_o(Tc_2^+–C_3H_4) > 32.7$, $D_o(Tc^+–C_2H_4) > 67$, and $D_o(Tc_2^+–C_6H_6) > 59.7$ kcal/mol] bond energy limits were estimated. The interaction of Tc^+ and Tc_2^+ with N_2O and O_2 was studied and the lower bond energy limits in oxide cations were determined [$D_o(Tc^+–O) > 40$, $D_o(Tc_2^+–O) > 118$, and $40 < D_o(Tc_2O_n^+–O) < 118$ kcal/mol, $n = 1–5$].

AN ION CYCLOTRON RESONANCE STUDY OF THE MECHANISM OF FORMATION OF METHANE COMPLEXES WITH MOLYBDENUM OXIDE CATIONS IN THE GAS PHASE

V.B. Goncharov

Russ. J. Phys. Chem., 78(10) (2004) pp. 1560-1571.

The reactions of Mo^+ and oxygen-containing molybdenum cluster ions $Mo_xO_y^+$ ($x = 1–3$ and $y = 1–9$) with methane, ethylene oxide, cyclopropane, and methanol were studied by ion cyclotron resonance. The formation of several organometallic ions, including $Mo_xO_y(CH_4)^+$ ($x =1–3$, $y = 2, 5, 8$), was observed. The upper and lower bond energy limits were estimated for oxometallocarbene complexes, $111 > D^0(Mo_xO_y^+–CH_2) > 82$ kcal/mol ($x = 1–3$ and $y = 2, 5, 8$), and for complexes with the methyl radical $D^0(MoO_y^+–CH_3) > 91.6$ kcal/mol ($y = 2, 3$), $D^0(Mo_2O_y^+–CH_3) > 91.6$ kcal/mol ($y = 4–6$), $D^0(Mo_3O_y^+–CH_3) > 91.6$ kcal/mol ($y = 8, 9$); methane $D^0(MoO_y^+–CH_4) > 89$ kcal/mol ($y = 2,3$), $D^0(Mo_2O_5^+–CH_4) > 89$ kcal/mol, $D^0(Mo_3O_8^+–CH_4) > 89$ kcal/mol, and hydrogen atom $D^0(MoO_3^+–H) > 104$ kcal/mol.

THE DETERMINATION OF INTERMEDIATE COMPOUNDS FORMED IN THE POLYCONDENSATION OF METHANOL IN THE GAS PHASE ON CHARGED MOLYBDENUM OXIDE CLUSTERS BY ION CYCLOTRON RESONANCE SPECTROMETRY

V.B. Goncharov

Russ. J. Phys. Chem., 78(12) (2004) pp. 1924-1928.

A set of oxygen-containing molybdenum clusters Mo_xO_y (x = 1-3, y = 1-9) was obtained using a Knudsen cell in combination with an ion confinement cell. Reactions of positively charged clusters with methanol were studied by ion cyclotron resonance. Several organometallic ions resulting from the initial insertion of molybdenum oxide ions into the C–O and C–H methanol bonds and methanol polycondensation products were observed. The key intermediate that initiated the polycondensation of methanol was shown to be the $Mo_3O_9CH_3^+$ ion. The lower bond energy limits for $Mo_xO_y^+$ complexes with the methyl radical were estimated to be $D^0(MoO_y^+\text{-}CH_3) > 91.6$ (y = 2, 3), $D^0(Mo_2O_y^+\text{-}CH_3) > 91.6$ (y = 4–6), and $D^0(Mo_3O_9^+\text{-}CH_3) > 91.6$ kcal/mol.

MECHANISM OF THE FORMATION OF MOLYBDENUM METALLOCARBENE COMPLEXES IN THE GAS PHASE

V.B. Goncharov

Kinet. Catal., 45(4) (2004) pp. 467-477.

The reactions of Mo^+ ions and $Mo_xO_y^+$ oxygen-containing molybdenum cluster ions (x = 1–3; y =1–9) with methane, ethylene oxide, and cyclopropane were studied using ion cyclotron resonance. The formation of a number of organometallic ions, including the metallocarbene $MoCH_2^+$ as well as molybdenum oxometallocarbenes $Mo_xO_yCH_2^+$ (x = 1–3; y = 2, 4, 5, or 8) and $Mo_xO_y(CH_4)^+$ ions (x = 1–3; y = 2, 5, or 8), was detected. The upper and lower limits of bond energies in oxometallocarbene complexes were evaluated: $111 > D^0\ (Mo_xO_y^+–CH_2) > 82$ kcal/mol (x = 1–3; y = 2, 5, 8).

MÖSSBAUER STUDIES OF THE PHASE COMPOSITION AND MICROSTRUCTURE OF THE $La_{1-x}Ca_xFeO_{3-y}$ SYSTEM AS RELATED TO THE REACTIVITY OF SURFACE AND BULK OXYGEN

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React. Kinet. Catal. Lett., 81(2) (2004) pp. 373-382.

The phase composition and microstructure of samples of the $La_{1-x}Ca_xFeO_{3-y}$ system prepared via a ceramic route were characterized by Mössbauer spectroscopy. In all cases, iron was found in the 3+ state. The ordering of anion vacancies in the samples with the composition in the range of $0.8 > x \geq 0.4$, which corresponds to a microheterogeneous solid solution, generates new distorted octahedral and fivefold/tetrahedral sites revealed by two typical sextets. The disordering of this solid solution and small (10-100 Å) sizes of domains with a perovskite, braunmillerite or Grenier phase structure caused the appearance of a superparamagnetic doublet, which grows with the Ca content up to x = 0.8 but disappears in the sample of pure braunmillerite. The appearance of Fe cations in a distorted coordination correlates with the increased activity of the samples with a microheterogeneous structure in the CO catalytic oxidation and with their reducibility by H_2.

OXYGEN STATES IN OXIDES WITH A PEROVSKITE STRUCTURE AND THEIR CATALYTIC ACTIVITY IN COMPLETE OXIDATION REACTIONS: SYSTEM $La_{1-x}Ca_xFeO_{3-y}$ (x = 0–1)

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Kinet. Catal., 45(3) (2004) pp. 446-452.

Oxygen states in the $La_{1-x}Ca_xFeO_{3-y}$ perovskites prepared using different procedures are studied by temperature-programmed reduction (TPR). Results are compared to data on the catalytic activity in the oxidation of methane and carbon monoxide. The activity of the samples in the CO and CH_4 oxidation over a wide temperature range (200–600°C) is shown to correlate with the amount of reactive surface and subsurface oxygen removable during TPR below 420°C. These oxygen states in the samples of the $La_{1-x}Ca_xFeO_{3-y}$ series can be associated with the domain or intergrain boundaries. No correlation is found between the amount of lattice oxygen removable during TPR and the activity of the $La_{1-x}Ca_xFeO_{3-y}$ samples in the complete oxidation of methane at temperatures of 450–600°C. It is suggested that catalytic complete oxidation is determined by the most reactive surface and subsurface oxygen states located at the interphase boundaries, whereas the lattice oxygen does not participate in these reactions.

MOBILITY AND REACTIVITY OF THE SURFACE AND LATTICE OXYGEN OF SOME COMPLEX OXIDES WITH PEROVSKITE STRUCTURE

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In: *"Mixed Ionic Electronic Conducting Perovskites for Advanced Energy Systems"*,
Eds. N. Orlovskaya, N. Browning, Kluwer Academic Publishers, Boston/Dordrecht/London,
2004, pp. 49-70.

Mobility and reactivity of the surface and bulk oxygen of perovskite-like mixed oxides including lanthanum manganite (I) and ferrite (II) systems modified by Ca (I,II) and fluorine (I), as well as some Co, Fe-containing complex perovskites known to be good mixed conductors were considered. Combination of thermal analysis data, dynamic and isothermal oxygen isotope exchange, O_2 TPD, isothermal pulse/flow samples reduction by CO, H_2 and CH_4 TPR, was applied to characterize the accessible surface/bulk oxygen mobility and reactivity. Comparison of these results with earlier obtained data on the real (defect) structure of these systems by TEM, EXAFS, XRD, FTIRS of lattice modes, SIMS allowed to elucidate factors determining the oxygen mobility and reactivity. Quantitative description of the experimental energetic spectrum of oxygen bound with regular and defect surface sites of perovskites was obtained by using semiempirical Interacting Bonds method with a due regard for the surface faces termination and relaxation. Analysis of the barriers for oxygen migration in the perovskite lattice by this method revealed pronounced effect of cation vacancies.

MICROHETEROGENEOUS SOLID SOLUTIONS IN PEROVSKITES: FORMATION, MICROSTRUCTURE, AND CATALYTIC PROPERTIES

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In: *"Mixed Ionic Electronic Conducting Perovskites for Advanced Energy Systems"*,
Eds. N. Orlovskaya, N. Browning, Kluwer Academic Publishers, Boston/Dordrecht/London,
2004, pp. 143-162.

Influence of the point and extended defects on the steady-state catalytic activity of perovskites in deep oxidation processes is discussed.

THIOPHENE HYDRODESULFURIZATION ACTIVITY OF MoS_2/Al_2O_3 CATALYSTS PREPARED VIA EXFOLIATION. THE EFFECT OF COBALT

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React. Kinet. Catal. Lett., 83(1) (2004) pp. 181-186.

In contrast to the bulk MoS_2, the structure of the active phase of the catalyst prepared via exfoliation is shown to exhibit a number of distortions, which form a superstructure of the type of the charge density waves with a quasi-period of 30 Å. Due to such distortions, the ions of cobalt firmly chemisorb on the basal plane of MoS_2 occupying, along the perimeter of the MoS_2 clusters, the regions with a lower energy of the Mo-S interaction. A synergetic increase in the catalyst activity due to the introduction of cobalt was observed up to the atomic ratios of Co/(Co+Mo) = 0.33, which is possible for the nanoparticles of MoS_2 with a diameter 200 Å, only if cobalt adsorbs on the basal plane.

PROPANE CARBONYLATION ON SULFATED ZIRCONIA CATALYST AS STUDIED BY ^{13}C MAS NMR AND FTIR SPECTROSCOPY

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J. Catal., 223(2) (2004) pp. 290-295.

Using *in situ* ^{13}C MAS NMR, it has been demonstrated that propane is carbonylated with carbon monoxide to produce isobutyraldehyde and isobutyric acid at 100-150°C on sulfated zirconia. Isobutyraldehyde represents the intermediate reaction product, almost completely converting into the acid at

150°C. Selective formation of isotyraldehyde indicates that the activation of propane by SZ is performed primarily toward secondary C-H bond rather than its C-C bond. This pathway of the alkane activation can be rationalized to occur either on the Lewis acid sites of SZ or by direct formylation by the formyl cation formed as equilibrated species from the formate. With the aid of IR spectroscopy the evidence was provided that the sulfate groups of SZ are accountable for the aldehyde oxidation, surface dithionate species being suggested to be formed as a result of sulfur reduction. The dithionate species are readily recovered to sulfate groups via oxidizing treatment in O_2 atmosphere.

STUDIES OF THE MECHANISM OF AMMONIA OXIDATION INTO NITROUS OXIDE OVER Mn-Bi-O/α-Al_2O_3 CATALYST

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J. Catal., 222(1) (2004) pp. 129-142.

Complex of kinetic and physicochemical methods: temperature-programmed surface reaction (TPSR), pulsing NH_3 or $NH_3/^{16}O_2$ ($^{18}O_2$) reaction mixture, Infrared and Photoelectron Spectroscopies was used for characterization of the high selective supported manganese-bismuth oxide catalysts and for the studying of the mechanism of the ammonia oxidation. Ammonia oxidation was demonstrated to proceed via alternating reduction and reoxidation of the catalyst surface with participation of the lattice oxygen. NH_3 interacts with weakly bonded oxygen species through hydrogen atom abstraction to form adsorbed [N] species, which are localized on Mn^{2+} and Mn^{δ} ($2<\delta<3$). Manganese ions with different oxidation degree (Mn^{3+} (Mn^{4+}) and $Mn^{\delta+}$) serve as active sites of the catalyst surface. The correlation between the selectivity towards N_2O and the portion of manganese in the Mn^{3+} (Mn^{4+}) state was established. Bismuth oxide plays an important role in consequence of increasing of the quantity, mobility and thermal stability of the subsurface oxygen. The reaction kinetic scheme is suggested based on the experimental results. Numerical simulation of TPSR data confirms the reliability of the proposed reaction mechanism.

THE ROLE OF SUPPORT IN FORMATION OF THE MANGANESE-BISMUTH OXIDE CATALYST FOR SYNTHESIS OF NITROUS OXIDE THROUGH OXIDATION OF AMMONIA WITH OXYGEN

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J. Catal., 221(1) (2003) pp. 213-224.

BET, XRD, XPS and TPR by hydrogen were used for investigation of supported Mn-Bi oxide catalysts for ammonia oxidation into nitrous oxide. The catalysts were synthesized by impregnation of γ–, α–Al_2O_3 and SiO_2 with solutions of manganese and bismuth nitrates. The character of phase transformations, surface concentration and state of the active component were shown to depend on the nature of the support. The sequence stabilization of active constituents of the Mn-Bi-O/α-Al_2O_3 catalyst and types of the stabilized species were determined. The activity of the Mn-Bi-O supported catalysts calcined at 400°C was established to be equal 95–97% and to be practically independent of the support nature, while the activity decreased with elevation of the calcination temperature. The Mn-Bi-O/α-Al_2O_3 catalysts exhibited the highest selectivity to N_2O (84.4%) under identical conditions. The correlation between the $Mn^{3+}/Mn^{\delta+}$ ($2<\delta<3$) ratio in the catalyst and the selectivity to N_2O was revealed.

SELECTIVE OXIDATION OF AMMONIA OVER Ru(0001)

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Surf. Sci., 555(1-3) (2004) pp. 83-93.

The decomposition and oxidation of NH_3 have been studied on the Ru(0001) surface in the temperature range from 150 up to 800 K. The results were compared to those found for Ir(110) and Ir(510). TDS results showed that most of the ammonia is dissociatively adsorbed between 150 and 300 K, with formation of H_2 around 300 K and N_2 between 600 and 800 K. N_2 desorption shifts to lower temperatures with increasing surface oxygen coverage. The products of ammonia oxidation observed were N_2, H_2O and N_2O. Formation of NO was not found.

Inhibition of the reaction presumably by *N* species was observed until 450 and 670 K, depending on the NH_3/O_2 ratios. Above those temperatures the reaction started as manifested by a decrease in the NH_3 and O_2 pressures and a simultaneous increase in the H_2O, N_2 and N_2O pressures.

MECHANISM AND KINETICS OF THE SELECTIVE NO REDUCTION OVER Co-ZSM-5 STUDIED BY THE SSITKA TECHNIQUE. II. REACTIVITY OF NO_X ADSORBED SPECIES WITH METHANE

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J. Catal., 225 (2004) pp. 179-189.

Steady-state isotopic transient kinetic analysis (SSITKA) was applied to study the reactivity of adsorbed NO_x species with methane over Co-ZSM-5 during CH_4-SCR of NO at different partial oxygen concentrations. Numerical analysis of the isotope responses after switching from $^{14}N^{16}O$ to $^{15}N^{18}O$, from $^{16}O_2$ to $^{18}O_2$, from $^{12}CH_4$ to $^{13}CH_4$, and from $C^{16}O_2$ to $C^{18}O_2$ in the feed gas was performed. This enables determination of (i) the concentration of surface intermediates resulting from the interaction of NO_x species with methane. The NO reduction with CH_4 in the presence of oxygen was shown to proceed by two different pathways with participation (1) $NO_2^{\delta+}$ species (formed on nanoclusters of cobalt oxide located inside the zeolite channels) and (2) NO_2^- nitrite complexes (formed on larger cobalt oxide particles located outside the zeolite channels), the reaction rate by the former being appreciably higher under the SCR reaction condition studied. Mononitrosil species appear not be directly involved in the overall process. Modeling results indicate that the rate of the first route is limited by the interaction of $NO_2^{\delta+}$ species and adsorbed methane, while in the second route the formation of nitrite species is a rate-determining step. Based on the obtained results, an overall reaction mechanism of the CH_4-SCR of NO in the presence of oxygen is proposed.

REACTION KINETICS AND MECHANISM OF SELECTIVE NO REDUCTION ON A CoZSM-5 CATALYST AS STUDIED BY SSITKA

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Kinet. Catal., 45(3) (2004) pp. 436-445.

The dynamics of ^{13}C transfer from methane to carbon dioxide was studied under the steady-state reaction conditions of selective NO reduction with methane on a CoZSM-5 catalyst at various reactant (NO, CH_4, and O_2) concentrations and temperatures. It was found that the reaction occurs by a two-pathway mechanism with the participation of Co^{2+} sites (or CoO_x clusters) and paired Co^{2+}–OH sites localized at the boundary between the clusters and the zeolite; in this case, the rate of the reaction at boundary sites was higher by more than one order of magnitude. Based on the numerical simulation of isotopic response curves, the concentrations of intermediate compounds and the rate constants of particular steps were evaluated; differences in the kinetics via the above reaction pathways were found and analyzed.

NO DECOMPOSITION OVER A NEW TYPE OF LOW METAL CONTENT FIBERGLASS CATALYSTS STUDIED BY TAP TECHNIQUE

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Catal. Commun., 5(11) (2004) pp. 691-695.

NO absorption and decomposition over novel type of leached fiberglass catalysts containing very small amounts of platinum were studied by means of the TAP technique. In the temperature range of 200-400°C NO was reversibly absorbed on the catalyst. At higher temperatures NO consumption and N_2 release occurred, indicating the proceeding of direct NO decomposition. However, in the temperature range of 400-500°C the rate of NO decomposition declined with the quantity of NO dosed, i.e. with the number of pulses introduced, so that steady-state NO conversion was close to zero. This drop in catalyst activity is related to the negligible oxygen desorption during NO decomposition in this temperature range, making it reasonable to assume a blocking of the catalyst active sites by accumulating oxygen. Nevertheless, as temperature was raised above 500°C, steady-state NO conversion increased sharply with temperature reaching a value of 45 % at 550°C. Apparently, a thermal desorption of oxygen beyond that temperature allows to free sites, which were covered during NO decomposition, sustaining in this way the overall reaction. Based on the obtained data activation energies of NO desorption and decomposition were estimated.

HIGH SELECTIVE FIBER GLASS WOVEN CATALYSTS DOPED BY NOBLE METALS IN THE REACTIONS OF AROMATIC NITRO-COMPOUNDS REDUCTION

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Chem. Eng. Transac., 3 (2003) pp. 285-289.

The features of liquid-phase hydrogenation of trinitrotoluene and trinitrobenzene over woven silica fiberglass (SFG) catalysts doped by Pt (Pt content 0,1 wt.%) were investigated. Specific surface area (SSA) of the catalysts was ranged from 1 to 15 m^2/g. The traditional Pd/C powdered catalyst (Pd content 5 wt.%, SSA of 500 m^2/g) was used as reference sample. The SFG catalysts showed a higher specific activity than conventional Pd/C one. An unexpected finding for SFG catalysts was that hydrogenation rates of second and third nitro-groups in trinitrotoluene and trinitrobenzene were, respectively, by one and two orders of magnitude less than that of the first one. The selectivity effect was found to decrease with increasing of SSA for SFG catalysts and wasn't revealed at all for Pd/C sample.

IN SITU FTIR STUDY OF PYRIDINE-3-CARBALDEHYDE ADSORPTION ON TiO_2 (ANATASE) AND V-Ti-O CATALYST

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React. Kinet. Catal. Lett., 83(2) (2004) pp. 353-360.

In situ FTIR spectroscopy was used to study the interaction of pyridine-3-carbaldehyde (3PyA) with the surface of TiO_2 and V-Ti-O catalyst in the temperature range of 120–300°C. 3PyA interacted with Lewis and Brønsted acid sites of TiO_2 and V-Ti-O catalyst to form nitrogen-coordinated complex and σ-bonded (through oxygen of CHO group) complex, as well as complex protonated at the N atom in the ring. Surface carboxylates (nicotinates) also were identified during interaction of 3PyA with the V-Ti-O catalyst at the temperature range of 200–300°C.

METHYLPYRAZINE AMMOXIDATION OVER BINARY OXIDE SYSTEMS. V. EFFECT OF PHOSPHORUS ADDITIVES ON THE PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF A VANADIUM-TITANIUM CATALYST IN METHYLPYRAZINE AMMOXIDATION

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Kinet. Catal., 45(1) (2004) pp. 104-113.

Oxide vanadium–titanium catalysts modified by phosphorus additives ($20V_2O_5$–(80-n)TiO_2–nP_2O_5, where *n*= 1, 3, 5, 10, and 15 wt %) are studied in methylpyrazine ammoxidation. Two regions of compositions are found corresponding to radically different catalytic properties, namely, catalysts with a low (≤ 5 wt % P_2O_5) and high (≥ 10 wt % P_2O_5) concentration of the additive. In the first case, the introduction of phosphorus is accompanied by a gradual increase in the activity. In the second case, an increase in the additive concentration results in a decrease in the activity and selectivity to the target product, pyrazineamide, and a simultaneous increase in the selectivities to by-products, pyrazine and carbon oxides. The catalysts are characterized by X-ray diffraction analysis, differential dissolution, IR, and NMR spectroscopic data. As in the binary system, the active sites of the samples with a low concentration of phosphorus contain V^{5+} cations in a strongly distorted octahedral oxygen environment, which are strongly bound to a support due to the formation of V–O–Ti bonds. The catalytic properties of the samples containing ≥ 10 wt % P_2O_5 are due to the presence of the phase of a triple V–P–Ti compound with an atomic ratio V : P : Ti approximately equal to 1 : 1 : 1. The V^{5+} cations in this compound occur in a weakly distorted tetrahedral oxygen environment and are bound to the tetrahedral P^{5+} cations.

KINETICS OF THE OXIDATION OF β-PICOLINE TO NICOTINIC ACID OVER VANADIA-TITANIA CATALYST. II. THE NETWORK OF THE REACTION AND THE EFFECT OF WATER

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React. Kinet. Catal. Lett., 82(1) (2004) pp. 191-197.

Over vanadia-titania catalysts, the oxidation of β-picoline into nicotinic acid proceeds under a parallel-consecutive network. Nicotinic acid is formed both directly from picoline and through pyridine-3-carbaldehyde as an intermediate. Products of total oxidation and nitrile are formed on a parallel path from picoline, and on a consecutive path via overoxidation of partial oxidation products. Introduction of water into the reaction mixture raises selectivity and activity due to an acceleration of the formation of carbaldehyde and nicotinic acid and not due to repressing the reactions of total oxidation.

HYDRODECHLORINATION OF TETRACHLOROMETHANE IN THE VAPOR PHASE IN THE PRESENCE OF Pd-Fe/SIBUNIT CATALYSTS

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Kinet. Catal., 45(2) (2004) pp. 183-188.

The hydrodechlorination of CCl_4 in the presence of Pd–Fe/Sibunit catalysts of different composition was studied. An optimum concentration of the metals (2.5% at the ratio Pd/Fe = 1:4) was determined, which corresponds to the highest stability of catalysts and selectivity of C_2–C_4 olefin and paraffin formation. With the use of TPR and magnetic measurements, it was found that the metals occurred in an oxidized state in the course of the reaction; it is likely that this resulted in the formation of C_2–C_4 hydrocarbons.

MECHANISM OF THE LOW-TEMPERATURE INTERACTION OF HYDROGEN WITH α-OXYGEN ON FeZSM-5 ZEOLITE

K.A. Dubkov, E.V. Starokon', E.A. Paukshtis, A.M. Volodin, G.I. Panov

Kinet. Catal., 45(2) (2004) pp. 202-208.

The mechanism of a low-temperature reaction of hydrogen with the radical anion surface oxygen species (α-oxygen, O_α) formed by decomposing N_2O over FeZSM-5 zeolite was studied using kinetic and isotope techniques. It was found that the reaction is of first order with respect to hydrogen and the rate of the reaction is proportional to the concentration of O_α. The activation energy of the reaction, which was measured for H_2 or D_2 over a temperature range from +20 to -100ºC, is equal to 3.2 or 5.3 kcal/mol, respectively. The reaction occurs with a considerable kinetic isotope effect (k_H/k_D), which varies over the range of 3.4–41 depending on the temperature. This fact indicates that the rate-limiting step of the reaction includes the dissociation of the hydrogen molecule. The temperature dependence of the isotope effect gave a value of 2.1 kcal/mol, which is close to the difference between the zero bond energies in the molecules of H_2 and D_2; this fact suggests that a tunnel effect does not significantly contribute to the reaction. The dissociative mechanism is consistent with data obtained by *in situ* IR spectroscopy. The interaction of hydrogen with α-oxygen is accompanied by the formation of new hydroxyl groups $O_\alpha H$ (absorption bands at 3635 and 3674 cm^{-1}) at the surface of the zeolite. The identification of these groups was supported by an isotope shift either on the replacement of H_2 by D_2 or on the replacement of $^{16}O_\alpha$ by $^{18}O_\alpha$. The stoichiometric ratio $H_2 : O_\alpha$ is consistent with the previously drawn conclusion on the paired arrangement of α-sites.

LIQUID PHASE OXIDATION OF ALKENES WITH NITROUS OXIDE TO CARBONYL COMPOUNDS

E.V. Starokon', K.A. Dubkov, D.E. Babushkin, V.N. Parmon, G.I. Panov

Adv. Synth. Catal., 346(2-3) (2004) pp. 268-274.

A variety of substrates including linear, cyclic, heterocyclic alkenes and their derivatives were tested in the liquid phase non-catalytic oxidation with nitrous oxide (N_2O). The structure and composition of alkenes have significant effect on the reaction selectivity. With many alkenes, N_2O oxidation provides a selective way for preparation of carbonyl compounds. Generation of carbene (or diazomethane) species is a remarkable feature of the oxidation of terminal alkenes.

METHANE OXIDATION IN A DIELECTRIC BARRIER DISCHARGE. THE IMPACT OF DISCHARGE POWER AND DISCHARGE GAP FILLING

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React. Kinet. Catal. Lett., 82(1) (2004) pp. 111-119.

The conversion of an air-methane mixture in a dielectric barrier discharge (DBD) was studied in a wide range of temperatures and discharge powers for different gap fillings. The impact of the gap filling surface area appears to be negligible at temperatures below 530 K, while being significant above 570 K. Some processes on the surface are countercurrent to those in the DBD plasma.

THE IMPACT OF A DIELECTRIC BARRIER DISCHARGE ON THE CATALYTIC OXIDATION OF METHANE OVER Ni-CONTAINING CATALYST

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React. Kinet. Catal. Lett., 82(1) (2004) pp. 131-137.

Methane oxidation with air was studied over a Ni-containing catalyst in a dielectric barrier discharge (DBD) at temperatures above 625 K. The DBD increases the methane conversion and shifts the process towards partial oxidation. This effect is related to a catalyst heating by the discharge.

A STUDY OF METHANE DECOMPOSITION OVER Ni-Si-CONTAINING CATALYSTS

A.A. Khassin, A.S. Kovalenko

Doklady Phys. Chem., 397(4-6) (2004) pp. 194-198.

The methane decomposition process over Ni-containing catalysts could be described by a scheme, which considers a gradual increase in the extent of the diffusion constrains (reaction rate control by kinetics → intraparticle diffusion control → deactivation → external kinetic regime) due to the accumulation of the filamentary carbon (FC) in the catalyst. The experimental values of the activation energy (190 ± 5 kJ/mol) and pre-exponential factor in the Arrhenius reaction rate equation ($3\cdot10^{13}$ s^{-1}) over Ni/MgO reference sample indicate that the RDS of the methane decomposition process is the H–CH_x bond cleavage. The Ni-Mg amesites showed low specific activity (30 time less than that for Ni/MgO) in the methane decomposition process and are therefore stable to coking in the methane decomposition reaction conditions.

COPRECIPITATED IRON-CONTAINING CATALYSTS (Fe-Al_2O_3, Fe-Co-Al_2O_3, Fe-Ni-Al_2O_3) FOR METHANE DECOMPOSITION AT MODERATE TEMPERATURES. I. GENESIS OF CALCINED AND REDUCED CATALYSTS

T.V. Reshetenko, L.B. Avdeeva, A.A. Khassin, G.N. Kustova, V.A. Ushakov, E.M. Moroz, A.N. Shmakov, V.V. Kriventsov, D.I. Kochubey, Yu.T. Pavlyukhin*, A.L. Chuvilin, Z.R. Ismagilov (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Appl. Catal., *A*, 268(1-2) (2004) pp. 127-138.

Genesis of the composition and structure of the active component of coprecipitated iron containing catalysts (Fe-Al_2O_3, Fe-Co-Al_2O_3, Fe-Ni-Al_2O_3) with high metal loadings (>50 wt.%) for methane decomposition at moderate temperatures (600–650°C) has been investigated by XRD, EXAFS, radial electron density distribution (REDD), TEM, FTIR and Mössbauer spectroscopy. The main stages of the catalyst genesis during drying, thermal decomposition and reduction have been studied. For bimetallic systems (Fe-Co-Al_2O_3, Fe-Ni-Al_2O_3) intermediate spinel phases with a composition $(M\ II, Fe)_3O_4$ (M =Co, Ni) have been shown to form during heat treatment and reduction. This leads to a decrease of the reduction temperature for iron oxides. Reduced bimetallic catalysts (Fe-Co-Al_2O_3, Fe-Ni-Al_2O_3) are composed of alloys.

The structure and parameters of their crystal lattices depend on the type and concentration of the added metal. Alumina has been shown to behave as a structural promoter. A model of the reduced catalysts consisting of highly dispersed (20–50 nm) metal and alumina particles with a spinel phase at their interface has been suggested.

COPRECIPITATED IRON-CONTAINING CATALYSTS ($Fe-Al_2O_3$, $Fe-Co-Al_2O_3$, $Fe-Ni-Al_2O_3$) FOR METHANE DECOMPOSITION AT MODERATE TEMPERATURES. II. EVOLUTION OF THE CATALYSTS IN REACTION

T.V. Reshetenko, L.B. Avdeeva, V.A. Ushakov, E.M. Moroz, A.N. Shmakov, V.V. Kriventsov, D.I. Kochubey, Yu.T. Pavlyukhin*, A.L. Chuvilin, Z.R. Ismagilov (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Appl. Catal., A, 270(1-2) (2004) pp. 87-99.

Coprecipitated $Fe-Al_2O_3$, $Fe-Co-Al_2O_3$ and $Fe-Ni-Al_2O_3$ catalysts is shown to be very efficient in carbon deposition during methane decomposition at moderate temperatures (600–650°C). The carbon capacity of the most efficient bimetallic catalysts containing 50-65 wt.% Fe, 5–10 wt.% Co (or Ni) and 25–40 wt.% Al_2O_3 is found to reach 145 g/g_{cat}. Most likely, their high efficiency is due to specific crystal structures of the metal particles and formation of optimum particle size distribution. According to the TEM data, catalytic filamentous carbon (CFC) is formed on them as multiwall carbon nanotubes (MWNTs). The phase composition of the catalysts during methane decomposition is studied using a complex of physicochemical methods (XRD, REDD, Mössbauer spectroscopy and EXAFS). Possible mechanisms of the catalyst deactivation are discussed.

A COMPARATIVE STUDY OF THE ACTIVITY OF OXIDE CATALYSTS IN THE OXIDATION OF METHANE AND 1,1-DIMETHYLHYDRAZINE

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Kinet. Catal., 45(5) (2004) pp. 722-729.

The catalytic oxidation of methane and 1,1-dimethylhydrazine ($(CH_3)_2N-NH_2$, unsymmetrical dimethylhydrazine (UDMH)) with air on oxide catalysts was studied. Two pairs of perovskites ($Ca_{0.7}Sr_{0.3}FeO_{2.5(3.0)}$ and $La_{0.7}Sr_{0.3}CoO_{2.5(3.0)}$, stoichiometric and superstoichiometric with respect to oxygen) and a supported spinel ($20\%(Cu_xMg_{1-x}Cr_2O_4)/v-Al_2O_3$, IC-12-73) were used as catalysts. The experiments were performed using two laboratory flow-type systems: in a catalytic fixed-bed reactor (the oxidation of CH_4) and in a gradientless vibrationally fluidized bed reactor (the oxidation of CH_4 and UDMH) at 150-700°C. In the oxidation of CH_4, the IC-12-73 catalyst was more active than the perovskite catalysts, although particular perovskite catalysts can exhibit higher activity in the region of low temperatures. In the oxidation of UDMH, the activity of perovskites in the test temperature region was lower than that of IC-12-73; this correlates with the higher activity of IC-12-73 in the oxidation of CH_4. The $Ca_{0.7}Sr_{0.3}FeO_{3.0}$ and $La_{0.7}Sr_{0.3}CoO_{2.5(3.0)}$ perovskites exhibited similar activities in the deep oxidation of UDMH, which were higher than the activity of $Ca_{0.7}Sr_{0.3}FeO_{2.5}$. A comparison between the selectivities of the conversion of fixed nitrogen, which is a constituent of UDMH, into nitrogen oxides S_{NOx}^N demonstrated that, on all of the perovskites, S_{NO}^N was higher and $S_{N_2O}^N$ was lower than the corresponding values on IC-12-73. Additional information on the possible mechanisms of intermediate formation in the adsorption and oxidation of UDMH on IC-12-73 was obtained using Fourier transform IR spectroscopy.

KINETICS OF THE MEDIUM-TEMPERATURE REDUCTION OF COPPER CHROMITE WITH HYDROGEN

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React. Kinet. Catal. Lett., 82(2) (2004) pp. 355-361.

The static volumetric method was used to study the kinetics of copper chromite $CuCr_2O_4$ reduction with hydrogen at 50-80 kPa and 498, 523 and 580 K. The rate of copper chromite reduction is maximal initially and decreases monotonically with time. This observation suggests that the reduction is not a topochemical process. The apparent activation energy of the reaction equals initially 107 kJ/mole. The results obtained argue for a particular mechanism of the copper chromite reduction via redox substitution of hydrogen for copper in the chromite and, therefore, agree with earlier data obtained by various structural and adsorption methods. Specific features of the reduction mechanism are discussed.

IN SITU XRD AND HRTEM STUDIES ON THE EVOLUTION OF THE Cu/ZnO METHANOL SYNTHESIS CATALYST DURING ITS REDUCTION AND RE-OXIDATION

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Phys. Chem. Chem. Phys., 6(18) (2004) pp. 4522-4526.

During the formation of the CuZnO solid solutions, the foreign anions in anion-modified (a.m.-) oxides give rise to: (i) extended stacking faults of (002) ZnO lattice plane, which are occupied by copper ions in the form of small clusters; and (ii) vacant inner holes of the a.m.-ZnO crystal. The main part of copper ions in the clusters is reduced to Cu^0 with hydrogen at 473 K. According to HRTEM studies, the reduction of $Cu_{0.08}Zn_{0.92}O$ results in the formation of copper metal species of two types: (i) particles of 3-10 nm in size on the a.m.-ZnO surface; and (ii) small (no more than 3 nm in size) atomic copper metal clusters in defect voids of the a.m.-ZnO structure. The copper metal clusters are coherent inclusions in the bulk of the ZnO, and the large copper metal particles are epitaxially bonded to the surface of the ZnO matrix. Copper metal particles on the surface of a.m.-ZnO are reoxidized to Cu^{+2} at 523 K in the helium flow containing 0.05 vol% oxygen, and they come back to the extended stacking faults. The copper metal clusters in the holes of a.m.-ZnO are inaccessible to the oxygen and are not reoxidized.

ACTIVE PHASES OF SUPPORTED COBALT CATALYSTS FOR 2,3-DIHYDROFURAN SYNTHESIS

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J. Mol. Catal. A: Chem., 215(1-2) (2004) pp. 95-101.

Dehydrogenation of 1,4-butanediol to 2,3-dihydrofuran over kaolin-supported Co and Co–Au catalysts has been investigated. Catalytic test and XRD analysis show that the presence of metallic cobalt with hexagonal structure is favourable for selectivity to 2,3-dihydrofuran of the reaction studied. It was established by XPS method that an optimal for the reaction selectivity Co^0/Co^{2+} ratio in Co/kaolin and Co–Au/kaolin catalysts exists. Quantum chemical calculations suggest that the initial step of 1,4-butanediol dehydrogenation on cobalt catalyst surface may be the cleavage of O---H bond to form alkoxide species on Co^{2+} ion. Based on the effect of metallic and ionic cobalt on the catalyst selectivity, it could be presumed that both cobalt species are involved in the rate-determining step in dehydrogenation of 1,4-butanediol into 4-hydroxybutanal intermediate.

ON THE EFFECT OF THE STRENGTH OF ACID SITES IN HETEROGENEOUS CATALYSTS ON THE ACTIVITY IN THE SKELETAL ISOMERIZATION OF *n*-BUTANE

V.P. Shmachkova, N.S. Kotsarenko, E.A. Paukshtis

Kinet. Catal., 45(4) (2004) pp. 554-557.

The catalytic activity of three groups of acid catalysts different in the nature and strength of acid sites in the skeletal isomerization of *n*-butane was studied. It was found that the strength of the sites did not correlate with the rate of the reaction.

THERMAL DECOMPOSITION OF NH_4-ANALCIME

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Phys. Chem. Miner., 31(5) (2004) pp. 306-312.

The thermal decomposition of ammonium-exhanged natural analcime is characterized by gas chromatography, IR spectroscopy and X-ray diffraction. The de-ammoniation and dehydroxylation proceed in parallel throughout the decomposition, which evidences the instability of the protonated analcime framework. The mechanism of degassing of NH_4-analcime changes throughout its decomposition. At the initial step, the mechanism of de-ammoniation consists in thermal dissociation of NH_4^+ molecule onto NH_3 and proton (framework OH group) and diffusion of NH_3 out of the structure. Subsequent decomposition and removal of the OH groups lead to a progressive loss of crystallinity. At this step, an apparent activation energy for NH_3 desorption is estimated to be 145(±13) kJ mol^{-1}. This value is within the upper limit of the activation energy characteristic for the NH_3 desorption from proton centres in large-pore zeolites. At the final step, the adsorption of NH_3 and protons onto the defect centres in the amorphosed aluminosilicate framework results in a significant increase of an apparent activation energy for the de-ammoniation and dehydroxylation up to 270(±20) kJ mol^{-1}.

METHANOL DEHYDROGENATION OVER COPPER-CONTAINING CATALYSTS MODIFIED BY CERIUM AND MANGANESE OXIDES

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Catal. Ind., 3 (2004) pp. 14-17.

For the purpose of improvement of the catalytic characteristics of copper-containing catalysts for methanol dehydrogenation, a possibility of modifying them with cerium and manganese oxides has been investigated. The X-ray phase analysis and derivatography were used for determination of phase composition and the nature of phase transformations at different stages of preparation of the catalysts on two types of carriers. Introduction of modifiers leads to decrease in activity and selectivity to methylformate for the samples based on sibunit and improves cited catalytic properties for the samples based on silicate composite. A possible mechanism of different action of additives on catalyst activity is discussed.

RADICAL GENERATION IN THE COURSE OF N-UNDECANE PYROLYSIS ON $BaCl_2$ AND THE DEFECT MAGNESIUM OXIDE

N.A. Vasilieva, R.A. Buyanov

Chem. Sustian. Devel., 12(6) (2004) p. 661-668.

Ethyl radical generation kinetics in the course of pyrolysis of n-undecane on $BaCl_2$ and defect magnesium oxides is studied using radical freezing in the resonator of an ESR spectrometer. $BaCl_2$ accelerates heterogeneous component, defect magnesium oxides accelerate homogeneous component of the process. $BaCl_2$ activation energy E = 192 kJ/mol is lower than one for the thermal pyrolysis E = 322 kJ/mol.

The phenomenon of surface “ignition” is found on the catalysts accelerating homogeneous component and making of the catalytic sphere. Thermal pyrolysis is performed between catalyst grains under temperature arising to a critical level. Then catalyst begins to generate additional radical, with activation energy typical of radical reactions E = 4 kJ/mol. Increase of the catalytic pyrolysis performance and selectivity through application of specific heterogeneous catalysts are suggested.

CHLORINATION OF METHANE OVER NANOCRYSTAL MAGNESIUM OXIDE

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Proceedings of the Tula State University, ser. “Chemistry”, 4 (2004) pp. 45-50.

In a range of temperatures 300-350°C vapour-phase chlorination of methane on a nanocrystal magnesium oxide has been investigated. It is shown that in comparison with industrial catalysts the nanocrystal MgO has much higher activity and selective action.

Application of Physicochemical Methods for Characterization of Catalysts, Supports, Synthesized Substances and Materials

SIMULATION OF X-RAY POWDER DIFFRACTION PATTERNS ON THE BASE OF THE MODELS OF IMPERFECT CRYSTALS

S.V. Cherepanova, S.V. Tsybulya

J. Mater. Sci. Forum, *Trans Tech Publications Inc.*,
Zurich, Switzerland,
443-444 (2004) pp. 87-90.

Software for the simulation of X-ray powder diffraction (XRPD) patterns for ultrafine grained materials with some kinds of imperfections has been developed. These calculations are performed on the base of the model of one dimensionally disordered crystal. Such a model can described stacking faults and other planar defects and also finite size of coherently scattering domains. Simulated XRPD pattern is compared with the experimental one and can be fitted to it. Potentialities of the software are illustrated by several examples.

PROTONATION SITE AND HYDROGEN BONDING IN ANHYDROUS AND HYDRATED CRYSTALLINE FORMS OF DOXAZOSINE MESYLATE FROM POWDER DATA

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Acta Crystallogr., Sect. B: Struct. Sci.,
B59(Part 6) (2003) pp. 787-793.

The three-dimensional solid-state structures of two modifications of doxazosin mesylate $(C_{23}H_{26}N_5O_5)^+(CH_3SO_3)^-$, 4-amino-2-[4-[(2,3-dihydro-1,4-benzodioxin-2-yl)carbonyl]piperazin-1-yl]-6,7-dimethoxyquinazoline methanesulfonate, a commonly used antihypertensive agent, have been determined by synchrotron X-ray powder diffraction. An anhydrous form (A) and a dihydrate form (dG) crystallize in monoclinic space groups. In both forms the doxazosin molecule is protonated at the N1 atom of the quinazoline bicycle. The N1 atom, and the amino H atoms and O atoms of the mesylate moieties are involved in three-dimensional hydrogen-bonding networks, while solvent water molecules and carboxamide O atoms are also incorporated in a hydrogen-bonding network in dG.

X-RAY DIFFRACTION STUDY OF ZIRCONIA PILLARED CLAYS

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React. Kinet. Catal. Lett., 81(1) (2004) pp. 137-142.

X-ray powder diffraction (XRPD) and X-ray radial electronic distribution density (RED) of initial and zirconia-pillared interlayered clays (Zr-PILC) were studied. After pillaring, the basal (001) spacing was found to increase from 11 Å in the initial clay kept under air to 17.7 Å in Zr-PILC. The structure of zirconium nanopillars was characterized. The interatomic distances with corresponding coordination numbers obtained from the RED curves were close to those in zirconium tetramers.

LOCAL STRUCTURE OF AMORPHOUS AND HIGHLY DISPERSED ZIRCONIUM HYDROXIDES AND OXIDES

D.A. Zyuzin, E.M. Moroz, A.S. Ivanova, A.N. Shmakov, G.N. Kustova

Kinet. Catal., 45(5) (2004) pp. 739-742.

The local structure of amorphous and highly dispersed hydroxide and oxide zirconium compounds prepared from zirconyl nitrate solutions by precipitation was studied by an X-ray diffraction technique of radial electron distribution. It was found that X-ray amorphous precipitates were formed at 383 K. These precipitates were polynuclear hydroxo complexes, whose short-range ordering was similar to the structure of a cubic ZrO_2 phase. A special feature of these formations, compared with the cubic oxide phase, is that the closest Zr–Zr distance in them is shortened by 0.2 Å, NO_3 and OH groups are the constituents of an anionic sublattice, and the coordination number of Zr–anion distances is increased. Calcination at 653 K followed by cooling to room temperature resulted in the appearance of a monoclinic ZrO_2 phase with a crystallite size of ~60 Å along with the cubic phase. The amount of the former phase depended on the pH of precipitation and on the presence of residual NO_3 and OH groups in precipitates.

CONSTITUTION AND PROPERTIES OF NANOCOMPOSITES PREPARED BY THERMAL DECOMPOSITION OF SILVER SALTS SORBED BY POLYACRYLATE MATRIX

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Colloid J., 65(6) (2003) pp. 720-725.

Constitution and dispersity of the products of thermal decomposition of silver nitrate ammonia complex sorbed by polyacrylate matrix are studied by the methods of small- and wide-angle X-ray scattering, optical, photoelectron and Auger-electron spectroscopies. It is shown that, at temperatures of 140–150°C, the complete decomposition of the complex occurs with the formation of nanoparticles and charged silver clusters in polymer bulk. No initial or intermediate products were observed. The average size of obtained nanoparticles is equal to 5 nm. The particles with the size less than 5 nm are amorphous according to X-ray data. The stabilization of nanoparticles occurs due to the adsorption of acrylic copolymer (presumably, via oxygen atoms) on their surfaces. Upon long-term storage in air, the self-diffusion of silver particles and clusters takes place from the surface to composite bulk caused by the detachment of oxygen-containing groups occurring at the metal–polymer interface.

CLEANING OF THE SURFACE OF SILVER CRYSTALS USED AS CATALYSTS OF GAS-PHASE OXIDATION OF ETHYLENE GLYCOL TO GLYOXAL

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Russ. J. Appl. Chem., 77(1) (2003) pp. 41-45.

The procedure for cleaning polycrystalline fibers of electrolytic silver used as a catalyst for gasphase oxidation of ethylene glycol to glyoxal was developed with the aid of X-ray photoelectron spectroscopy.

PLASMA CHEMICAL SYNTHESIS OF SILICON CARBONITRIDE FILMS

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Investigated in Russia, 147 (2004) pp. 1607-1615.

Silicon carbonitride thin films were synthesised with RP CVD process using the novel single-source precursors $Me_2HSiNHNMe_2$ and $Me_2Si(NHNMe_2)_2$, which are derivative of 1,1-dimethylhydrazine. The films were characterized by XPS, FTIR, UV-vis and XANES spectroscopy as well as ellipsometry. Electrophysical properties were investigated using test MIS (metal-insulator-semiconductor) structures. Spectroscopy data showed that Si-N, Si-C and C-N are the main bonds for the films deposited from $Me_2HSiNHNMe_2$ whereas Si-N and C-N are basic bonds for the films obtained using $Me_2Si(NHNMe_2)_2$. The films represent $Si_xN_yC_z$ alloys of variable composition. Chemical composition, optical and electrophysical properties of the films and MIS structures are dependent on the deposition conditions.

APPLICATION OF SCANNING TUNNELING MICROSCOPY AND X-RAY PHOTOELECTRON SPECTROSCOPY IN THE INVESTIGATION OF THE SINTERING OF Ag/Al_2O_3 MODEL SUPPORTED CATALYSTS

A.V. Nartova, R.I. Kvon

Kinet. Catal., 45(5) (2004) pp. 730-734.

The results of a study of a specially prepared Ag/Al_2O_3 model system by scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) are presented. The surface morphology of a model support (a thin alumina film on a conducting support) and a model supported catalyst (Ag/Al_2O_3) was characterized using STM. The first experimental results obtained in the STM and XPS study of the sintering of supported catalysts are reported, which demonstrate the capabilities of these techniques for studies of this kind.

NANOWIRE ARRANGEMENTS OF $PbS-Sb_2S_3$-COMPOUNDS

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J. Cryst. Growth, 267(3-4) (2004) pp. 745-750.

In analogy to $PbS–Sb_2S_3$-minerals nanowires of synthetic boulangerite ($Pb_5Sb_4S_{11}$) with diameters ranging from 100 to 500 nm and lengths up to 100 μm were crystallized from the melt. In most cases these nanowires are arranged like bundles and microtubes, which are inspected by scanning electron microscopy. The chemical composition of these materials was analysed by electron microprobe and transmission electron microscope adapted energy dispersive X-ray analysis. The lattice parameters of natural and synthetic boulangerite nanomaterials were determined by powder X-ray diffraction. The crystal structure was examined by means of high resolution transmission electron microscopy, whereby the relation between structure and morphology was studied and the material was checked regarding cation ordering.

X-BAND PERPENDICULAR-MODE EPR SPECTRA OF ‘EPR SILENT’ MANGANESE(III) PORPHYRINS

E.P. Talsi, K.P. Bryliakov

Mendeleev Commun., 14(3) (2004) pp. 111-112.

The X-band perpendicular-mode EPR spectra of manganese(III) porphyrins were detected for the first time.

INVESTIGATION OF FRAGMENTATION PATTERN OF BIS(TRIMETHYLSILYL) ESTER OF 3-MERCAPTOPROPIONIC ACID

A.I. Potapov, A.V. Vorontsov

Intern. J. Mass Spectrom., 235(2) (2004) pp. 163-170.

The routes of fragmentation of the parent molecule resulting from electron impact ionization have been studied in a quadrupole ion trap using collision induced dissociation (CID) of fragments. Fragmentation of the parent molecular ion *m*/*z* 250 results in major ions 235, 178, 163, 135, 129, 75, 73, and 55. While some fragments are easily assigned according to literature - *m*/*z* 235 to $[M - CH_3]^+$, *m*/*z* 73 to $[Si(CH_3)_3]^+$, *m*/*z* 75 to $[Si(CH_3)_2OH]^+$, and *m*/*z* 55 to $[CH_2CHCO]^+$ - other ions required CID to obtain their structure. Fragment *m*/*z* 178 was found to emerge from breaking of Si---S bond and hydrogen rearrangement in the molecular ion. Fragment *m*/*z* 163 is formed by elimination of CH_3 group from ion *m*/*z* 178. Elimination of H_2S from ion *m*/*z* 163 leads to formation of the ion *m*/*z* 129. Another route is elimination of molecule CO from ion *m*/*z* 163 to form ion *m*/*z* 135. Fragmentation of ion *m*/*z* 129 by elimination of neutral molecule CO_2 leads to emerging of ion *m*/*z* 85. For supporting the assumed structure of ions *m*/*z* 178, 163, 135, quantum chemical calculations were performed using methods PM3 and DFT. The calculations demonstrated that these ions have TMS group attached to the carboxyl group. The stability of the ions is associated with forming cyclic structures containing new bonds S---O (*m*/*z* 178), O---Si (*m*/*z* 163) and S---Si (*m*/*z* 129). Molecular dynamics calculations confirmed that these structures are the most stable conformations of the ions.

NMR DETERMINATION OF THE TOTAL COMPOSITION OF COMMERCIAL ABSORBENTS BASED ON MONOETHANOLAMINE

V.P. Talzi

Russ. J. Appl. Chem., 77(3) (2004) pp. 430-434.

The composition of aqueous solution of monoethanolamine used in various units of gas treatment of the Omsk Oil-Refining Plant, Joint-Stock Company, was studied by the ^{13}C NMR spectroscopy. The components of the gases to be purified and the reactions producing the impurities were established.

OLIGOMERIC FORMS OF TIN(IV) IN THE $Rb_2Sn(OH)_6-H_2O-H_2O_2-Rb_2Sn(OOH)_6$ SYSTEM AS PROBED BY ^{119}Sn AND ^{17}O NMR

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Russ. J. Inorg. Chem., 49(10) (2004) pp. 1562-1567.

Solutions of the $Rb_2Sn(OH)_6–H_2O–H_2O_2–Rb_2Sn(OOH)_6$ system with different $[H_2O_2]/[H_2O]$ ratios were studied by ^{119}Sn and ^{17}O NMR. A broad ^{119}Sn NMR signal in the range from –590 to –610 ppm was assigned to Sn(IV) oligomeric forms with bridging peroxo groups. The conditions of their formation and stability range were determined. The first ^{17}O NMR characteristics of the peroxo groups coordinated to the tin(IV) atom were obtained.

HYDROLYSIS OF VOLATILE AMMONIUM OXOFLUOROTITANATE ACCORDING TO ^{19}F, ^{17}O, AND ^{49}Ti NMR DATA

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J. Struct. Chem., 45(1) (2004) pp. 74-82.

Hydrolysis of $NH_4TiO_xF_{5-2x}$ ($x \leq 0.4$) (I) was investigated by ^{19}F, ^{17}O, and ^{49}Ti NMR. The interaction of complex I with water is accompanied by the formation of $[TiF_6]^{2-}$ and multinuclear titanium forms. The composition of the main forms resulting from hydrolysis of I has been established. The bonding of titanium octahedra into dimers and other oligomers occurs by formation of hydroxyl bridges, considerably lowering the pH of the solution. Close analogy has been found between hydrolysis of the title complex and that of titanium tetrafluoride.

STATE OF MOLECULES AND IONS IN THE STRUCTURAL CHANNELS OF SYNTHETIC BERYL WITH AN AMMONIUM IMPURITY

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J. Struct. Chem., 45(1) (2004) pp. 56-63.

The contents of the structural channels of beryl, grown hydrothermally from an ammonium-containing solution, were investigated by IR and EPR spectroscopy. Using IR spectroscopy it was found that water molecules, ammonium ions, and a small number of HCl molecules enter the structural channels of beryl in the course of mineral growth. In these beryls, the ammonium ions play the role of alkali cations. The ammonium ions are as rigidly fixed in the lattice as are water molecules; they are eliminated by calcination at high temperatures close to the decomposition temperature. On exposure to g radiation at 77 K, the paramagnetic NH_3^+ and H^0 radicals are stabilized in the structural channels of beryl. In addition to the known H^0 radical, other states of atomic hydrogen, interacting with medium protons, are observed as well. For one of the additional radicals, H_b, the model of atomic hydrogen stabilized at the center of a silicon-oxygen ring with two water molecules in adjacent cavities is suggested.

FERROMAGNETIC RESONANCE OF NICKEL NANOPARTICLES IN AN AMORPHOUS OXIDE MATRIX

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Kinet. Catal., 45(5) (2004) pp. 735-738.

The formation of a ferromagnetic phase in the thermal decomposition of a layered lithium–aluminum double hydroxide with intercalated nickel–EDTA complexes was studied using ferromagnetic resonance (FMR) spectroscopy. The FMR spectra were simulated based on a superparamagnetic narrowing model. Data on the size and shape of the resulting nickel nanoparticles were calculated.

SYNTHESIS AND ADSORPTION PROPERTIES OF INTIMATELY INTERMINGLED MIXED METAL OXIDE NANOPARTICLES

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J. Mater Chem., 14(4) (2004) pp. 757-763.

A series of intimately intermingled mixed metal oxide nanoparticles were prepared *via* a modified aerogel procedure (MAP). These mixed oxides were composed of alkaline earth oxides and aluminas. It was found that the surface area and reactivity of these materials decreased on going from magnesium to barium in these intimately intermingled metal oxides. The samples were analyzed by HRTEM and the images obtained illustrate the degree of mixing throughout each of the intermingled mixed metal oxides. As well as synthesizing and characterizing these samples, standardized adsorption tests were also carried out and compared to those of individual metal oxide nanoparticles and physical mixtures of metal oxide nanoparticles. The following tests have been shown to be effective in determining the adsorption properties of metal oxide nanoparticles: (i) destructive adsorption of paraoxon (a surrogate of the chemical warfare nerve agent, VX) and (ii) the adsorption of acid gases. The data clearly show enhanced kinetics and capacities for the intermingled AP-$MgAl_2O_4$ and indeed, the data suggest that surface reactivities can be tailored by the aerogel mixing process.

THE STATUS OF THE KEDR ASHIPH SYSTEM

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Nucl. Instrum. Methods Phys. Res., *Sect. A*, 518(1-2) (2004) pp. 597-601.

Cherenkov counters based on Aerogel, wavelength SHIfter, and PHotomultipliers (ASHIPH) for the KEDR detector are described. As compared with the direct light collection on PMT, the ASHIPH method allows us to diminish the number of PMTs essentially. The quality of the particle identification with the ASHIPH counters was tested. The small π/K separation is 4.5σ for the momentum 1.2 GeV/c. The mass production of the ASHIPH counters was organized in Budker Institute of Nuclear Physics (Novosibirsk, Russia). 80 counters filled with 500 ls of aerogel have been produced and tested with cosmic muons. These counters were installed into the KEDR detector in 2003. The stability of the micro-channel PMTs without protecting layer was studied. The first results on a long-term stability of the ASHIPH counters filled with the hygroscopic aerogel are presented.

IR SPECTRA OF PARACETAMOL AND PHENACETIN. I. THEORETICAL AND EXPERIMENTAL STUDIES

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J. Struct. Chem., 45(1) (2004) pp. 64-73.

IR spectra of paracetamol and phenacetin have been measured for powder crystals of these compounds and for their solutions in chloroform and dimethylsulfoxide. *Ab initio* calculations of their equilibrium geometry and vibrational spectra were carried out for spectrum interpretation. Differences between the experimental IR spectra of solutions and crystalline samples have been analyzed. Variations of molecular structure from the isolated state to molecular crystal were estimated based on the difference between the optimized molecular parameters of free molecules and the experimental bond lengths and angles evaluated for the crystal forms of the title compounds. The role of hydrogen bonds in the structure of molecular crystals of paracetamol and phenacetin is investigated, and spectral ranges with maximal intermolecular interactions are determined.

A STRONG ACID THAT DOES NOT PROTONATE WATER

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J. Phys. Chem. A, 108(42) (2004) pp. 9310-9315.

The nature of solvated acids in benzene and chlorinated hydrocarbon solvents is sensitively revealed by IR spectroscopy. Two similarly strong, structurally related acids, triflic acid (CF_3SO_3H) and the N-H acid bis(trifluoromethylsulfonyl) imide ($(CF_3SO_2)_2NH$), behave quite differently toward water in these media. Triflic acid protonates water at the one-equivalent level to give the hydronium ion, H_3O^+. By contrast, bis(trifluoromethylsulfonyl) imide forms a simple hydrate, $(CF_3SO_2)_2NH\cdots OH_2$, even with water at the two-equivalent level. The difference arises from the differing abilities of the conjugate base anions to engage in H-bonding and ion pairing. It illustrates how acidity in low-dielectric media is critically dependent on the nature of the conjugate base anion. νO-H and νN-H stretching frequencies indicate that the H-bonding acceptor ability for solvents toward acidic protons increases in the order carbon tetrachloride < benzene ~ 1,2-dichoroethane < water. With benzene, a marked tendency for acidic protons to H-bond to the π-face of the arene ring is noted and an IR signature of this solvation mode is observed.

UNEXPECTED IR CHARACTERISATION OF HYDROGEN BONDS IN THE 18-CROWN-6-ETHER COMPLEX OF THE H_3O^+ HYDRONIUM ION. CAN THE LOCATION OF THE PROTONS BE SPECIFIED?

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J. Phys. Chem. A, 108(5) (2004) pp. 907-913.

The ν_{as}(C-O-C) IR spectral signatures of polyethers in H-bonded hydronium ion complexes have been established in studies of H_3O^+ and $H_5O_2^+$ complexes with 15-crown-5, 18-crown-6, dibenzo-18-crown-6, and their open chain poly(ethylene glycol) analogues in 1,2-dichoroethane solutions. When experiment meets theory in the structure of the $H_3O^+ \cdot 18$-crown-6 complex, there is disagreement. While DFT calculations at the BLYP/II'//BLYP/6-31G* level indicate a C_{3v} structure with three normal, static linear H bonds to alternate O atoms of the crown ether, IR spectroscopy in the ν(C-O-C) region indicates that all six O atoms are equivalent. A new type of low-barrier H-bonding involving rotational mobility of H_3O^+ is proposed to rationalize the experimental observations.

NANOCLUSTERS AS PRECURSORS TO $(MoVW)_5O_{14}$: *IN SITU* AND CHEMICAL CHARACTERIZATION OF THE SYSTEMS OF A SINGLE PHASE OXIDATION CATALYST

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Phys. Chem. Chem. Phys., 5(23) (2003) pp. 5343-5348.

The ternary oxide $(MoVW)_5O_{14}$ is considered to be highly significant for catalytic, mild selective oxidation reactions. By using UV/Vis, EPR, ^{95}Mo NMR spectroscopies and conductivity measurements the coordination chemistry of the molybdate species in the precursor solutions was studied. This work has established that mixing the precursor solutions (ammonium heptamolybdate, ammonium metatungstate and vanadyl oxalate) forms a polymeric network in which the vanadyl species act as a linker between the molybdate species. The addition of tungsten atoms significantly enhances the polymerisation process.

LINEAR NANOSCALE CLUSTERS OF CuO IN Cu-ZSM-5 CATALYSTS

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Appl. Surf. Sci., 226(1-3) (2004) pp. 88-93.

The electron states of copper have been studied by ESR and UV-Vis as a function of the method used for preparation of Cu-ZSM-5 (ion-exchange, wet impregnation, and deposition), synthesis conditions (pH of copper solution, copper precursor, temperature, etc.) and copper loading.

For calcined Cu-ZSM-5 samples treated under vacuum at 400°C, axial ESR spectra of O^- ion radicals ($g_\perp$=2.05, $g_\parallel$=2.02), which are presumably assigned to linear ---O^----Cu^+---O^----Cu^+---O^--chains in zeolite channels, are observed. The same samples treated under vacuum at 150–400°C, exhibit UV-Vis absorption bands at the unexpected region of 18,000–23,000 cm^{-1}. They are assigned to the ligand–metal charge transfer bands in ---O^{2-}---Cu^{2+}---O^{2-}---Cu^{2+}---O^{2-}-like chains in the zeolite channels. Along with these states, isolated octahedral Cu^{2+} ions with different extents of tetragonal distortion (absorption band (a.b.) 12,500–14,000 cm^{-1}) and clustered copper oxide species (charge transfer band (CTB) 27,000–32,000 cm^{-1}) are also observed.

FORMATION OF NANOCRYSTALLINE STRUCTURES IN A Co-Al SYSTEM BY MECHANICAL ALLOYING AND LEACHING

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J. Alloys Compd., 351(1-2) (2003) pp. 101-105.

Phase composition of the materials obtained by mechanical alloying of system Co–Al (Al concentration ranges from 50 to 70 at.%) and removal of aluminum from such alloys was investigated by differential dissolution, X-ray phase analysis and TEM with a resolution of 0.4 nm. The intensive mechanical alloying provides formation of the nanocomposite material containing both amorphous phase Co_2Al_5 and nanocrystalline particles of phase CoAl. Leaching of amorphous phase Co_2Al_5 results in the amorphous cobalt containing admixtures of alumina and hydroxide. Nanocomposite amorphous phase Co_2Al_5 and CoAl convert into nanocomposite amorphous Co and b.c.c. Co.

A NEW MESOPOROUS TITANIUM-SILICATE Ti-MMM-2: A HIGHLY ACTIVE AND HYDROTHERMALLY STABLE CATALYST FOR H_2O_2-BASED SELECTIVE OXIDATIONS

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Catal. Today, 91-92 (2004) pp. 205-209.

Physico-chemical characterisation and catalytic properties of a new hydrothermally stable mesoporous mesophase titanium-silicate, denoted as Ti-MMM-2, synthesised under moderately acidic conditions are reported. Structure and texture were characterised by using X-ray diffraction, N_2 adsorption and TEM. The state of titanium was characterised using DRS-UV and XANES techniques. Catalytic properties of Ti-MMM-2 were tested in oxidation of three large organic substrates, 2,3,6-trimethylphenol, caryophyllene, and methyl phenyl sulfide, and compared with catalytic properties of TS-1 and Ti-MMM (titanium-silicate of the MCM-41 type synthesised under weakly alkaline conditions). The catalytic activity of Ti-MMM-2 is considerably higher compared to the activity of microporous TS-1 and similar to that of Ti-MMM. The performed physico-chemical study implicated that Ti-MMM-2 combines marked accessibility of titanium and its high dispersion that ensure high catalytic activity of this material. By contrast to Ti-MMM, Ti-MMM-2 is hydrothermally stable and can be used repeatedly without deterioration of catalytic properties. A blend of high catalytic activity and hydrothermal stability allows to consider Ti-MMM-2 as a promising catalyst for the selective oxidation of large organic molecules with aqueous H_2O_2.

PATHWAYS OF DIRECTED SYNTHESIS OF IRON(II) CLATHROCHELATES AND POLYCLATHROCHELATES WITH NON-EQUIVALENT CAPPING GROUPS STARTING FROM ANTIMONY- AND GERMANIUM-CONTAINING PRECURSORS

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Inorg. Chim. Acta.,
357(11) (2004) pp. 3187-3204.

Alternative methods for directed syntheses of clathrochelates and polyclathrochelates with two non-equivalent capping fragments using semiclathrochelate precursors and capping group reactions are described. The lability of antimony-capped iron(II) clathrochelates in remetallation (a capping group exchange) reactions allowed to obtain of mono- and bis-clathrochelates of a general formula $FeNx_3X^1X^2$ and $(FeNx_3X^1)_2X^2$ (where Nx^{2-} is cyclohexanedione-1,2-dioxime dianion; X^1, X^2 are different capping groups). The first and unique dioximate $[Fe(HN_x)_3(Sb(C_6H_5)_3)](ClO_4)$ semiclathrochelate was isolated and characterized. The reaction of this complex with differing mono- and bifunctional cross-linking agents (Lewis acids) led to the formation of clathrochelates molecules with non-equivalent capping groups. The clathrochelates with a labile triethylantimony capping group underwent remetallation in the presence of silicon dioxide as a catalyst. The first stage led to the formation of a surface-immobilized mixed SbSi-capped clathrochelate, which under the action of another capping agent desorbed from the surface gives a mono- or bis-clathrochelate depending on the nature of this agent. An alternative pathway using the bis-capping agents has been implemented for synthesis of bis-clathrochelates when reactive fragments of an initial azomethine ligand demonstrate essentially different chemical properties. The oximehydrazonate germanium-capped iron(II) bis-clathrochelate was synthesized starting from a bis-semiclathrochelate, which was initially isolated with bis-capping germanium(IV) tetraethoxide. A further H^+-catalyzed macrocyclization with triethyl orthoformate produced germanium-capped bis-clathrochelate. The obtained mono- and bis-clathrochelates have been characterized using elemental analysis, PD mass, IR, UV–Vis and ^1H and ^{13}C NMR spectra, and X-ray crystallography (for $FeNx_3(Sb(C_2H_5)_3)_2$ complex), as well as by cyclic voltammograms. The distortion angle φ values and the main distances in the clathrochelate frameworks have been deduced using ^{57}Fe Mössbauer parameters, and EXAFS data and molecular mechanics calculations, respectively.

ANALYTICAL CHEMISTRY OF PHASES OF VARIABLE COMPOSITION AND THE PRINCIPLES OF STOICHIOGRAPHIC DETERMINATION OF SUCH PHASES IN MULTIELEMENT MULTIPHASE SAMPLES

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J. Analyt. Chem., 59(11) (2004) pp. 1016-1026.

The general problems of determining the stoichiometry and content of solid phases of variable composition in multielement multiphase substances are discussed. The possibilities and conditions of application of a reference-free stoichiographic method based on the differential dissolution (DD) of components for the analysis of samples containing spatially homogeneous and inhomogeneous phases are considered. The results of mathematical modeling of the DD process for a mixture of phases of constant and variable composition are presented. These data substantiate the use of the stoichiogram affinity criterion for the identification of spatially inhomogeneous phases of variable composition. Examples of applying the DD method to the phase analysis of various substances containing phases of variable composition are given.

STRUCTURE, STOICHIOMETRY, AND MAGNETIC PROPERTIES OF THE LOW DIMENSIONAL STRUCTURE PHASE $LiCuVO_4$

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J. Solid State Chem., 177(9) (2004) pp. 3131-3139.

A systematic investigation of a series of single- and polycrystalline $LiCuVO_4$ samples by means of X-ray diffraction, X-ray photoelectron spectroscopy, differential dissolution analysis, and magnetic susceptibility measurement were performed. This study reveals a noticeable difference in stoichiometry and structure of the samples prepared in different ways. The magnetic properties are discussed with respect to phase inhomogeneity, non-stoichiometry and structural defects.

CHEMICAL COMPOSITION OF SURFACE LAYERS OF ATMOSPHERIC AEROSOLS OF BAIKAL REGION BY METHOD OF SECOND IONIC MASS-SPECTROMETRY

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Chem. Sustain. Devel.,
12(1) (2004) pp. 165-173.

Secondary ion mass spectrometric technique was used to study elemental and phase composition of surface layers of two types of atmospheric aerosols drawn in Irkutsk (Listvyanka village) and at the high-level station Mondy. The first type aerosols were the ones sampled by pumping air through filters, and another type aerosol particles were captured during snowfalls and collected by pumping the melted snow through filters. The action of water was established to result in “leaching” Na, Ca and Ti from the surface layers to form hydroaluminosilicates. Therefore, the considerable dispersion of element concentrations in the surface layers of air aerosols may be accounted for by the action of atmospheric moisture on the aerosols which depends on the residence time of the aerosols in the atmosphere.

DISSOCIATION CONDITIONS OF METHANE HYDRATE IN MESOPOROUS SILICA GELS IN WIDE RANGES OF PRESSURE AND WATER CONTENT

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J. Phys. Chem. B, 108(42) (2004) pp. 16540-16547.

The temperature of methane hydrate dissociation in silica mesopores has been monitored within a wide range of pressures from 10 MPa to 1 GPa. Because the determination of pore size appears to be crucial for the studied phenomenon, several methods of calculation have been applied. According to our findings, the size that corresponds to the mean size of the most representative pores is to be considered as the most reliable. It was concluded that the shape of hydrate particles replicates a host space of pores and may have a complex (e.g., fractal) shape. An attempt to simulate the curvature of hydrate particles by globular (quasi-spherical), elongated (quasi-cylindrical), or any intermediate models has been done. The quasi-spherical model seems to be more adequate for hydrate particles in small pores (<8 nm), while the quasi-cylindrical model fits better the experimental data for hydrate particles in larger pores. According to experimental results, the hydrate can be formed in pores only by capillary condensate, without in-volving the water layers tightly bound by the surface, and pressure has an insignificant effect on the decrease of the dissociation temperature of the confined hydrate. A new effect of the formation of hydrates at a temperature higher than the bulk hydrate dissociation temperature has been observed for silica gels with the narrowest pores studied.

Fundamental and Practical Approaches to Catalyst Preparation

MECHANOCHEMICAL SYNTHESIS OF YTTRIUM AND LANTHANUM TANTALATES

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Inorg. Mater., 40(1) (2004) pp. 83-89.

The phase changes in the Y_2O_3–Ta_2O_5 and La_2O_3–Ta_2O_5 systems during mechanical activation and subsequent heat treatment are investigated. Y_2O_3 and Ta_2O_5 are shown to react during mechanical activation to form Y_3TaO_7. Calcination of activated mixtures leads to the formation of $YTaO_4$ and $LaTaO_4$. The observed processes are interpreted in terms of transformations of the fluorite structure. A new method is proposed for the synthesis of rare-earth tantalates for applications in diagnostic X-ray contrast media. The method has a number of important advantages over the conventional ceramic route.

MECHANOCHEMICAL SYNTHESIS OF INTERMETALLIC HYDRIDES AT ELEVATED HYDROGEN PRESSURES

V.V. Goidin, V.V. Molchanov, R.A. Buyanov

Inorg. Mater., 40(11) (2004) pp. 1165-1168.

An apparatus is described for producing gas pressures of up to 10 MPa in the grinding vessels of a planetary mill. Mechanochemical reactions are carried out for the first time at gas pressures above 1 MPa. A novel approach to the synthesis of intermetallic hydrides is proposed which involves mechanical activation of a metal mixture at a high hydrogen pressure. Using this approach, two new hydrides are synthesized: Mg_2NiH_6 and a magnesium copper hydride with the approximate composition $MgCuH_2$.

EFFECT OF MECHANOCHEMICAL ACTIVATION ON THE CATALYTIC PROPERTIES OF ZINC OXIDE

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Kinet. Catal., 45(5) (2004) pp. 684-693.

The reasons for changes in catalytic activity as a function of the time of mechanochemical activation in a planetary mill were studied with the use of a set of physicochemical techniques. The dependence of the specific rate of CO oxidation on the time of mechanochemical activation exhibited an extremal character. Small-angle interblock boundaries, disordered dislocations, and shear defects were formed in the sample with maximum activity because of mechanochemical activation. The linear dependence of the specific rate of CO oxidation on the value of microstresses suggested that the above defects were responsible for an increase in the catalytic activity. It is likely that oxygen atoms situated at the sites of the outcrop of defects on the surface served as elementary active centers.

MECHANOCHEMICAL SYNTHESIS AND REACTIVITY OF $La_{1-x}Sr_xFeO_{3-y}$ PEROVSKITES

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J. Mater. Sci., 39(16-17) (2004) pp. 5517-5521.

Mechanochemical synthesis of $La_{1-x}Sr_xFe_{3-y}$ ($0 \le x \le 1$) perovskites was carried out from simple oxides. Undoped lanthanum ferrite samples calcined at 900 and 1100°C for 4 hours are nearly single-phase systems, while some substituted ones (samples with $0.3 \le x \le 0.8$ calcined at 900°C and samples with x=0.3, x=0.4 and x=0.8 calcined at 1100°C) are two-phase systems consisting of orthorhombic perovskite $La_{1-x}Sr_xFeO_{3-y}$ (A) and tetragonal perovskite $Sr_zLa_{1-z}FeO_{3-y}$ (B) phases. In CO and CH_4 oxidation processes the specific catalytic activity (SCA) of samples calcined at 1100°C varies non-monotonously with the Sr content. In CO oxidation SCA reaches a maximum in the range of La substitution by Sr where phase transition occurs and samples are comprised of two coexisting phases (x=0.3 and 0.8). In CH_4 oxidation SCA decreases with the Sr content.

THE EFFECT OF HYDROTHERMAL CONDITIONS ON THE MESOPOROUS STRUCTURE OF TiO_2 NANOTUBES

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J. Mater. Chem., 14(22) (2004) pp. 3370-3377.

A systematic analysis of the influence of preparation conditions in the alkali hydrothermal synthesis on the morphology of TiO_2 nanotubes is performed using HRTEM and low temperature nitrogen adsorption. The possible mechanisms of nanotube formation are reviewed and a mechanism based on the key stage of wrapping of intermediate multilayered titanate nanosheets is suggested. The driving force for wrapping is considered to be the mechanical stress arising during crystallisation/dissolution. The average diameter of the nanotubes was found to depend on the temperature and on the ratio of weight of TiO_2 to the volume of sodium hydroxide solution. An increase in the temperature from 120 to 150°C results in an increase in the average nanotube diameter. Subsequent increases in the temperature result in the formation of non-hollow TiO_2 nanofibers with an average diameter of 75 nm, a wide distribution in diameter and a length in excess of 10 µm. The increase of the TiO_2 : NaOH molar ratio results in an increase in the average diameter of nanotubes and a decrease of surface area. The average inner diameter of TiO_2 nanotubes varied between 2 and 10 nm. The pore-size distribution was evaluated from TEM, and low-temperature nitrogen adsorption data using the BJH method. It was shown that nitrogen adsorption is a suitable method for characterisation of the pore morphology of nanotubes.

POROUS COMPOSITES BASED ON OXIDE-ALUMINUM CERMETS (SYNTHESIS AND PROPERTIES)

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Manuscript,
Publishing House of SB RAS, "Geo" Branch,
Novosibirsk, 2004, 205 p.

The manuscript is devoted to the physicochemical fundamentals of synthesis of porous ceramometals (cermets): Al_2O_3/Al, $Me/Al_2O_3/Al$, $MeO_x/Al_2O_3/Al$, as well as ceramic composites on their bases, prepared through hydrothermal oxidation of powdered aluminum followed by calcination. The manuscript includes a detailed description of all stages of the preparation and the main properties of the composites (mechanical, textural, thermophysical, and catalytical). Special attention was paid to the relation between the parameters of synthesis and properties of cermets. A series of kinetic and balance equations has been obtained, which permit one to predict the properties of composite materials. The manuscript has no analogs in Russia and abroad as it is based upon the authors' results obtained for the last 15 years. The manuscript is partially a reference book as it includes summarizing figures, diagrams, and tables. The manuscript is useful for specialists in the field of the preparation of porous materials as well as for engineers and students.

POROUS Al_2O_3/Al METAL CERAMICS PREPARED BY THE OXIDATION OF ALUMINUM POWDER UNDER HYDROTHERMAL CONDITIONS FOLLOWED BY THERMAL DEHYDRATION. IV. EFFECT OF OXIDE ADDITIVES ON THE COMPOSITION AND TEXTURE CHARACTERISTICS OF $MO_x/Al_2O_3/Al$ COMPOSITES

S.F. Tikhov, Yu.V. Potapova, V.B. Fenelonov, V.A. Sadykov, A.N. Salanov, S.V. Tsybulya, L.F. Melgunova

Kinet. Catal., 45(4) (2004) pp. 607-617.

The synthesis, structure, and texture of metal ceramics based on Al_2O_3/Al with powdered oxide additives (CaO, MgO, Al_2O_3, La_2O_3, and TiO_2) were studied. Analytic expressions were derived to relate the main macroscopic characteristics of the composites.

THE EFFECT OF SUPPORT NATURE AND THE TEMPERATURE OF PRELIMINARY CALCINATION ON THE ATOMIC CATALYTIC ACTIVITY OF SUPPORTED PALLADIUM CATALYSTS FOR THE COMPLETE OXIDATION OF HYDROCARBONS

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Kinet. Catal., 45(3) (2004) pp. 406-413.

It is shown that for palladium catalysts supported on various supports, there is no effect of thermal activation consisting of an increase in the turnover number (TON) of palladium with an increase in the temperature of sample calcination from 500 to 700°C, as was observed in the case of similar supported platinum catalysts; for two palladium–alumina catalysts calcined at 500°C and differing in the concentration of palladium and dispersity, the TON of low-dispersity palladium is substantially higher than the TON of high-dispersity palladium; all other conditions being the same, the TON of supported palladium is determined by the support nature.

FORMATION OF THE PORE STRUCTURE OF OXIDE VANADIUM-TITANIUM-PHOSPHORUS CATALYSTS IN THE COURSE OF THERMAL TREATMENT

V.Yu. Gavrilov, G.A. Zenkovets, O.V. Zalomaeva, S.V. Tsybulya

Kinet. Catal., 45(5) (2004) pp. 702-707.

The effect of the conditions of the thermal treatment of vanadium–titanium–phosphorus catalysts on the formation of the pore structure and phase composition was studied. It was found that the optimum doping of catalysts with phosphorus (5 wt % P_2O_5) was favorable for retention of the high dispersity of primary particles up to 450°C. The main change in the texture of the catalysts occurred within the range of micropores and mesopores with $D < 10$ nm. The formation of the coarsely dispersed well-crystallized phase of a vanadium–titanium–phosphorus compound was detected.

DEVELOPMENT OF NOVEL CATALYSTS AND PROCESSES FOR SELECTIVE REDUCTION OF NITROGEN OXIDES BY HYDROCARBON IN EXCESS OXYGEN

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In "*Green Chemistry in Russia*", Eds. V. Lunin, P. Tundo, E. Lokteva, Moscow Lomonosov State University, 2004, pp. 64-100.

The authors summarize results of multiyear Russian investigations in the field of the development of catalysts for selective reduction of nitrogen oxides by hydrocarbons in excess oxygen, including the results obtained under international cooperative programs. Understanding of the limiting stages of the reactions and the nature of active sites responsible for activation and stabilization of reactants makes it possible to resolve deliberately the problems of controlling catalytic behavior of the systems, where transition metal cations are fixed on the surface of various supports including the supports based on partly stabilized dispersed zirconia and montmorillonite clays pillared with zirconia nanocolumns. The influence of clustering of transition metal cations and of strong cation-support interaction on the species and bond strength of the reactants involved in the key stages. Practically promising systems are identified; the experience in preparation of variously shaped monolith catalysts based on these systems is discussed.

STUDY OF THE INFLUENCE OF THE PREPARATION METHOD ON THE FORMATION OF THE PHASE COMPOSITION AND STRUCTURE OF V-Ti-O AND W-Ti-O CATALYSTS FOR SELECTIVE CATALYTIC REDUCTION OF NO BY NH_3

G.V. Odegova, E.M. Slavinskaya

Kinet. Catal., 45(1) (2004) pp. 133-140.

The influence of the preparation method on the structure and phase composition of V–Ti–O and W-Ti–O catalysts for selective catalytic reduction of NO by NH_3 was studied. The preparation conditions were found to insignificantly affect the structure of the resulting V–Ti–O catalysts, whereas in the case of W-Ti-O catalysts, such an influence was distinctly observed. The introduction of tungsten ions into the lattice of titanium dioxide leads to the formation of both local defects (solid solutions of the substitution type) and extended, so-called Wadsley's defects in the framework of TiO_2. The concentrations of the defects of both types depend on the catalyst preparation conditions.

SYNTHESIS OF MESOPOROUS COMPLEX FRAMEWORK ZIRCONIUM PHOSPHATES VIA ORGANIC-INORGANIC NANOCOMPOSITES: GENESIS OF STRUCTURE, ADSORPTION AND CATALYTIC PROPERTIES

Yu.V. Frolova, V.A. Sadykov, S.N. Pavlova, S.A. Veniaminov, R.V. Bunina, E.B. Burgina, V.N. Kolomiichuk, T.V. Larina, N.V. Mezentseva, M.A. Fedotov, A.M. Volodin, E.A. Paukshtis, V.B. Fenelonov, R. Roy*, D. Agrawal* (**Materials Research Laboratory, Pennsylvania State University, University Park, PA, USA*)

Mat. Res. Soc. Symp. Proc., 788 (2004) pp. 215-220.

This work presents the first results of synthesis of framework binary phosphates of zirconium and transition metal cations (Co, Cu, Ce) via nanocomposites of starting inorganic salts with citric acid and studies of their structure genesis. Nanoparticles of layered Zr phosphates with typical sizes in the range of 18-24 Å are formed at the mixing stage. Less basic Cu and Co cations are mainly octa-coordinated with both phosphate groups of those nanoparticles and citric acid molecules. At subsequent thermal treatment, Cu and Co cations are incorporated within Zr phosphate nanoparticles acquiring a low coordination approaching a tetrahedral one while rearranging the nuclei structure into that of a framework type. Removal of citric acid by heating under air at 200-300°C preserves the size of nanoparticles while their ordered stacking forms mesoporous structure with a narrow pore size distribution ~ 50 Å and specific surface area up to 200 m^2/g after calcination at 600°C. The binary phosphates promoted by a small amount of Pt were found to be effective catalysts of NO_x selective reduction by decane in the oxygen excess not subjected to coking with a high and stable performance at high space velocities in the presence of steam.

EXPERIMENTAL AND THEORETICAL STUDIES OF THE ELECTRONIC SPECTRA OF MIXED FRAMEWORK PHOSPHATES OF Zr AND Co

**Yu.V. Frolova, V.I. Avdeev, S.Ph. Ruzankin,
G.M. Zhidomirov, M.A. Fedotov, V.A. Sadykov**

J. Phys. Chem. B, 108(22) (2004) pp. 6969-6980.

Electronic Diffuse Reflectance Spectra were acquired for samples of mixed framework phosphates of zirconium and cobalt calcined in a broad temperature range (40-900°C). Analysis of the spectral features and their comparison with available data for different cobalt phosphates and CoAPO revealed that in complex framework phosphates the nearest coordination sphere of Co cations mainly corresponds to the oxygen polyhedra with a low coordination number such as tetrahedron, pyramid etc.

In the frames of the time-dependent DFT method (TDDFT), the electronic excitation energies for cobalt cations in different oxygen environment have been calculated. The obtained results allowed to describe the spectra of mixed cobalt-zirconium phosphates of various crystallinity both in the d-d transition and charge transfer ranges with a due regard for simultaneous presence of Co cations in different coordination polyhedrons and spin states. In prediction of the spectral features, the approach used in this work was shown to reasonably agree with the traditional concepts and experience in analysis of the electronic spectra of transition metal cations in their complexes and inorganic frameworks.

PREPARATION AND MICROSTRUCTURAL AND TEXTURAL CHARACTERIZATION OF SINGLE-PHASE ALUMINUM OXIDES

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G.N. Kryukova, S.V. Tsybulya**

Kinet. Catal., 45(5) (2004) pp. 714-721.

Conditions for the preparation of single-phase θ-, η-, and χ-aluminas were determined. The structures of η- and χ-aluminas were characterized. With the use of high-resolution electron microscopy, it was found that η-Al_2O_3 particles exhibited the most developed {111} face and consisted of coherently joined domains with a pronounced platelet shape. Planar defects in the (111) plane occurred in the η-Al_2O_3 particles. Microstructural differences between single-phase η-Al_2O_3 and ν-Al_2O_3 with a defect spinel structure were revealed. It was found that the η-Al_2O_3, χ-Al_2O_3, and θ-Al_2O_3 oxides are characterized by uniformly porous structures with average pore diameters of 47, 55, and 110 Å, respectively.

THE EFFECT OF MODIFICATION ON THE STRUCTURAL, ACIDIC, AND CATALYTIC PROPERTIES OF A LAYERED ALUMINOSILICATE

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Kinet. Catal., 45(5) (2004) pp. 708-713.

The effect of modification on the structural, acidic, and catalytic properties of a natural layered aluminosilicate containing 90% montmorillonite was studied. With the use of low-temperature nitrogen adsorption and XRD analysis, it was found that the addition of hydroxo complexes of aluminum prevents the silicate layers of the layered aluminosilicate from closing upon heating and results both in the formation of stable micropores and in a considerable increase in the specific surface area. The acidic properties of the H, Na, and Al forms of the layered aluminosilicate were studied by IR spectroscopy of adsorbed CO molecules and by the indicator method. After modification with hydroxo complexes of aluminum, the number of Lewis acid sites and the accessibility of acidic OH groups to CO adsorption increased. The total number and strength of acid sites increased as the calcination temperature of the layered aluminosilicate was increased. A correlation between catalytic activity in the reaction of acetone dimerization and the number of acid sites in different forms of the layered aluminosilicate was obtained.

PROPERTIES OF THE SOL-GEL TiO_2-SiO_2 SELECTIVE OXIDATION CATALYSTS PREPARED USING ETHYL SILICATE 40 AS A SILICA PRECURSOR

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Appl. Catal. A, 273(1-2) (2004) pp. 47-53.

It has been shown that the effective titania-silica sol-gel catalysts can be obtained from a modified version of the two-stage, acid-base sol-gel procedure with tetraethoxysilane (TEOS) and ethyl silicate 40 used as silica precursors in the first and second step, respectively. Porous texture of these materials appeared to be similar or superior to those of the corresponding ones synthesized using TEOS or TMOS and this plus excellent surface homogeneity positively affected their catalytic properties which proved to be very attractive in the oxidation of 2,3,6-trimethylphenol (TMP) to 2,3,5-trimethyl-1,4-benziquinone (TMBQ) using aqueous H_2O_2.

INTRODUCTION TO PHYSICOCHEMICAL CHEMISTRY OF SUPRAMOLECULAR STRUCTURE OF ADSORBENTS AND CATALYSTS

V.B. Fenelonov

Monograph, Publishing House of SB RAS, Novosibirsk, 2004, 414 p.

The monograph is first in the available world literature which deals with physicochemical basis of a new interdisciplinary scientific area, namely supramolecular structures (textures) of porous materials, the mechanisms of their formation and application of adsorption methods for their characterization. Here, the term *supramolecular* relates to the structures with elements of no less then one nanometer in size (without top size limits). These structures differ in many features from objects of molecular chemistry because such elements as surface curvature, topological element connectivity, morphology are the key elements here. Weaker and less specific forces (Van der Waals and electrostatic forces) of *intermolecular interaction* substitute for the forces of covalent *intramolecular* interaction. The monograph will be useful to specialists who work in the fields of synthesis, characterization or application of porous and dispersed materials (from biologists to geologists) including, naturally, specialists in heterogeneous catalysis and adsorption.

FORMATION OF Ru-M/SIBUNIT CATALYSTS FOR AMMONIA SYNTHESIS

N.B. Shitova, N.M. Dobrynkin, A.S. Noskov, I.P. Prosvirin, V.I. Bukhtiyarov, D.I. Kochubey, P.G. Tsyrulnikov, D.A. Shlyapin

Kinet. Catal., 45(3) (2004) pp. 414-421.

The effects of the nature of ruthenium and alkaline promoter precursor compounds and support properties on the activity of Ru–(Cs, K)/Sibunit catalysts in the reaction of ammonia synthesis were studied. The formation of active centers in the catalysts was studied with the use of EXAFS, XPS, and electron microscopy. It was found that ruthenium and a portion of cesium occurred in metallic states in the reduced catalysts. The most active catalysts containing 4 wt % ruthenium at the atomic ratios [K] : [Ru] = 4.5 and [Cs] : [Ru] = 2.5 were obtained with the use of the $[Ru(dipy)_3](OH)_2$ complex.

NEW Y(La)–M–O BINARY SYSTEMS (M = Ca, Sr, or Ba): SYNTHESIS, PHYSICOCHEMICAL CHARACTERIZATION, AND APPLICATION AS THE SUPPORTS OF RUTHENIUM CATALYSTS FOR AMMONIA SYNTHESIS

A.S. Ivanova, E.S. Kalyuzhnaya*, G.S. Litvak, E.M. Moroz, S.M. Yunusov*, V.S. Lenenko*, B.L. Moroz, V.B. Shur*, V.A. Likholobov (**Nesmeyanov Institute of Organoelement Compounds, Moscow, Russia*)

Kinet. Catal., 45(4) (2004) pp. 541-546.

The effect of the nature of the alkaline-earth metal on the phase composition and specific surface area of new Y(La)–M–O binary oxide compositions (M = Ca, Sr, or Ba) prepared by coprecipitation was studied. These systems were found to contain mixed compounds ($M_2Y_2O_5$, MY_2O_4, and MLa_2O_4), which are different in thermal stability, in addition to individual La_2O_3 or Y_2O_3 phases. The Y(La)–M–O compositions calcined at 450°C were characterized by a more developed specific surface area, as compared with that of individual La_2O_3 or Y_2O_3. An increase in the calcination temperature to 650°C was accompanied by a decrease in the specific surface area of binary compositions. Catalysts prepared by supporting $K_2[Ru_4(CO)_{13}]$ onto the Y(La)–M–O systems were active in ammonia synthesis at 250-400°C and atmospheric pressure. The most active of these catalysts, $K_2[Ru_4(CO)_{13}]$/Y–Ba–O, provided a higher yield of NH_3 at 250-300°C than analogous catalysts prepared with the use of well-known supports (Sibunit, CFC-1, and C/MgO).

Selective Methane Oxidation to Syngas

SELECTIVE CATALYTIC OXIDATION OF METHANE TO SYNGAS OVER SUPPORTED MIXED OXIDES CONTAINING Ni AND Pt

S.N. Pavlova, N.N. Sazonova, V.A. Sadykov, O.I. Snegurenko, V.A. Rogov, E.M. Moroz, I.A. Zolotarskii, A.V. Simakov, V.N. Parmon

Kinet. Catal., 45(4) (2004) pp. 589-597.

The activity of Ni, Pt, and $LaNiO_3$ supported on α-Al_2O_3 is studied in the selective catalytic oxidation of methane to syngas at 900°C and a contact time of ~0.002 s using dilute mixtures (1000 ppm CH_4 + 500 ppm O_2 in He). The grain size was ~100 μm. The method of X-ray phase analysis shows that supported $LaNiO_3$, both pure and containing Pt, has a perovskite hexagonal structure with altered lattice parameters. Using temperature-programmed reduction by hydrogen, it was found that the reduction of supported $LaNiO_3$ is simplified in the presence of Pt and/or $Ce_{0.2}Zr_{0.8}O_2$. The activity and selectivity of the catalysts in the reaction of selective catalytic oxidation of methane depends on their composition and oxidative–reductive treatment. It was found that, in the presence of catalysts based on $LaNiO_3$ and containing Pt and/or $Ce_{0.2}Zr_{0.8}O_2$, the reaction occurs with an induction period. It was assumed that the value of the induction period depends both on the dynamics of phase $LaNiO_3$ reduction to Ni, which is associated with the accumulation of carbonate complexes and surface hydroxylation, and on slow changes in the defect structure of $Ce_{0.2}Zr_{0.8}O_2$, which are associated with oxidation–reduction.

SELECTIVE METHANE OXIDATION INTO SYN-GAS AT SHORT CONTACT TIMES OVER MONOLITH CATALYSTS

S.N. Pavlova, V.A. Sadykov, I.I. Bobrova, N.F. Saputina, O.I. Snegurenko, R.V. Bunina, A.N. Salanov, V.A. Kuzmin, Z.Yu. Vostrikov, I.A. Zolotarskii

Catal. Ind., Special issue (2004) pp. 12-17.

Catalysts based on $Ce_xZr_{1-x}O_2$ solid solutions promoted by Pt and Rh and applied on corundum honeycombs of cellular structure were investigated in the reaction of selective catalytic oxidation (SCO) of methane into synthesis gas. The effect of preparation method and catalyst composition, thickness of catalytic layer on activity of catalysts in SCO reaction including that in the presence of water vapors and CO_2 (automatic mode), reactions of vapor and carbon-dioxide conversion of methane (isothermal mode) has been investigated. The produced catalysts are shown to provide CH_4 conversion and selectivity to synthesis gas more than 90 % in SCO reaction at contact times $\tau \sim 0{,}1$ s, and they are of high activity in reactions of vapor and carbon-dioxide methane conversion. Introduction of $Ce_xZr_{1-x}O_2$ into catalysts helps prevent carbonization and allows replacing rhodium by more inexpensive platinum. Variation of the composition of starting reaction mixture makes it possible to produce synthesis gas of different H_2/CO ratios. Pilot tests of honeycomb catalysts showed that conduction of SCO in the automatic mode in the reaction mixture of composition 25–30 vol. % CH_4 in the air at $T_{\text{inlet}} = 400$°C and $\tau = 0{,}1 \div 0{,}25$ s provides methane conversion ~ 90 % and synthesis gas output ~50 vol. %.

PARTIAL OXIDATION OF METHANE TO SYNTHESIS GAS OVER SUPPORTED CATALYSTS BASED ON Pt-PROMOTED MIXED OXIDES

S.N. Pavlova, N.N. Sazonova, J.A. Ivanova, V.A. Sadykov, O.I. Snegurenko, V.A. Rogov, I.A. Zolotarskii, E.M. Moroz

Catal. Today, 91-92 (2004) pp. 299-303.

Alumina supported catalysts comprised of a ceria–zirconia solid solution and lanthanum nickelate promoted by Pt were tested in the partial oxidation of methane into synthesis gas under conditions (high temperature, short contact time, highly diluted gas mixture, small catalyst grains) providing acquisition of a catalyst intrinsic activity. The phase composition and reducibility of catalysts were characterized with XRD and TPR. The influence of the catalyst chemical composition, type of redox pretreatment and support phase composition on the activity has been studied. Prolonged relaxations of catalytic activity have been observed, and their nature is discussed taking into account the catalyst properties.

MONOLITH COMPOSITE CATALYSTS BASED ON CERAMOMETALS FOR PARTIAL OXIDATION OF HYDROCARBONS TO SYNTHESIS GAS

S.N. Pavlova, S.F. Tikhov, V.A. Sadykov, Yu.N. Dyatlova, O.I. Snegurenko, V.A. Rogov, Z.Yu. Vostrikov, I.A. Zolotarskii, V.A. Kuzmin, S.V. Tsybulya

Stud. Surf. Sci. Catal., 147 (2004) pp. 223-228.

Microchannel ceramometal monoliths of a high thermal and mechanical stability have been synthesized via hydrothermal treatment of powdered mixtures containing aluminum and additives (oxides or/and Ni-Cr(Co) alloy) followed by calcination. The phase composition and textural properties of monoliths depend on the additive nature affecting the aluminum reactivity toward oxidation as well as their interaction with remaining Al^0. Microchannel ceramometal monoliths and catalysts based on them ensure a high performance and stability in CPO of hydrocarbons at short contact times.

CERIA-BASED FLUORITE-LIKE OXIDE SOLID SOLUTIONS AS CATALYSTS OF METHANE SELECTIVE OXIDATION INTO SYNGAS BY THE LATTICE OXYGEN: SYNTHESIS, CHARACTERIZATION AND PERFORMANCE

V.A. Sadykov, T.G. Kuznetsova, G.M. Alikina, Yu.V. Frolova, A.I. Lukashevich, Yu.V. Potapova, V.S. Muzykantov, V.A. Rogov, V.V. Kriventsov, D.I. Kochubey, E.M. Moroz, D.A. Zyuzin, V.I. Zaikovskii, V.N. Kolomiichuk, E.A. Paukshtis, E.B. Burgina, V.V. Zyryanov, N.F. Uvarov*, S. Neophytides, E. Kemnitz*****
(**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*; ***Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece; ***Institute of Chemistry, Humboldt-University, Berlin, Germany*)

Catal. Today, 93-95 (2004) pp. 45-43.

Polymerized precursor route [M.P. Pechini, US Patent 3, 330 (1967) 697] was applied for synthesis of dispersed ceria-based solid solutions $Ce_{1-x}Me_x^{3+}O_{3-y}$ ($Me^{3+}= Sm^{3+}$ or Bi^{3+}, x up to 0.5). The surface properties of those samples were modified by supporting Pt. Their bulk and surface structural features were characterized by using XRD, TEM, EXAFS, X-ray wide angle scattering (RED), UV–vis, Raman, FTIRS of lattice modes and adsorbed CO. To elucidate factors controlling the surface/bulk oxygen mobility and reactivity, these results were compared with the data of the oxygen isotope exchange and/or H_2/CH_4 temperature-programmed reduction (TPR). Single-phase fluorite-like solid solutions with a nanodomain microstructure are characterized by distortion of the coordination polyhedra caused by dopants followed by the lattice local rearrangement into that of a lower symmetry at a high dopant content. The highest performance in methane selective oxidation into syngas by the lattice oxygen is found for samples where isolated oxygen vacancies dominate. Earlier studied Pt/Ce–Zr–La–O system has a lower oxygen mobility, is less stable in redox cycles and less selective for syngas. Bi–Ce–O system mainly combusts methane and is irreversibly decomposed by deep reduction due to metallic Bi evaporation.

METHANE SELECTIVE OXIDATION INTO SYNGAS BY THE LATTICE OXYGEN OF CERIA-BASED SOLID ELECTROLYTES PROMOTED BY Pt

V.A. Sadykov, V.V. Lunin*, T.G. Kuznetsova, G.M. Alikina, Yu.V. Frolova, A.I. Lukashevich,

Yu.V. Potapova, V.S. Muzykantov, S.A. Veniaminov, V.A. Rogov, V.V. Kriventsov, D.I. Kochubey, E.M. Moroz, D.A. Zyuzin, V.I. Zaikovskii, V.N. Kolomiichuk, E.A. Paukshtis, E.B. Burgina, V.V. Zyryanov, N.F. Uvarov**, S. Neophytides***, E. Kemnitz****** (**Moscow Lomonosov State University, Moscow, Russia*; ***Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*; ****Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece; ****Institute of Chemistry, Humboldt-University, Berlin, Germany*)

Stud. Surf. Sci. Catal., 147 (2004) pp. 241-246.

Nanocomposites based upon ceria doped by Zr, Zr+La or Sm with supported Pt nanoparticles efficiently convert methane into syngas by their lattice oxygen. In red-ox cycles with pure methane as reagent, the surface carbon build-up is observed, which is lower for Sm-doped samples possessing a higher surface and lattice oxygen mobility. When stoichiometric amounts of CO_2 or H_2O are present in the feed, the catalysts efficiently operate in methane steam and dry reforming at high space velocities without deactivation.

METHANE TRANSFORMATION INTO SYNGAS OVER Ce–Zr–O SYSTEMS: ROLE OF THE SURFACE/BULK PROMOTERS AND OXYGEN MOBILITY

T.G. Kuznetsova, V.A. Sadykov, S.A. Veniaminov, G.M. Alikina, E.M. Moroz, V.A. Rogov, O.N. Martyanov, V.F. Yudanov, I.S. Abornev, S. Neophytides* (**Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece*)

Catal. Today, 91-92 (2004) pp. 161-164.

The surface and bulk oxygen mobility and reactivity of ceria-based solid solutions as related to the process of methane conversion into syngas can be tuned in a broad limits by bulk and surface promoters. Variation of the surface/bulk real structure of those complex oxides and their strong interaction with the surface promoters (Pt, Ni) appear to be responsible for those effects.

REACTIVITY OF SURFACE AND BULK OXYGEN IN $La_{1-x}Ca_xFeO_{3-y}$ SYSTEM WITH RESPECT TO METHANE OXIDATION

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React. Kinet. Catal. Lett., 81(2) (2004) pp. 393-398.

The reactivity and mobility of the surface and lattice oxygen in a $La_{1-x}Ca_xFeO_{3-y}$ system prepared via a ceramic route were studied by using CH_4-TPR. While the middle-temperature (400-700^{o}C) oxygen lattice mobility reaches maximum for samples with disordered anion vacancies, the high-temperature lattice oxygen flux appears to be controlled by a rapid transfer along disordered domain walls. In the high-temperature range, a high selectivity to syngas of methane oxidation by the lattice oxygen was achieved both for pure lanthanum ferrite and for samples with a microdomain structure.

Carbon and Carbon-Related Processes

MECHANISM OF CARBON FILAMENTS AND NANOTUBES FORMATION ON METAL CATALYSTS

V.L. Kuznetsov

In *"Nanoengineered Nanofibrous Materials"*,
Eds. S.I. Guceri, Y. Gogotsi, V.L. Kuznetsov,
Kluver Academic Book Publishers,
Dordrecht, The Netherlands,
Vol. 169, 2004, pp. 19-34.

The consideration of the formation mechanisms of carbon deposits on surface metal catalysts led to conclusion that the majority of these mechanisms include some common steps, the most important of which are the formation of metal or metal carbide particle oversaturated with carbon atoms and the nucleation of carbon deposits on the metal surface. A thermodynamic analysis of the carbon nucleation on the metal surface was performed. The master equation for the dependence of critical radius of the carbon nucleus on the reaction parameters, such as the reaction temperature, the catalyst nature, the supersaturation degree of catalyst particle by carbon was obtained. This equation and the phase diagram approach were used for a discussion of the different scenarios of carbon deposit formation, namely, encapsulated metal particles, carbon fibers and filaments, bamboo-like nanotubes, multi-wall and single-wall carbon nanotubes.

ELECTRONIC STRUCTURE OF THE FLUORINATED HIPco NANOTUBES

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In *"Nanoengineered Nanofibrous Materials"*,
Eds. S.I. Guceri, Y. Gogotsi, V.L. Kuznetsov,
Kluver Academic Book Publishers,
Dordrecht, The Netherlands,
Vol. 169, 2004, pp. 143-151.

Single-wall carbon nanotubes (SWNTs) produced by high pressure CO decomposition (HiPco) process has been fluorinated using a volatile mixture of BrF_3 and Br_2. The composition of the fluorinated material was estimated by X-ray photoelectron spectroscopy to be C_4F. Raman spectroscopy showed the narrower tubes are more readily fluorinated. Comparison between CKα-spectrum of the fluorinated SWNTs and theoretical spectra obtained for the (8,8) tube models with different fluorine pattern revealed the fluorine atoms preferably form the chains around a tube circumference.

CARBON FILAMENT ROPE FORMATION

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In *"Nanoengineered Nanofibrous Materials"*,
Eds. S.I. Guceri, Y. Gogotsi, V.L. Kuznetsov,
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Carbon filament growth via CO disproportionation on cobalt supported catalyst was investigated. For the first time the formation of the carbon filament ropes on Co catalysts was observed.

SELF-ASSEMBLING CARBON FILAMENT ROPES FORMATION

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Carbon, 42(5-6) (2004) pp. 1037-1042.

The process of carbon nanotubes and filaments production via catalytic decomposition of CO on SiO_2-modified Co catalyst was investigated. It was demonstrated that variation in carbon nucleation conditions could be used for the production of different type of carbon deposits over the same catalyst. Carbon nucleation conditions were altered by varying reaction temperature and/or catalyst pretreatment procedure. The formation of carbon filament ropes was observed for the first time.

FIELD EMISSION FROM PRODUCTS OF NANODIAMOND ANNEALING

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Carbon, 42(5-6) (2004) pp. 1099-1102.

Field emission characteristics were measured for the samples produced by controlled annealing of nanodiamonds (ND) leading to the formation of

sp^2/sp^3 composites containing diamond core encapsulated in curved graphitic scales, onion-like carbon, and hollow graphite polyhedrons. The sequential raise in the ND annealing temperature was found to result in no monotonic change of emission threshold value of the products. The experimental data were interpreted using results of quantum-chemical AM1 calculation of density of occupied states of carbon structures.

CARBON REDISTRIBUTION PROCESSES IN NANOCARBONS

V.L. Kuznetsov, Yu.V. Butenko, V.I. Zaikovskii, A.L. Chuvilin

Carbon, 42(5-6) (2004) pp. 1057-1061.

Here are presented the results on carbon atom redistribution processes in the closed systems leading to etching of the carbon nanostructures with a high surface energy and to simultaneous formation of bulk graphitic structures. The TEM study of the products produced by treatment of nanodiamond and their annealing products in closed vessels at 2140 K and controlled pressure of CO, CO_2, and H_2O gases shows formation of the low surface area graphitic ribbon structures and polygonized graphitic particles. It has been proposed that in a closed system carbon atoms redistribute due to the reversible reactions of carbon and different hydrogen- and oxygen-containing gases. Thus, these reactions are considered as carbon transport reactions. Intermediates of the growing structures were characterized with high resolution TEM. The basal plane edges and arched basal planes formed on the graphite crystal edges are suggested to be growing centers.

FILAMENTOUS CARBONS AS A SUPPORT FOR HETEROPOLY ACID

M.N. Timofeeva, M.M. Matrosova, T.V. Reshetenko, L.B. Avdeeva, A.A. Budneva, A.B. Ayupov, E.A. Paukshtis, A.L. Chuvilin, A.V. Volodin, V.A. Likholobov

J. Mol. Catal. A: Chem., 211(1-2) (2004) pp. 131-137.

Different kinds of catalytic filamentous carbons (CFC) were used as a support for a few heteropoly acids (HPAs), $H_6P_2W_{21}O_{71}(H_2O)_3$, $H_6As_2W_{21}O_{69}(H_2O)$, Dawson type $H_6P_2W_{18}O_{62}$ (P_2W_{18}) and Keggin type $H_3PW_{12}O_{40}$ (PW). The properties of support determining the interaction between HPAs and supports were studied. Concentration of Brønsted acidic sites in PW and PW/support was determined from ESR studies of the stable nitroxyl radical 4-hydroxy-2,2',6,6'-tetramethylpyperidin-N-oxyl (TEMPOL) adsorbed from hexane. The reaction of 2,6-di-tert-butyl-4-methylphenol (DMBP) with toluene as tert-butyl acceptors was studied using bulk and supported PW and P_2W_{18}. It has been found that P_2W_{18} is more active than PW. The catalytic activities of HPAs supported on SiO_2 and CFC were similar. The activity of the surface protons in HPA/support increased monotonically with increasing the total HPA loading, reaching a maximum for the bulk HPA.

NEW FLUORINATED CARBON SUPPORT FOR CATALYST

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J. Mol. Catal. A: Chem., 217(1-2) (2004) pp. 155-160.

The adsorption of $H_3PW_{12}O_{40}$ on carbon mesoporous materials, Sibunit and fluorinated Sibunit (F-Sibunit), from water and organic solvents (acetone and acetonitrile) was studied. The concentration of Brønsted acidic sites in $H_3PW_{12}O_{40}$ and 8% $H_3PW_{12}O_{40}$/F-Sibunit was determined from ESR studies of the stable nitroxyl radical 4-hydroxy-2,2',6,6'-tetramethylpyperidin-N-oxyl (TEMPOL) adsorbed from hexane. For $H_3PW_{12}O_{40}$ and 8% $H_3PW_{12}O_{40}$/F-Sibunit, the concentration was equal to 4 and 12 $\mu mol \cdot g^{-1}$, respectively. A correlation between the rate constant of cyclohexene dimerization in the hexane solution and the strength of the interaction between HPA and support was determined.

CATALYTIC FILAMENTOUS CARBON AS SUPPORTS FOR NICKEL CATALYSTS

T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, A.L. Chuvilin

Carbon, 42(1) (2004) pp. 143-148.

Ni catalysts supported on catalytic filamentous carbon (CFC) were studied in the model reaction of methane decomposition at 525°C. The supports (CFC) were synthesized by decomposition of methane over metal catalysts (Ni, Ni–Cu, Co and Fe–Co–alumina) at 500–675°C. The yield of secondary carbon was shown to reach 224 g/g_{Ni} on the Ni/CFC (Ni–Cu, 625°C) catalyst. The stability and activity of the

Ni/CFC catalysts for deposition of the secondary carbon at 525°C depend both on textural properties of the support and on the surface structure of the CFC filaments. It seems that highly porous carbon supports are more suitable for development of Ni/CFC catalyst for methane decomposition. The catalytic properties of the supported Ni/CFC systems may be accounted for by generation of weak dispersive interactions between specifically shaped Ni crystallites 30–70 nm in size and basal planes on the surface of the carbon filament.

GASIFICATION BEHAVIOR OF CATALYTIC FILAMENTOUS CARBON

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Carbon, 42(12-13) (2004) pp. 2501-2507.

The paper reports on the effect of the catalytic filamentous carbon (CFC) gasification on its textural properties. CFC samples were prepared by methane decomposition over metal catalysts (Ni, Co, Ni–Cu, Fe–Co-alumina) at 500–625°C. With respect to the ease of hydrogasification, CFC samples of different types can be arranged in the following order: CFC (Co) > CFC (Fe–Co) = CFC (Ni) >> CFC (Ni–Cu, 575°C). The order of their activity in oxidation with CO_2 is: CFC (Co) > CFC (Ni) > CFC (Ni–Cu, 575°C) >> CFC (Fe–Co). When all studied types of CFC are activated in the presence of CO_2 or H_2, changes in the volume of micropores and fine mesopores (3–4 nm) are minimal and do not depend on the treatment conditions. The main observed changes are related to the development of large mesopores, macropores and increase of the CFC surface area by a factor of 1.1-1.5. The development of large mesopores with D>10 nm appears to result from gasification of less ordered graphene packages of the filaments with sizes about 10–30 nm. A slight increase of the microporosity is observed after the CFC treatment with HNO_3 at 100°C.

STAGES OF FILAMENTARY CARBON GROWTH FROM HYDROCARBONS ON NICKEL-CONTAINING CATALYSTS AND CAUSES OF THEIR DEACTIVATION

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Eurasian Chem. Tech. J., 5(4) (2003) pp. 253-260.

Methane decomposition to carbon and hydrogen has been studied using the Ni/Al_2O_3, $Ni\text{-}Cu/Al_2O_3$ and Ni-Cu/MgO catalysts at 550°C. The S-shaped kinetic curves of carbon formation from methane exhibit the following periods: induction, acceleration, stationary state and deactivation. The induction period is characterized by oversaturation of metal or alloy particles with carbon atoms and predominant formation of the graphite phase at the (111) faces of the catalyst particles. After formation of the graphite crystallization centers, the acceleration period is accompanied by the growth of graphite filaments and simultaneous reconstruction of the metal particles. After termination of the above processes, the carbon deposition rate becomes constant. Deactivation of the catalyst is caused by blocking of the front side of the metal particle with a carbon film. When the reaction temperature increases to 700°C, deactivation of the nickel-containing catalyst follows a different mechanism. During the growth of the filamentary carbon, the metal particle becomes viscous-flowing. This fact allows for its partial capturing by the inner filament channel. As a result, the formed carbon filament has an internal channel filled either with metal or its alloy. Hydrogen addition to methane leads to a decrease in the carbon formation rate on the catalyst and a change in the filamentary carbon morphology: now it contains a hollow channel.

CARBON DISPERSION AND MORPHOLOGY IN CARBON-COATED NANOCRYSTALLINE MgO

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Langmuir, 19(24) (2003) pp. 10426-10433.

Nanoscale carbon/MgO composite adsorbents have been prepared by chemical vapor deposition (CVD) of carbon over aerogel-prepared nanocrystalline MgO with propylene as the carbon precursor, and by pyrolysis of $Mg(OH)_2$ aerogels modified with resorcinol. A new textural approach including adsorption methods and HREM has been applied for comprehensive characterization of their textural properties. Carbon has been found to form twisted isolated graphite-like fragments designated as nanoislands (1-2 graphite-like monolayers) coating the MgO surface in the case of carbon CVD and a thicker (2-3 graphitelike monolayers) coating in the case of pyrolysis of resorcinol-modified $Mg(OH)_2$ aerogels. The average number of carbon nanoislands grows with an increase of carbon loading whereas their mean size remains approximately the same. The nanoislands have very high specific surface areas close to the maximum surface area possible for carbon. The discovered peculiarities of carbon deposition allow one to achieve controlled carbon/mineral (hydrophobic/hydrophilic) composition of the surface in the surface coverage range of 20-70%.

ESR AND HRTEM STUDY OF CARBON-COATED NANOCRYSTALLINE MgO

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J. Phys. Chem. B, 108(10) (2004) pp. 3140-3144.

Carbon coated nanocrystalline MgO samples were prepared by butadiene pyrolysis at 500°C over aerogel-prepared MgO samples. Samples with carbon loadings of 1.2, 3.2, 5.0, 10.0 and 15.9 wt. % were prepared. Initial carbon formation rate was about 2 wt. % per hour. According to HRTEM, the structure of the mineral component in the carbon-mineral materials was not altered by the carbon deposition. At low loading of carbon, it was found to deposit only inside the MgO aggregates 5-10 nm from their outside surface forming thin individual bands 1.5-2 nm long. At the highest loading, carbon deposits form three-dimensional graphite-like multilayer structures filling the pore volume of the MgO aggregates and cover the outside surface of the aggregates with a thin monolayer coating. A single symmetric Lorentzian line with g = 2.0029 attributable to carbon deposits has been observed in the ESR spectra of the carbon-mineral materials. It gradually narrows from 5.0 to 1.9 G as the carbon loading increases from 1.2 to 15.9 wt. %. Nitroxyl radicals formed after dinitrobenzene adsorption on MgO nanocrystals have been used as a spin probe for estimation of the concentration of strong basic sites present on the surface of the carbon-mineral materials and degree of their coverage with carbon. The sample with the carbon loading of 15.9 wt. % has practically all such sites blocked with carbon, while samples with the carbon concentration between 5 and 10 wt. % seem to be the most promising candidates for practical application as destructive adsorbents.

NEW GENERATION OF POROUS CARBON MATERIALS FROM PETROLEUM COKE AND COMPOUNDS MODELING ITS STRUCTURE

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Petroleum Chem., 44(6) (2004) pp. 403-406.

The results of a study on new highly porous carbon materials obtained from petroleum coke and aromatic compounds are presented. These materials are characterized by a high specific surface area and a high micropore volume. It was shown that they adsorb up to 180 mg of methane per gram of a sample at room temperature and a pressure of 4 MPa.

Catalysis by Metal Complexes and Heteropolycomplexes

THE FIRST ISOLATED ACTIVE TITANIUM PEROXO COMPLEX: SYNTHESIS, CHARACTERIZATION AND THEORETICAL STUDY

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Inorg. Chem., 43(7) (2004) pp. 2284-2292.

The protonated titanium peroxo complex, $[Bu_4N]_4[HPTi(O_2)W_{11}O_{39}]$ (**1**), has been first prepared *via* interaction of the μ-oxo dimeric heteropolytungstate $[Bu_4N]_8[(PTiW_{11}O_{39})_2O]$ with an excess of 30% aqueous H_2O_2 in MeCN. Peroxo complex **1** has been characterized by using elemental analysis, UV-vis, IR, resonance Raman (RR), ^{31}P and ^{183}W NMR spectroscopy, cyclic voltammetry, and potentiometric titration. The electronic and vibrational spectra of **1** are very similar to those of the well-known unprotonated titanium peroxo complex $[Bu_4N]_5[PTi(O_2)W_{11}O_{39}]$ (**2**), while ^{31}P and ^{183}W NMR spectra differ significantly. A compilation of the physico-chemical techniques supports a monomeric Keggin type structure of **1** bearing one peroxo ligand attached to Ti(IV) in a η^2-coordination mode. The protonation of the titanium peroxo complex results in an increase of the redox potential of the peroxo group,

$E_{1/2}$ = 1.25 and 0.88 V relative to Ag/AgCl reference electrode for **1** and **2**, respectively. In contrast to **2**, **1** readily reacts with 2,3,6-trimethylphenol (TMP) at 40°C in MeCN to give 2,2′,3,3′,5,5′-hexamethyl-4,4′-biphenol (BP) and 2,3,5-trimethyl-*p*-benzoquinone (TMBQ). The proportion between BP and TMBQ in the reaction products depends on the TMP/**1** ratio. When a 2-fold excess of TMP is used, the main reaction product is BP (90%), while using a 2-fold excess of **1** leads to TMBQ (95%). Based on the product study, a homolytic oxidation mechanism that implicates the formation of phenoxyl radicals is suggested. The RR deuterium labeling experiments show that the activating proton is most likely localized at a Ti–O–W bridging oxygen rather than at the peroxo group. Theoretical calculations carried out at the DFT level on the protonated and unprotonated titanium peroxo derivatives also propose that the most stable complex is formed preferentially after protonation of the Ti–O–W site, however, both Ti–OH–W and TiOO–H protonated anions could coexist in solution.

AEROBIC FORMALDEHYDE OXIDATION UNDER MILD CONDITIONS MEDIATED BY Ce-CONTAINING POLYOXOMETALATES

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In *"Catalysis of Organic Reactions"*, Ed. J.R. Sowa, Marcel Dekker, NY, 2004.

Various Ce-POMs have been synthesized and evaluated as catalysts for the aerobic oxidation of formaldehyde at ambient conditions along with simple Ce-compounds. The most active catalyst was the monosodium acid salt of the Ce(IV)-monosubstituted silicotungstate, $NaH_3SiW_{11}CeO_{39}\cdot 7H_2O$ (**1**). Optimization of the reaction conditions led to a system that afforded 30 turnovers of **1** after 5 h. Based on both IR and UV-vis, the Ce-POM retains its structure under the turnover conditions. The formic acid product inhibits the reaction. The kinetic data obtained are consistent with a chain radical mechanism of oxidation. POM **1** can be heterogenized on NH_2-functionalized supports such as xerogels, fibers, etc., and in this form used repeatedly without significant loss of catalytic activity.

Co-CONTAINING POLYOXOMETALATE-BASED HETEROGENEOUS CATALYSIS FOR THE SELECTIVE AEROBIC OXIDATION OF ALDEHYDES UNDER AMBIENT CONDITIONS

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R.I. Maksimovskaya, T.A. Trubitsina,
M.S. Melgunov, E.B. Burgina, J. Mrowiec-Białoń*,
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J. Catal., 226(2) (2004) pp. 363-371.

Tetra-n-butylammonium (TBA) salts of the cobalt-monosubstituted Keggin polyoxometalate (Co-POM), $TBA_4HPW_{11}CoO_{39}$ (I) and $TBA_5PW_{11}CoO_{39}$ (II), have been prepared and characterized by using elemental analysis, potentiometric titration, IR, UV–vis, ^{31}P NMR, and cyclic voltammetry. Different modes of heterogenization of the Co-POM, including anchoring to both NH_2- and NH_3-modified mesoporous silica surfaces and sol–gel synthesis, have been performed. The resulting solid catalysts were characterized by N_2-adsorption measurements, elemental analysis, DR-UV–vis, and FT-IR spectroscopy. The activity of the solid Co-POM materials to catalyze aerobic oxidation of two representative aldehydes, isobutyraldehyde (IBA) in MeCN and formaldehyde in H_2O under mild conditions (20–40^{0}C, 1 atm of air), was assessed and compared with the catalytic activity of the corresponding homogeneous Co-POMs. An emphasis has been placed on leaching tests and catalyst recycling. The effect of protonation of the amine-modified silica surface or the Co-POM on the loading, stability, and activity of the Co-POM solid catalyst was evaluated.

2,6-DIMETHYL-γ-PYRONE AS A ^{13}C NMR INDICATOR FOR ESTIMATING THE ACIDITY OF HETEROPOLYACID SOLUTIONS

G.M. Maksimov, A.V. Golovin

Russ. J. Inorg. Chem., 49(8) (2004) pp. 1256-1259.

^{13}C NMR of solutions containing 2,6-dimethyl-γ-pyrone as a ^{13}C NMR indicator were used to estimate the acidity of aqueous solutions of ordinary acids (HCl, HNO_3, $HClO_4$) and heteropolyacids (HPA) (13HPA of five structural types were used). In the concentration range $[H^+]$ = 0–1.7 mol/l, the change in the signal positions in the spectra reaches 10 ppm, which enables the use of this method to compare the solution acidities of ordinary acids. In HPA solutions, indicator–HPA anion and, probably, indicator–H^+–HPA anion interactions were detected. It was concluded that the indicator method is inapplicable for acidity determinations in HPA solutions.

HYDROFORMYLATION OF 1-HEXENE CATALYZED BY WATER SOLUBLE $CoCl_2(TPPTS)_2$ IN BIPHASIC MEDIUM

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J. Mol. Catal. A: Chem., 211(1-2) (2004) pp. 83-87.

$CoCl_2(TPPTS)_2$ catalyzed hydroformylation of 1-hexene was studied in an aqueous biphasic medium. The effect of temperature, pressure, and concentration of cobalt catalyst on the reaction was studied. At elevated temperatures and pressures, it gave >90% conversion with 68% selectivity for aldehyde and *n*/*iso* ratio of 3.0 for the aldehyde.

SOLID SUPERACIDS FOR HALIDE-FREE CARBONYLATION OF DIMETHYL ETHER TO METHYL ACETATE

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Stud. Surf. Sci. Catal., 147 (2004) pp. 403-408.

The production of methyl acetate directly from dimethyl ether was performed by halide-free carbonylation. The solid superacid catalysts with high density of Brønsted acid sites $Rh/Cs_xH_{3-x}PW_{12}O_{40}$ were compared with $Rh/SO_4/ZrO_2$ and $Rh/WO_x/ZrO_2$. The correlation between the nature of acid sites and activity and selectivity of the catalysts in halide-free carbonylation of DME was found.

PREPARATION OF COLLOIDAL SOLUTIONS OF NOBLE METALS STABILIZED BY POLYOXOMETALATES AND SUPPORTED CATALYSTS BASED ON THESE SOLUTIONS

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Kinet. Catal., 45(6) (2004) pp. 870-878.

Conditions for the preparation of stable aqueous monometallic and bimetallic colloidal solutions (sols) of noble metals (Ru, Rh, Pd, Pt, Ir, Ag, and Au) in the presence of polyoxometalates containing W, Mo, V, and Nb were found. The stability of sols against coagulation at room temperature was studied. The metal/C samples prepared by metal adsorption from sols were studied by powder X-ray diffraction analysis and transmission electron microscopy. The following factors of importance for the preparation of a stable sol are discussed: (1) the formation of a sol of a metal polyhydroxo complex stabilized by a polyoxometalate (preliminary stage) and (2) the formation of polyoxometalate–metal clusters in the course of reduction of polyhydroxo complexes.

SYNTHESIS AND CHARACTERIZATION OF THE HETEROPOLYANION $SiW_{11}CeO_{39}{}^{4-}$

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Russ. J. Inorg. Chem., 49(9) (2004) pp. 1325-1330.

The heteropolyanion $[SiW_{11}CeO_{39}]^{4-}$ (**I**) has been synthesized in solution by electrodialysis method. It was isolated as acid sodium and cesium salts and characterized by ^{183}W and ^{17}O NMR and IR spectroscopy. The ^{183}W NMR spectrum of **I** contains six lines. ^{183}W and ^{17}O NMR spectra were also recorded for $[(SiW_{11}O_{39})_2Ce]^{12-}$ (**II**), which had been obtained earlier. The ^{183}W NMR spectrum of **II** shows 11 lines. Assignment of the ^{183}W NMR spectra of **I** and **II** was carried out. The thermal stability of $NaH_3SiW_{11}CeO_{39}$ was studied.

NEW AMMONIA SYNTHESIS CATALYSTS BASED ON SUPPORTED POTASSIUM CARBONYL RUTHENATES AS PRECURSORS OF CATALYTICALLY ACTIVE RUTHENIUM PARTICLES AND POTASSIUM PROMOTER

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J. Mol. Catal. A: Chem., 219(1) (2004) pp. 149-153.

New supported single-component ruthenium catalysts for ammonia synthesis are reported. For preparation of the catalysts, various potassium carbonyl ruthenates such as $K_2[Ru_6(CO)_{18}]$ (K/Ru = 1/3), K_4 $[Ru_4(CO)_{12}]$ (K/Ru = 1/1), $K_6[Ru_6(CO)_{16}]$ (K/Ru = 1/1), $K_6[Ru_4(CO)_{11}]$ (K/Ru = 1.5/1) and $K_2[Ru(CO)_4]$ (K/Ru = 2/1) were used as precursors of both catalytically active ruthenium particles and potassium promoter while graphite-like active carbon “Sibunit” was utilized as a support. The studied catalysts have been compared in their activity with the previously described $K_2[Ru_4(CO)_{13}]$-based catalyst (K/Ru = 1/2) on “Sibunit” carbon. It has been established that the rate of the ammonia synthesis at 300ºC over these catalysts increases with the increase in the K:Ru ratio in the starting carbonyl metallate, reaching a maximum in the case of the $K_6[Ru_4(CO)_{16}]$-based sample. On further enhancement in the K:Ru ratio, i.e. when the $K_2[Ru(CO)_4]$ catalyst is used, the rate of the ammonia formation noticeably diminishes. The activity of the $K_2[Ru(CO)_4]$-based catalyst in the ammonia synthesis can be considerably augmented on the replacement of “Sibunit” by CFC-II carbon or MgO. The use of γ-Al_2O_3 or carbon-coated γ-Al_2O_3 as supports decreases the reaction rate. An introduction of metallic potassium into the $K_2[Ru(CO)_4]$ catalysts on carbons “Sibunit” and CFC-II accelerates strongly the process of the ammonia synthesis. The highest activity is exhibited by the $K_2[Ru(CO)_4]$ + K system on “Sibunit” at the metallic potassium to carbon molar ratio of 0.08. On using this catalyst (3.55 g), the steady ammonia concentration in the gas flow at 300ºC and 1 atm amounts to 71.1% of the equilibrium value while at 350 and 400ºC the process of the ammonia synthesis fully reaches the equilibrium. In its efficiency in the ammonia production at 250-300ºC, the $K_2[Ru(CO)_4]$ + K catalyst on “Sibunit” carbon significantly exceeds the previously developed $K_2[Ru_4(CO)_{13}]$ + K catalyst on the same support.

REGENERATION OF CATALYSTS BASED ON AQUEOUS SOLUTIONS OF Mo-V PHOSPHOROUS HETEROPOLY ACIDS UNDER OXYGEN PRESSURE

E.G. Zhizhina, M.V. Simonova, V.F. Odyakov, K.I. Matveev

Chem. Sustain. Devel.,
12(6) (2004) pp. 683-688.

Oxidation with oxygen of 0.2 M $H_{7+m}P(V^{IV})_m(V^V)_{4-m}Mo_8O_{40}$ (H_mHPA-4) at temperatures 373-433 K and O_2 pressure up to 8 atm (810 kPa) was studied. Maximal reaction rate s observed at 433 K. Partially oxidized 2 M H_mHPA-4 solutions are thermally unstable at higher temperatures. Apparent activation energy is increased with the increase of oxidation state.

CATALYTIC SYNTHESIS OF 1,4-NAPHTHO- AND 9,10-ANTHRAQUINONES BY REACTION OF DIENE SYNTHESIS FOR PULP AND PAPER INDUSTRY

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Chem. Sustain. Devel.,
12(1) (2004) pp. 47-51.

Adducts of the diene synthesis of 1,4-benzo- and 1,4-naphthoquinones with butadiene are established to be oxidized to 1,4-naphtho- and 9,10-anthraquinones under the action of Mo-V-P heteropolyacids (HPA) and salts of these acids. Prospectively, the multistage catalytic synthesis of 1,4-quinones can be reduced to one stage in the presence of HPA.

REACTIONS OF NITROSOARENES CONTAINING ELECTRON-WITHDRAWING SUBSTITUENTS WITH COORDINATED CO. SYNTHESIS AND STRUCTURE OF COMPLEXES $Pd_2(OAc)_2(p\text{-}ClC_6H_4N[p\text{-}ClC_6H_3NO])_2$ AND $Pd_2(OAc)_2(o\text{-}ClC_6H_4N[o\text{-}ClC_6H_3NO])_2$

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Russ. Chem. Bull.,
53(4) (2004) pp. 819-824.

The reaction of tetranuclear $Pd_4(\mu\text{-}COOCH_3)_4(\mu\text{-}CO)_4$ cluster (1a) with *p*- and *o*-chloronitrosobenzenes was found to give dinuclear nitrosoamide complexes, $Pd_2(OAc)_2(p\text{-}ClC_6H_4N[p\text{-}ClC_6H_3NO])_2$ (4) and $Pd_2(OAc)_2(o\text{-}ClC_6H_4N[o\text{-}ClC_6H_3NO])_2$ (5), respectively. The formation of complexes 4 and 5 is accompanied by evolution of CO_2, resulting from oxidation of CO coordinated in cluster 1. Complexes 4 and 5 were characterized by elemental analysis and IR and ^1H NMR spectroscopy; their structures were studied by EXAFS. The reactions of dinuclear complex 4 with molecular hydrogen and CO were studied. The major products of reduction of 4 with hydrogen include metallic palladium, acetic acid, cyclohexanone, and molecular nitrogen. Treatment of complex 4 with CO under mild conditions (1 atm, 20°C) affords *p*-chlorophenyl isocyanate.

Photocatalytic and Related Processes

CHEMICAL REACTIONS IN TROPOSPHERE

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Ocean Atmosph. Optics, 16(5-6) (2003) pp. 447-453.

Primary gas-phase chemical reactions initiated by tropospheric solar irradiation are briefly overviewed. The work also encompasses the survey of investigations in the field of photo-induced heterogeneous chemical processes that proceed on the surface of basic phase components of tropospheric aerosols. The processes are suggested to divide into groups with different types of absorption of the irradiation quanta. Based on the division, the experimentally observed processes can be identified and classified as photoadsorption, photocatalytic reactions, interaction of gas-phase molecules with a solid surface under the action of irradiation quanta, and surface photochemical reactions.

HETEROGENEOUS CATALYSIS IN THE FENTON-TYPE SYSTEM FeZSM-5/H_2O_2

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Appl. Catal. B, 51(3) (2004) pp. 165-170.

The work deals with Fe-containing zeolites for the catalytic oxidation of water-dissolved organic substances by H_2O_2. A detailed study of the system FeZSM-5/H_2O_2 meant to reveal the nature of the catalysis is presented. For this purpose, the following characteristics of the system were determined: the iron concentration in the filtrate of the catalyst suspension in several reaction runs; Fe content changes in the repeatedly used heterogeneous catalyst; the catalytic activities of the filtrate and of the heterogeneous catalyst in several runs. It has been shown that in the system FeZSM-5/H_2O_2, the heterogeneous catalysis makes the main contribution to the catalyst activity in the H_2O_2 decomposition and oxidation of organic substrates. Additionally, in the presence of the iron ions complexing agents, FeZSM-5 showed a significantly different behavior in comparison to the homogeneously dissolved iron cations. For example, in the presence of the $P_2O_7^{4-}$ anions, the rate of the H_2O_2 decomposition increased by several times in the FeZSM-5 suspension, while it is totally reduced in a homogeneous iron solution.

THE CATALYTIC AND PHOTOCATALYTIC OXIDATION OF ORGANIC SUBSTANCES USING HETEROGENEOUS FENTON-TYPE CATALYST

E.V. Kuznetsova, E.N. Savinov, L.A. Vostrikova, G.V. Echevsky

Wat. Sci. Technol.,
49(4) (2004) pp. 109-115.

This paper deals with catalytic and photocatalytic oxidation of organic substances using H_2O_2 over heterogeneous Fenton-type catalysts. In the study a series of Fe-containing catalysts was experienced. A zeolite named as FeZSM-5 was selected as the most active heterogeneous Fenton-type catalyst. The FeZSM-5 reported was prepared by hydrothermal crystallization in the presence of iron salt. In contrast to the homogeneous Fenton system the catalyst prepared had minimal, if any, leaching of iron ions, was stable during 30 catalytic runs and did not lose its activity in the presence of complexing agents, e.g. $P_2O_7^{4-}$. The catalyst was active in oxidation of organic substances at pH from 1.5 to 8, maximum activity was observed at pH = 3. The FeZSM-5 effectively oxidized a simulant of the warfare agent, diethylnitrophenil phosphate, which is hardly detoxified by other methods. It appeared that the rate of oxidation of formic acid, ethanol and benzene over FeZSM-5 increased under the action of visible light (λ>436 nm), quantum efficiency being 0.06-0.14.

CATALYTIC VAPOUR-PHASE HYDROLYSIS AND PHOTOCATALYTIC OXIDATION OF DIMETHYL METHYLPHOSPHONATE ON A TiO_2 SURFACE

D.A. Trubitsyn, A.V. Vorontsov

Mendeleev Commun., 14(5) (2004) pp. 197-198.

The products of dimethyl methylphosphonate (DMMP) hydrolysis and photocatalytic oxidation on TiO_2 were identified and quantified by a FTIR technique at different relative air humidities and concentrations of DMMP.

SELECTIVITY OF PHOTOCATALYTIC OXIDATION OF GASEOUS ETHANOL OVER PURE AND MODIFIED TiO_2

A.V. Vorontsov, V.P. Dubovitskaya

J. Catal., 221(1) (2004) pp. 102-109.

The rates of the two main stages of photocatalytic ethanol destruction - oxidation of ethanol to acetaldehyde and oxidation of acetaldehyde to CO_2 - were studied under varied concentrations of ethanol and acetaldehyde and photocatalyst irradiance, at different temperatures, and over different photocatalysts. The rates followed the semiempirical three sites Langmuir–Hinshelwood model that envisages sites for ethanol and acetaldehyde adsorption and additional sites for competitive adsorption of ethanol and acetaldehyde. The increase in irradiance gave rise to higher selectivity toward CO_2 via increased concentrations of gaseous intermediate acetaldehyde. However, the rate of ethanol oxidation rose faster than the rate of acetaldehyde oxidation. The selectivity toward CO_2 monotonically decreased with temperature over TiO_2 and the rate of oxidation reached a maximum at 80°C. Among platinum-doped catalysts, the best activity was found for 1.1% Pt/TiO_2. Platinum addition to TiO_2 resulted in a 1.5- to 2-fold increased overall rate of oxidation. The selectivity to CO_2 over Pt/TiO_2 catalyst monotonically increased with temperature. Separate studies in a batch reactor demonstrated that addition of platinum changed the product distribution. Acetic acid, instead of carbon monoxide, was formed in copious quantities over the Pt/TiO_2 catalyst.

PATHWAYS OF PHOTOCATALYTIC GAS PHASE DESTRUCTION OF HD SIMULANT 2-CHLOROETHYL ETHYL SULFIDE

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J. Catal., 220(2) (2003) pp. 414-423.

Photocatalytic oxidation of HD simulant, 2-chloroethyl ethyl sulfide (CEES), was studied in a specially designed coil and flow photocatalytic reactor by means of GC-MS and FTIR techniques. TiO_2 Hombikat UV 100 photocatalyst was deactivated after a few hours of operation, which was signaled by the appearance of incomplete oxidation products in the reactor effluent and accumulation of incomplete oxidation products on the TiO_2 surface. Complete reactivation of the photocatalyst was achieved by washing the photocatalyst with water. Compared to diethyl sulfide, CEES showed lower reactivity in photocatalytic oxidation and was accumulated on the TiO_2 surface after catalyst deactivation. Without UV irradiation, hydrolysis of CEES proceeded on the TiO_2 surface. Major gaseous products of CEES incomplete photocatalytic oxidation are acetaldehyde, chloroacetaldehyde, SO_2, diethyl disulfide, and chloroethylene. Surface products extracted from the TiO_2 surface with acetonitrile and water include mainly 2-chloroethyl ethyl sulfoxide and ethanesulfinic and ethanesulfonic acids, as well as diethyl di-, tri-, and tetrasulfides mono and disubstituted in the β-position with a chlorine or hydroxyl group. While surface monodentate sulfates can be removed upon washing, surface bidentate species stayed on the surface and possibly contribute to the permanent catalyst deactivation.

COMPARATIVE STUDY ON PHOTOCATALYTIC OXIDATION OF FOUR ORGANOPHOSPHORUS SIMULANTS OF CHEMICAL WARFARE AGENTS IN AQUEOUS SUSPENSION OF TITANIUM DIOXIDE

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J. Photochem. Photobiol., A., 162(2-3) (2004) pp. 503-511.

Photocatalytic oxidation by oxygen of air was carried out for dimethyl methyl phosphonate (DMMP), trimethyl phosphate (TMP), triethyl phosphate (TEP), and diethyl phosphoramidate (DEPA) in different concentration. The initial rate of organophosphorus compounds consumption increases with the initial concentration at relatively low concentrations but decreases at higher initial concentrations. If the concentration is higher than the concentration in maximum, the rate decreases because of the lack of adsorbed oxygen. These summit-like dependencies are well approximated by one site Langmuir–Hinshelwood equation with competitive adsorption of oxygen and organophosphorus compound. Parameters of the Langmuir–Hinshelwood equation are reported. Complete mineralization of the organophosphorus compounds at the end of reaction was evidenced by the total organic carbon concentration profiles. These profiles have sigmoidal shape. GC–MS technique was used to identify intermediates of TEP and TMP oxidation. The main intermediates are dimethyl phosphate and methyl phosphate in the case of TMP and diethyl phosphate and ethyl phosphate in the case of TEP. The set of intermediates shows that photocatalytic oxidation proceeds primarily at α carbon atoms of TEP. The distribution of intermediates corroborates that photocatalytic oxidation is initiated by reaction with hydroxyl radicals.

Electrocatalysis and Electrochemical Processes

INFLUENCE OF PARTICLE AGGLOMERATION ON THE CATALYTIC ACTIVITY OF CARBON-SUPPORTED Pt NANOPARTICLES IN CO MONOLAYER OXIDATION

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Phys. Chem. Chem. Phys.,
7(2) (2005) pp. 375-383.

Fuel cell electrocatalysts usually feature high noble metal contents, and these favour particle agglomeration. In this paper a variety of synthetic approaches (wet chemical deposition, electrodeposition and electrodeposition on chemically preformed Pt nuclei) is employed to shed light on the influence of nanoparticle agglomeration on their electrocatalytic properties. Pt loading on model glassy carbon (GC) support is increased systematically from 1.8 to 10.6 μg Pt cm^{-2} and changes in the catalyst structure are followed by transmission electron microscopy. At low metal loadings (≤5.4 μg Pt cm^{-2}) isolated single crystalline Pt nanoparticles are formed on the support surface by wet chemical deposition from H_2PtCl_4 precursor. An increase in the metal loading results, first, in a systematic increase of the average diameter of isolated Pt nanoparticles and, second, in coalescence of nanoparticles and formation of particle agglomerates. This behaviour is in line with the previous observations on carbon-supported noble metal fuel cell electrocatalysts. The catalytic activity of Pt/GC electrodes is tested in CO monolayer oxidation. In agreement with the previous studies, it was found that the reaction is strongly size sensitive, exhibiting an increase of the reaction overpotential as the particle size decreases below *ca*. 3 nm. At larger particle sizes the dependence levels off, the catalytic activity of particles with diameters above 3 nm approaching that of polycrystalline Pt. Meanwhile, Pt agglomerates show remarkably enhanced catalytic activity in comparison to either isolated Pt nanopraticles or polycrystalline Pt foil, catalysing CO monolayer oxidation at *ca*. 90 mV lower overpotential. Enhanced catalytic activity of Pt agglomerates is ascribed to high concentration of surface defects. CO stripping voltammograms from Pt/GC electrodes, comprising Pt agglomerates along with isolated single crystalline Pt nanoparticles from 2 to 6 nm size, feature double voltammetric peaks, the more negative corresponding to CO oxidation on Pt agglomerates, while the more positive to CO oxidation on isolated Pt nanoparticles. It is shown that CO stripping voltammetry provides a fingerprint of the particle size distribution and the extent of particle agglomeration in carbon-supported Pt catalysts.

INFRARED SPECTROSCOPIC STUDY OF CO ADSORPTION AND ELECTRO-OXIDATION ON CARBON-SUPPORTED Pt NANOPARTICLES: INTERPARTICLE VERSUS INTRAPARTICLE HETEROGENEITY

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J. Phys. Chem. B, 108(46) (2004)
pp. 17893-17904.

In this paper, Fourier transform infrared (FTIR) spectroscopy and stripping voltammetry at saturation and submonolayer CO coverages is used to shed light on the influence of size on the CO adsorption and electro-oxidation on Pt nanoparticles. Pt nanoparticles supported on low surface area (~1 $m^2 \cdot g^{-1}$) carbon (Sibunit) are used throughout the study. The vibrational spectra of adsorbed CO are dominated by interparticle heterogeneity (contribution of particles of different size in the range from 0.5 to 5 nm) rather than intraparticle heterogeneity (contribution of different adsorption sites). CO stripping voltammetry exhibits two peaks separated by approximately 0.25 V (at 0.02 V s^{-1}), which are attributed to the CO oxidation from "large" (~3.6 nm) and "small" (~1.7 nm) Pt nanoparticles. Using stepwise oxidation, it was possible to separate the contributions of "large" and "small" nanoparticles and obtain their infrared and voltammetric "fingerprints". Considerable differences are observed between "large" and "small" nanoparticles in terms of (i) the vibrational frequencies of adsorbed CO molecules (ii) their vibrational coupling, and (iii) CO oxidation overpotential.

SIZE EFFECTS ON REACTIVITY OF Pt NANOPARTICLES IN CO MONOLAYER OXIDATION: THE ROLE OF SURFACE MOBILITY

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Faraday Discuss., 125 (2004) pp. 357-377.

The reactivity of model Pt nanoparticles supported on glassy carbon has been studied. The particle size effect is rationalized for CO monolayer oxidation exploring electrochemical methods (stripping voltammetry and chronoamperometry) and modelling. Significant size effects are observed in the particle size interval from *ca.* 1 to 4 nm, including the positive shift of the CO stripping peak with decreasing particle size and a pronounced asymmetry of the current transients at constant potential. The latter go through a maximum at low CO_{ads} conversion and exhibit tailing, which is the longer the smaller the particle size. Neither mean field nor nucleation & growth models give a coherent explanation of these experimental findings. It was, therefore, suggested a basic model employing the active site concept. With a number of reasonable simplifications a full analytical solution is obtained, which allows a straightforward comparison of the theory with the experimental data. A good correspondence between experiment and theory is demonstrated. The model suggests restricted CO_{ads} mobility at Pt nanoparticles below *ca.* 2 nm size, with the diffusion coefficient strongly dependent on the particle size, and indicates a transition towards fast diffusion when the particle size exceeds *ca.* 3 nm. Estimates of relevant kinetic parameters, including diffusion coefficient, reaction constant *etc.* are obtained and compared to the literature data for extended Pt surfaces.

POISONING OF PtRu/C CATALYSTS IN THE ANODE OF A DIRECT METHANOL FUEL CELL: A DEMS STUDY

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Electrochim. Acta, 49(22-23) (2004) pp. 3927-3936.

Poisoning of a commercial PtRu/C electrocatalyst with the products of methanol dehydrogenative adsorption has been studied in a membrane electrode assembly of a liquid fed direct methanol fuel cell at different electrode potentials in the temperature range between 30 and 110°C using a newly designed DEMS setup. In all cases CO_{ads} is identified as the stable methanol dehydrogenation product. The adsorbate coverage versus the electrode potential follows a bell-shaped curve, reaching a maximum around 0.1/0.2 V RHE. During methanol oxidation, the adsorbate coverage remains high and increases with temperature ($\theta \sim 0.6$ at 90°C in 1 M methanol solution). Kinetics of methanol adsorption has been studied at the open circuit potential (between 0 and 20 mV versus RHE). The coverage of the adsorbate and the rate of adsorption rise with temperature. The adsorption isotherms are of Temkin type with an adsorption rate constant k_{ad} increasing from 1.6 ± 0.1 cm^3 mol^{-1} s^{-1} at 30°C to 73 ± 11 cm^3 mol^{-1} s^{-1} at 110°C and a temperature-dependent inhomogeneity parameter αf ranging from 35 ± 1 at 30°C to 8.3 ± 0.2 at 110°C. The apparent activation energy of methanol adsorption at the OCP and zero coverage is estimated as ca. 45 ± 2 kJ mol^{-1}.

HYDROXIDE ADSORPTION ON Ag(110) ELECTRODES: AN *IN SITU* SECOND HARMONIC GENERATION AND *EX SITU* ELECTRON DIFFRACTION STUDY

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J. Phys. Chem. B, 108(48) (2004) pp. 18640–18649.

The adsorption of hydroxide on the Ag(110) surface has been studied with cyclic voltammetry, *in situ* second harmonic generation (SHG), and *ex situ* low energy electron diffraction (LEED) and reflection high energy electron diffraction (RHEED). OH^- is found to be adsorbed on the Ag(110) surface at potentials negative of the potential of zero charge, forming small antiphase domains of c(2 × 6) symmetry. Further adsorption leads to longer-range order and the removal of antiphase domain boundaries and is associated with a current peak in the cyclic voltammogram (CV). Concurrently, a change in symmetry patterns is observed in SHG. A c(2 × 2) pattern gradually replaces the c(2 × 6) pattern as the potential, and the OH^- coverage, is increased. At the beginning of the second current wave, another symmetry change takes place which is accompanied by a sharp change in the LEED pattern from a c(2 × 2) pattern to a (1 × 1) pattern with strong background, indicating a disordered adlayer. However, RHEED results show that some patches of c(2 × 2) structure remain on the surface. The correlation between SHG and diffraction measurements and comparison of the information obtained from each technique allow to develop a detailed picture of the structures and electronic effects at the Ag(110) alkaline electrolyte interface.

A COMPARATIVE STUDY OF HYDROXIDE ADSORPTION ON THE (111), (110) AND (100) FACES OF SILVER WITH CYCLIC VOLTAMMETRY, *EX SITU* ELECTRON DIFFRACTION AND *IN SITU* SECOND HARMONIC GENERATION

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Langmuir, 20(25) (2004) pp. 10970–10981.

Hydroxide adsorption on the (111), (110), and (100) faces of silver electrodes from mixed NaOH/NaF solution is studied using cyclic voltammetry and *in situ* second harmonic generation (SHG). Cyclic voltammograms for the three low index silver planes in alkaline electrolytes are for the first time compared. They show two pairs of anodic and cathodic peaks in the potential interval below the equilibrium Ag/Ag_2O potential. These are attributed to the specific adsorption of hydroxide ions followed by submonolayer oxide formation. The differences in the cyclic voltammograms for the (111), (110), and (100) planes are attributed to different (i) work functions, (ii) surface atomic densities, and (iii) corrugation potentials for these surfaces. *Ex situ* low energy electron diffraction (LEED) and reflection high energy electron diffraction (RHEED) show that disordered adlayers are formed on Ag(111) and Ag(100), in contrast to Ag(110), where ordered structures are produced in the region of the first pair of current peaks. In the region of the second pair of peaks, LEED indicates disordered oxide phases on each crystal plane and RHEED shows the presence of small islands of *c*(2 × 2) structure at some potentials on (110) and (100). SHG measurements were performed (i) in the potential scan mode at constant rotational angle and (ii) at constant potential as a function of the rotational angle. The isotropic (for the (111), (110), and (100) planes) and anisotropic (for the (110) and (111) planes) contributions to the SHG intensity were calculated by fitting the experimental data and are discussed in terms of their dependence on the charge density at the interface, on hydroxide adsorption, and on submonolayer oxide formation.

METHANE OXIDATION ON THE SURFACE OF MIXED-CONDUCTING $La_{0.3}Sr_{0.7}Co_{0.8}Ga_{0.2}O_{3-\delta}$

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Catal. Commun., 5(6) (2004) pp. 311-316.

Mixed-conducting $La_{0.3}Sr_{0.7}Co_{0.8}Ga_{0.2}O_{3-\delta}$ (LSCG) possesses substantial oxygen permeability, but exhibits a high activity to complete CH_4 oxidation, thus making it necessary to incorporate reforming catalysts in the membrane reactors for methane conversion. Dominant CO_2 formation is observed for the steady-state conversion of CH_4 by atmospheric oxygen (methane/air ratio of 30:70) in a fixed bed reactor with LSCG as catalyst, and for the oxidation of CH_4 pulses supplied in helium flow over LSCG powder. The conversion of dry CH_4 by oxygen permeating through dense LSCG ceramics, stable operation of which under the air/CH_4 gradient is possible due to the surface-limited oxygen transport, yields CO_2 concentrations higher than 90%. The prevailing mechanism of total methane combustion is probably associated with weak Co–O bonding in the perovskite-related LSCG lattice, in correlation with data on oxygen desorption, phase stability and ionic transport.

ALKYLATING AGENTS STRONGER THAN ALKYL TRIFLATES

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J. Amer. Chem. Soc., 126(39) (2004) pp. 12451-12457.

A new class of potent electrophilic "R$^+$" alkylating agents has been developed using weakly nucleophilic carborane anions as leaving groups. These reagents, R($CHB_{11}Me_5X_6$) (R = Me, Et, and *i*-Pr; X = Cl, Br), are prepared via metathesis reactions with conventional alkylating agents such as alkyl triflates, using the high oxophilicity of silylium ion-like species, Et_3Si(carborane), as the driving force to obtain increased alkyl electrophilicity. The crystal structure of the isopropyl reagent, *i*-Pr($CHB_{11}Me_5Br_6$), has been determined, revealing covalence in the alkyl-carborane bonding. This contrasts with the free *i*-Pr$^+$ carbocation observed when the anion is less coordinating (e.g. $Sb_2F_{11}^-$) or with tertiary alkyl centers, as in [*tert*-butyl][carborane] salts. In solution, the reagents exist as equilibrating isomers with the alkyl group at the 7-11 or 12 halide positions of the CB_{11} icosahedral carborane anion. These alkylating agents are so electrophilic that they (a) react with alkanes at or below room temperature via hydride extraction to produce carbenium ions, (b) alkylate benzene without a Friedel-Crafts catalyst to give arenium ions, and (c) alkylate electron-deficient phosphorus compounds that are otherwise inert to conventional alkylating agents such as methyl triflate.

Olefin Polymerization

RECENT DATA ON THE NUMBER OF ACTIVE CENTERS AND PROPAGATION RATE CONSTANTS IN OLEFIN POLYMERIZATION WITH SUPPORTED Zn CATALYSTS

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Macromol. Symp., 213(1) (2004) pp. 19-28.

Data on the number of active centers (Cp) and propagation rate constants (Kp) have been obtained by means of polymerization quenching with ^{14}CO of propylene and ethylene polymerization with supported titanium-magnesium catalysts (TMC) with different composition. In the case of propylene polymerization the Cp and Kp values have been measured separately for isospecific, aspecific and low stereospecific centers. Effects of $MgCl_2$ support, internal and external donors are discussed on the basis of data obtained. Data on the strong effect of diffusion limitation at ethylene polymerization with number of TMC have been obtained and a set of methods have been used to exclude this effect. Data on Cp and Kp values at ethylene polymerization with low stereospecific and highly stereospecific catalysts are presented.

SILICA-SUPPORTED ZIRCONOCENE/(PERFLUOROPHENYL)BORATE CATALYST FOR PROPYLENE POLYMERIZATION: DRIFTS STUDY OF THE CATALYST FORMATION AND SURFACE SPECIES

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J. Mol. Catal. A: Chem., 225(2) (2005) pp. 271-277.

IR spectroscopy has been used to study the interaction of silica with $PhNEt_2$ (N) and $B(C_6F_5)_3$ (B) and subsequent interaction of the support SiO_2/[N+B] with dimethylzirconocene $Me_2Si(2\text{-}Me\text{-}Ind)_2ZrMe_2$ (“Zr”). The data were obtained on the composition of the surface compounds appeared at both stages of catalyst synthesis.

It has been shown that (B) and (N) interact with OH groups of silica to form ionic pair $[H\text{-}NR_3]^+[(C_6F_5)_3B\text{-}O\text{-}Si{\equiv}]^-$ (IP-1). Cation fragment of this pair contains highly reactive N-H bond with a.b. at 3230 cm^{-1}. It has been found that N-H groups in a part of IP-1 complexes react with neighboring OH groups of silica by hydrogen bonding that gives complexes IP-2. It has been shown that “Zr” complexes interact both with complexes IP-1 and IP-2. As “Zr” reacts with IP-1, zirconium ionic complexes IP-3 containing Zr-Me bond are formed on silica. These complexes are suggested to be the precursor of the polymerization active sites. The reaction of “Zr” with IP-2, most likely, produces surface zirconium compound containing no Zr-Me bonds and inactive for propylene polymerization.

AN IR-SPECTROSCOPIC STUDY OF THE STATE OF ZIRCONIUM IN SUPPORTED ZIRCONOCENE CATALYSTS

V.N. Panchenko, I.G. Danilova, V.A. Zakharov, E.A. Paukshtis

Kinet. Catal., 45(4) (2004) pp. 547-553.

The surface compounds of zirconium in $SiO_2/MAO/Cp_2ZrMe_2$ (**I**) and SiO_2/Cp_2ZrMe_2 (**II**) catalysts were studied by the IR spectroscopy of adsorbed CO at 93–293 K. It was found that the bridging and terminal complexes of CO were formed on the surface of the catalysts at 93 K; the adsorption of CO was reversible. At 293 K, CO was irreversibly inserted into the Zr–Me bond with the formation of various acyl compounds of zirconium; these compounds were characterized by absorption bands in the region 1495–1750 cm^{-1} in the IR spectrum. These data suggested the heterogeneity of the surface composition of zirconocene catalysts **I** and **II**. Catalyst **I**, which was active in ethylene polymerization, contained surface zirconium complexes that can be considered as the precursors of active centers for ethylene polymerization.

FERROUS RATHER THAN FERRIC SPECIES ARE THE ACTIVE SITES IN BIS(IMINO)PYRIDINE IRON ETHYLENE POLYMERIZATION CATALYSTS

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Catal. Commun., 5(1) (2004) pp. 45-48.

^{1}H NMR and EPR spectroscopic studies show that the iron centers in bis(imino)pyridine iron(II) and bis(imino)pyridine iron(III) olefin polymerization pre-catalysts $LFeCl_2$ and $LFeCl_3$ (L=bis(imino)pyridine) are converted upon treatment with methylaluminoxane (MAO) into ferrous complexes of the type $[L(Me)Fe(II)(\mu\text{-}Me)_2AlMe_2]$ or $[LFe(II)(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$.

THE ACTIVE INTERMEDIATES OF ETHYLENE POLYMERIZATION OVER 2,6-BIS(IMINO)PYRIDYL IRON COMPLEX ACTIVATED WITH ALUMINUM TRIALKYLS AND METHYLALUMINOXANE

K.P. Bryliakov, N.V. Semikolenova, V.A. Zakharov, E.P. Talsi

Organometallics, 23(22) (2004) pp. 5375-5378.

The intermediates of olefin polymerization over homogeneous catalysts based on bis(imino)pyridine iron(II) chloride ($LFeCl_2$, L=2,6-bis[(1-2,6-dimethylphenylimino)ethyl]pyridine) with different activators (trimethyl-, triisobutyl-, trioctylaluminum and MAO) have been studied by ^{1}H and ^{2}H NMR. In conditions approaching real polymerization, neutral species of the type $[LFe(II)Cl(\mu\text{-}R)_2AlR_2]$ or $[LFe(II)R(\mu\text{-}R)_2AlR_2]$ dominate in the reaction solution in $LFeCl_2+AlR_3$ systems, whereas in $LFeCl_2/MAO$ systems, ion pairs $[LFe(II)(\mu\text{-}Me)(\mu\text{-}Cl)AlMe_2]^+[Me\text{-}MAO]^-$ (at Al/Fe < 200) and $[LFe(II)(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$ (at Al/Fe > 500) are the predominant species.

MODIFICATION OF POLYETHYLENE BY SELECTIVE OXIDATION OF END DOUBLE BONDS TO CARBONYL GROUPS

S.V. Semikolenov, K.A. Dubkov, L.G. Echevskaya, M.A. Matsko, E.B. Burgina, D.E. Babushkin, V.A. Zakharov, G.I. Panov

Polymer Sci. Ser. B, 46(9-10) (2004) pp. 308-311.

It was demonstrated that the treatment of polyethylene by nitrous oxide (N_2O) at 230–250°C leads to selective oxidation of end double bonds of the polymer and their quantitative conversion into carbonyl groups. Oxidation has an insignificant effect on the molecular mass distribution of the polymer and may be regarded as a new method of PE modification.

COPOLYMERIZATION OF TRIFLUOROCHLOROETHYLENE AND ALKYL VINYL ETHERS

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Polymer Sci. Ser. B, 46(9-10) (2004) pp. 255-258.

The copolymerization of trifluorochloroethylene and alkyl vinyl ethers, a process that is widely used for manufacturing of protective coatings, was investigated. In order to raise efficiency in the use of trifluorochloroethylene–alkyl vinyl ether–hydroxyalkyl vinyl ether ternary copolymers, the possibility of eliminating copolymer structuring during polymerization through the addition of small amounts of primary alcohols or hydroxyamines was suggested and experimentally verified. Some properties of coatings based on these copolymers that were cured by toluylene diisocyanate additives were studied.

NEW BIS(ARYLIMINO)PYRIDYL COMPLEXES AS COMPONENTS OF CATALYSTS FOR ETHYLENE POLYMERIZATION

S.S. Ivanchev, G.A. Tolstikov*, V.K. Badaev, I.I. Oleinik*, N.I. Ivancheva, D.G. Rogozin, I.V. Oleinik*, S.V. Myakin (**Vorozhtsov Institute of Organic Chemistry, Novosibirsk, Russia*)

Kinet. Catal., 45(2) (2004) pp. 176-182.

A new series of 2,6-bis(arylimino)pyridineiron(II) complexes with cycloaliphatic (cyclopentyl, cyclohexyl, cyclooctyl, and cyclododecyl) substituents in the *ortho* position of the aryl ring are synthesized and studied as components for ethylene polymerization catalysts. Methylaluminoxane is used as an activator for the complexes. The resulting catalytic systems are more active in polymerization at elevated temperatures (60-80°C) than previously described systems based on substituted 2,6-bis(arylimino)pyridines. The influence of the number of CH_2 groups in a cycloaliphatic substituent on the efficiency of the catalytic system is studied. Polymers formed are characterized by an increased molecular weight, high density, and high crystallinity.

ANIMATE ETHYLENE POLYMERIZATION OVER CATALYTIC SYSTEM *BIS*[N-(3-*TRET*-BUTYLSALICILIDEN)ANILINEATO]TITANDICHLORIDE – METHYLALUMOXANE

S.S. Ivanchev, V.K. Badaev, N.I. Ivancheva, S.Ya. Khaikin

Doklady Chem., 394(5) (2004) pp. 639-642.

Kinetics of the polymerization of ethylene over a catalytic system *bis*[N-(3-*tert*-butylsalicylidene) anilinato]titanedichloride – methylalumoxane was studied. The shapes of the polymerization rate curves indicated the stable operation of the catalytic systems for long enough time (more than 30 min) at the temperature as high as 50°C. The obtained time dependencies of the molecular mass of synthesized polyethylene allowed the mechanism of animated polymerization to be established. This mechanism also was supported by calculations. Another evidence was that the addition of hexane to the ethylene feed resulted in the formation of ethylene-hexene block-copolymer. The animated polymerization of ethylene was observed for the first time with this comparatively simple and available catalytic system.

DESIGN OF ARYLIMINE POSTMETALLOCENE CATALYTIC SYSTEMS FOR OLEFIN POLYMERIZATION.
I. SYNTHESIS OF SUBSTITUTED 2-CYCLOALKYL- AND 2,6-DICYCLOALKYLANILINES

I.I. Oleinik*, I.V. Oleinik*, I.B. Abrakhmanov, S.S. Ivanchev, G.A. Tolstikov*** (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia; **Institute of Organic Chemistry, Ufa, Bashkortostan, Russia*)

J. General Chem., 74(9) (2004) pp. 1423-1427.

An easy approach to synthesis of substituted 2-cycloalkyl- and 2,6-dicycloalkylanilines, included catalytic hydrogenation in methanol over nickel-Reney of available o-cycloalkenylanilines, produced by interaction of cyclic allyhalogenides with anilines, has been designed.

DESIGN OF SCHIFF BASE-LIKE POSTMETALLOCENE CATALYTIC SYSTEMS FOR POLYMERIZATION OF OLEFINS.
II. SYNTHESIS OF 2,6-BIS(ARYLIMINOALKYL)PYRIDINES WITH CYCLOALKYL SUBSTITUENTS

I.I. Oleinik*, I.V. Oleinik*, I.B. Abrakhmanov, S.S. Ivanchev, G.A. Tolstikov*** (**Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia; **Institute of Organic Chemistry, Ufa, Bashkortostan, Russia*)

J. General Chem., 74(10) (2004) pp. 1575-1579.

Reactions of substituted cycloalkylanilines with 2,6-diacetylpyridine in methanol in the presence of formic acid afforded a wide series of the corresponding bis(cycloalkylaryliminoalkyl)pyridines which can be used as ligands for the preparation of iron and cobalt complexes.

SPECTROSCOPIC INVESTIGATION OF PRODUCTS OF ULTRADISPERSED POLYTETRAFLUOROETHYLENE SUBLIMATION

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(**Institute of Chemistry, Vladivostok, Russia*)

J. Struct. Chem., 45(5) (2004) pp. 830-836.

IR-spectroscopy was used to study structure of the fractions, evolved in the process of thermal sublimation of UPTFE powder. Fractions consisted of highly amorphous fragments formed by branched chains with end olefin groups condensed at temperatures 50-160°C. Fractions, isolated at temperatures ≥300°C have the structure similar to PTFE and are highly crystalline. It is suggested, that amorphism of the samples is caused by irregular distribution of fragments with end olefin and side fluoromethyl groups in the structure.

PECULIARITITES OF THERMAL DESTRUCTION AND CALORIMETRY OF SUPERDISPERSED POLYTETRAFLUOROETHYLENE

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T.S. Kukhlevskaya, A.K. Tsvetnikov**,**
A.V. Kartashev*** (**Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institute of Chemistry, Vladivistok, Russia; ***Kirenskii Institute of Physics, Krasnoyarsk, Russia*)

Chem. Sustain. Devel., 12(5) (2004) pp. 605-610.

Derivatography, mass-spectrometry and differential scanning microcalorimetry were used to study ultradispersed powder of terafluoroethylene, prepared by thermal gas-dynamic method (material FORUM®). The process of FORUM thermal decomposition and its thermal physical properties differs significantly from the industrial PTFE. Temperature range of the decomposition process increased more than 4 times: 465-595◦C for PTFE and 70-550◦C for FORUM. FORUM evolved wide spectrum of molecular fragments with atomic masses from 31 to 881 upon thermal decomposition. Phase transitions in crystal phase, typical for industrial PTFE, are missed.

MECHANOCHEMICAL METHODS TO OBTAIN COMPOSITE MATERIALS METAL-CERAMICS-POLYTETRAFLUOROETHYLENE

O.I. Lomovskii*, A.A. Politov*, D.V. Dudina*,
M.A. Korchagin*, V.M. Buznik (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Chem. Sustain. Devel., 5 (2004) pp. 619-626.

Solid phase mechanochemical methods to obtain new materials – metalfluoropolymer and metal-ceramic-fluoropolymer composites have been developed. Composite materials with high electroconductivity and low friction constant, stable to abrasion were prepared on the base of W-Cu, WC-Cu, Cu-TiB_2 and ultradispersed polytetrafluoroethylene (UPTFE). Thermal stability of pure mechanically treated UPTFE and PTFE in the composite differs and depends on the nature of the main composite component.

Biotechnology and Biology Related Catalysis

KINETIC PECULIARITIES OF α-PINENE OXIDATION BY MOLECULAR OXYGEN

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V.A. Semikolenov (**Aventis Animal Nutrition S. A., France*)

Appl. Catal., A, 272(1-2) (2004) pp. 109-114.

Kinetic peculiarities of α-pinene oxidation by molecular oxygen were studied. The process proceeds selectively at a low a-pinene conversion and the main products are verbenyl-hydroperoxide and α-pinene epoxide. The products ratio depends slightly on temperature, oxygen pressure and α-pinen conversion. The kinetic equation for the reaction rate was suggested.

KINETIC STUDY ON ISOMERIZATION OF VERBENOL TO ISOPIPERITENOL AND CITRAL

N.V. Maksimchuk, I.L. Simakova,
V.A. Semikolenov

React. Kinet. Catal. Lett., 82(1) (2004) pp. 165-172.

Thermal isomerization of verbenol in the gas and liquid phases is discussed. The effect of temperature and residence time on the reaction mixture composition was studied (at 460-600°C and a residence time τ of about 10^{-3} min for the gas phase conditions; at 200-350°C and τ = 10-80 min for the liquid phase process). The kinetic behavior and the reaction mechanisms are presented.

HETEROGENEOUS BIOCATALYSTS AND REACTORS FOR INNOVATIVE PROCESSES OF ENZYMATIC PROCESSING OF STARCH AND SUGAR

G.A. Kovalenko, O.V. Komova, I.L. Simakova, L.V. Perminova, A.V. Simakov, V.V. Khomov, S.V. Sukhinin* (**Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia*)

Catal. Ind., 2 (2004) pp. 41-47.

The domestic innovative developments analyzed in this article concern the biocatalysis and describe alternative technological approach to heterogeneous processes of enzymatic hydrolysis of starch-containing raw material and sugar into starch treacle of various composition, and invert syrups. Their essence is in production and use of highly-stable biocatalysts on the basis of ferments: glucoamylase and invertase immobilized on carbon-containing macrostructured ceramic supports. A rotary-inertial bioreactor designed for these heterogeneous biocatalysts allows increasing efficiency of the processes of enzymic hydrolysis of starch and sugar as compared with the conventional bioreactor with steady layer.

ROTOR-INERTIAL BIOREACTOR FOR HETEROGENEOUS BIOCATALYTIC PROCESSES. I. STARCH ENZYMATIC HYDROLYSIS

G.A. Kovalenko, S.V. Sukhinin*, A.V. Simakov, L.V. Perminova, O.V. Komova, V.V. Khomov, O.Yu. Borovtsova (**Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia*)

Biotechnology, 1 (2004) pp. 83-90.

Comparative studies of enzymatic hydrolysis of dextrinized corn and wheat starch in innovative rotor-inertial bioreactor (RIB) were carried out using heterogeneous biocatalyst obtained by adsorptive immobilization of glucoamilase on carbon-containing foam-like ceramics. Principle of RIB operation and structure, and also some characteristics in comparison with traditional fixed-bed bioreactor are given. Under optimal conditions (rotational speed of container not less than 80 turn/minute, rate of substrate feeding not more than 0,2 l/h) it was shown that efficiency of the process of corn dextrines hydrolysis and activity of heterogeneous biocatalyst in the RIB was 1,5-2 times and 3-3,5 times, correspondingly, higher than that in the traditional fixed-bed bioreactor.

CATALYTIC FILAMENTOUS CARBONS (CFC) AND CFC–COATED CERAMICS FOR IMMOBILIZATION OF BIOLOGICALLY ACTIVE SUBSTANCES

G.A. Kovalenko, D.G. Kuvshinov, O.V. Komova, A.V. Simakov, N.A. Rudina

In *"Nanoengineered Nanofibrous Materials"*,
Eds. S.I. Guceri, Y. Gogotsi, V.L. Kuznetsov,
Kluver Academic Book Publishers,
Dordrecht, Netherlands, Vol. 169, 2004, pp. 251-256.

Adsorption properties of bulk catalytic filamentous carbon (CFC) granules and CFC-coated macrostructured ceramics (honeycomb monoliths, foams) have been studied for adsorptive immobilization of biologically active substances, including enzymes (glucoamylase, invertase) and non-growing cells of bacteria. The effects of morphology of surface carbon layer on the adsorption efficiency of the supports and on the biocatalytic properties (activity and stability) of immobilized enzymes have been investigated.

HYDROXYAPATITE FORMATION IN HUMAN BLOOD

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Proceedings of the International Congress on Applied Mineralogy,
Eds. Picchio et. al, ICAM-BR, San-Paulo,
2004, pp. 207-210.

In existing models of the soft tissue mineralization the role of blood is limited to transport of calcium and phosphorus ions. In present study it is proved a tissue mineralization mechanism starting that hydroxyapatite (HAP) is produced in the blood plasma. This mechanism is based on the observation of HAP microcrystalls, which are similar to hydroxyapatite calcificates on heart valves and the bone apatite, in the dry blood rests of healthy donors. Modeling experiments were carried out under adjustable conditions (T = 37°C, pH = 7.4) with respect to the ionic composition of the main elements (Ca, P, Mg, and NaCl) in aqueous solution close to their contents in the blood plasma. The basic blood protein albumin was used as a biological component. Serum bovine albumin was used as the modeling protein. On the basis of experimental data it was concluded that the blood proteins promote the formation of hydroxyapatite microcrystalls. Albumin plays a special role in this process.

Study of Nucleation Processes

A COMPUTER ALGORITHM FOR NUCLEATION RATE SURFACE CONSTRUCTION

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In *"Nucleation and Atmospheric Aerosols 2004"*,
Eds. M. Kasahara, M. Kulmala,
Kyoto University Press, Japan, pp. 205-209.

A computer algorithm for nucleation rate surface design is developed. An obvious advantage of the computer semi-empirical design of nucleation rate surfaces is the ability to construct this surface over the full interval of nucleation parameters that are unavailable for any experiments. Examples of conditions that are difficult to achieve include very low temperatures, high-pressures and/or very high-temperature medium (such as stars) etc. It is assumed that the current algorithm can be further developed for the semi-empirical design of nucleation rate surfaces for one- and two-component systems.

EXPERIMENTAL PROOF OF THE TWO-CHANNEL NUCLEATION NEAR THE TRIPLE POINT

M.P. Anisimov, P.K. Hopke* (**Clarkson University, Potsdam, USA*)

J. Aerosol Sci., 1 (2004) pp. 107-108.

An important result is following from the idea of semiempirical construction of the nucleation rate surfaces over diagram of phase equilibria. One can see two nucleation rate surfaces for two different phase states of the critical embryos in the vicinity of triple point. Each nucleation rate surface related with one independent channel of nucleation. Measurements of the aerosol size distribution, which have been done in the present research, show the existence of two nucleation rate surfaces, i.e. one surface for each phase state of critical embryos. In the present research the first measurements have been done of the relative location of the nucleation rate surfaces on the example of crystal and droplet nucleation.

SOME GENERAL REQUIREMENTS FOR VAPOR NUCLEATION RATE EXPERIMENTS

M.P. Anisimov, P.K. Hopke* (**Clarkson University, Potsdam, USA*)

In *"Nucleation and Atmospheric Aerosols 2004"*,
Eds. M. Kasahara, M. Kulmala,
Kyoto University Press, Japan, pp. 173-177.

One of the reasons for the problems of nucleation theory development is the inconsistencies among experimental measurements as well as the assumptions used to interpret the experimental results. Some general requirements for nucleation experiments associated with any phase transformation of the first order are formulated. Measurement of the single-channel nucleation rate plays the key role in comparison of the experimental data on nucleation rate and one-channel nucleation theory. Interpretation of multy channel nucleation in the approximation of one channel nucleation produce the unsolvable problem of theory and experiment consistency.

GENERALIZATION OF THE OSTWALD'S RULE ON THE EXAMPLE OF THE MULTI-CHANNEL VAPOR NUCLEATION

M.P. Anisimov, V.S. Akimov* (**Fare Eastern University of Communication, Khabarovsk, Russia*)

In *"Nucleation and Atmospheric Aerosols 2004"*,
Eds. M. Kasahara, M. Kulmala,
Kyoto University Press, Japan, pp. 260-263.

The current generalization of the Ostwald rule for the formation of phases is proved on the basis of common results on nucleation. The present consideration uses the qualitative prove on the base of several plausible assumptions. The chemical reactions presented there should obey the main conclusions of the present consideration.

TOPOLOGIES OF THE NUCLEATION RATE SURFACES CONSTRUCTED OVER SOME DIAGRAMS OF PHASE EQUILIBRIA

M.P. Anisimov

In *“Nucleation and Atmospheric Aerosols 2004”*,
Eds. M. Kasahara, M. Kulmala,
Kyoto University Press, Japan, pp. 200-204.

Treatment of multiple nucleation rate surfaces in the one surface approximation can be mentioned as one of the reasons of the nucleation theory inconsistence and experimental results on nucleation. Unfortunately the most experimental data (possible from two or more nucleation rate surfaces) are interpreted in one-surface approximation of Classical Nucleation Theory. The experimental detection of nucleation rate from individual nucleation rate surface is available only in the resent time. The present research illustrates several examples of nucleation rate surface topologies which are designed over diagrams of phase equilibria. It can be shown the continuum of nucleation rare surfaces for binary system.

DESIRABLE CONDITIONS FOR VAPOR NUCLEATION RATE MEASUREMENTS

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J. Aerosol Sci., 1 (2004) pp. 209-210.

Agreement between experimentally measured vapor nucleation rates and current theoretical predictions exists for only a limited number of systems. One of the reasons for this problem is the inconsistencies among experimental measurements as well as the assumptions used to interpret the experimental results. Usually the causes of these disagreements cannot be identified. The current state-of-the-art is such that experimental results using different methods can lead to very different interpretations for the same phenomenon. Some of the problems in nucleation can be created by inconsistencies in the models used to interpret the experimental results.

Composite Sorbents and Catalysts

SELECTIVE WATER SORBENTS FOR SOLID SORPTION CHILLER: EXPERIMENTAL RESULTS AND MODELLING

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Int. J. Refrig., 27(3) (2004) pp. 284-293.

In this paper the experimental results of a lab-scale chilling module working with the composite sorbent SWS-1L (mesoporous silica gel impregnated with $CaCl_2$) are presented. The interesting sorption properties of this material yield a high $COP = 0.6$ that gives a promising alternative to the common zeolite or silica gel for application in solid sorption units driven by low temperature heat ($T \leq 100^{o}C$). The measured low specific power of the device is a result of not optimised geometry of the adsorber and of the pelletised shape of the adsorbent. Heat transfer optimisation is currently under progress to increase the specific power.

The experimental results are compared with those of a mathematic model able to describe the dynamic behaviour of the system. The model is used to study the influence of the main operating parameters on the system performance.

ENVIRONMENTALLY APPROPRIATE ADSORPTIVE COOLER BASED ON THE ECOLOGICALLY SOUND “WATER–SWS-1K ADSORBENT”: LABORATORY PROTOTYPE

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Chem. Sustain. Devel.,
12(2) (2004) pp. 211-216.

Test results on a laboratory prototype of the adsorptive cooler based on the ecologically sound “water–SWS-1K adsorbent” working pair are discussed. The adsorbent relates to the family of selective water sorbents; this is a mesoporous silica gel KSK modified with calcium chloride. The device produces cold water (at the temperature of 5–10°C) to be used for air conditioning, food storage etc. The testing demonstrates coefficient of performance (COP) of the device as high as 0.6 at a low temperature of water desorption (90–95°C); as a result, the adsorbent may be a real alternative to the traditional materials (silica gel, zeolites) which are used for ecologically friendly adsorption systems to utilize low potential heat (T 100°C).

SOME ECOLOGICAL AND ECONOMIC ASPECTS OF APPLICATION OF SORPTIVE HEAT PLANTS IN RUSSIA

Yu.I. Aristov

Chem. Sustain. Devel., 12(6) (2004) pp. 751-755.

Ecological and economic aspects of application of sorptive heat plants (refrigerators and heat pumps) in Russia, as well as competitiveness of these devices against the traditional systems are considered. The utilization of heat wastes (or solar energy) is shown to make the sorptive refrigerators more ecologically sound and economically profitable than the compressive ones. When regenerated through combustion of natural gas, the sorptive plants can only provide no ecological damage as an exceptional case; therefore, it seems reasonable to advance the compressive devices with high coefficients of performance (COP ≥ 4) to minimize wastes of greenhouse gases. The sorptive heat pumps with coefficients of augmentation $COA > 1$ are more ecologically sound and economically profitable than gas heaters. The natural gas consumption is decreased by 41 and 33% at $COA_{abs} = 1.7$ and 1.5, respectively. These results are of considerable practical interest.

SELECTIVE WATER SORBENTS FOR AIR DEHYDRATION: FROM TEST-TUBE TO INDUSTRIAL ADSORBER

Yu.I. Aristov

Catal. Ind., 6 (2004) pp. 36-41.

Properties of industrial desiccant IK-011-1 based on aluminum oxide modified by calcium chloride are described. The desiccant was developed in Boreskov Institute of Catalysis for removal of water out of process air and other gases. This material is characterized by high dynamic sorptive capacity, low dew point of desiccated gas and good hydrothermal stability. In a short time it will pass from laboratory studies of structure and properties to its pilot tests, organization of its production and supply to customers.

KINETICS OF CARBON DIOXIDE SORPTION BY THE COMPOSITE MATERIAL K_2CO_3 IN Al_2O_3

V.E. Sharonov, A.G. Okunev, Yu.I. Aristov

React. Kinet. Catal. Lett., 82(2) (2004) pp. 363-369.

The kinetics of the CO_2 sorption by a composite sorbent K_2CO_3 in Al_2O_3 was studied in a gradientless adsorber at 295 K. The order of the sorption rate with respect to the CO_2 concentration was found to be $n = 1.04 \pm 0.07$. The sorption rate constants were evaluated for sorbent grains of various sizes between 0.25 and 2.1 mm. It was shown that the rate constant is proportional to the grain reciprocal radius. The dynamic capacity was obtained as a function of the CO_2 concentration. The maximum sorption capacity was found to be 83 mg of CO_2 per 1 g of the sorbent.

Ecology Related Catalysts

DEVELOPMENT OF MONOLITHIC CATALYSTS WITH LOW NOBLE METAL CONTENT FOR DIESEL VEHICLE EMISSION CONTROL

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Top. Catal., 30(31) (2004) pp. 293-298.

Monolith washcoated catalysts with potential for diesel emission control have been developed. Two types of catalysts have been prepared for further study: (1) MnO_x supported on granulated γ-Al_2O_3, (2) MnO_x supported on cordierite monolith washcoated with γ-Al_2O_3. Both catalysts have been calcined at 500 and 900°C and subsequently modified by doping with 0.1–1.0 wt% of Pt or Pd. The influence of the concentration of both manganese oxide (0–10 wt%) and noble metals Pt and Pd in the range 0–1.0 wt% on the catalytic activity in methane oxidation has been studied. Comparison of the catalytic activity of MnO_x/Al_2O_3 and MnO_x + Pt(Pd)/Al_2O_3 with that of a standard 1 wt% Pt/Al_2O_3 catalyst shows the existence of a synergetic effect. This effect is more pronounced for the samples calcined at 900°C. The developed monolithic catalysts MnO_x + Pt(Pd)/Al_2O_3 demonstrate higher activity and thermal stability (up to 900°C) compared to the commercial monolithic catalyst (TWC's).

OXIDATION DESTRUCTION OF CHLORINATED ORGANICS ON FIBER GLASS CATALYSTS

B.S. Bal'zhinimaev, E.A. Paukshtis, L.G. Simonova, L.V. Malysheva, A.N. Zagoruiko, V.N. Parmon

Catal. Ind., 5 (2004) pp. 21-27.

Glass fiber based Pt-containing catalysts for oxidizing destruction of chlorinated organics including vent gases from vinyl chloride production were developed. The catalyst modification with Al (to increase acidity) as well as doping with Mn, Cu and Co, in particularly, provide the complete and highly selective oxidation of different chlorine hydrocarbons into HCl, CO_2 and H_2O under the reaction conditions mild enough without formation of highly hazardous by-products, for example, molecular chlorine, phosgene and chlorinated dioxins. An addition of propane and water substantially improves the destructive efficiency of polychlorided compounds. Long term testing (more than 100 h) at temperatures lower than 550°C showed high stability of glass fiber catalysts.

OXIDATIVE NEUTRALIZATION OF ALKALINE SULFIDE DRAINS

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B.S. Bal'zhinimaev, O.L. Elin*,
Ch.Ch. Rakhimov*, A.S. Noskov
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Catal. Ind., Special issue (2004) pp. 32-40.

The process of liquid-phase oxidation of sulfide-containing waste water by oxygen over porous Sibunit graphitic material used as a catalyst and an adsorbent has been investigated. The process of purification comprises two successive stages. Initially toxic sulfides are neutralized by catalytic oxidation into sulfates. Then organic substances, being in the water phase and capable to be isolated out of waste waters at increased temperatures, are successively adsorbed from the solution and oxidized in catalytic manner into carbon dioxide and water. The experiments were carried out in the full-mixed static installation with a high-pressure reactor and in the continuous flow installation. Conversion and selectivity of sulfides-to-sulfates oxidation were determined under different modes of operation. It is shown that sulfite-ions and thiosulfate-ions are formed upon sulfide-ions oxidation at temperature < 80°C and sulfates are formed in temperature range of T = 100¸ 130°C. It was found that Sibunit possesses the highest catalytic activity in sodium sulfide to sulfate oxidation, activity of metal sulfides and cobalt phthalocyanine supported on Sibunit being lower than the initial Sibunit. As for supported catalysts, selectivity of oxidation to sodium sulfate increases upon the decreasing of the content of active component, approaching the characteristics for pure Sibunit. Use of Sibunit as a catalyst in oxidation reactions as well as an adsorbent for extraction of organic substances from waste waters allows oxidation of sulfide-ions to sulfates at T = 110¸ 130°C and oxidation of sulfur-organic and organic components at T = 200¸ 240°C and solves a problem of neutralization of toxic substances containing in alkaline sulfide waste waters.

Catalysis for Petrochemical Industry

AROMATIZATION OF LIGHT NAPHTHA FRACTIONS ON ZEOLITES.
II. MODEL OF CATALYST DEACTIVATION

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G.V. Echevsky (**Omsk State University, Omsk, Russia*)

Hemijska Industrija, 58(3) (2004) pp. 104-108.

A model of catalyst deactivation in the "Zeoforming" process was developed. The deactivation rate constant and activation energies were estimated. The role of adsorbed oligomers in the reaction and deactivation kinetics were examined. The model is intended for further modeling and optimization of the process.

DIRECT INSERTION OF METHANE INTO C_3–C_4 PARAFFINS OVER ZEOLITE CATALYSTS: A START TO THE DEVELOPMENT OF NEW ONE-STEP CATALYTIC PROCESSES FOR THE GAS-TO-LIQUID TRANSFORMATION

G.V. Echevsky, E.G. Kodenev, O.V. Kikhtyanin, V.N. Parmon

Appl. Catal. A, 258(2) (2004) pp. 159-171.

The paper demonstrates that utilization of the well-known concept of the ability of the same catalytic centers to catalyze both forward and backward reactions can result in the development of a process of the direct one-step insertion of methane into heavier hydrocarbons. The insertion seems to proceed as a part of linear alkanes dehydrocyclization reactions at rather mild pressure and temperature conditions (at 773–823 K) over Zn- or Ga-promoted zeolite catalysts. The experimental study of the process evidences in its potential practical applicability for the natural gas-to-liquid conversion.

THIOPHENE CONVERSION IN THE BIMF PROCESS

D.G. Aksenov, O.V. Klimov, G.V. Echevsky, E.A. Paukshtis, A.A. Budneva

React. Kinet. Catal. Lett., 83(1) (2004) pp. 187-194.

Catalytic conversion of an oil distillate with the added extra amounts of thiophene over a zeolite catalyst was studied. The rate of the catalyst deactivation was found to increase with the increase in the thiophene concentration in the feed. A possible pathway of the thiophene conversion is discussed.

BIPHENYL OXIDATION WITH NITROUS OXIDE ON MFI ZEOLITES

D.P. Ivanov, L.V. Piryutko, V.I. Sobolev

Petroleum Chem., 44(5) (2004) pp. 322-327.

The gas–phase reaction of biphenyl oxidation with nitrous oxide on iron-containing zeolite MFI was studied. It was shown that the main products of this reaction were monosubstituted phenylphenols, which were represented predominantly by *para*- and *meta*-isomers. Optimal reaction conditions, ensuring a high selectivity for phenylphenols (~95%), were found. The initial catalyst productivity was ~1.5 mmol of PhPhOH/(g h). The activity decreased in the course of the reaction as a result of catalyst deactivation by coking.

HYDROGENATED Zr-Fe ALLOYS CAPSULATED IN Al_2O_3/Al MATRIX AS CATALYSTS FOR FISCHER-TROPSCH SYNTHESIS

S.F. Tikhov, V.I. Kurkin*, V.A. Sadykov, E.V. Slivinsky*, Yu.N. Dyatlova, A.E. Kuzmin*, E.I. Bogolepova*, S.V. Tsybulya, A.V. Kalinkin, V.B. Fenelonov, V.P. Mordovin* (**Topchiev Institute of Petrochemical Synthesis, Moscow, Russia*)

Stud. Surf. Sci. Catal., 147 (2004) pp. 337-342.

The genesis of the ZrFe intermetallides with different atomic ratios during preparation of $Zr_yFe_zH_y/Al_2O_3$/Al catalysts and their performance in Fischer-Tropsch synthesis have been studied. The effect of structural, surface and textural properties on their activity has been discussed.

HYDROGENATION OF DIALKYL DISULFIDES ON SUPPORTED SULFIDE CATALYSTS

A.V. Mashkina, L.N. Khairulina

Petroleum Chem., 44(1) (2004) pp. 52-57.

The reduction of dimethyl and diethyl disulfides by hydrogen under atmospheric pressure in the presence of sulfide catalysts with different compositions was studied. Methanethiol or ethanethiol, respectively, was the main reaction product on all catalysts at T = 200°C. The same behavior was observed for the hydrogenation of dimethyl and diethyl disulfides, but the rate of transformation of diethyl disulfide on most catalysts was higher than that of dimethyl disulfide. In the formation of alkanethiols, alumina-supported metal sulfides were more active than those supported on carbon or silica gel. Among the alumina-based catalysts, tungsten sulfide was least active and rhodium sulfide was most active. In the presence of the aluminorhodium sulfide catalyst, the reaction rate increased with temperature and with an increase in the initial concentrations of hydrogen and dimethyl disulfide in the reaction mixture to 15 vol % and 2 vol %, respectively.

Mathematical Simulation of Processes and Reactors. Chemical Engineering

MODELING OF THE OXIDATION OF ORGANIC COMPOUNDS IN SUPERCRITICAL WATER

A. Yermakova, V.I. Anikeev

Theor. Found. Chem. Engin.,
38(4) (2004) pp. 333-340.

A system for oxidation of organic impurities in supercritical water is proposed. Models are formulated and calculations are performed to determine the characteristics of the main apparatuses of the system, namely, heat exchangers, a chemical reactor, and a separator. The models take into account specific features of processes under supercritical conditions, specifically, the changes in the thermodynamic properties (enthalpy, specific heat, critical parameters) of the reaction mixtures with changes in pressure and temperature, and also the variations of the compositions of the mixtures along the lengths of the apparatuses. The thermodynamic properties are calculated by methods of nonequilibrium thermodynamics. A numerical analysis is performed of one of the variants of a system for acetic acid oxidation by oxygen in supercritical water, which can be a prototype of a pilot plant. The fuel is chosen to be an aqueous methanol solution, and the oxidant is taken to be hydrogen peroxide. Replacement of the reactant, the fuel, or the oxidant does not fundamentally change the methods for calculating the characteristics of the apparatuses and the entire system.

EFFECT OF PRESSURE ON THE RATE CONSTANT OF THE DECOMPOSITION OF ALIPHATIC NITROCOMPOUNDS IN SUPERCRITICAL WATER

V.I. Anikeev, A. Yermakova, A.V. Golovizin, M. Hoto* (**Kumamoto University, Kumamoto, Japan*)

Russ. J. Phys. Chem.,
78(10) (2004) pp. 1553-1559

It was found that the observed first-order rate constant for the decomposition of aliphatic nitrocompounds RNO_2 in supercritical water at constant temperature increases exponentially with the pressure. The volumes of activation for the reactions under study were determined. The experimental data were described within the framework of the transition-state theory. Conclusions on the nature of the activated complex have been drawn. The calculated values of the volume of activation for the decomposition of nitromethane, nitroethane, and 1-nitropropane in supercritical water are similar, a result indicative of the same nature of the activated complex in all three cases. The true rate constant for the decomposition of these nitrocompounds in supercritical water decreases virtually linearly in the series NM > NE > NP.

THE USE OF CUBIC EQUATIONS OF STATE FOR CALCULATING THE THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF MULTICOMPONENT NONIDEAL MIXTURES

A. Yermakova, A.V. Golovizin, V.I. Anikeev

Russ. J. Phys. Chem.,
78(11) (2004) pp. 1723-1728.

Calculations of the enthalpy and heat capacity of a multicomponent mixture in the critical region of its parameters with the use of cubic equations of state are considered. The possibility of describing the anomalous behavior of these mixture properties in the supercritical region is demonstrated. Examples that illustrate the behavior of the partial molar properties of components and averaged mixture properties such as heat capacity and enthalpy close to the critical point of the mixture are given. The influence of nonideality characteristic of mixtures in the near-critical state on the heat effects of chemical transformations and adiabatic mixture heating values was determined.

KINETICS AND THERMODYNAMICS OF 2-PROPANOL DEHYDRATION IN SUPERCRITICAL WATER

V.I. Anikeev, A. Yermakova, J. Manion*, R. Huie* (**National Institute of Standards and Technology, Gaithersburg, MD, USA*)

J. Supercrit. Fluids, 32(1-3) (2004) pp. 123-135.

Kinetics and thermodynamics of 2-propanol dehydration in supercritical water (SCW) and the effect of density on this reaction have been investigated in a batch reactor. The studies were performed at water densities between 0.24 and 0.58 g/cm^3 and temperatures between 654 and 686 K.

The main reaction products of 2-propanol dehydration were propene and water. Rate of the reaction was found to depend essentially on the water density.

Two models are used to predict the effect of SCW density on the rate constant of 2-propanol dehydration reaction: a thermodynamic model (the model of activated complex) and a model of acid-catalyzed reaction. Redlich–Kwong–Soave equation of state was used for calculation of the partial molar volumes of the reaction participants in SCW including a transition state and activation volume of the reaction. Application of the activated complex model demonstrated that the calculated values of the activation volume depend strongly on pressure at fixed temperature, which contradicts the experimental data where the activation volume is independent of pressure. At the same time, the mechanism of 2-propanol dehydration reaction in SCW was shown to correlate well with the acid-catalyzed mechanism in solutions. Rate of the reaction is directly proportional to the concentration of 2-propanol and H_3O^+ ions. An increase in the H_3O^+ concentration in SCW with density correlates unequivocally with an increase in the reaction rate.

KINETIC MODEL OF THE REACTION OF METHANOL WITH HYDROGEN SULFIDE

A. Yermakova, A.V. Mashkina

Kinet. Catal., 45(4) (2004) pp. 522-529.

The kinetics of the reaction of methanol with hydrogen sulfide in the presence of an IKT-31 catalyst was experimentally studied. The experiments were performed in a fixed-bed flow reactor under the following conditions: $T = 598–653$ K, $P = 0.1–1.0$ MPa, and $P^0_{H_2S}/P^0_{Me} = 0.4–15.0$. Rate equations were derived which describe the rates of formation of methanethiol as the main product and dimethyl sulfide and dimethyl ether as by-products. The rate constants and activation energies were found by the mathematical Treatment of experimental data. The model proposed can be used for reactor design.

KINETICS OF INTERACTION OF TOLUENE WITH A PRE-OXIDIZED VANADIA/TITANIA CATALYST

E.A. Ivanov, S.I. Reshetnikov, D.A. Bulushev*
(**Swiss Federal Institute of Technology, Lausanne, Switzerland*)

React. Kinet. Catal. Lett., 82(1) (2004) pp. 199-206.

A kinetic model for the interaction of toluene with a pre-oxidized vanadia/titania catalyst has been developed. The model is based on two types of oxygen sites and includes 5 steps. It describes satisfactorily the transient behavior of toluene and products (benzaldehyde, CO_2) in the temperature range of 523-633 K.

STUDY OF BENZENE SORPTION IN H-ZSM-5 ZEOLITE UNDER CATALYTIC CONDITIONS

S.I. Reshetnikov, S.B. Ilyin, A.A. Ivanov, A.S. Kharitonov

React. Kinet. Catal. Lett.,
83(1) (2004) pp. 157-164.

The equilibrium of the sorption of benzene in an H-ZSM-5 zeolite has been investigated in the temperature range of 100-400°C and at partial pressures 0.11÷0.57 atm. The data on the sorption under these conditions could be fitted with the Langmuir isotherms taking into account a linear decrease in heats of sorption with the increase in the sorbate loading. The equilibrium constants and heat of the sorption have been determined.

NEW LARGE-CAPACITY PROCESS OF PRODUCING NITROUS OXIDE

A.S. Noskov, I.A. Zolotarskii, S.A. Pokrovskaya, E.M. Slavinskaya, V.V. Mokrinsky, V.N. Kashkin, V.N. Korotkikh, I.A. Polukhina

Catal. Ind., 1 (2004) pp. 5-11.

The article is devoted to development of large-capacity process to produce nitrous oxide by selective oxidation of ammonia with oxygen over oxide catalysts MnO_2-Bi_2O_3/α-Al_2O_3 developed in the Boreskov Institute of Catalysis. The kinetic studies carried out at $T = 270÷400$°C and $P = 0,1÷ 0,6$ MPa have shown that oxidation of ammonia over the mentioned catalysts proceeds in two main parallel routes with formation of N_2O and N_2. Selectivity to nitrous oxide was 88–90 % in the temperature range of $T = 340÷360$°C and selectivity to NO does not exceed 1 % within the whole range of the experimental conditions. The kinetic data obtained were used for mathematical modeling of the process to produce nitrous oxide in fluidized-bed reactors and in tubular reactors. It was shown that in spite of significant thermal effects, the reaction mixture with the ratio ammonia : oxygen = 1 : 1 may be used in fluidized bed reactor. Design nitrous oxide selectivity was 85,6 % at ammonia conversion of 98 %. The mathematical modeling of the process in a tubular reactor showed the maximum permissible ammonia concentration at the inlet of the reactor upon stable thermal operation modes are realized to increased from 4,5 to 8 vol. % when passing from spherical catalyst to grains in the form of Rashig rings. Pilot tests of the process were carried out in reactors of fixed bed and fluidized bed and their total time period was ~ 700 h. As a result, the catalyst was shown to maintain activity and selectivity both in the fluidized-bed and in a tubular reactors during all the test time. In both reactor types, selectivity to nitrous oxide was 86-88 % with ammonia conversion of 95–98 %. Based on the mathematical modeling and the pilot tests, a process flowsheet was developed. It provides production of nitrous oxide of ~ 3 ruble/kg in first cost with content of the purpose product no less than 86 % (the rest is nitrogen)

THERMAL PROCESSES STUDY IN CATALYTIC SOOT FILTERS FOR DIESEL EXHAUST TREATMENT

T.L. Pavlova, N.V. Vernikovskaya.
N.A. Chumakova, A.S. Noskov

J. "Combustion, Explosion and Shock Waves",
40(3) (2004) pp. 14-21.

For a catalytic diesel particulate filter with quartz foam structure, mathematical modeling of both the soot particles filtration and the catalytic oxidation regeneration are presented. Two different operation modes are under consideration, first of them is successive filtration and regeneration, while the second one is combining filtration at a higher temperature and simultaneous catalytic combustion of the soot particles. The influence of process parameters on the system dynamics was studied. It was shown that in the case of rather small particles it is efficient to follow the first operation mode, while for the diesel exhaust treatment with bigger soot particles one should prefer the second strategy.

UTILIZATION OF REACTION HEAT IN PROCESS OF METHANE OXIDATION FROM VENT GASES OF COAL MINES: PILOT TESTS

N.A. Chumakova, O.P. Klenov, D.A. Stepanov,
V.N. Korotkikh, P.G. Tsyrulnikov, A.S. Noskov

Catal. Ind., Special issue (2004) pp. 45-53.

Some results of pilot tests of a catalytic reactor for oxidation of lean methane-air mixtures that simulate the vent gases from coal mines are presented. The main goal of the study is the experimental verification whether the catalytic reverse-process is efficient for utilization of such gases and simultaneous high-temperature heat production. The experiments have shown the efficiency of unsteady state process in a fixed-bed reactor with 0,5 wt % Pd/γ-Al_2O_3 catalyst and inert packing at the reactor ends. In this case, a periodical reverse of the gas flow in the reactor takes place and a part of the gas flow can be withdrawn from the central part of the high-temperature zone of the layer into an outer heat exchanger. Autothermal operation of the apparatus with methane concentration of no less than 0,4 vol. % and a possibility of utilization of more than 80 % of reaction heat at methane concentration of 0,61 vol. % was shown.

THE KINETIC MODEL OF FORMATION OF NANOFIBROUS CARBON FROM CH_4–H_2 MIXTURE OVER A HIGH-LOADED NICKEL CATALYST WITH CONSIDERATION FOR THE CATALYST DEACTIVATION

S.G. Zavarukhin, G.G. Kuvshinov

Appl. Catal. A, 272(1-2) (2004) pp. 219-227.

A mathematical model is suggested for the process of formation of nanofibrous carbon from the mixture of methane and hydrogen over a high-loaded nickel catalyst (90 wt.% Ni-Al_2O_3) to describe the observed process kinetics involving the catalyst deactivation. The experimental kinetic data obtained at hydrogen volume fraction of 0 to 40%, 490-590°C and atmospheric pressure are analyzed to suggest the formula for calculation of the maximal rate of the carbon formation and the equation of the catalyst deactivation. The suggested kinetic model relates to the mechanism when the cleavage of the first hydrogen atom from a methane molecule adsorbed on the catalyst surface is the rate limiting stage. The model is appropriate for the qualitative and quantitative description of the process under consideration. The calculations in terms of the model are exemplified with synthesis of nanofibrous carbon in an isothermal perfect-mixing reactor at a constant methane consumption. The calculated results agree well with the experimental data.

ALGORITHM BIDIMS FOR AUTOMATED SYSTEMATIZATION OF DATA ARRAY. CASE STUDY: REDISCOVERING MENDELEEV'S PERIODIC TABLE OF CHEMICAL ELEMENTS

A.N. Zagoruiko, N.G. Zagoruiko* (**Institute of Mathematics, Novosibirsk, Russia*)

Int. J. "Inform. Theor. & Applic.", 11(4) (2004) pp. 309-318.

The method (algorithm BIDIMS) of multivariate objects display to bidimensional structure in which the sum of differences of objects properties and their nearest neighbors is minimal is being described. The basic regularities on the set of objects at this ordering become evident. Besides, such structures (tables) have high inductive opportunities: many latent properties of objects may be predicted on their coordinates in this table. Opportunities of a method are illustrated on an example of bidimentional ordering of chemical elements. The table received in result practically coincides with the periodic Mendeleev table.

THREE-DIMENSIONAL NUMERICAL SIMULATION OF A NONSTATIONARY GRAVITATING *N*-BODY SYSTEM WITH GAS

V.N. Snytnikov, V.A. Vshivkov*,*, E.A. Kuksheva, E.V. Neupokoev**,***, S.A. Nikitin****, A.V. Snytnikov**,***** (**Institute of Computational Technologies, Novosibirsk, Russia; **Novosibirsk State Technical University, Novosibirsk, Russia; ***Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russia; ****Institute of Nuclear Physics, Novosibirsk, Russia*)

Astronomy Lett., 30(2) (2004) pp. 134-146.

A three-dimensional numerical model to investigate nonstationary processes in gravitating *N*-body systems with gas has been developed. Efficient algorithms were used for solving the Vlasov and Poisson equations that included the evolutionary processes under consideration, which ensures rapid convergence at high accuracy. Examples of the numerical solution of the problem on the growth of physical instability in the model of a flat rotating disk with a gaseous component and its three-dimensional dynamics under various initial conditions including a nonzero velocity dispersion along the rotation axis are given.

ION-ACOUSTIC TYPE INSTABILITY IN PROTOPLANETARY DISK

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In *"Plasma in the Laboratory and in the Universe"*, AIP Conference Proceedings Series: N.Y., Vol. 703, 2004, pp. 280-283.

The computer simulations showed that gravitational instability development in the two-phase medium of gas-dust circumstellar disk is the mechanism of protoplanets formation. At the non-linear stage of instability development, the soliton density waves of high gas density form.

MAGNETIC FIELDS IN PROTOPLANETARY AND GALACTIC DISKS

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In *"Plasma in the Laboratory and in the Universe"*, AIP Conference Proceedings Series: N.Y., Vol. 703, 2004, pp. 284-287.

Time dependent 3D distributions of magnetic field generated by electrical currents in galactic/circumstellar discs of various spatial structures (the rings, spirals and matter clusters and others) have been obtained via 3D self-consistent numerical modeling using nonstationary Vlasov-Liouville's equation for particles and the Poisson's equation for self-consistent potential.

FLUIDIZED-BED REACTOR FOR DIRECT HYDROGEN SULFIDE OXIDATION TO ELEMENTAL SULFUR: EXPERIENCE OF CREATION OF EXPERIMENTAL INDUSTRIAL INSTALLATION AT BAVLINSKOE OILFIELD (TATARSTAN REPUBLIC)

Z.R. Ismagilov, S.R. Khairulin, M.A. Kerzhentsev, A.N. Golovanov*, A.A. Golovanov*, A.M. Mazgarov, A.F. Vil'danov**, Sh.F. Takhautdinov***, F.A. Zakiev***** (**JSC "TATNIINEFTEMASH", Kazan, Tatarstan; **State Unitary Enterprise "VNIIUS", Kazan, Tatarstan; ***JSC "TATNEFT" Almetievsk, Tatarstan*)

Catal. Ind., Special issue (2004) pp. 50-54.

The description of an experimental-industrial installation for catalytic process of direct hydrogen sulfide oxidation to elemental sulfur in fluidized bed reactor for purifying of casing-head oil-gases at Bavlinskoe Oilfield (Tatarstan Republic) is given. The structure of the fluidized-bed reactor and plant processing characteristics are given.

NEW APPROACHES TO THE FISCHER-TROPSCH SYNTHESIS PROCESS. ADVANTAGES OF MEMBRANE REACTORS

A.A. Khassin

Russ. Chem. J., 47(6) (2003) pp. 36-47.

The analysis of the specific features of the Fischer-Tropsch synthesis helps formulating the most important requirements to the FTS reactor. Membrane reactor designs can be useful for the FTS process application. Semi-permeable hydrogen-selective distributors allow to control the H_2:CO ratio along the catalyst bed and thus enhance the selectivity of the process. Membranes of extractor type can help to improve the FTS performance by selective removing water from the reaction volume. On the other hand, plug-through contactor membrane reactor design (PCM) seems to meet all the other requirements, ensuring the high concentration of the catalyst, isothermicity, high gas-liquid interface area, small effective diffusion length and reasonable hydraulic resistance. Varying the membrane composition and conditions of its preparation leads to the changes in porous structure parameters of the PCM membrane. This allows to weaken the diffusion constrains in a predictable way and, therefore, to control the productivity and selectivity of the Fischer-Tropsch process.

NEW DATA ON THE MECHANISM OF THE METHANE STEAM REFORMING OVER NICKEL AND RUTHENIUM CATALYSTS

I.I. Bobrova, N.N. Bobrov, V.V. Chesnokov, V.N. Parmon

Chemical Engineering Transaction,
Ed. S. Pierucci, Italy, Vol. 4, 2004 – H2www
Proceedings.

The kinetics of the steam reforming and pyrolysis of methane on Ni-Al_2O_3 and Ru/Al_2O_3 (T = 650-750°C, P_{CH_4} = 0.001-0.030 MPa) via an improved flow-recycling method has been studied. The values of the rates and activation energies are compared. It is shown that the steam reforming may proceed by either a heterogeneous or heterogeneous-homogeneous mechanism depending on the process conditions. The comparative activities of nickel and ruthenium catalysts at the occurrence of the process in both heterogeneous and heterogeneous-homogeneous modes are discussed.

EXPERIMENTAL STUDY OF HEAT REGIMES ON A DRY, PARTIALLY OR COMPLETELY WETTED AND LIQUID FILLED CATALYST PARTICLE

V.A. Kirillov, A.V. Kulikov, N.A. Kuzin, A.B. Shigarov

Chem. Eng. J., 98(3) (2004) pp. 219-235.

Steady-state and dynamic-heat regimes on the dry, partially wetted, and completely filled catalyst particles were studied using the model reactions of benzene, α-methylstyrene and octene hydrogenation over the several catalysts with different porous structures, apparent catalytic activities, and heat conductivities. A rise in the particle temperature at the external limitation regime was studied and the effective diffusion coefficients of limiting species were determined.

The regime of particle preheating, gas temperature, hydrogen saturation of AMS or octene vapors, and the liquid mass flow rate on the top of a catalyst particle were varied. The phase equilibrium between the vapor saturated hydrogen and the partially wetted catalyst particle is found to essentially affect for dynamic runaway of the particle. According to the measured center and surface temperatures of each particle, there are two significantly different steady states in the range of liquid flow rates. A catalyst wetted by liquid and blown off with dry hydrogen provides a temperature hysteresis phenomenon. This phenomenon is characterized by the regime when the catalyst particle is almost liquid filled and its temperature is lower than that of gas. Another high-temperature regime occurs if a catalyst particle is almost dry and its temperature is higher than that of gas. Ignition and extinction dynamics of the catalyst particle were studied under conditions of the combined evaporation and hydrogenation processes.

OPTIMIZATION OF THE ACTIVE COMPONENT DISTRIBUTION THROUGH THE CATALYST BED

V.M. Khanaev, E.S. Borisova, A.S. Noskov

Chem. Eng. Sci., 59(6) (2004) pp. 1213-1220.

A variational problem was formulated to determine the optimal axially non-uniform catalyst activity distribution along the fixed catalyst bed. It was observed that the mass transport limitations or non-isothermal temperature profile are necessary conditions for potential optimization of the catalyst distribution along the bed length. Under isothermal conditions with linear dependence of the reaction rate on concentration at a constant mass transfer coefficient, the uniform distribution is optimal. Analytical solution for the first-order reaction and numerical solutions for power-law kinetics were found.

IMPROVEMENT OF THE CATALYTIC MONOLITHS EFFICIENCY FOR CO OXIDATION USING NON-UNIFORM ACTIVE COMPONENT DISTRIBUTION ALONG THE MONOLITH LENGTH

V.M. Khanaev, E.S. Borisova, L.I. Galkina, A.S. Noskov

Chem. Eng. J., 102(1) (2004) pp. 35-44.

It is shown that the efficiency of catalytic packages can be improved using two approaches. The monotone increase of the active component concentration towards the monolith outlet is shown optimal for minimization of the total active component loading at the preserved purification degree. To resolve the problem of achieving the maximal purification degree at a fixed quantity of the active component, it is preferable to concentrate the active component near the duct entrance.

COMPACT RADIAL REACTOR WITH A STRUCTURED METAL POROUS CATALYST FOR CONVERSION OF NATURAL GAS TO SYNTHESIS GAS: EXPERIMENT AND MODELING

V.A. Kirillov, A.S. Bobrin, N.A. Kuzin, V.A. Kuzmin, A.B. Shigarov, V.B. Skomorokhov, E.I. Smirnov, V.A. Sobyanin

Ind. Eng. Chem. Res.,
43(16) (2004) pp. 4721-4731.

To perform the catalytic conversion of natural gas to synthesis gas, a compact radial reactor supplied with a structured porous metal catalyst has been designed. The reactor was tested at normal pressure using natural gas and air. The reactor can operate without preheating of the inlet gas mixture. A novel structured porous metal catalyst was developed on the basis of the 7% Ni/α-Al_2O_3 commercial catalyst and Ni-Cr powders. The catalyst is characterized by a low hydraulic pressure drop and a high tortuosity coefficient of the regular structure. The coefficient of heat conductivity of the structured catalyst and the coefficient of mass transfer between a gas flow and the catalyst were determined in special experiments. The catalyst temperature and outlet gas concentrations were experimentally investigated with respect to the gas-air flow rate and methane concentration in the mixture. The catalyst temperature drop along the reactor radius was no higher than 230°C. The maximum catalyst temperature does not exceed 1090°C for all runs. At volumetric flow rates of the gas mixture of 4000-40000 h^{-1} and O_2/CH_4 ratios of 0.6-0.9, methane is completely converted, and the maximum space time yield (STY) of the reactor is about 1 L of CH_4 per second per liter of reactor. A mathematical model for this process was developed. The results of modeling agree well with the experimental data. One possible application of the developed syngas generator in internal combustion engines is discussed.

CHEMICAL MICROREACTORS IN CATALYSIS

N.P. Belyaeva

Catal. Ind., 2 (2004) pp. 21-27.

The article is devoted to a new trend in the sphere of chemical synthesis: synthesis in the reactors of submillimetric dimensions named as "microreactors". They are characterized by an extremely great surface/volume ratio and exclusively high mass and heat transfer rates. Because of these properties, catalytic processes with participation of toxic and explosive substances may safely proceed in such microreactors. Highly-exothermal and highly-endothermic processes regulation is possible. The microreactors expand possibilities of kinetic studies and combinatorial catalysis. Examples of their application in catalysis are given.

CENTRIFUGAL FLASH-REACTOR FOR THERMO-SHOCK TREATMENT OF POWDER MATERIALS AT THE STAGES OF SYNTHESIS OF SUPPORTS AND CATALYSTS

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Catal. Ind., Special Issue (2004) pp. 60-67.

A concept of centrifugal thermo-shock treatment (activation) of powder materials over solid heat-carrier has been developed and the proper instrumentation of the process has been proposed. The centrifugal flash-reactor provides: heating of powders of 10-150 mm in size up to *T* = 100÷700 ° C with the rate >1000 degree/s; time of thermal treatment not more than 1,5 s; control of thermal treatment by changing the rotary speed and heat-carrier configuration, controllable flow of initial material in the range of 5-40 kg/h; removal of gaseous products, and quenching of solid products. Reactor is used for heat treatment of hydrargillite. According to data of physical-chemical analysis the product is characterized by high reactivity and can be used for preparation of alumina catalysts, supports, and other functional materials on the basis of γ-and η-Al_2O_3

SCIENTIFIC PUBLICATIONS

JOURNAL PUBLICATIONS AND MONOGRAPHS

1. **D.G. Aksenov, O.V. Klimov, G.V. Echevsky, E.A. Paukshtis, A.A. Budneva,**
   Thiophene Conversion in the BIMF Process,
   React. Kinet. Catal. Lett.,
   83(1) (2004) pp. 187-194.
2. **(E.Ya. Aladko, Y.A. Dyadin), V.B. Fenelonov, (E.G. Larionov), M.S. Melgunov, (A.Yu. Manakov, A.N. Nesterov, F.V. Zhurko),**
   Dissociation Conditions of Methane Hydrate in Mesoporous Silica Gels in Wide Ranges of Pressure and Water Content,
   J. Phys. Chem. B.,
   108(42) (2004) pp. 16540-16547.
3. **(J.E. Ancel), N.V. Maksimchuk, I.L. Simakova, V.A. Semikolenov,**
   Kinetic Peculiarities of α-Pinene Oxidation by Molecular Oxygen,
   Appl. Catal. A,
   272(1-2) (2004) pp. 109-114.
4. **V.I. Anikeev, A. Yermakova, A.V. Golovizin, (M. Hoto),**
   Effect of Pressure on the Rate Constant of the Decomposition of Aliphatic Nitrocompounds in Supercritical Water,
   Russ. J. Phys. Chem.,
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260. **V.A. Sadykov, V.A. Sobyanin**,
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263. **A.N. Salanov, A.I. Titkov, V.N. Bibin,**
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266. **E.R. Savinova,**
Electrocatalysis at Supported Metal Nanoparticles: Nanoparticles versus Extended Surfaces,
University of Leeds, September 2004, Invited lecture.

267. **E.R. Savinova,**
FTIR and Electrochemical Study of CO and Methanol Oxidation on Model Pt Nanoparticle Electrodes,
Max-Planck-Institut fuer Kohlenforschung (Coal Research), April, Muelheim, Germany. Invited lecture.

268. **E.R. Savinova, P.A. Simonov, (V. Rao), D.I. Kochubey, (U. Stimming),**
Novel PtRu/Sibunit Anode Catalysts for DMFCs: An Electrochemical, and *in situ* XAS Study,
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271. **N.V. Semikolenova, I.G. Danilova, E.A. Paukshtis, V.A. Zakharov,**
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273. **(V.I. Sharypov, B.N. Kuznetsov, N.G. Beregovtseva, S.V. Baryshnikov), A.N. Startsev,**
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274. **D.A. Shlyapin, D.I. Kochubey, P.G. Tsyrulnikov, N.M. Dobrynkin, A.A. Vedyagin,**
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275. **V.P. Shmachkova, N.S. Kotsarenko, G.N. Kryukova, V.V. Kanazhevskii, D.I. Kochubey, (J. Vedrine),**
Supported Sulfated Zirconia with Regulated Size Nanoparticles as Catalyst of Alkane Skeletal Isomerization,
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276. **V.P. Shmachkova, N.S. Kotsarenko, L.S. Dovlitova, V.V. Malakhov, D.I. Kochubey,**
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278. **V.N. Sidelnikov, Yu.V. Patrushev,**
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279. **V.I. Simagina, I.V. Stoyanova, A.G. Gentsler, S.V. Tsybulya, O.V. Netskina,**
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280. **I.L. Simakova,**
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281. **I.L. Simakova, V.A. Semikolenov,**
3-Carene Isomerization in the Presence of Na/C Catalyst,
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288. **M.Yu. Smirnov, A.V. Kalinkin, A.V. Pashis, A.M. Sorokin, I.P. Prosvirin, A.S. Noskov, V.I. Bukhtiyarov,**
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290. **V.A. Sobyanin**,
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291. **V.A. Sobyanin, (S.V. Korenev),**
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292. **A.M. Sorokin, (A.I. Timoshin), V.V. Kaichev, (A.A. Rastorguev, A.M. Badalyan),**
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293. **A.I. Stadnichenko,**
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298. **E.V. Starokon', K.A. Dubkov, D.E. Babushkin, G.I. Panov,**
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300. **A.G. Stepanov, M.V. Luzgin, S.S. Arzumanov, (D. Freude, M. Hunger),**
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306. **V.M. Tapilin,**
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307. **(K.A. Tarasov, E.V. Starikova, V.P. Isupov, V.V. Boldyrev), M.M. Yulikov, (A.E. Ermakov),**
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309. **S.F. Tikhov, (V.E. Romanenko), V.A. Sadykov, V.N. Parmon, (A.I. Rat'ko),**
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316. **(A.K. Tsvetnikov, V.G. Kuryavyi, Yu.M. Nikolenko), V.M. Buznik,**
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317. **S.V. Tsybulya, G.N. Kryukova, S.V. Cherepanova, A.S. Ivanova,**
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320. **G.G. Volkova, L.M. Plyasova, L.N. Shkuratova, A.A. Budneva, E.A. Paukshtis, M.N. Timofeeva, A.N. Salanov, V.A. Likholobov,**
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