



BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

ANNUAL
REVIEW
2001

ANNUAL REVIEW

of Activities in Fundamental Areas

2001



BORESKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

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

Phone: (007) 383 2 34 32 69
FAX: (007) 383 2 34 30 56
E-mail: bic@catalysis.nsk.su
http: [//www.catalysis.nsk.su](http://www.catalysis.nsk.su)

© Boreskov Institute of Catalysis, 2002



Dear Colleagues,

This book is already the eighth issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities which covers the year 2001.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and CIS, but also in many western and oriental countries. Since the sixties it remains the largest chemical research institution in the Asian part of Russia and has many deep and stable traditions in providing research in nearly all fields of catalysis. The interests of BIC spread from the sophisticated areas of purely academic research to the real applied problems, including commercial catalysts and catalytic technologies.

The current features of BIC are the result of dramatic changes in Russia during the last decade and its stepwise approach to the market economy. In spite of general economic instability in the country, the Institute appears to be able to survive as a high quality specialized organization. Moreover, the intensity and quality of the research and engineering activity at the Institute became at that period even higher. 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. Hope, the readers will feel that themselves, when comparing the materials of this and previous issues of the Annual Review.

The year 2001 was very important for the life of BIC in many aspects. First of all, the Institute has managed to sustain successfully in the extremely high financial instability of Russia in the mid of 1998. This appeared possible only due to a very high professional value of the Institute among the industries both in Russia and abroad that helped financial self-maintenance of the Institute. Thus, since 1996 nearly one quarter of the Institute's budget originates as royalties or license fees from the industries, mainly the western ones. The total income from the Russian and foreign industries into the overall budget of the Institute has approached the value of 75 % in 1999. Also, since the mid 1990's there was established a really strategic partnership with some Russian and world leading industrial companies. The situation remained nearly the same for year 2001, an extremely important feature being a rapid growing of the collaboration with the Russian industries.

Since 1998 the Institute has been operating 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. From that year the Institute succeeded also in reestablishing the National Russian R&D program in new generation of catalysts and catalytic technologies sponsored by the Ministry of Industry, Science and Technologies of the Russian Federation.

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). The general director of the UIC is the director of the Boreskov Institute of Catalysis. Now the United Institute of Catalysis includes the Boreskov Institute of Catalysis with its Omsk and St. Petersburg Divisions, the Research and Engineering Institute for Technical Carbon in Omsk as well as Scientific-Engineering Center “Zeosit” in Novosibirsk and Volgograd Scientific-Engineering Center on the Volga River. The facilities of the UIC include now three powerful semi-industrial plants capable of providing manufacturing of the first industrial batches of various catalysts and specialty chemicals. Thus, UIC has appeared to be now one of the most powerful Russian specialized R&D organizations of the industry-oriented chemistry. Indeed, current management of the Institute is recognizing well all the existing problems and trying to take care in the maintenance of high activity and productivity of R&D of both BIC and UIC in both fundamental and applied areas as the goals 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’s capacity 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 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 Borekov 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. Borekov (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. Borekov.

In 1976 Professor Kirill I. Zamaraev has been invited by Academician G.K. Borekov 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 Borekov Institute of Catalysis. Now the United Institute of Catalysis (UOC) includes the Borekov Institute of Catalysis with its Omsk and St. Petersburg Divisions, the Research and Engineering Institute for Technical Carbon in Omsk as well as Scientific-Engineering Center “Zeosit” in Novosibirsk and Volgograd Scientific-Engineering Center on the Volga River.

STRUCTURE OF THE INSTITUTE

The Institute of Catalysis with its Omsk and St. Petersburg Divisions currently has 1000 employees, of these 2 Corresponding Members of the RAS, about 60 Professors, more than 200 have a Ph.D. degree, and 40 Ph.D. students. The Institute presents the unique society of 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 7 scientific-research departments, Department of Applied Catalysis Problems, 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.

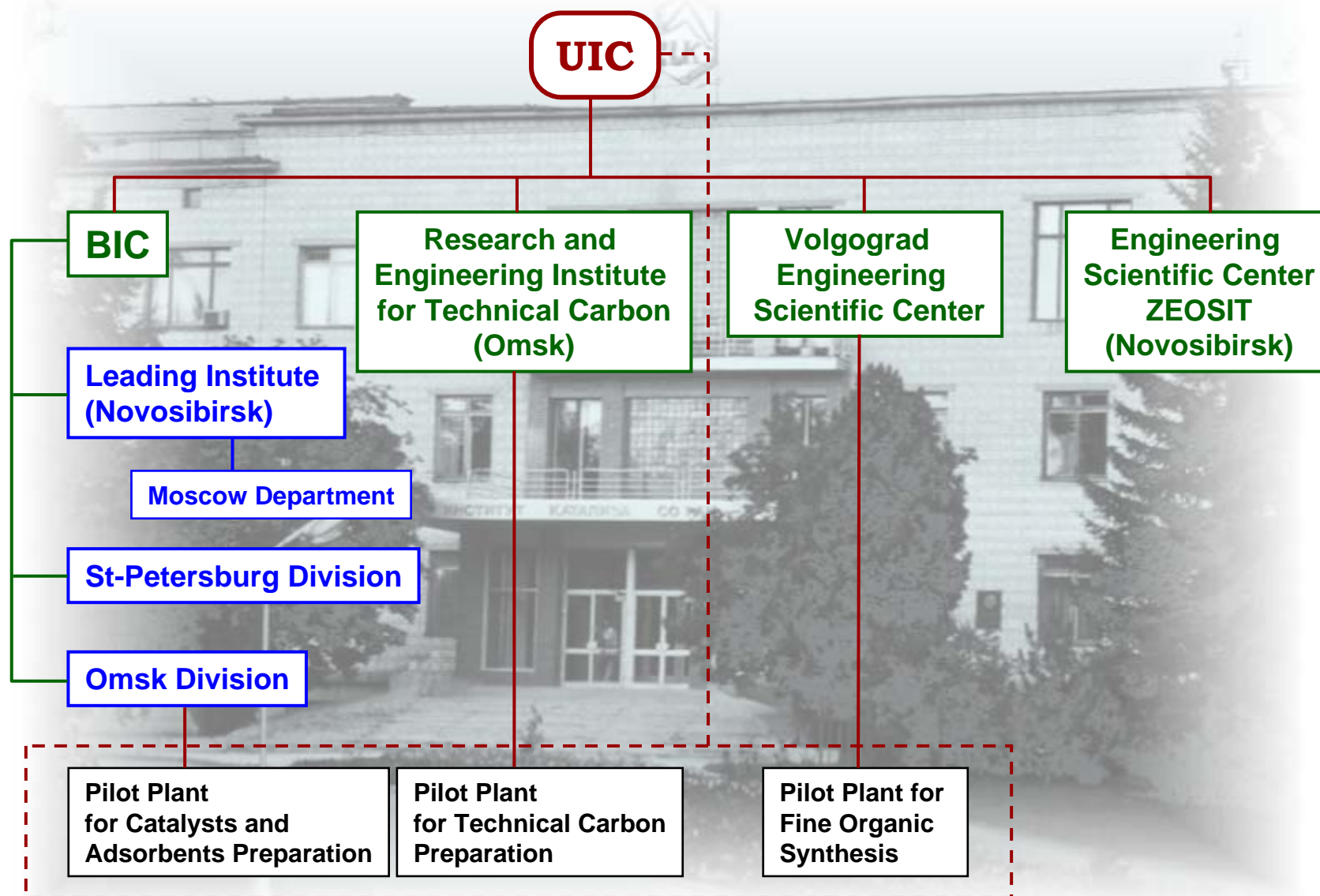
The Information Center of the Institute comprises the Library of Scientific Literature and the Group of mathematical and program support.

The Information Center was established to support WWW-server of the Institute <http://www.catalysis.nsk.su> and the United server SB RAS on Chemical Sciences <http://www.catalysis.nsk.su/chem>.

Data bank include 8 Databases on Russian and foreign catalysts, catalyst supports, catalytic processes, etc.

Department of Applied Catalysis Problems 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)





STRUCTURE OF THE INSTITUTE

Directorate:

S.E. Glaznev, S.P. Kildyashev, A.S. Noskov,
V.A. Sobyenin, I.A. Kamolkin, O.N. Martyanov,
V.A. Likholobov, R.A. Buyanov, V.N. Parmon,
B.S. Bal'zhinimaev

DIRECTOR

Directorate

Scientific Council

Research Departments



DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
8 laboratories and 5 groups Head: Prof. D.I. Kochubey



DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES AND TECHNOLOGIES
3 laboratories and 6 groups Head: Acad. V.N. Parmon



DEPARTMENT OF HETEROGENEOUS CATALYSIS
8 laboratories and 7 groups Head: Prof. V.A. Sobyenin



DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS
3 laboratories and 3 groups Head: Prof. V.A. Likholobov



DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS
2 laboratories and 4 groups, Center for Catalyst Characterization and Testing Head: Prof. Bair S. Bal'zhinimaev



DEPARTMENT OF CATALYTIC PROCESS ENGINEERING
8 laboratories and 1 group Head: Prof. A.S. Noskov



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



DEPARTMENT OF APPLIED CATALYSIS PROBLEMS
Head: I.A. Zolotarskii



THE INFORMATION CENTER OF THE INSTITUTE
Head: Dr. V.L. Kuznetsov



Scientific-Supportive Units



Manufacturing Facilities



Administration and Services

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

HEAD OF THE DEPARTMENT PROF. DIMITRII I. KOCHUBEY



**Laboratory of Structural Methods
Head: Dr. Sergey V. Tsybulya**



**Laboratory of Adsorption
Head: Prof. Valerii F. Yudanov**



**Laboratory of Analytical Chemistry
Head: Prof. Vladislav V. Malakhov**



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



**Laboratory of Quantum Chemistry
Head: Prof. Georgii M. Zhidomirov**



**Surface Science Laboratory
Head: Prof. Valerii I. Bukhtiyarov**



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



**Group of the Mechanisms of Radical-Catalytic Reactions
Head: Dr. Vladimir A. Rogov**



**Group of Scanning Spectroscopy
Head: Dr. Aleksey N. Salanov**



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



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



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



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

DEPARTMENT OF NONTRADITIONAL CATALYTIC TECHNOLOGIES

HEAD OF THE DEPARTMENT ACAD. VALENTIN N. PARMON



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



Laboratory of Energy Transforming Materials
Head: Dr. Yurii I. Aristov



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



Group of Photocatalysis on Semiconductors
Head: Prof. Eugenii N. Savinov



Laboratory of Catalytic Processes for Desulfurization
Head: Prof. Nikolai N. Kundo



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



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



Group of Biocatalysis
Head: Dr. Galina A. Kovalenko



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

DEPARTMENT OF HETEROGENEOUS CATALYSIS

HEAD OF THE DEPARTMENT PROF. VLADIMIR A. SOBYANIN



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



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



Group of Synthesis of Nanodispersed Materials
Head: Prof. Oleg P. Krivoruchko



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



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



Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov



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



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



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



Group of Direct Catalytic Hydrogen Sulfide Oxidation
Head: Dr. Mikhail A. Kerzhentsev



Laboratory of Catalytic Conversion of Carbon Oxides
Head: Prof. Tamara M. Yurieva



Group of Reactions of Oxidation on Metals
Head: Prof. Aleksandr V. Khasin



Group of Dynamics of Surface Transformations
Head: Dr. Andrei V. Simakov



Group of Catalytic Synthesis of Oxygen-Containing Compounds
Head: Dr. Galina G. Volkova



Group of Catalytic Synthesis of Hydrocarbons
Head: Dr. Aleksandr A. Khassin

DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS

HEAD OF THE DEPARTMENT PROF. VLADIMIR A. LIKHOLOBOV



**Laboratory of Catalysis by Complex Metal Compounds
Head: Prof. Vladimir A. Likholobov**



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



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



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



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



**Group of Catalysts on Carbon Supports
Head: Prof. Vladimir A. Semikolenov**

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS

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



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



Department of Applied Catalysis
Il'ya A. Zolotarskii



Laboratory of Catalysts Activity Testing
Head: Dr. Nikolai N. Bobrov



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



Group of Catalysts Preparation
Head: Vasiliy Yu. Kruglyakov



Group of Catalysts Testing
Head: Aleksandr S. Bobrin



Group of Pilot Installations and High Pressure
Head: Viktor N. Korotkikh



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

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING

HEAD OF THE DEPARTMENT PROF. A.S. NOSKOV



Laboratory of Kinetics of Catalytic Processes
Head: Dr. Sergei I. Reshetnikov



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



Laboratory of Industrial Catalytic Processes
Head: Il'ya A. Zolotarskii



Laboratory of Dynamics of Catalytic Processes
Head: Dr. Andrey N. Zagoruiko



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



Group of Mathematical Methods for Catalytic and Adsorption Processes Modeling
Head: Dr. Natalia A. Chumakova



Laboratory of Catalytic Conversion of Solid Fuels and Wastes
Head: Dr. Aleksandr D. Simonov



Laboratory of Multiphase Processes Modeling
Head: Prof. Valerii A. Kirillov



Laboratory of Catalytic Processes in Dynamic Bed
Head: Prof. Gennadii G. Kuvshinov

RESEARCH AND PRODUCTIVE DEPARTMENT

ACTING HEAD OF THE DEPARTMENT PROF. Z.P. PAI



Group of Catalytic Synthesis of Biologically Active Compounds
Head: Prof. Aleksandr G. Tolstikov



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

OMSK DIVISION OF THE BORESKOV INSTITUTE OF CATALYSIS



DIRECTOR PROF. VLADIMIR A. LIKHOLOBOV



SCIENTIFIC MANAGER PROF. VALERII K. DUPLYAKIN

SCIENTIFIC-RESEARCH SUBDIVISIONS



Laboratory of Deep Petroleum Refining
Head: Prof. Valerii K. Duplyakin



Group of Carbon Materials
Head: Prof. Georgii V. Plaksin



Laboratory of Catalytic Methods for Atmosphere Protection
Head: Prof. Pavel G. Tsyrunikov



Laboratory of Catalysis by Supported Metals
Head: Dr. Aleksandr S. Belyi



Laboratory of Kinetics and Modeling of Petrochemical Processes
Head: Prof. Nikolai M. Ostrovskii



Group of Zeolite-Containing Catalysts for Petrochemistry and Petroleum Refining
Head: Dr. Vladimir P. Doronin



Group of Catalytic Synthesis of Hydrocarbon from Natural Gas
Head: Dr. Aleksandr I. Oruzhenikov

SUBDIVISION OF PHYSICOCHEMICAL METHODS OF INVESTIGATION



Group of Adsorption
Head: Dr. Vladimir A. Drozdov



Group of X-Ray and Electron Microscopy Technique
Head: Dr. Aleksandr I. Nizovskii



Group of Spectral Methods
Head: Dr. Valentin P. Talsi



Analytical Group
Head: Tatiana V. Kireeva

EXPERIMENTALLY-MANUFACTURING DEPARTMENT



HEAD: KONSTANTIN V. KOLMOGOROV

**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 rate 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.

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.

In 1999 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.

In the context of future research program, the Institute will continue to study the mechanisms and kinetics of actually important catalytic reactions, improve physicochemical and quantum-chemical methods used in catalysis, develop the research basis for purposeful synthesis of a number of catalysts, supports and sorbents (including non-traditional mechanochemical, plasma, radiation-thermal methods, etc.), study the regularities of formation of new materials (carbon-carbon composite materials of globular and fibrous structure, polymer-inorganic composites, composite membranes, etc.) as well as supports and adsorbents with the optimum geometry and controlled structure and mechanical properties (monolith multichannel ceramics, honeycomb carbon and ceramic monoliths); design new and improve the existing catalytic processes (cracking, alkylation, polymerization, etc.) and novel reactors, study the possibilities of using catalysis in such non-traditional fields as thermocatalytic conversion of solar and other types of energy; design of adsorption materials for freon-free air conditioners, accumulators of low-potential heat, active cooling systems; technologies with the use of low-energy fuels; various types of heaters with catalytic fuel cells, etc.

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 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*
VUV electron spectroscopy
UV-VIS electron spectroscopy
Vibrational spectroscopies (IR, including *in situ*, and RAMAN)
HREELS
LEED
X-Ray and NMR tomography.

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 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.

The Institute of Catalysis invites all researchers interested in collaboration for mutual-benefit cooperation in the field of catalysis.

During the year 2001 97 scientists took part in 41 international scientific measures abroad.

**Visits of the specialists from the Boreskov Institute of Catalysis
to foreign institutions**

Australia	1	India	1	Portugal	2
Canada	2	Ireland	10	South Arabian Republic	2
China	1	Israel	1	Spain	7
Czech Rep.	2	Italy	14	Sweden	1
Finland	25	Japan	4	Switzerland	1
France	17	Malaysia	3	Thailand	3
Germany	23	Netherlands	14	Turkey	2
Greece	2	Norway	1	UK	2
Hungary	1	Poland	6	USA	14

Visits of foreign specialists to the Boreskov Institute of Catalysis

Bulgaria	1	Italy	4	South Arabian Republic	1
Finland	2	Japan	5	Spain	1
France	15	Netherlands	6	UK	1
Germany	4	Poland	2	USA	9
Greece	5	Portugal	1		

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:

– **Institute of Energy Conversion and Storage, TAE**, Messina – **BIC**, Novosibirsk, “*Catalysis for Solving the Energy Problems*”.

FRANCE

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

– **Institute de Recherches sur la Catalyse**, Villeurbanne on the BIC-IRC Twinning Program:

1. Membranes in Catalysis.

2. Studying of Reaction Mechanism of a) Selective Oxidation, b) NO Reduction with Methane in Oxygen Excess over Fiber Glass Materials, c) Monte-Carlo Modelling of Reactions of Selective Oxidation.
3. Studying of Reaction of Hexachloro-Benzene Hydrodechlorination over Pd-Ni, Pd-Cu, Pd-Pt Catalysts.
4. Molecular Dynamics in Zeolites.

– **Université Pierre et Marie Curie**, Paris

POLAND

In the frame of RAS-PAS agreement **BIC** cooperates with the **Institute of Chemical Technology**, Glivitse.

COOPERATION WITH FOREIGN ORGANIZATIONS IN THE FRAMEWORK OF BILATERAL AGREEMENTS

GERMANY

Cooperation in the frame of RAS-DFG agreement with the **Fritz-Haber-Institut MPG**, Berlin.

USA

Cooperation with the **Kansas University**, “*Catalytic Reaction of Halogen-Containing Compounds over Alkaline-Earth Oxides*”.

THE NETHERLANDS

Grant provided by **Dutch Organization for Scientific Research (NWO)** “*Clusters in Zeolite Materials*”. Project Coordinator: **Prof. R.A. van Santen**, Eindhoven University of Technology, Eindhoven. Participants: **Prof. G. Zhidomirov**, BIC, Novosibirsk; **Prof. V. Kazansky**, Zelinsky Institute of Organic Chemistry, Moscow.

COOPERATION IN THE FRAMES OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

I. Electronic, Magnetic and Adsorption Properties of Carbon Nanostructured

Project Coordinator:

Prof. J. Marc-Bonard, Ecole Polytechnique Federale de Lausanne, Switzerland.

Participants:

Dr. V. Kuznetsov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. O. Klein**, Ecole Polytechnique, Palaiseau, France; **Dr. A. Okotrub**, Institute of Inorganic Chemistry, Novosibirsk, Russia; **Dr. T. Kononenko**, General Physics Institute, Moscow, Russia.

II. Novel Nanostructured Catalysts for the Selective Reduction of NO_x by Heavy Hydrocarbons

Project Coordinator:

Prof. J. Ross, University of Limerick, Ireland.

Participants:

Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. A. Rosovskii**, Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; **Prof. V. Matyshak**, Semenov Institute of Chemical Physics, Moscow, Russia; **Prof. B. Andersson**, Chalmers University of Technology, Göteborg, Sweden.

III. Theoretical and Experimental Studies on the Catalytic Activity of the V₂O₅-TiO₂ System

Project Coordinator:

Prof. K. Jug, Universität of Hannover, Germany.

Participants:

Prof. O. Lapina, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Borovkov**, Institute of Organic Chemistry, Moscow, Russia; **Prof. C. Minot**, Université Pierre et Marie Curie, Paris, France.

IV. Ethanol Combustion in a Solid Oxide Fuel Cell for Electrical Power Generation Aided Study

Project Coordinator:

Prof. Tsiakaras, University of Thessaly, Greece.

Participants:

Prof. V. Sobyenin, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Dr. S. Kirillov**, Institute of Technological and Information Innovations, Kiev, Ukraine; **Dr. A. Demin**, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia; **Dr. V. Antonucci**, Institute of Transformation and Accumulation of Energy, CNR, Messina, Italy.

V. Experimental and Theoretical Studies of Temporal and Spatial Self-Organization

Processes in Oxidative Reactions over Platinum Group Metals. An Approach to Bridge the Gap between Single Crystals and Nano-Size Supported Catalyst Particles

Project Coordinator:

Prof. B. Nieuwenhuys, Leiden University, The Netherlands.

Participants:

Prof. N. Jager, University of Bremen, Germany; **Prof. R. Imbihl**, University of Hannover, Germany; **Prof. V. Gorodetskii**, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. M. Vasiliev**, Physical Institute, Kiev, Ukraine; **Dr. M. Slin'ko**, Institute of Physical Chemistry, Moscow, Russia.

VI. Catalytic Materials

Project Coordinator:

Prof. P. Siffert, EMRS, Strasbourg, France.

Participants:

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Dr. R.L. Keiski**, University of OULU, Linnanmaa, Finland; **Prof. J. Santamaria**, University of Zaragoza, Zaragoza, Spain; **Prof. P.G. Menon**, University of Gent, Belgium.

VII. Development and Study of New Catalytic Systems Based upon Microdomain Textured Perovskites for Efficient Lean DeNO_x Process, CO Removal and C₂H₆ Conversion

Project Coordinator:

Prof. R. Schloegl, Fritz-Haber-Institut, Berlin, Germany.

Participants:

Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. N. Lyakhov**, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Prof. Z. Mansurov**, Al'-Farabi Kazakh State University, Almaty, Kazakhstan; **Prof. V. Corbean**, Institute of Catalysis and Petrochemistry, Madrid, Spain.

VIII. Nanostructured Catalysts for Ultra-Deep Cleaning of Motor Fuels

Project Coordinator:

Prof. J. Moulijn, Delft University of Technology, Delft, The Netherlands.

Participants:

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

IX. The Nature of Sulfated Zirconia Strong Acidity

Project Coordinator:

Prof. J. Vedral, University of Liverpool, Liverpool, United Kingdom.

Participants:

Prof. G. van Tendeloo, University of Antwerpen RUCA, Antwerpen, Belgium; **Prof. D. Kochubey**, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. A. Kokorin**, Institute of Chemical Physics, Moscow, Russia; **Prof. A. Kulak**, Institute of General and Inorganic Chemistry, Minsk, Belarus.

X. Catalytic Oxidation of Organic Pollutants in Waste Waters

Project Coordinator:

Dr. P. Gallezot, Institut de Recherches sur la Catalyse, Villeurbanne, France.

Participants:

Prof. M. Sheintuch, Technion-Israel Institute of Technology, Haifa, Israel; **Prof. V. Parmon**, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. B. Laskin**, Research Scientific Center for Applied Chemistry, St.-Petersburg, Russia.

Grants provided by INTAS-RFBR

I. Silica and Zirconia Based Mesoporous Mesophases: Synthesis, Structure, and Catalytic Properties

Project Coordinator:

Prof. G. Poncelet, Universite Catholique de Louvain, Belgium.

Participants:

Prof. V. Fenelonov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. F. Schuth**, Universität Frankfurt, Germany; **Prof. S. Kirik**, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia.

II. Study of Microstructure of Free Volume in High Permeability Polymers: Comparison with Microporous Sorbents

Project Coordinator:

Prof. D. Hofmann, GKSS Research Centre, Institute of Chemistry, Teltow, Germany.

Participants:

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

III. Oxygen Mobility and Catalytic Activity of Anion Modified Complex Oxides with Perovskite and Fluorite Type Structures in the Unsteady-State Conditions of Selective Oxidation-Reduction Processes

Project Coordinator:

Prof. E. Kemnitz, Humboldt University of Berlin, Germany.

Participants:

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

IV. Theoretical Investigations of Selective Hydrocarbon Oxidation Catalyzed by Transition Metal Oxide, Peroxide and Hydroxide Substances

Project Coordinator:

Prof. N. Roesch, Munich Technical University, Munich, Germany.

Participants:

Prof. G. Zhidomirov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

COPERNICUS

I. Natural Gas Fuelled Solid Oxide Fuel Cells (SOFCs) for Cogeneration of Electricity and Chemicals

Project Coordinator:

Prof. S.G. Neophytides, Institute of Chemical Engineering and High Temperature Chemical Processes, Platani Achaïas, Greece.

Participants:

Prof. R.M. Ormerod, Keele University, Staffordshire, United Kingdom; **Dr. A. Demin**, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia; **Prof. C. Comninellis**, Swiss Federal Institute of Technology, Lausana, Switzerland; **Prof. V. Sobyanin**, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Khukharov**, University of Chemical Technology and Metallurgy, Sofia, Bulgaria; **Dr. N. Zakharina**, Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakhstan.

II. Feasibility Study of Novel Technology for Natural Gas Liquefaction Based on Plasma Catalysis and the Fischer-Tropsch Synthesis

Project Coordinator:

Prof. M. Heintze, Institut für Niedertemperatur-Plasmaphysik eV, Greiswald, Germany.

Participants:

Prof. V. Kirillov, **Prof. V. Parmon**, **Prof. T. Yurieva**, Boreskov Institute of Catalysis, Novosibirsk, Russia.

III. Recovery of Methane from Vent Gases of Coal Mines and its Efficient Utilization as a High Temperature Heat Source

Project Coordinator:

Prof. Dr.-Ing. G. Eigenberger, Institute of Chemical Process Engineering, Stuttgart University, Germany.

Participants:

Prof. A. Noskov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Babkin**, Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia; **Prof. K. Gosiewski**, Group of the University of Czestochowa, Czestochowa, Poland; **Prof. K. Warmuzinski**, Institute of Chemical Engineering of the Polish Academy of Sciences, Gliwice, Poland; **Prof. P. Forzatti**, Research Group at Department of Industrial Chemistry and Chemical Engineering "Natta" at Politecnico di Milano, Milano, Italy.

IV. Development of the Environmentally Benign Technology for Deep Recovery of Elemental Sulphur from Technological Off-Gasses of Metallurgical Coke Plants and Chemical Refineries of Crude Oil

Project Coordinator:

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

Participants:

Prof. J.A. Moulijn, Delft University of Technology, Delft, The Netherlands.

NATO PROGRAMME: SCIENCE FOR PEACE

I. Catalytic and Electrochemical Processes for SO₂ and NO_x Emission Abatement

NATO Country Project Director:

Dr. S. Boghosian, Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece.

Partner Country Project Director:

Prof. B. Bal'zhinimaev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

II. Development of Shape Steam Reforming Catalysts

NATO Country Project Director:

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

Partner Country Project Director:

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

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

NATO Country Project Director:

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

Partner Country Project Director:

Prof. E. Savinov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

IV. Synthesis of Ordered Mesoporous Aluminas and Their Application as Catalyst Supports

NATO Country Project Director:

Dr. T. Blasco, Instituto de Tecnologia Quimica, Valencia, Spain.

Partner Country Project Director:

Prof. H. Calderaru, Institute of Physical Chemistry "I.G. Murgulescu", Bucharest, Romania.

Participants:

Prof. A. Startsev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)

I. Development of Technology of Catalytic Fluidized Bed Destruction of Mixed Liquid Organic Wastes from Radio-Chemical and Chemical Metallurgy Plants

Project Manager:

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

Participating Institutions:

Pacific Northwest National Laboratory, USA; **Lawrence Livermore National Laboratory**, USA; **Siberian Chemical Complex**, Seversk, Russia; **Novosibirsk Chemical Concentrates Plant Ltd.**, Novosibirsk, Russia; **Novosibirsk State Design-Exploratory Institute VNIPIET**, Novosibirsk, Russia.

II. Development of Technology of Catalytic Fluidized Bed Destruction of Components of Rocket Fuels

Project Manager:

Dr. M. Kerzhentsev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

Project Scientific Leader

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

Participating Institutions:

Netherlands Energy Research Foundation, The Netherlands; **LERCSI Laboratory**, Louis Pasteur University, France; **State Rocket Center's Makeyev Design Bureau**, Miass, Russia; **Novosibirsk State Design-Exploratory Institute VNIPIET**, Novosibirsk, Russia; **Russian Applied Chemistry Research Center**, St. Petersburg, Russia; **Federal Research & Production Corporation "Altai"**, Biisk, Russia.

CONFERENCE AND EXHIBITION ACTIVITIES

Solution of many specific problems requires joint efforts in order to promote its fastest accomplishing. International congresses, symposia, conferences, and seminars are most productive to familiarize scientists with innovations outside their own research and to disseminate the information about the results achieved to a wider audience.

EXHIBITION ACTIVITY

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.

Our Institute, while owing numerous items in the field of applied catalysis, exercises the attending at exhibitions to promote its developments to the consumer market, to advertise its R&D activities and search for potential customers.

In 2001, the most important BIC's achievements in the area of applied catalysis were presented at the next exhibitions and fairs:

- ❑ **The First Moscow International Salon of Innovations and Investments** (*Inventions, Investment-Attractive Innovations, High Technologies*), 7-10 February, Moscow - **Golden Medal** for the Reforming Catalysts of the "PR" Series, Catalytic Heating Plant, Hemosorbent VNIITU-1 and Electroconductive Carbon.
- ❑ **International Salon of Industrial Property "Archimedes"**, 22-26 March, Moscow - **Golden Medal and Diploma** for "SULFACRYLATE" – medical glue for surgery; **Golden Medal and Diploma** for Selective Water Sorbents; **Diploma** for Active Participation.
- ❑ Exhibition-Fair "**The North of Russia-2001**", 3-6 April, Novosibirsk.
- ❑ Exhibition "**New Chemical Technologies and Materials**", 16-29 April, Belgrad, Yugoslavia; Hungary, Budapest.
- ❑ Exhibition of **Military Land Equipment and Armament "VTTV-Omsk-2001"**, 6-9 June, Omsk.
- ❑ "**High Technologies. Investments. Innovations**", "**HI-TECH-2001**", 12-15 June, St. Petersburg - **Diploma and Medal** for "Technology for Preparation of Reductive Atmospheres"; **Diploma** for Revival of Scientific and Industrial Complex of Russia and Active Participation.
- ❑ 11th International Exhibition "**CHEMISTRY-2001**", 10-14 September, Moscow.
- ❑ The Siberian Fair "**SibSecurity, SpasSib-2001**", 18-21 September, Novosibirsk.
- ❑ "**Science of Siberia-2001**", 23-26 October, Novosibirsk - **Big Golden Medal** for Design and Organization of Production of Catalysts for Petroleum Refining and Chemistry, Ensuring Refusal of Large-Scale Purchases.
- ❑ International Exhibition-Seminar "**Innovation Technologies in Petrochemistry, Catalysis and Waste Water Purification**", 30 October-2 November, Kuala Lumpur, Malaysia - the Catalogue "*Innovation Technologies in Petrochemistry, Catalysis, and Environment Protection. Research and Developments. Malaysia, 2001*" and the Book of Abstracts "*Innovation Technologies in Petrochemistry, Catalysis, and Environment Protection*" have been issued.
- ❑ Exhibition-Fairy "**GASIFICATION-2001**", 30 October-2 November, Tomsk - **Diploma** of "**Siberian Athens**" for «Bicyclar» Technology for Aromatic Hydrocarbons Production.
- ❑ Exhibition of Scientific and Technological Achievements of the Cities - Members of the World Association of Technopolices "**Technomart**", 7-9 November, Taejon, Korea. It has

to be stressed that Novosibirsk was the sole Russian city admitted to WAT. Among exciting events was start-up of an enlarged laboratory installation for synthesis of high-octane gasoline in Taejon. The installation was designed at the Borekov Institute of Catalysis by the team headed by Prof. K. Ione under the Samsung Project, fabricated and assembled by Korean specialists.

The high scientific and engineering level of developments of our Institute suggested for such fields as chemistry, petroleum refining, medicine, environmental protection, heat power engineering, the manner of presenting them at the exhibitions attracted the attention of many Russian large-scale enterprises and foreign companies.

CONFERENCE ACTIVITY

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 CIS, but International as well.

XV International Conference on Chemical Reactors, "CHEMREACTOR-15"

June 5-8, Helsinki, Finland

The Borekov Institute of Catalysis organized the first Russian conference on this subject in Novosibirsk (former USSR) in 1960. Since that time the conferences devoted to the Chemical Engineering Science in the field of chemical reactors took place in different cities of the former USSR every 3 years. They gained International status starting since 1996. Such outstanding scientists in this subject as **Prof. M. G. Slinko**, **Acad. G. K. Borekov**, **Acad. G. I. Marchuk** (Russia), **Prof. K. R. Westerterp** (The Netherlands), **Prof. G. Froment** (Belgium), **Prof. A. Renken** (Switzerland) helped a lot in conferences organizing and formation. This time the conference was held in Helsinki in the Russian Scientific and Cultural Center. Representatives of industrial enterprises and companies engaged in chemical technology took part in the conference and in the exhibition as part of the conference.

Conference organizers:

- Borekov Institute of Catalysis
- Finnish Catalytic Society
- Russian Center of International Scientific and Cultural Cooperation under RF Government
- Ministry of Industry, Science and Technologies of the Russian Federation
- Scientific Council on Catalysis of RAS
- European Federation on Chemical Technologies
- Russian Scientific and Cultural Center in Helsinki.

120 Specialists from 14 countries attended the conference. The support of the Ministry of Industry, Science and Technologies of Russian Federation (Moscow), Sibakadembank

(Novosibirsk) and JSC “Nizhnekamskneftehim (Nizhnekamsk) have provided the circle of the Russian participants of the conference to be expanded.

Scientific program included 7 plenary lectures:

V. N. Parmon, Z.R. Ismagilov, V.A. Kirillov, D.V. Simonov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – “*Environmentally Benign Catalytic Methods of Heat Production*”

A. Renken (Swiss Federal Institute of Technology, Lausanne, Switzerland) – “*Catalytic Microreactors*”

M. P. Duduković, Shantanu Roy*, M.H. Al-Dahhan (Washington University, St. Louis, USA; *Process Engineering and Modeling, Corning Incorporated, Corning, NY, USA) – “*Flow Mapping and Modeling of Liquid-Solid Risers*”

A. Bridgwater (Bio-Energy Research Group, Aston University, Birmingham, UK) – “*Renewable Fuels and Chemicals by Thermal Processing of Biomass*”

D. W. Agar (University of Dortmund, Germany) – “*Regenerative & Reactive Enhancement of Temperature & Concentration Profiles in Chemical Reactors*”

M.G. Slinko, **D.Yu. Murzin*** (SRC “Karpov NIPCI”, Moscow, Russia; *Process Chemistry Group, Åbo Akademi, Turku, Finland) – “*Reaction Kinetics – Basis for Modelling of Catalytic Processes*”

E. Tirronen, T. Salmi* (Kemira, Finland; *Process Chemistry Group, Åbo Akademi, Turku, Finland) – “*Process Development in the Fine Chemical Industry*”



Presented oral contributions (46) and posters (32) covered the following subjects:

- ◆ Physico-Chemical and Mathematical Bases of Processes Occurring on Catalysts Surface
- ◆ Processes in Chemical Reactors
- ◆ New Types of Chemical Processes and Reactors
- ◆ Chemical Reactors for Solving the Fuel and Energy Production Problems
- ◆ Waste Detoxication and Processing.



Special Workshop on the INTAS Project “*Experimental and Theoretical Studies of Temporal and Spatial Self-Organization Processes in Oxidative Reactions over Platinum Group Metals*” was adjoined to the first topic.

The conference became interesting both for researchers, and for representatives of the chemical industry.

The Organizing Committee organized a Helsinki city-tour and an excursion to the island Suomenlinna-Sveaborg during the conference.

NATO ARW “Magnetic Resonance in Colloid and Interface Science”

June 26-30, St. Petersburg, Russia

Joining their efforts, the Boreskov Institute of Catalysis and Pierre and Marie Curie University have held NATO ARW "Magnetic Resonance in Colloid and Interface Science" at the House of Scientists, St. Petersburg. It has attracted great attention of the experts – 130, among them 50 scientists from Russia, Estonia and Ukraine and 79 foreign participants from 21 west countries, and 20 NATO experts.

Organizers:

- > NATO
- > Université Pierre et Marie Curie
- > Centre National de la Recherche Scientifique (CNRS)
- > Boreskov Institute of Catalysis
- > Russian Foundation for Basic Research
- > International Association for the Promotion of Cooperation with Scientists from the New Independent States of the Former Soviet Union (INTAS)
- > Bruker Analytik GMBH
- > St. Petersburg Scientific Centre
- > Consulat Général de France a Saint-Petersbourg
- > Meriya of St. Petersburg

The Scientific Program of the Symposium comprised 17 plenary lectures, 10 keynote lectures, 21 oral communications and 75 poster presentations. The scope covered the following topics:

- ◆ NMR in the Adsorbed State
- ◆ Innovative Techniques in NMR and EPR
- ◆ NMR and EPR Applied to Microporous Compounds and Catalysts
- ◆ EPR in Coordination Chemistry
- ◆ NMR in Microemulsions
- ◆ ²H NMR in Liquid Crystals and Membranes
- ◆ Structure and Dynamics of Polymers
- ◆ NMR of Metal Nanoparticles
- ◆ NMR Imaging
- ◆ Diffusion in Heterogeneous Systems

Plenary Lectures were given by:

O. Söderman (University of Lund, Lund, Sweden) – “*NMR in Colloid Science with Special Emphasis on Self-Aggregating Systems*”

Z. Luz (The Weizmann Institute of Science, Rehovot, Israel) – “*Mesomorphism, Isomerisation, Dynamics and Density Undulation in Some New Columnar Liquid Crystalline Phases: A Solid State NMR Study*”

J. Kärger (University of Leipzig, Leipzig, Germany) – “*NMR Diffusion Studies of Molecules in Nanoporous Materials*”



J.-P. Amoureux, M. Pruski*, F. Taulelle**, Z. Gan*** (Université des Sciences et Technologies de Lille, Lille, France; *Iowa State University, Ames, USA; **Universite Louis Pasteur, Strasbourg, France; Tallahassee, Florida, USA) – “*High-Resolution Methods in Solid-State NMR of Quadrupolar Nuclei: Enhanced Sensitivity with CPMG-ANAFOR*”

A. Pines (University of California, Berkeley, USA) – “*Lighting UP*” NMR and MRI for Colloids and Interfaces”

D. Müller (Bruker Analytic GmbH, Rheinstetten, Germany) – “*Recent Achievements on NMR Tomography for Material Science and Catalysis*”



D. Michel, J. Roland (University of Leipzig, Leipzig, Germany) – “ *^1H NMR Spectroscopy of Molecules Adsorbed in Porous Media and on Interfaces at Ultra High Magnetic Field*”

H. W. Spiess (Max-Planck-Institut für Polymerforschung, Mainz, Germany) – “*High-Resolution Double Quantum MAS NMR of Solids: A New Tool for Structural and Dynamic Investigations*”

J. H. Strange (University of Kent, Kent, UK) – “*Characterization of Porous Materials by NMR*”

A. Samoson (National Institute of Chemical Physics and Biophysics, Tallinn, Estonia) – “*Dynamic MAS NMR*”

I. Moudrakovski, A. Nossou, S. Lang, E. Brouwer, D. Soldatov, C. Ratcliffe, **J. Ripmeester** (Stacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Canada) – “*Applications of Hyperpolarized ^{129}Xe NMR Spectroscopy to the Study of Materials*”

H. Eckert (Institute für Physikalische Chemie Wesfälische Wilhelms, Universität Münster, Münster, Germany) – “*Quantifying Structural and Dynamic Disorder in Solid Electrolyte Materials: New NMR Approaches and Strategies*”

P. Sozzani, A. Comotti, R. Simonutti (University of Milan “Bicocca”, Milan, Italy) – “*NMR Study of Organic-Inorganic Interfaces in Materials*”

M. Pruski (Ames Laboratory, Iowa State University, Iowa, USA) – “*Progress in High Resolution Solid State NMR of Quadrupolar Nuclei: Applications to Porous Materials and Catalysts*”

B. Blümich (Institut für Technische Chemie und Makromolekulare Chemie, RWTH Aachen, Aachen, Germany) – “*Multidimensional Exchange NMR in k Space*”

H.J. Jakobsen, H. Bildsøe, J. Skibsted, T. Giavani (Instrument Centre for Solid-State NMR Spectroscopy, University of Aarhus, Aarhus, Denmark) – “*¹⁴N MAS NMR Spectroscopy. An Instrumental Challenge and Informatory Technique*”

F. Pedrazzini (NATO Scientific Affairs Division, Brussels, Belgium) – “*The NATO Scientific Program*”.

Scientific INTAS Session was organized on June 27 and included oral communications and poster presentations on 14 INTAS Projects.

Extension Courses in the Field of Catalysts and Catalytic Processes

September 23-30, Novosibirsk, Russia

The Borekov Institute of Catalysis received experts from different industrial enterprises and organizations – JSC “Yarsintez” (Yaroslavl), NZK, Ltd (Novokuibyshevsk), JSC “LUKoil-Perm nefteorgsintez” (Perm), JSC “Achinsk Oil Refinery Plant (Achinsk), JSC “Sibneft-ONPZ” (Omsk), JSC “Cherepovets AZOT” (Cherepovets), JSC “Nizhnekamskneftehim” (Nizhnekamsk), “METANOL Co” (Tomsk), JSC “Invist” (Tver region), JSC “Promkataliz” (Ryazan), JSC “Kaustik” (Sterlitamak), JSC “Kirovo-Chepetsk’s Chemistry Plant” (Kirovo-Chepetsk), Kazan’ State Technological University (Kazan’), Ural Electrochemical Plant (Novouralsk), JSC “Katalizator” (Novosibirsk) who wished to expand their knowledge in the field of catalysis. In a week 38 persons finished the *Extension Courses in the Field of Catalysts and Catalytic Processes* and after solemn receiving of appropriate documents have come back to their workplaces in complete reliance that they visited Novosibirsk not in vain.



The organizers of the courses were the Borekov Institute of Catalysis, Novosibirsk State University and Zamaraev International Charitable Scientific Foundation.



The Programme included 15 lectures by the leading researches of the Institute and Novosibirsk State University, practical training in research laboratories and computer center of the Institute.

The lectures were given by:

1. **V.A. Likholobov**, *“Catalysis. Introduction and Main Conceptions”*
2. **V.B. Fenelonov**, *“Fundamentals of Adsorption and Theory of Catalysts Texture Control”*
3. **V.A. Semikolenov**, *“Supported Metal Catalysts”*
4. **V.A. Sadykov**, *“Oxide Catalysts”*
5. **D.I. Kochubey**, *“Catalysis and Physicochemical Methods”*
6. **N.N. Bobrov**, *“Experimental Methods for Catalyst Testing”*
7. **N.A. Pakhomov**, *“Scientific Bases for Catalysts Preparation. Catalyst Supports”*
8. **A. Yermakova**, *“Rate of Catalytic Transformations and Macrokinetic Models of Catalytic Reactions”*
9. **A.N. Zagoruiko**, *“Fundamental Basis for Design of Catalytic Reactors. Heat(Mass) Transfer in Catalytic Reactors”*
10. **A.S. Shmelev, I.A. Zolotarskii, S.I. Reshetnikov**, *“Computational Systems for Chemical Technological Schemes Calculation”*
11. **V.P. Doronin**, *“Modern Trends in Development of Catalytic Petroleum Refining”*
12. **G.V. Echevsky**, *“Application of Zeolite Catalysis for Petroleum Chemistry and Petroleum Refining”*
13. **I.A. Zolotarskii**, *“Modern Trends in Development of Catalytic Processes in Nitric Industry”*
14. **Z.R. Ismagilov**, *“Progress Trends in Development of Catalytic Processes for Environmental Protection”*
15. **S.N. Zagrebelnyi**, *“Enzymes in Chemical Industry”*.

BORESKOV INSTITUTE OF CATALYSIS AS AN EDUCATIONAL CENTER

With deep belief that people are a decisive factor and the best way to study yourself is to teach others, many researchers of the Institute participate in the training of specialists in chemistry and, of course, in catalysis. The majority of them ensure closest and time-tested links of the Institute with the main source of researchers – Novosibirsk State University (NSU). The others develop dynamic contacts with other Siberian schools, primarily, with Novosibirsk State Technical University (NSTU).

BIC – NSU

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

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

Boreskov Institute of Catalysis is a key element in the training of specialists in chemistry at NSU. More than 35 researchers of the Institute are currently part-time teachers at the Department of Natural Sciences (DNS) at NSU. They present lectures, give seminars and practical classes, participate in the organization and renovation of the educational process at four out of eight chemical chairs of DNS, namely, chairs of physical chemistry, general chemistry, analytical chemistry, adsorption and catalysis.

The chair of adsorption and catalysis is of special importance for the Institute. It is only 5 years younger than Novosibirsk State University itself. The organization of the chair was initiated in 1964 by Academician G.K. Boreskov – the founder and first director of the Boreskov Institute of Catalysis SB RAS. The chair is located at the Institute, which provides it with everything required for efficient training of students specializing in catalysis and technology of catalytic processes. Twenty five to thirty students of the IV, V and VI years of the Chemical Department of DNS are trained at the chair annually. Its graduates obtain Bachelors, Specialists and Masters diplomas. Graduation works of the students are conducted at the laboratories of the Institute and are supervised by experienced researchers. Their results are usually published in scientific journals and form the basis of their future Ph.D. theses.

From the first years, the strategy of the training of students at the chair is formed by leading scientists of BIC and harmonically combines two aspects. On the one hand, curricula provide the students with deep theoretical and practical knowledge in catalysis, theory of the prevision of the catalytic action of substances, kinetics of catalytic reactions, scientific bases of the preparation of catalysts, bases of the technology of catalytic processes, application of modern physical and mathematical methods for investigation of catalysts and catalysis. On the other hand, the curricula allow for a significant widening of the sphere of the working activity of its graduates. They can work as technologists, production managers, researchers at various research organizations, teach at universities.

All this allows the students to prepare their graduation study at the highest scientific level and become widely informed specialists in chemistry and catalysis. The graduates of the chair of adsorption and catalysis are the principal source of recruitment of the personnel of the Institute.

BIC – NSTU

Training of the personnel in the field of technology of catalytic processes is of special importance for practical application of fundamental knowledge in the field of catalysis. To meet this task, work in two main directions is under way. First, corresponding courses ("Bases of chemical technology", "Mathematical modeling of catalytic reactors") are prepared for students studying at the chair of adsorption and catalysis. Further progress in this direction is connected with the training of students specializing in "Engineering environment protection" started at NSTU in 1998. It is one of the steps in realization of the program of joint training of specialists at NSTU and institutes of the Siberian Branch of RAS. The basic training is conducted by a chair founded at the Boreskov Institute of Catalysis. Researchers of BIC present courses on industrial ecology and technology of the environment protection, basics of manufacturing and catalytic methods.

BIC – graduate school

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

There is a great demand for specialists in catalysis trained at the Boreskov Institute of Catalysis, both graduates of the chair of adsorption and catalysis and of the graduate school. Many of them apply their knowledge in these fields at various research centers, universities and manufacturing companies.

SCIENTIFIC SOCIAL LIFE

In the middle of February at the Boreskov Institute of Catalysis the Scientific Council meeting dedicated to the 85th anniversary of Professor Anatolii P. Karnaukhov, prominent specialist in the field of physical chemistry of surface phenomena, adsorption, texture studies of disperse and porous solids, was held. He already has ceased working by virtue of venerable age, but more than thirty years he has worked "for the sake of catalysis", have strongly linked him to the Institute, colleagues and followers.



February, 21 at the Presidential Hall of the Presidium of the Russian Academy of Sciences the solemn handing of the honorary diplomas to the winners of the Charity foundation for Assistance to Domestic Science of the Presidium of the Russian Academy of Sciences, the "SibNeft" and the "Russian Aluminum" companies has been held. Among the other 11 Siberian scientists, winners in nomination "Young Doctors of Sciences" – **Prof. Valerii I. Bukhtiyarov**, now the deputy director of the Institute.



Dr. D.E. Babushkin was among the young talented scientists who have been awarded with the State Scientific Scholarships of 2000 according to the SB RAS Presidium decree.



The following scientists of the Institute have been awarded with the State Scientific Scholarships of 2000 pursuant to the SB RAS Presidium enactment according to the Russian Federation Presidential Decree "On the measures for material support of Russian scientists":

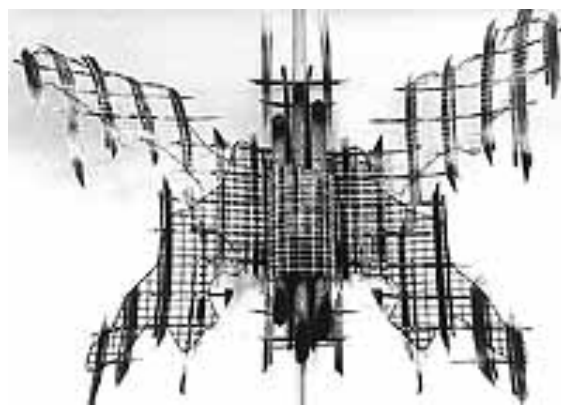
Prof. Anna Yermakova, Prof. Georgii M. Zhidomirov, Prof. Vladimir A. Zakharov, Prof. Zinifer R. Ismagilov, Prof. Valerii A. Kirillov, Prof. Vladimir A. Likhobov, Prof. Vladislav V. Malakhov, Prof. Ella M. Moroz, Prof. Aleksandr S. Noskov, Prof. Boris N. Plakhutin, Prof. Vladimir A. Semikolenov, Prof. Vladimir A. Sobyenin, Prof. Eugenii P. Talsi, Prof. Gennadii I. Panov.



Developing the line "Scientific bases of processing of natural gas, oil, coal, as well as restored and non-traditional chemical raw materials, in particular, vegetative biomass", the body of the Institute of Chemistry and Chemical Engineering of the Krasnoyarsk Scientific Center of the SB RAS has fulfilled a number of fundamental works of priority character, with a block of applied proposals. Among them the works on quantum-chemical calculations of different reactions carried out jointly with the Munich Technical University and **the Boreskov Institute of Catalysis**.



Two rather exotic exhibitions have been opened in the beginning of April in foyer of the Exhibition Center of the Siberian Branch. **Acad. Valentin Parmon**, Director of the Borezskov Institute of Catalysis and **Dr. Alexandr Kulikov**, employee of the same Institute, have presented the collections "*Sugars of the world*" (more than 500 exhibits from different countries) and "*Unusual angelica*".



April, 20 is the field day in the life of the Institute of Catalysis. It is birthday of **Academician Georgii K. Borezskov**, the founder of the Institute. To date for this day the problem seminars where post-graduates and young researchers of the Institute report on their work has become a tradition. At the last seminar the works in the field of heterogeneous catalysis, priority field of Borezskov's activity have been presented.



May, 31 the "Gasprom" Delegation visited Novosibirsk Scientific Center, and three institutes of the Center – the Borezskov Institute of Catalysis, Institute of Oil and Gas and Institute of Theoretical and Applied Mechanics. At the Exhibition Center of the Siberian Branch they became interested in many developments of the Institutes of the SB RAS.



June, 9 the solemn meeting of the SB RAS Presidium, Administration of the Novosibirsk Region, Novosibirsk City Administration, scientific community and Higher Education institutes dedicated to the 70th anniversary of **Academician Valentin A. Koptuyg** has been held at the House of Scientists of the Novosibirsk Scientific Center. V. Koptuyg was the Chairman of the Siberian Branch for 17 years. The epoch of V. Koptuyg in the SB RAS is characterized by development and final formation of the Siberian Branch, and then by the period of system crisis in our country, the time of catastrophes and destructions. He had a quality very

valuable to the people surrounding him, which at the same time complicated hardly his own life. He worked always to his full capacity.



August, 21 the Novosibirsk Scientific Center has accepted eminent guests: the Second General Assembly of the Association of Asian Academies of Sciences and the Third International Symposium "Transfer and Adaptation of Advanced Technologies in Asia" has been opened at the House of Scientists. **Academician Valentin N. Parmon** gave a report.



At the end of October the House of Scientists has received the participants of the International Conference "University, Science, Business in Conditions of Contemporary Open Information Society", held by joint efforts of the Ministry of Education of Russian Federation, the Novosibirsk State University, the SB RAS, Administration of Novosibirsk Region, the "Open Society" Institute and the leading software companies.

The urgency of cooperation of representatives of educational, scientific and business areas to resolve problems of equal importance is commonly recognized. It is the Professor Parmon's opinion that the Conference is ten years late. However, now is just the time of reasonable approach to the problem. V.N. Parmon agrees with the attitude of the Administration of Novosibirsk region that the economical upturn should be predominantly based on high-tech innovations. He states that the progress needs experts in the areas of science and business. That is why the master-education system must be developed to allow physicists and mathematicians to be trained in economics.



Presidium of RAS resolved: gave a purse in the name of A.A. Balandin of 2001 year to **Prof. T. Andrushkevich, Dr. V. Bondareva, Dr. G. Popova** for the series of works "*Heterogeneous-Catalytic Oxidation of Alkaline Organic Substances to Carbon Acids: Mechanism, Kinetics and Catalyst Design*".



During the XXXVIII Annual BIC's Competition of the Research Works the 1 Prize has got the work by Yu.I. Aristov, N.M. Bukhavtsova, N.V. Vernikovskaya, V.P. Doronin, L.Yu. Il'ina, K.V. Kolmagorov, I.V. Koptuyug, V.N. Korotkikh, A.G. Okunev, N.M. Ostrovskii, T.P. Sorokina, M.M. Tokarev, N.A. Chumakova "*Selective Water Sorbents for Gas Dehydration*".



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 «Altay», Biysk
- «Ecogeochem Ltd.», Moscow
- Association «Russian House for International Scientific and Technological Cooperation»
- Other scientific, commercial and financial institutions.

The Foundation is supported by IUPAC and some Russian sponsors.

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. During November 1997 - January 2001 Zamaraev International Charitable Scientific Foundation conducted 7 competitions between young Russian scientists working in the field of chemical catalysis and physical chemistry. The results of these competitions had been summed up, 30 winners received Zamaraev post-graduate scholarships, 20 scholars – student scholarships. These scholarships will help to support young scientists in their researching work.

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. The following students, who made diploma in the Institute of Catalysis, have got the Student Scholarships –2001

A. Lysova (NSU, Novosibirsk)

A. Matveev (NSU, Novosibirsk)

A. Moseichuk (TSU, Tomsk)

A. Panchenko (NSU, Novosibirsk)

P. Snytnikov (NSU, Novosibirsk)

Next post-graduates have got the post-graduate scholarships-2001:

N. Trukhan, A. Vedyagin, I. Mishakov



9 Ph.D. students and scientific employees of the Institute and also representative of the students 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. Geogii 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 were 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 Mepodium to G.K. Boreskov. Visitors can see an unusual exposition displaying the full attributes of ceremonies of awarding the HONORIS CAUSA titles to Gerogii 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.

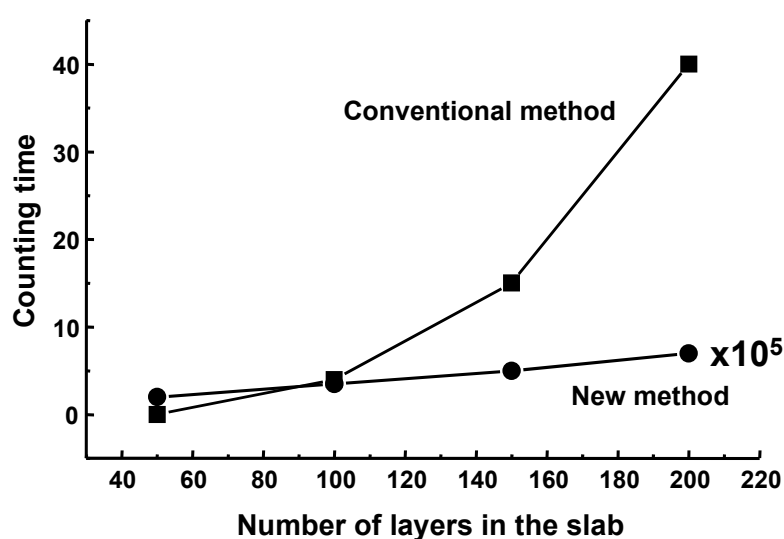
Everyone, who knew personally Kirill Ilyich, remember his exceptional ability not to loose courage at any, even very severe, circumstances. He had a really iron character, and it was not without vain that the sport he went in for was mountaineering.

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

**IMPORTANT RESULTS OF THE R&D
BY THE BORESKOV INSTITUTE
OF CATALYSIS FINISHED IN 2001**

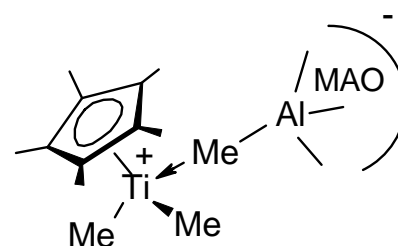
➤ New methods for quantum chemical calculations were developed to allow the expenses of computing to be considerably decreased. A special and accurate presentation of electron wave functions in the form of incident and reflected from the surface Bloch waves was proposed for slabs. That made it possible to derive a set of equations determining the wave function, whose order being independent on the thickness of the processed slab. The given approach allows the time of quantum chemical computing of an extended class of tasks to be reduced by several orders of magnitude. For example, the time taken to compute a 50-layer crystal slab using the new method is reduced by almost 5 orders of magnitude.

Thus, the tasks allowed now to resolve only using supercomputers can be processed with ordinary computers, while supercomputers can be used for essentially new problems.

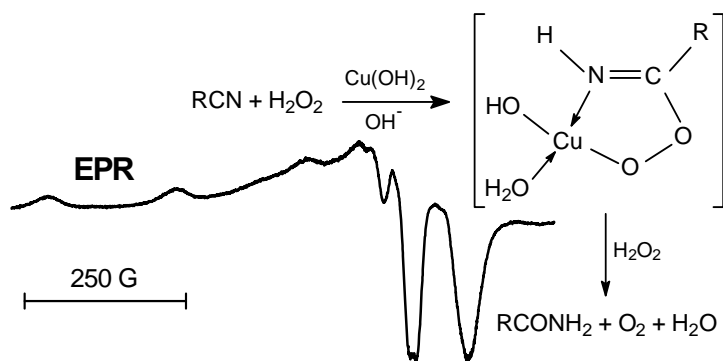


Laboratory of Quantum Chemistry, Head: Prof. Georgii M. Zhidomirov

➤ Titanium complexes formed in practically important catalytic systems for production of syndiotactic polystyrene $C_5(CH_3)_5TiMe_3+MAO$ and $C_5(CH_3)_5TiCl_3+MAO$ was first characterized using ^{13}C NMR spectroscopy. The cationic intermediates $C_5(CH_3)_5Me_2Ti^+ \leftarrow Me^- - Al \equiv MAO$ (Fig.) were found to predominate in reaction mixture (jointly with the Laboratory of Catalytic Polymerization).



Cu(II) complex with peroxy imino-acid formed upon acetonitrile reaction with hydrogen superoxide in alkaline solution was first determined and characterized using EPR (jointly with the Laboratory of Catalytic Methods of Solar Energy Conversion)



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

- The connection between spatial-temporal surface transformations and generation of self-oscillations in the reaction of carbon oxide oxidation over palladium has been established.

Group of Scanning Spectroscopy, Head: Dr. Aleksey N. Salanov

- A new research area – *Physicochemical basis of formation of supramolecular structure of heterogeneous catalysts and porous materials*, a division of the general theory of catalyst preparation – was formulated and validated. It seems reasonable to consider it as an independent discipline because theoretical and practical approaches to formation of chemical and phase composition of catalysts are essentially different from the approaches to formation of their supramolecular structure. The former mainly refer to methods and laws of molecular chemistry, while the latter are based on supramolecular physical chemistry including the theory of surface and capillary phenomena, statistical thermodynamics and mechanics of small-sized objects, a number of special divisions of geometry, as well as modern supramolecular organic chemistry and biochemistry.

Laboratory of the Texture Studies, Head: Prof. Vladimir B. Fenelonov

- By using *in situ* solid state ¹³C MAS NMR and *ex situ* GC-MS, the analysis of the mechanism of n-butane isomerization over sulfated zirconia catalyst (SZ) has been performed. It is shown that upon n-butane-1-¹³C conversion on SZ at 20°C two parallel processes occur: (1) labels scrambling in n-butane and (2) skeleton isomerization of n-butane to iso-butane. No formation of the products of butane disproportionation (propane and pentanes) was detected at the initial stage (a few hours) of the reaction. The analysis of ¹³C label distribution in butanes after reaction revealed that the label scrambling in n-butane proceed via intra- (or mono-) molecular pathway, whereas n-butane isomerization to iso-butane occurs via bimolecular mechanism (formation of C₄⁺, its dimerization, β-elimination).

➤ 1. The electronic peculiarity of the Pt(100)-(1×1) surface affected by different adsorbates was studied by Disappearance Potential Spectroscopy. Two below types of features were revealed in DAP spectra:

(i) The first type of features corresponds to the ordinary threshold excitation of the platinum core electron to available vacant state. These features are mainly attributed to the substrate properties and faintly depend on the adsorbate origin. The peak locations are in good agreement with LDOS calculations that related to platinum unoccupied states;

(ii) The second type of features evidences for the conjugate electron transition, which includes the above excitation of the substrate core electron and excitation of the valence electron of adsorbed species to vacuum level. The location of the respective satellites in DAP spectra strongly depend on the adsorbate origin.

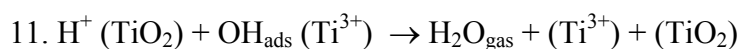
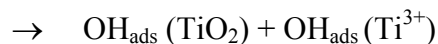
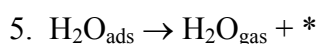
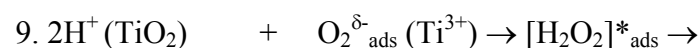
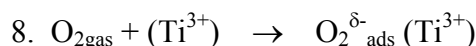
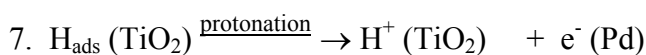
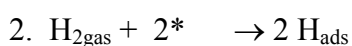
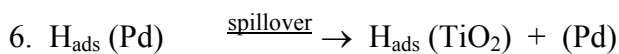
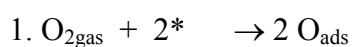
The present results testify to the substantial unity of the substrate and adsorbate electronic structure and display potentials of the DAPS technique to reveal the peculiarities of the surface unoccupied states and valence states corresponding to both the substrate and adsorbate.

2. A dual-site mechanism of H₂ dissociation on the Pd particles and then migration H_{ads} across the TiO_x surface to the active sites with the O₂^{δ-}_{ads} species have been studied on the defects of Ti³⁺-□_O/TiO₂ and Pd-Ti³⁺-□_O/TiO₂ types with XPS, UPS, TDS, mass-spectrometry and pre-adsorbed oxygen photodesorption techniques. The effect of spillover phenomena (H_{ads}/Pd → O_{2ads}/Ti³⁺/TiO₂) on the overall rate of H₂ oxidation have been studied as well. The role of defects (Ti³⁺ sites) in the adsorption centres formation, their stabilization by the palladium particles and then defects participation in H₂ + O₂ reaction have been studied on the TiO_x surface. The results obtained with H₂ + O_{ads} reaction over Pd (110) single crystal surface have been compared. The process of hydrogen oxidation can proceed on two kinds of sites of the Pd model catalyst, *i.e.* on Pd and Ti³⁺/TiO₂, due to the hydrogen spillover from Pd to Ti³⁺/TiO₂.

The mechanism of H₂ + O₂/Pd-Ti³⁺/TiO₂ reaction with participation of spillover effect:

H₂ oxidation on Pd crystallites

Spillover effect in H₂ oxidation on Ti³⁺/TiO₂



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

➤ Simple in realization and very effective in resolution MQMAS method has become very popular in solid state NMR spectroscopy. Spectacular results have been obtained with a number of nuclei, among them: ^{27}Al , ^{23}Na , ^{11}B , ^{87}Rb . However, it is commonly admitted that small value of quadrupolar moment and large value of chemical shielding anisotropy are a limitation to MQMAS and, in particular, prevent its application to vanadium nucleus. In cooperative work with French colleagues it has been demonstrated that MQMAS technique can also be successfully applied to vanadium nucleus. The results obtained show that combination of ultra high rotation frequency (30-35 kHz) with low power radio-frequency excitation allows the application of MQMAS to vanadium nucleus at all vanadium coordination, specially for complex spectra with overlapping lines. In the latter case MQMAS has significant privilege among other techniques. Figs 1, 2, and 3 demonstrate 3QMAS spectra for different vanadium coordination.

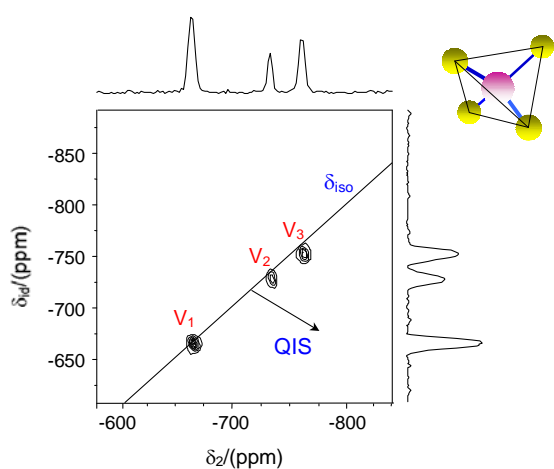


Figure 1. 1D and 2D 3QMAS ^{51}V NMR spectra of AlVO_4 . Isotropic (δ_{iso}), and quadrupolar-induced shift (QIS) axes as well as three nonequivalent vanadium sites (V_1 , V_2 and V_3) of Q^0 type are marked.

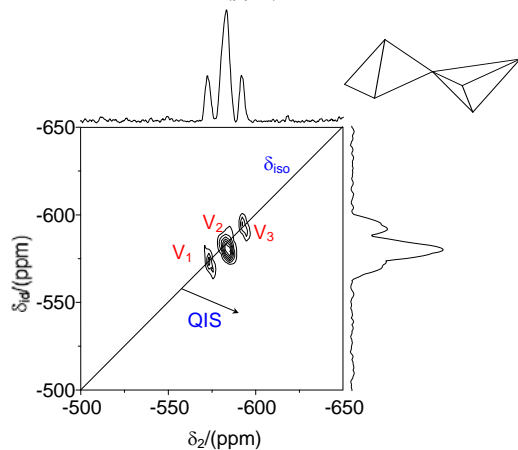


Figure 2. 1D and 2D 3QMAS ^{51}V NMR spectra of $\text{Ba}_2\text{V}_4\text{O}_7$. Isotropic (δ_{iso}), and quadrupolar-induced shift (QIS) axes as well as three nonequivalent vanadium sites (V_1 , V_2 and V_3) of Q^2 type are marked.

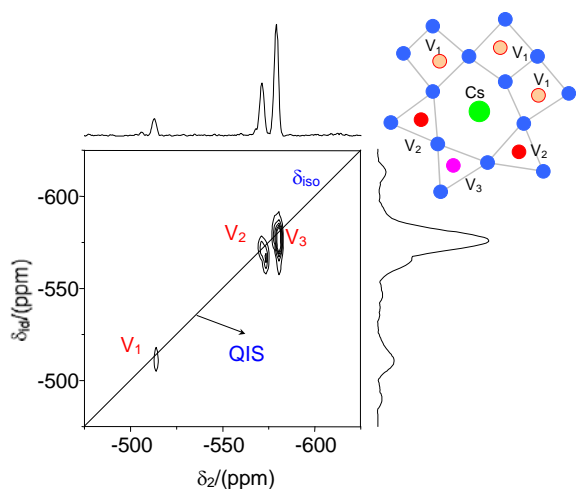
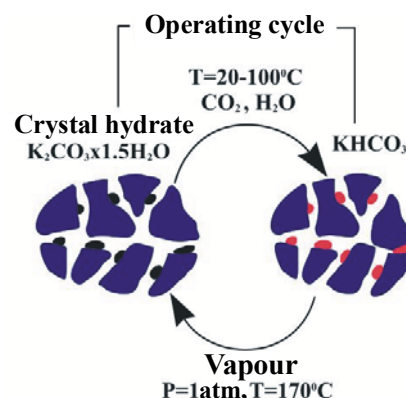


Figure 3. 1D and 2D 3QMAS ^{51}V NMR spectra of $\text{Cs}_4\text{V}_2\text{O}_{11}$. Isotropic (δ_{iso}), and quadrupolar-induced shift (QIS) axes as well as three nonequivalent vanadium sites (V_1 , V_2 and V_3) tetrahedral and pentahedral coordination are marked.

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

➤ Composite sorbents “potassium carbonate in a porous matrix” were developed for removal of carbon dioxide from wet gases. For five sorbents the influence of matrix nature and preparation procedure on their dynamic sorption capacity was studied at $T=40\text{-}170^\circ\text{C}$. As a result, the sorbent $\text{K}_2\text{CO}_3/\text{Al}_2\text{O}_3$ was found to have at 40°C the dynamic capacity of 0.4 g of CO_2 per 1 gram of the sorbent under conditions of high humidity of the inlet air. For this sorbent its composition as well as preparation and regeneration procedures were optimized to reach its stable operation under multiple cycles “sorption-desorption”. The sorption capacity of the composite was found to decrease with temperature, however even at 170°C it is still 30% higher than the capacity of zeolites. The study of mechanism of carbon dioxide sorption demonstrated that high capacity can be reached only in the presence of crystallization water in the sorbents.



Laboratory of Energy Transforming Materials, Head: Dr. Yurii I. Aristov

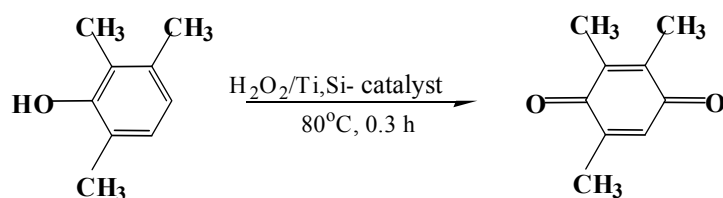
➤ NMR and IR spectroscopic techniques were used to study the structure of active sites of catalysts V_2O_5 supported on Al_2O_3 , TiO_2 , or the $\text{Al}_2\text{O}_3\text{-TiO}_2$ mixture. Critical phenomena were observed during oxidation of hydrogen sulfide in solutions (pH 10-13). Kinetic and physicochemical studies made it possible to establish general features of the mechanism of H_2S oxidation in solutions and over solid catalysts and to suggest the reaction mechanism.

A new method for catalytic gas purification from hydrogen disulfide was developed based on gas-phase oxidation of major quantity of H_2S followed by liquid-phase afteroxidation of rest non-oxidized hydrogen disulfide. The concentration of H_2S in the purified gases can be attained as low as 10 ppm.

Laboratory of Catalytic Processes for Desulfurization, Head: Prof. Nikolai N. Kundo

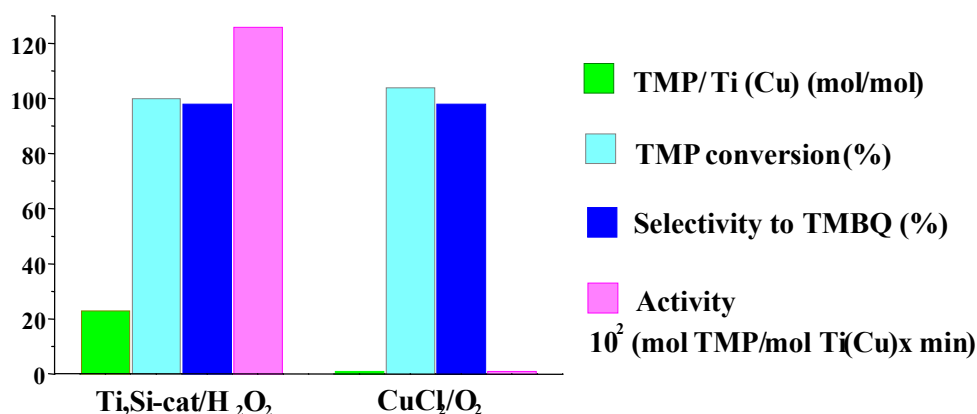
➤ Mesoporous TiO₂-SiO₂ mixed oxides with varied titanium content and porosity (aerogels and xerogels) were synthesized and characterized by elemental analysis, N₂ adsorption and IR-spectroscopy.

Parallel testing of catalytic properties of well-organized mesoporous mesophase materials (Ti-MMM) and amorphous TiO₂-SiO₂ mixed oxides in oxidative reactions of methyl-phenyl-sulfide to sulfoxide and sulfone and 2,3,6-trimethylphenol (TMP) to 2,3,5-trimethyl-1,4-benzoquinone



(TMBQ) with aqueous H₂O₂ has been performed. All the materials study have been proved to operate as truly heterogeneous catalysts. No titanium leaching occurs from the solid matrixes

during the oxidation process. For samples with similar titanium loading, both the catalytic activity and TMBQ yield appeared to fall in the order TiO₂-SiO₂ aerogel > Ti-MMM > TiO₂-SiO₂ xerogel and correlate with average mesopore diameter and mesopore volume. The selectivity to TMBQ attains 98% at 100% TMP conversion under optimal reaction conditions.

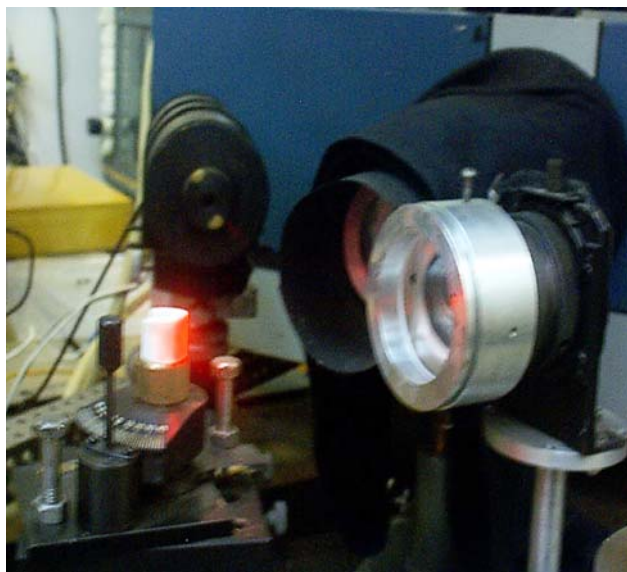


Titanium content in Ti-MMM determines the state of active catalytic site and influences on the structure regularity, thus effecting the catalytic behavior. Factors effecting the catalyst stability and catalytic activity after re-cycling have been studied. Some loss of catalytic properties observed after recycling may occur due to collapsing of the catalyst structure caused by water.

Group of Stereoselective Catalysis, Head: Dr. Oxana A. Kholdeeva

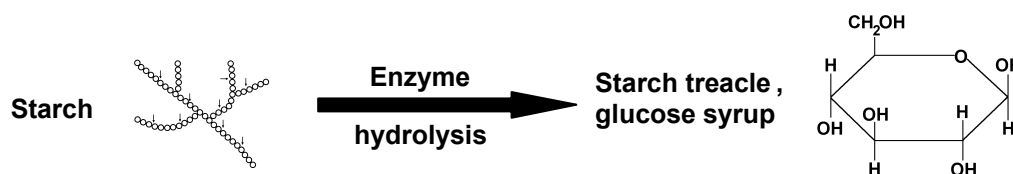
➤ Experiments on recording luminescent UV spectra through the long-wavelength infrared region were carried out with samples of alumina, silica, zirconium oxide, titanium oxide, as well as other supports, catalysts based thereon and metals. Luminescence of the sample surface was excited by radiation of a pulse ultraviolet ArF laser at a high density of radiation power on the sample at atmospheric conditions over a large temperature range. It was discovered that the recorded spectra

are high sensitive to the nature and phase composition of the sample, as well as to compounds adsorbed by the surface. In particular, appearance of octahedrally and tetragonally coordinated atoms of impurities was detected in metastable alumina species. It was confirmed that luminescent lines of $\alpha\text{-Al}_2\text{O}_3$ and $\theta\text{-Al}_2\text{O}_3$ phases with trace concentrations of impurity ions are at their own characteristic wavelengths. Therefore, laser induced fluorescence spectroscopy based on a pulse excimer laser can be used for remote control of variations in the phase composition of catalysts. This method also can be used, among others, to studying heterogeneous chemical reactions under real conditions of high-pressure chemical reactors on the time of micro- or nanoseconds.



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

➤ Macrostructured carbon-containing ceramic supports were comprehensively studied as adsorbents for immobilization of various enzymes to develop heterogeneous biocatalysts for biotechnology. As a result, a high-stable heterogeneous biocatalysts for the process of continuous starch hydrolysis were developed. The highly stable biocatalyst was obtained via adsorption of glucoamylase on the supports covered by a surface layer of the *catalytic filamentous carbon (CFC) morphology*. The stability of immobilized glucoamylase increased by an order of magnitude against that of the soluble enzyme. Study of the activity of the developed biocatalysts at flow reactor conditions revealed that the rate of starch hydrolysis was restricted by starch/dextrins diffusion. The pore-diffusion resistance depended strongly on the morphology of the surface carbon layer and can be decreased using intentionally synthesized supports with transport pores larger than 1 μm in size. Macrostructured CFC-coated ceramics supports of complex geometric shape (honeycomb monolith, foam-like materials) were undoubtedly promising adsorbents for the applications in biocatalysis and biotechnology.

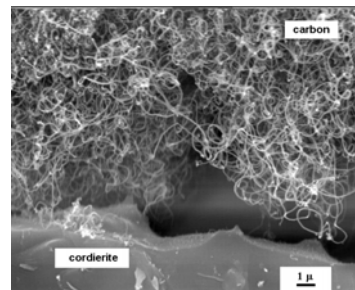


Enzymes Glucoamylase from *Aspawamori*

Support Macrostructured inorganic supports, covered by catalytic filamentous carbon

Stability of heterogeneous biocatalyst

1.5 year without loss of activity



Group of Biocatalysis, Head: Dr. Galina A. Kovalenko

➤ The new thermodynamic model and a solution algorithm are proposed for calculation of partial molar volumes of reactants and activated complex, and of the reaction rate constant dependence on supercritical fluids density. A thermodynamic approach was developed based on the concept of equilibrium of reactants and activated complex formed via interaction of reacting molecule with the solvent.

The analysis of stationary states for reactions of benzene hydrogenation and liquid-phase methanol synthesis in the batch reactors has been made.

The catalytic regularities of thiophene gas phase hydrogenation over sulfide-palladium catalyst IC-73-4 have been studied and the reaction rate constants and activation energies have been estimated.

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

➤ An active catalyst was suggested for the new process for synthesis of thioles by hydrogenation of organic di- and polysulfides. Small-scale method of its preparation was developed. Selective hydrogenation of dialkyldisulfides and di- and polysulfides of spatially hindered phenols over this catalyst was achieved at the yields up to 90 mol %.

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

➤ The outer surface of nickel particles formed during the growth of carbon filaments is built-up by crystallographic 111, 110 and 100 faces in the proportion depending on the conditions of carbon formation. These particles behave as active components of metal-carbon systems for hydrogenation reactions. Hydrogen chemisorption by 111 and 100 faces results in formation of hydride species of hydrogen, which is responsible for complete hydrogenation of dienes and

acetylenes into paraffins. The chemisorption by 110 faces produces atomic hydrogen species active to selective hydrogenation of dienes and acetylenes into olefins.

A phenomenological model of mechanochemical activation (MCA) was proposed based on the concept of the solution of various types of defects in the crystal lattice, the defect concentration and equilibrium between them being dependent on the energetic strain, i.e. on the dissipation level. The Gibbs-Folmer concept on critical sizes and conditions of a crystal nucleus growth were expanded to the processes of dispersing, multiplication of defects in the course of MCA, conditions of condensation of point and dispersed defects into linear and planar defect structures. The role of dissipative structures generated at MCA of different intensities was discussed.

Laboratory of Dehydrogenation, Head: Prof. Roman A. Buyanov

➤ Unique honeycomb catalysts were developed for selective oxidation of natural gas into syn-gas at millisecond contact times and 800–1000°C. Application of innovative approaches to synthesis of corundum-based monolithic supports, as well as the proper choice of the active component composition – platinum metals with complex perovskite-like and fluorite-like oxide systems - allowed the high activity and selectivity of the catalysts to be provided at a considerably lower loading of the noble metals compared to that in the known analogues. The developed catalysts maintain their high activity and selectivity during long life tests with mixtures containing natural gas and air, they also are resistant to thermal shocks and carbonization. The new process allows the capital costs to be decreased by a factor of 5 to 10 and the current cost by 30 to 50% against those of the processes known before.



The process was scaled-up for designing the first industrial plant at the Norilsk Mining and Smelting Co. The technology for manufacturing of commercial prototypes of thin-wall monoliths and catalysts based thereon was tested. A semicommercial batch of the catalysts (100 l) was synthesized. An industrial reactor for generation of syn-gas at short contact times for direct reduction of dispersed oxides (nickel oxide) into the metal powder was developed, assembled and supplied to the customer. The low cost of syn-gas produced by the selective oxidation of natural gas makes it a promising feedstock for chemistry, metallurgy and electronics.

Laboratory of Catalysts for Deep Oxidation, Head: Prof. Vladislav A. Sadykov, Department of Applied Catalysis, Head: Il'ya A. Zolotarskii

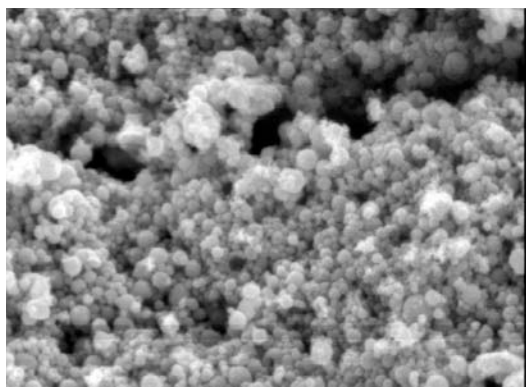
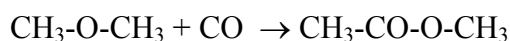
➤ Processes of formation of phyllosilicates of nickel and nickel-magnium-aluminium, as well as nickel-magnium phylloaluminosilicates structured as amesite and hydrochlorite were thoroughly studied. Regularities were established for transformations of the formed silicate and

aluminosilicate structures during temperature elevation in reductive and inert atmospheres, as well as in the presence of water vapor and H₂O + CO + H₂ mixture.

The results obtained allowed us to choose conditions for preparation of nickel-silicon-containing catalysts for steam reforming of methane. The catalysts are free of silica, stable under hydrothermal conditions and under conditions of steam reforming of methane and light hydrocarbons. They are highly active to steam reforming of hydrocarbons but low active to formation of carbonaceous deposits. Of particular importance are their specific rheological properties that makes it possible to produce complex shaped granules of the catalyst.

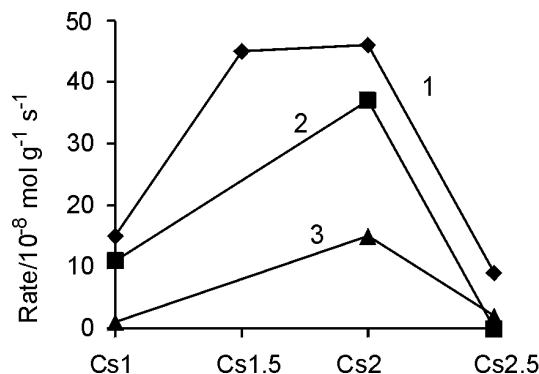
Laboratory of Catalytic Conversion of Carbon Oxides, Head: Prof. Tamara M. Yurieva

➤ It was found that halide-free carbonylation of dimethyl ether (DME) to methyl acetate occurs on Rh/Cs_xH_{3-x}PW₁₂O₄₀ (1.5 ≤ x ≤ 2 and Rh ≥ 0.1%) catalysts:



1% Rh/Cs₂HPW₁₂O₄₀

S = 100 m² g⁻¹



1 - rate of methyl acetate formation

2 - rate of isopentane formation
[B.B. Bardin, R.J. Davis, Topics in Catalysis, 6 (1998) 77]

3 - rate of isobutane formation
[N. Essayem, G. Coudurier, M. Fournier and J.C. Vedrine, Catal. Lett., 34 (1995) 223]

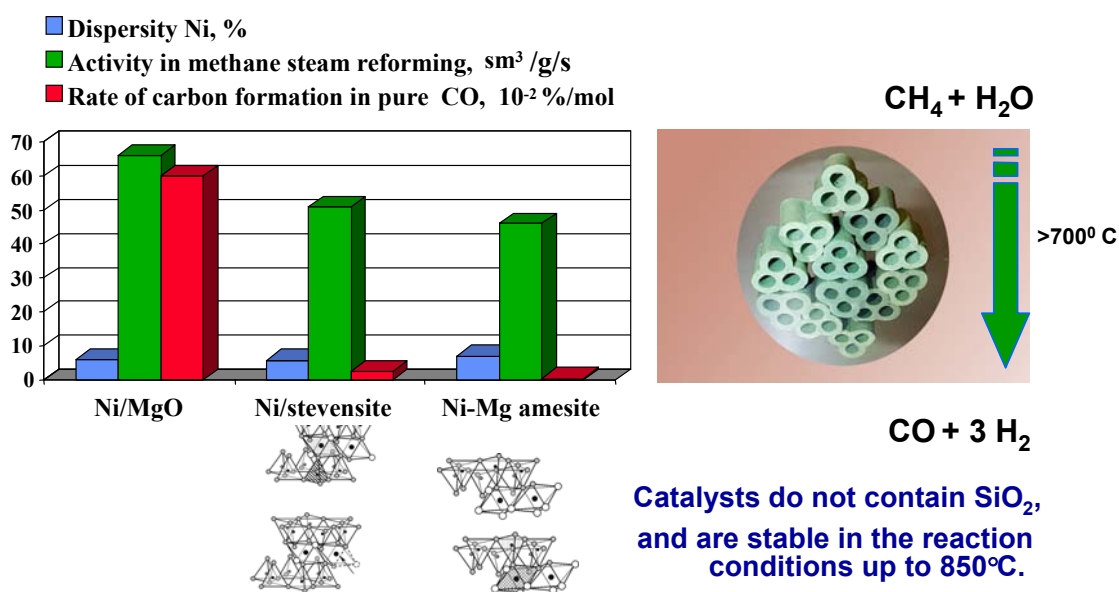
The best catalysts Cs1.5 and Cs2.0 can activate C-O bond (E=350 kJ/mol) in DME that is similar to activation of the C-C bond (E=344 kJ/mol) in alkanes. This stage replaced the activation C-I bond (E=240 kJ/mol) in methyl iodide - first step in typical carbonylation reactions (for example, industrial methanol carbonylation to acetic acid).

Group of Catalytic Synthesis of Oxygen-Containing Compounds, Head: Dr. Galina G. Volkova

➤ Ni-based catalysts are known to be very active in methane steam reforming. The most critical disadvantage of these catalyst is the occurrence of carbonization processes in the target reaction

conditions, which significantly shortens the term of the catalyst operation and may cause the death of the industrial methane conversion reactor. In literature, there were reported some indications that Ni-containing catalysts on the Si-containing supports are not active in the undesirable reactions of carbonaceous phase formation. However, using of these supports is not spread to the methane steam reforming, since they are not stable in the reaction conditions. In these conditions (i.e. at above 700°C) silica readily reacts with water vapor giving volatile compound Si(OH)₄, which then is condensed in the heat-exchangers as SiO₂.

Several Ni-Si-containing catalysts were developed, where silicon is stabilized either in the structure of the layered silicate of Mg (stevensite) or in that of Ni-Mg aluminosilicate (Ni-Mg chlorite-vermiculite). The methods for the synthesis of the precursor compounds (i.e. Ni-Mg hydroxycarbonate supported by Ni-Mg stevensite and Ni-Mg amesite) were developed as well. The so obtained catalysts do not contain SiO₂, they are stable in the reaction conditions up to 850°C. In their active state, catalysts contain Ni as dispersed particles with a dispersion of *ca.* 5-7 %, which are highly active in methane steam reforming. At the same time, these catalysts are significantly more stable in respect to coke formation comparatively to their Si-free analogues. For example, the rate of graphite-like carbon formation in the pure CO flow at 1 bar is 20-70 times lower over the designed catalysts with respect to that over Si-free Ni-containing catalysts.



The additional advantage of the developed Ni-Si-containing catalysts are their excellent rheological properties (which are caused by their layered (clay) structure). This allows producing the grains of complicated shape, which is necessary to achieve the optimal heat and mass transfer in the catalyst bed.

**Laboratory of Catalytic Conversion of Carbon Oxides, Head: Prof. Tamara M. Yurieva;
Group of Catalytic Synthesis of Hydrocarbons, Head: Dr. Alexander A. Khassin**

➤ High-active and selective catalysts (aqueous solution of palladium with Mo-V-P heteropolyacid) were developed for oxidation of C₂ – C₄ olefins into corresponding carbonyl compounds such as acetaldehyde, acetone or methylethylketone (MEK). The work on synthesis of MEK is of practical importance and commercially promising.

Group of Catalysts and Processes Based on Heteropoly Acids

Head: Prof. Klavdii I. Matveev

➤ ¹H and ²H NMR techniques were used for studying the influence of the nature of organoaluminium activators of different compositions on catalytic properties for ethylene polymerization and the structure of intermediates formed in the *bis*(imino)pyridineiron(cobalt) (II) chloride based systems. The obtained experimental data revealed for the first time that active sites in these systems are neutral but not ionic complexes.

This idea was the basis for developing preparation procedures and compositions of supported catalysts containing *bis*(imino)pyridine complexes of Fe(II). New highly-active and stable catalysts were synthesized using SiO₂ and MgCl₂ as supports.

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

➤ Development of functionally new digital gas flowcontrollers was accomplished. The devices currently used everywhere for physicochemical studies are analog heat mass flowcontrollers. The digital devices employed instead of analog ones enable to expand the dynamic range, to improve the batching accuracy and reproducibility of the gas feeding, to make the cost of automatic gas meters several times lower.

Creation of digital flowcontrollers is the most important achievement at the Laboratory. Accomplishment of this work allows a number of unique devices competitive to the best foreign analogues to be proposed. For example, a kinetic installation of new generation, a new adsorption apparatus for measuring specific surface area (in cooperation with the Institute of Semiconductor Physics), several versions of high-precision devices for preparation of reference gas mixtures etc. were developed in 2001 based on the digital flowcontrollers. Examination of new tools demonstrated that they are much superior in accuracy and efficiency to the devices used before.

Laboratory of Catalysts Activity Testing, Head: Dr. Nikolai N. Bobrov

➤ The nature of products deactivating surface of sulfated zirconium oxides during alkylation of isobutane with butylenes was studied. It was concluded that the deactivation results from formation of surface zirconocene complexes behaving as polymerization sites.

The process of chlorination of paraffin hydrocarbons with chlorine and carbon tetrachloride was studied. It was shown that there is the active chlorination of paraffins under the action of chlorine at the temperature range of 50 to 200°C to add chlorine to predominantly terminal

carbon atoms. With carbon tetrachloride, paraffins are chlorinated over H-ZSM-5 zeolites at the temperature as low as 350°C, aromatic compounds, tetrachloroethylene and trichlorodivinyll being observed along with chloroform among the reaction products formed from the propane-butane fraction.

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

➤ Laboratory of Catalytic Conversion of Hydrocarbons has developed a process of one-stage conversion of middle distillates, heavy oil fractions and non-stable gas condensates into high-octane gasoline, winter diesel and liquefied gas C₃-C₄ (**Bi-MF process**).

- The process proceeds in a continuous flow reactor with a fixed bed of not containing noble metals zeolite catalyst (IC-30-1M) at T= 350-450⁰C and P<10 atm. Hydrogen presence during the reaction is not necessary.

- Both non-stable gas condensates and straight-run oil fractions (starting boiling point – 35⁰C, final boiling point – 350-370⁰C) without their preliminary distillation can be used as initial raw material.

- A total sulfur content in the initial stuff is not limited.

- A sulfur content in the reaction products – high-octane gasoline and diesel – makes up less than 0.05 %wt. During the process sulfur compounds are converted to hydrogen sulfide.

- The catalyst is regenerated using a mixture of nitrogen with air making oxygen content 0.5-1.5% in a regular manner. Duration of the stage is not exceeded 80 hours.

- Duration of Time-On-Stream of the catalyst with reaction temperature increase makes up 120 hours at least.

- The catalyst is produced in an industrial scale on JSC “NZHK” (Novosibirsk, Russia under a license owing to Boreskov Institute of Catalysis.

- A main advantage of the developed process is considerable both simplification and reduction of prices of oil processing along with simultaneous increase of gasoline and diesel fuels yield. Processes of hydrotreating, reforming and dewaxing are not required.

- During August 2001 Boreskov Institute of Catalysis and “Plasmokhim Ltd. Co.” (Kazan) have carried out experiments using a pilot installation (reactor volume 1500 cm³) on a synthesis of motor fuels from oil distillates (boiling end 350⁰C, S content 3.75% wt.). The results obtained previously on a laboratory installation in BIC were totally confirmed.

➤ The next reaction conditions in the pilot experiments were used:

Initial reaction temperature - 350⁰C

Reaction pressure – 10 atm

WHSV – 3 h⁻¹

➤ The results obtained in the course of experiments:

Yield of liquid product – 80-85%

Motor octane number of gasoline fraction – 80-85

Benzene content doesn't exceed 1% at total aromatics content 30-40%

Diesel fraction corresponds to winter grade

S content doesn't exceed 0.05% wt.

Below is a material balance of the process of production of gasolines with motor octane numbers 78-80 and 85-90 calculated on the base of results of pilot experiments (%wt.).

	H ₂	H ₂ S	C ₁ -C ₂	C ₃ -C ₄	Including olefins C ₂ -C ₄	Gasoline	Motor octane number	Diesel fuel
Raw material (boiling end 360 ⁰ C)		3.75(S)		0.35		47.8	58	48.1
Product 1	1.0	3.7	1.1	11.2	3.5	47	78-80	36
Product 2	1.7	3.7	0.8	14.8	1.0	53	85-88	26

The Bi-MF process doesn't requires working out of non-standard equipment and can be realized using standard equipment of refineries. Reaction block represents two lines each constituting from one to three reactors in dependence on the installation productivity. The Bi-MF process is endothermic and requires intermediate heating of reaction mixture. During the process one line of the reactors is in "reaction" conditions, while other line is in "regeneration" conditions. Such technology is used, for example, in Zeoforming process – production of gasolines from gas condensates and straight gasoline fractions. The Bi-MF process uses another catalyst, this let to increase boiling end of raw material from 200⁰C to 360⁰C along with a small change of reaction conditions (comparatively with Zeoforming process). Thus, the same technological scheme let to obtain both high-octane gasoline and winter diesel fuel in ratios variable in dependence on reaction conditions (Products 1 and 2 in the Table).

The Bi-MF process can use other raw materials as well. The next reaction was investigated on a laboratory scale in BIC. Heavy vacuum gasoil (fraction 350-500⁰C) is underwent by mild hydrocracking using a hydrotreatment catalyst (T=400-450⁰C, P=20-30 atm, WHSV=0.7-1.0 h⁻¹) to obtain fraction with boiling end 360⁰C. The resulting product is used as a raw material for Bi-MF process. The reaction products in this case are the same as described above.

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

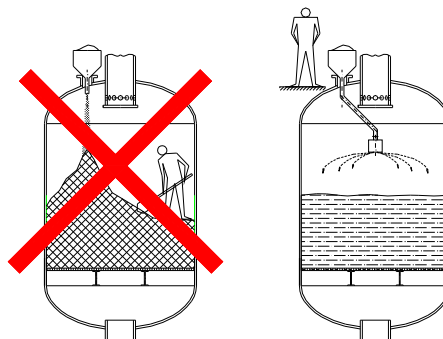
➤ The technology of synthesis of catalyst IC-27-42 for treatment of Claus tale gases from hydrogen sulfide was successfully adapted for industrial production by Boreskov Institute of Catalysis in cooperation with Katalizator Co. A semicommercial batch of the catalyst was manufactured by Katalizator Co. and supplied to Omsk Oil Processing Plant.

Laboratory of Dynamics of Catalytic Processes, Head: Dr. Andrey N. Zagoruiko

➤ Experimental studies were carried out using benches modeling conditions attained in contact apparatuses: formation of fixed beds and filtration of reaction flow through the bed. Based on the

results obtained, methods for loading of the fixed catalyst beds into multiple-shelf and tube reactors were developed.

The method is underlain by the principle of free fall of catalyst particles into the produced bed. Key parameters determining the quality of the fixed bed (bulk density, degree of spatial inhomogeneity) are experimentally chosen. In order to put into practice the methods of loading into tube reactors with longer than 12 m tubes (reactors of steam methane conversion for production of ammonia and methanol), coefficients of aerodynamic resistance are studied and chosen for differently shaped catalyst particles in flowing air.



A) Multiple-shelf reactors

Technology and devices for close loading of a granulated catalyst into multiple-shelf reactors are developed. In the technology, the particles are distributed uniformly with compressed air over the loaded bed and then allowed to fall. The developed devices enable two times shorter loading time, controlled increase (5 to 12%) in the bulk density of the fixed bed and provide arrangement of the bed of a uniform structure for the flow to be filtered.

The technology was put into practice in 2001. The reactors loaded in 2001 are 14 in total number, the loaded amount is more than 400 t of the catalyst. Employing of the close packing provides an increase by 8 to 12% in average in the useful reactor volume that results in the potential productivity of the reactors. The loading methods are mainly used for oil processing (Ufa Oil Processing Plant, UfaNefteKhim) and for production of nitric acid (Azot Co. in Berezniki and “Akron” in Novgorod).

B) Tube reactors

The experimental data were used for computing the fall of particles in the counterflow air to propose the technology for loading of granulated catalysts into tube reactors. The technology is based on controlled retardation of the falling catalyst particles by contradirectional air flow to provide the close particle packing in the tubes at equal hydraulic resistance in each tube. The developed method enables charging of the tube reactors without additional making them vibrating for condensing the bed that allows 2-2.5 fold reduction of the charging time.

A device for the technology implementation was designed. Large-scale testing of the device was carried out using a reactor of steam methane reforming at Metanol Co. (Tomsk, Russia).

Laboratory of Unsteady-State Catalytic Methods for Gas Purification,

Head: Prof. Alexander S. Noskov

➤ A demonstration pilot heating unit of 230 kWt capacity was designed and tested. The installation is based on catalytic combustion of solid fuel. It is equipped with peripheral facilities to provide the continuous operation mode.

Laboratory of Catalytic Conversion of Solid Fuels and Wastes, Head: Prof. Aleksandr D. Simonov

➤ In virtue of a number of advantages provided by fuel cells against other kinds of devices for transformation of fuel chemical energy into electric energy, development of fuel cells becomes of urgent importance to scientific community and leading companies engaged in the field.

Among the problems of interest of the Institute of Catalysis is development of a fuel processor for production of hydrogen from hydrocarbon-containing raw materials including natural gas. The first stage of this process is steam reforming of methane. A new type reactor was developed for this stage based on the idea of heat conjunction of the endothermic reaction of steam methane conversion and exothermic reaction of hydrogen oxidation modeling the anodic gas of the fuel cell. The reactor is designed to provide cocurrent feeding of the reactants in the endothermic and exothermic channels. Experimental studies of the operation modes achieved in the reactor showed the provided effectiveness for hydrogen as high as $540 \text{ nm}^3 \text{ H}_2/\text{h}\cdot\text{m}^3$ reactor that corresponded to the expected electric power of 1 kWt/l of the fuel cell. This is much higher than the values obtained with reactors based on separated exothermic and endothermic reactions. Essential advantages of straight-flow against counterflow were demonstrated. Optimal conditions of the heat conjugate reactions were determined. It was shown theoretically that the highest hydrogen yield could be attained using the straight-flow at preheating of the inlet gases in a counterflow recuperative heat exchanger. In this case 1.5 to 3 moles of hydrogen in syn-gas could be produced from one mole of combusted hydrogen (depending on the degree of heat recuperation).

Laboratory of Multiphase Processes Modeling, Head: Prof. Valerii A. Kirillov

➤ Methods were developed for computing periodical process of synthesis of filamentous carbon (FC) from methane/hydrogen mixtures in a fluidized bed reactor at gas flow recirculation. The use of recirculating gas flow was shown to provide ca. 1.5 times specific yield of carbon.

Tools of mathematical modeling were used for studying the influence of temperature gradient in the reactor, fluctuations in temperature and inlet gas mixture flow rate on the preparation process and FC characteristics.

Laboratory of Catalytic Processes in Dynamic Bed, Head: Prof. Gennadii G. Kuvshinov

➤ Efficiency of a new medication Klatiram was studied for dam cow stocks in cattle-breeding farms of Novosibirsk Region. It was established that the recommended doses of the medication for prophylaxis and treatment of pathologies and functional abnormalities in reproductive organs are 150–300 μg ADV depending on the nutritional state and hormone preparations applied before.

**Group of Catalytic Synthesis of Biologically Active Compounds,
Head: Prof. A.G. Tolstikov**

➤ a) Theoretical studies aimed at revision of validation of the possibility to determine excess energy of critical nuclei from experimental data on nucleation were accomplished to derive the relevant equation. Experimental values are mainly included in the equation but the assumptions are in the minimal number allowed by the current status of investigations. The principal distinctive feature of the approach used is no unreliable estimations of the critical nuclei density necessary for the droplet model. Application of the proposed algorithm made it possible to discover a considerable decrease (one second or one third of that given by the droplet model) in the excess energy of the critical nuclei while the cluster diameter approaches one-two nanometers (Fig. 1).

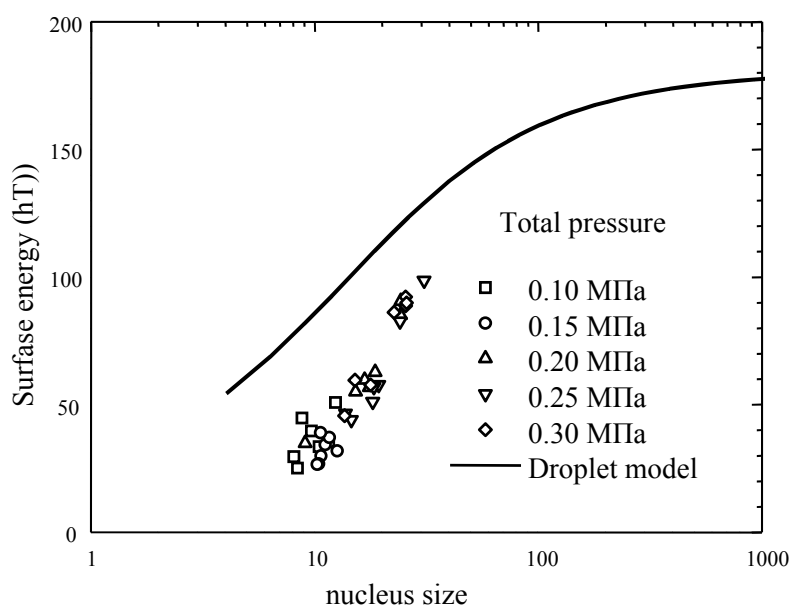


Fig. 1. Surface energy for cluster droplet model (line) and excess energy (points) in dependence of nucleus size (number of molecules in a critical nuclei) for *octanol-SF₆* nucleation

б) To provide experimental validation of the semiempirical method for construction of nucleation rate surfaces, an experiment was undertaken to reveal existence of two nucleation rate surfaces about a triple point as was predicted before (M. Anisimov. *Metastable vapor states diagram*. J. Aerosol Sci., 21(1) (1990) pp. 23-25) (Fig. 2). Bimodality of the particle size distribution (see Fig. 3) resulting from the difference of accommodation coefficients of molecules that impinge the cluster surface of different phase states is a direct evidence of the existence of two nucleation surfaces about a triple point. There is no analogue of the said result worldwide.

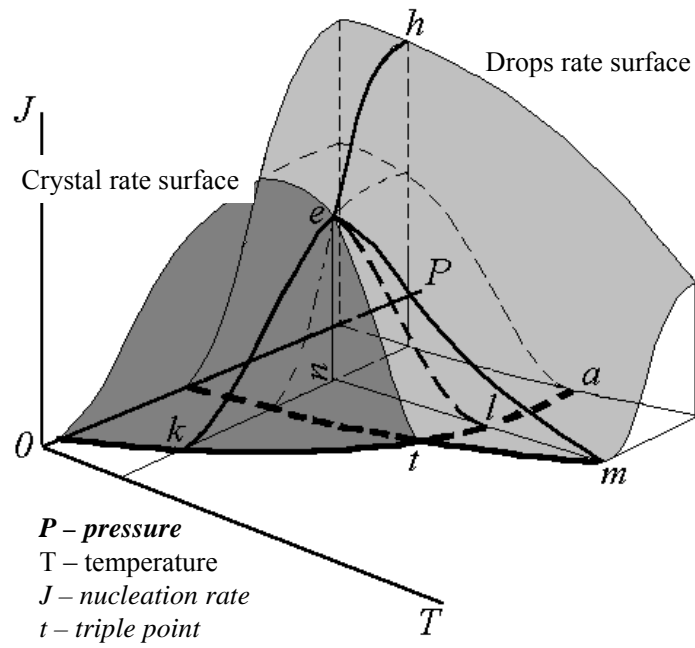


Fig. 2. Topology of the nucleation rate surfaces in the vicinity of triple point

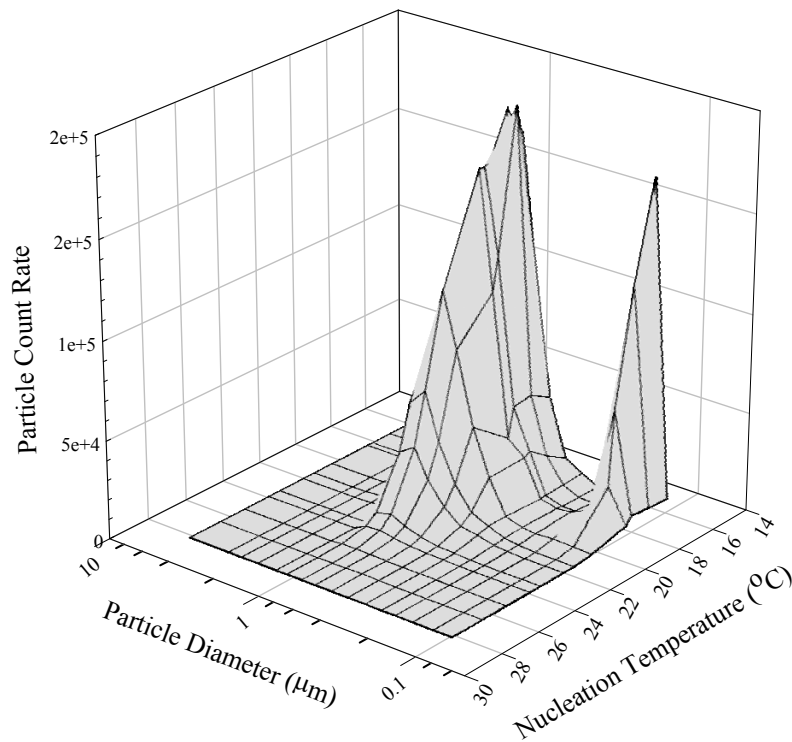


Fig.3. Particle size distribution upon glycerin vapours nucleation near triple point

в) The studies on intercalibration of experimentally measured nucleation rates were carried out. Necessity of transition from the routine task resolved at constant flow mass for a static diffusion chamber to the task with non-preserved flow mass was demonstrated. If so,

experimental data on the nucleation rate obtained by different methods can be brought to an agreement. At present the Laboratory is among the leaders worldwide in the field of development of verifying standards for nucleation rates to allow the commensurable data to be obtained by different teams.

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

➤ Novel derivatives of bis-imines and bis(imino)pyridines as components for a new class of postmetallocene catalysts are synthesized jointly with Vorozhtzov Institute of Organic Chemistry (Novosibirsk). Complexes with methylaluminumoxane cocatalyst prepared therefrom are studied as ethylene polymerization catalysts. A possibility for using some substituted bis(imino)pyridine complexes at elevated temperatures (60–70°C) is demonstrated for the first time. Feasibility of obtaining polyethylenes with various molecular weight values from oligomers to super-high-molecular PE is also shown.

Polymerizations in the conditions close to commercial processes (70°C) are successfully performed without comonomers using derivatives of 1,2-bis(arylimino)acenaphthyl-NiBr₂ complexes as the catalysts components resulting in polyethylenes with molecular weights from oligomers to high molecular polymers with various branching degree.

First silica gel supported catalysts based on bis(imino)pyridines are obtained followed by the beginning of studying their efficiency at gas phase ethylene polymerization using a model installation at Share Holding Company “Kazanorgsynthes”.

Samples of Ti-monocyclopentadienyl derivatives are prepared for the application in styrene-divinyl copolymerization.

Group of the Study of New Catalytic Systems for Ethylene Polymerization and Copolymerization with α -olefins

First in Russia (and probably in the CIS) research and technological approaches to obtaining latexes comprising nano- and microsized hollow particles via synthetic methods (emulsion polymerization) are developed. The main factors responsible for hollow particle geometry are revealed. The synthesized latexes are shown to be useful in pigment polymeric composites. This novel polymer pigments are found to be advantageous over conventional inorganic counterparts such as titania, litopon etc. These studies are performed jointly with Neste Chemicals Co. (Finland). The research activities are supposed to be further developed in the area of functionalization of hollow polymer particle latexes in order to apply them as microreactors with permeable walls to carry out chemical reactions.

Jointly with The Dow Chemical Co. (USA) methods for obtaining asymmetric latex films (with variable chemical composition over the film cross-section) from latex blends are developed. Factors responsible for the degree of latex polymer stratification during the film formation are revealed.

Jointly with The Dow Chemical Co. (USA) several techniques for obtaining hybrid polymer dispersions on the basis of polyurethanes and styrene-butadiene (SB) copolymers are developed. Up to 40% of cheap SB copolymer is successfully incorporated into hybrid polyurethane particles without any deterioration in mechanical properties of the films obtained from the prepared dispersions compared to those formed from merely polyurethane dispersions.

Group of the Study of Emulsion Processes

A possibility for obtaining Aerosil nanostructures in polypropylene matrix in situ in extruder via the hydrolysis of vinylalkoxysilanes sorbed in the matrix was studied jointly with Borealis GmbH (Austria). The formation of SiO₂ nanoparticles in polypropylene is confirmed by electron microscopy. A structuring activity of Aerosil nanoparticles providing the improvement of impact and modulus performances of PP at the filler concentrations less than 1% wt. is revealed. However achievement of the enhanced polymer properties requires precise maintaining of the synthesis conditions to reproduce the formed nanostructures that is hardly attained at processing.

Group of the Modification of Polymer Structure and Properties

St-Petersburg Division of the Boreskov Institute of Catalysis

➤ Development of new technology for co-processing of natural gas and oil fractions to produce motor fuels (Biforming)

Pilot studies were carried out to develop a new technology for co-processing of C₃-C₄ hydrocarbons and gasoline fractions into high-octane motor fuels. The process provides 6-8 wt % increase in the yield of gasoline with RON 95. The results obtained were used to reconstruct conventional reforming installations for the biforming mode. The compiled initial and technical data were used for preparation of the project of re-equipment of the typical reforming installation available at the Ryazan Oil Processing Plant affiliated by Tyumen Oil Co. The Project was to be accomplished by the end of 2001. A fixed run in the biforming mode is planned for the first Quarter of 2002 to assess the cost efficiency against the conventional reforming mode.

Laboratory for Catalysis by Supported Metals

Development of a new type reforming and biforming catalyst to be used in fixed catalyst bed installations

A new technology for preparation of PR-series reforming and biforming catalysts was developed as applied to production at the Angarsk Catalyst and Organic Synthesis Plant. The technology provides remarkable improvement of textural, strength and catalytic properties of the catalysts. A pilot batch of the support (2 t) was manufactured in 2001 and then a commercial batch of PR-51A catalyst (24 t). Comparative pilot testing of the new catalyst modification and

the one manufactured before (Ryazan Industrial Catalyst Co., an affiliate of Tyumen Oil Co.) in the reforming and biforming processes were performed. Superior performance was observed with the new catalyst modification, PR-51A, *i.e.* a higher activity (5 to 7%) and selectivity (an increase in the yield of RON 95 reformat by 2 to 3%). The biforming test also demonstrated improved parameters such as the conversion of *n*-propane as high as 65% at the reaction temperature of 490°C and 5–6 wt % higher yield of liquid biformate.

A commercial batch of PR-51A catalyst was loaded in an installation LG-35-11/300 in Drogobych (Ukraine). At the inlet temperature 494°C, the reformat with RON 95–96 was synthesized at the yield of 86–87 wt % that is superior to the results obtained worldwide before.

Application for formulation and procedure for preparation of the new support and catalyst modification is filed to the Russian Patent Agency.

Laboratory for Catalysis by Supported Metals

Studies of the nature of high-temperature dispersing of oxides of transition metals and platinoids in supported catalysts MnO_x/ZrO_2 , $Pt(Pd)/CeO_2$, $Pt(Pd)/ZrO_2$, $Pt(Pd)CeO_2/Al_2O_3$, $Pt(Pd)/ZrO_2/Al_2O_3$.

The effect of thermoactivation was discovered for platinum and palladium catalysts supported on Al_2O_3 , ZrO_2 , CeO_2 . The atomic catalytic activity to reactions of complete oxidation of methane and *n*-pentane increased considerably upon elevation of their precalcination temperature from 500 to 700°C

Laboratory for Catalytic Methods of Atmosphere Protection

Development of new supports and sorbents

A new inexpensive support was developed for preparation of IC-11-01 type desiccant from ample feedstocks. The pore volume of ca. 0.6 cm³/g (from moisture capacity data) and a high mechanical strength are characteristic of the support. The industrial technology for the support synthesis was adapted using experimental and production facilities of the Omsk Department of the Institute of Catalysis. A pilot batch (500 kg) of the support was manufactured. The use of the support will allow the desiccant to be produced at a high profitability (no less than 100%)

Group of Zeolite-Containing Catalysts for Petrochemistry and Oil Processing

Omsk Division of the Boreskov Institute of Catalysis

COMMERCIAL CATALYSTS AND TECHNOLOGIES OWNED BY THE BORESKOV INSTITUTE OF CATALYSIS

CATALYSTS FOR CONVERSION OF LIQUID
ORTHO-HYDROGEN TO PARA-HYDROGEN

1970 - Uzbekistan

VANADIUM CATALYSTS FOR
SULFURIC ACID PRODUCTION

1970 - Russia

CATALYSTS FOR ENVIRONMENTAL
PROTECTION

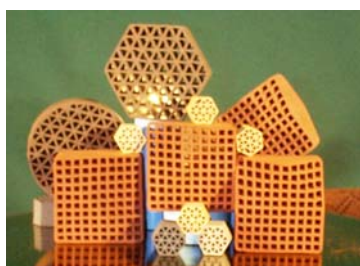
1990 - Russia

FORMALDEHYDE PRODUCTION FROM
METHANOL OVER OXIDE CATALYST

1972 - Russia
1982 - Czech Republic, Bulgaria

DEHYDROGENATION CATALYSTS
FOR ELASTOMERS PRODUCTION

1974 - Russia



TECHNOLOGY OF ALUMINA PRODUCTION:
NITRATE-AMMONIA TECHNOLOGY, THERMAL
DECOMPOSITION WITH THE USE OF CH₄,
THERMOCHEMICAL AND MECHANOCHEMICAL
ACTIVATION

1975 - Germany, 1990 - Kazakhstan,
1992 - Russia



CATALYSTS FOR PROPYLENE
POLYMERIZATION

1980 - Kazakhstan, 1987 - Russia
1995 - The Netherlands, USA

CATALYST FOR NITROUS GASES
PURIFICATION FROM OXYGEN
IN HYDROXYLAMINE SULFATE
PRODUCTION

1981 - Russia, 1995 - Germany

TECHNOLOGIES AND REACTORS
BASED ON REVERSE-PROCESS

1982 - Russia, 1985 - Kazakhstan,
1989 - Japan, 1990 - Bulgaria,
1991 - Uzbekistan, 1993 - China,
1995 - USA, 1998 - Australia

CATALYTIC HEATING PLANTS

1982 - Russia

NEW CARBON MATERIAL - SIBUNIT
AND SIBUNIT BASED CATALYSTS

1984 - Russia

CATALYSTS FOR METHIONINE
PRODUCTION

1986 - Russia

"ZEOFORMING" PROCESS FOR
THE PRODUCTION OF HIGH-OCTANE
GASOLINES (BIC - SEC "ZEOSIT")

1992 - Russia, 1997 - Poland

NONPLATINUM HONEYCOMB
CATALYSTS TO PRODUCE NITRIC ACID

1995 - Russia

CATALYSTS FOR CLAUS PROCESS

1996 - France



Industrial Reverse-Plant for processing
of waste gases of metallurgy to H₂SO₄.
Capacity up to 100 000 m³/h
("Pechenganickel" Metallurgy Plant)

CATALYSTS FOR LOW-TEMPERATURE
CONVERSION OF CARBON MONOXIDE
IN AMMONIA PRODUCTION

1996 - Kazakhstan



Reactor for ammonia oxidation with IC-42-1
catalyst (AO "Azot", Berezniki)

DEVELOPMENTS OF THE BORESKOV INSTITUTE OF CATALYSIS AT SEMI-COMMERCIAL SCALE

TECHNOLOGIES BASED ON
"CATALYTIC HEAT GENERATORS" - COMBUSTION,
DRYING AND THERMAL TREATMENT

1984 - Russia, Ukraine, Lithuania

DEVICES AND INSTALLATIONS
FOR CATALYSTS TESTING

1985 - Russia, 1992 - USA

ENVIRONMENTALLY FRIENDLY
AIR HEATER

1986 - Russia, Uzbekistan

CATALYSTS FOR PLANT OILS
HYDROGENATION, PRODUCTION OF
MEDICINES (LIDOCAIN, SULPIRID)

1988 - Russia

PROCESSES FOR GASES AND WASTE
WATER PURIFICATION FROM
SULFUR-CONTAINING SUBSTANCES

1989 - Russia

CATALYTIC NEUTRALIZER FOR
PURIFICATION OF AUTOMOTIVE
EXHAUSTS

1990 - Russia

NOVEL COMPOSITE SORBENTS
BASED ON CARBON MATERIALS,
ALUMINAS, SILICA GELS FOR WASTE
WATER PURIFICATION,
PRECIOUS METALS EXTRACTION,
FRESH WATER RECOVERY

1995 - Russia

CATALYSTS FOR ACRYLIC
ACID PRODUCTION

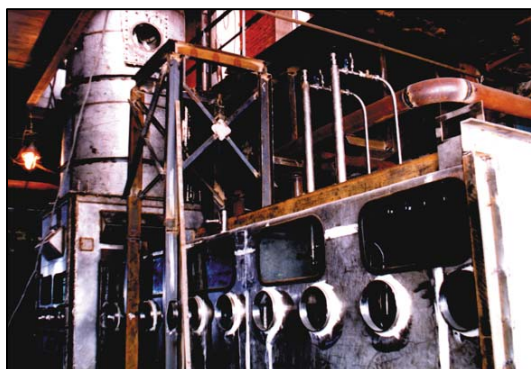
1992 - Russia

ALKYLATION OF AROMATICS
OVER ZEOLITE CATALYSTS

1990 - Russia

CATALYSTS FOR PRODUCTION OF
ULTRA-HIGH MOLECULAR WEIGHT
POLYETHYLENE (UHMWPE) AND
ETHYLENE-PROPYLENE COPOLYMERS

1997 - Russia



Industrial plant for destruction of mixed organic wastes containing natural uranium with a capacity of 50 t/y (Novosibirsk Chemical Concentrates Plant Ltd.)



Pilot plant for synthesis of phenol from benzene, with nitrous oxide used as the oxidant (ALPHOX, USA)

CATALYTIC PROCESS TO DESTRUCT
ORGANIC RADIOACTIVE WASTES

1995 - Russia

ONE-STAGE PROCESS OF BENZENE
TO PHENOL OXIDATION (ALPHOX)

1996 - USA

Catalytic Processes from Molecular Level to Industrial Plants



RESEARCH ACTIVITY

Quantum-Chemical Studies

BASIS FUNCTIONS WITH POLYNOMIAL TAILS FOR BAND STRUCTURE CALCULATIONS

V.M. Tapilin

J. Struct. Chem., 42(3) (2001) pp. 411-417.

The electronic structure of copper crystal has been calculated in the basis of standard atomic fractions and in the basis of functions with polynomial tails. Comparison of the results of calculations reveals that in the basis of functions with polynomial tails the accuracy of calculation may be achieved comparable to those in the basis of common functions at approximately twofold time shortening.

A DFT QUANTUM CHEMICAL APPROACH TO THE REAL STRUCTURE OF POLYMETHYLALUMOXANE

I.I. Zakharov, V.A. Zakharov

Macromol. Theory & Simul., 10 (2001) pp. 108-116.

A DFT quantum chemical calculations have been performed in order to optimize the geometric and electronic cage structure of polymethylalumoxane (MAO) with oligomerization degree $n = 9-15$ and find such structures that fit most closely the existing experimental data on the MAO composition and structure. The following peculiarities of the MAO structure were found:

i) In “classic” MAO ($n = 9, 12, 15$; Al:CH₃:O = 1:1:1), which has triple-layer cage structure, the inner layer contains highly reactive bonds Al-O.

ii) Reaction between “classic MAO” and trimethylaluminium (TMA) proceeds by the concerted mechanism with the insertion of Al-CH₃ groups into these Al-O bonds. The reaction produces “true” MAO showing ratio Al:CH₃:O = 1:1.5:0.75. Calculated geometry and electronic structures of “true” MAO with $n=6, 9, 12$ are presented.

iii) “True” MAO and “classic” MAO exist in equilibrium. Driving force for the formation of “true” MAO is the decrease of enthalpy, and of “classic” MAO is the increase of entropy in the equilibrium reaction between “classic” MAO and TMA.

THEORETICAL STUDY OF METHANE ADSORPTION ON Zn(II) ZEOLITES

L.A.M.M. Barbosa*, G.M. Zhidomirov, R.A. van Santen* (*Eindhoven University of Technology, Eindhoven, The Netherlands)

Phys. Chem. Chem. Phys., 2(17) (2000) pp. 3909-3918.

The adsorption of methane on Zn-exchanged zeolites was studied theoretically by density functional theory (DFT). Diverse types of active sites were employed, such as: a Zn(II) cation, which was placed on different rings (4T and 5T), a ZnO (in tetramer configuration) cluster and a [Zn-O-Zn]²⁺ dimer complex. The Zn(II) cation is the most exposed to probe molecules when situated on the “4T ring” of zeolites. In this position, the cation activates strongly two IR bands of methane (ν_1 and ν_3). This activation is not observed when Zn(II) sits on larger rings. The assignment of the band shifts found in the experimental IR spectra of methane adsorption, which were associated with the cation position in the zeolite framework, had to be revised following the results for the calculated shifts. Larger shifts are associated with the cationic position at small rings. Methane prefers to adsorb physically in a 3-fold configuration on Zn(II) at both 4T and 5T rings. This is not the case for ZnO and [Zn-O-Zn]²⁺ sites, in which the dissociative adsorption is more favorable. In the last two cases, the dissociation is in good agreement with the “alkyl path”, described previously in the literature. The [Zn-O-Zn]²⁺ site appears to be one of the active forms of the Zn cation on zeolites with a low Si/Al ratio. This site is more thermodynamically stable than both Zn(II) on 5T and (ZnO)₄. In the absence of Brønsted sites, (ZnO)₄ does not decompose into Zn(II) or [Zn-O-Zn]²⁺. Owing to its size, this oxide cluster may only be stable in special positions inside the pores. Different adsorption configurations and loadings were tested in order to understand the large shift observed experimentally for the ν_1 band of methane. The largest shifts calculated here were found for 3-fold physisorption on ZnO and Zn(II) (“4T ring”), as well as in dissociative adsorption on the [Zn-O-Zn]²⁺ site. None of these models, however, could describe this large experimental shift. The same results were also observed when these systems were embedded in a

solvent cage, which mimicked the framework environment around the active site.

THEORETICAL STUDY OF THE MOLECULAR HYDROGEN ADSORPTION AND DISSOCIATION ON DIFFERENT Zn(II) ACTIVE SITES OF ZEOLITES

L.A.M.M. Barbosa*, **G.M. Zhidomirov**,
R.A. van Santen* (*Eindhoven University of
Technology, Eindhoven, The Netherlands)

Catal. Lett., 77(1-3) (2001) pp. 55-62.

The adsorption and dissociation of hydrogen on Zn-exchanged zeolites has been studied theoretically by density functional theory (DFT). Diverse types of active sites have been employed for the Zn cation, such as: placed on different rings (4T and 5T), in the (ZnO)₄ (in a cubic configuration cluster) and in the [Zn–O–Zn]²⁺ dimer complex. The Zn(II) cation is most exposed to probe molecules when situated on 4T ring of zeolites. In this position, the cation activates the infrared stretching band of the hydrogen molecule, which is not observed when Zn(II) sits on 5T rings. The assignment of the band shifts found in the experimental IR spectra of hydrogen adsorption, which were associated to the cation position in the zeolite framework, had to be revised following the results for the calculated shifts. Larger shifts are associated to the cationic position at small rings. In the case for (ZnO)₄ the dissociative adsorption is more favorable. The calculated activation energy is the lowest among all sites studied. The results have also confirmed the current proposal that ZnO microparticles are responsible for the large H–H stretching shift and the H₂ dissociation on Zn(II) sites in zeolites.

DFT STUDY OF OXYGEN-BRIDGED Zn²⁺ ION PAIRS IN Zn/ZSM-5 ZEOLITES

A.L. Yakovlev*, **A.A. Shubin**, **G.M. Zhidomirov**,
R.A. van Santen* (*Eindhoven University of
Technology, Eindhoven, The Netherlands)

Catal. Lett., 70(3-4) (2000) pp. 175-181.

A cluster model for Zn/ZSM-5 zeolite is proposed, which consists of an oxygen-bridged [Zn–O–Zn]²⁺ moiety attached to two framework aluminum ions of two adjacent ZSM-5 5-rings. Its stability and catalytic activity in ethane dehydrogenation were considered using the DFT method and compared with those for single Zn²⁺ ions

in the same rings. It is shown that the oxygen-bridged Zn²⁺ pair is rather reactive towards ethane dissociation and that the rate-limiting step is release of hydrogen.

COMPARATIVE QUANTUM CHEMICAL STUDY OF STABILIZATION ENERGIES OF Zn²⁺ IONS IN DIFFERENT ZEOLITE STRUCTURES

A.A. Shubin, **G.M. Zhidomirov**, **A.L. Yakovlev***,
R.A. van Santen* (*Eindhoven University of
Technology, Eindhoven, The Netherlands)

J. Phys. Chem. B, 105(21) (2001)
pp. 4928-4935.

Cluster model quantum chemical calculations have been performed to compare stabilization energies (E_{st}) of Zn²⁺ ions in four-, five-, and six-membered zeolitic rings. E_{st} was evaluated as energy of the reaction $Zn^{2+}/Z + H_2 \Rightarrow 2H^+/Z + Zn^0$. It was found that E_{st} substantially decreases in the series six-, five-, and four-membered ring, and this trend is essential to the understanding of the comparative adsorption ability and reactivity of Zn²⁺ in cationic sites of different zeolites. This conclusion was proved in calculations of the heterolytic dissociation of ethane. The molecular structure of active sites in ZnHY and AZXnHZSM-5 zeolites and the question of the stability of small intrazeolite zinc oxide species are discussed.

N₂O DECOMPOSITION CATALYZED BY TRANSITION METAL IONS

A.L. Yakovlev*, **G.M. Zhidomirov**,
R.A. van Santen* (*Eindhoven University of
Technology, Eindhoven, The Netherlands)

Catal. Lett., 75(1-2) (2001) pp. 45-48.

The direct N₂O decomposition catalyzed by 5-coordinated transition metal ions Fe, Co, and Rh was studied using the DFT method. The cluster model has the formula M(OH)₃(H₂O)₂. Energies of intermediates and transition states were computed. The results show that Co and Rh sites are more active than Fe, the former two being very similar.

ETHYLENE AND OXYGEN SPECIES ADSORBED ON A DEFECT OXIDIZED SURFACE Ag(111): THEORETICAL ANALYSIS BY DFT METHOD

V.I. Avdeev, G.M. Zhidomirov

Surf. Sci., 492(1-2) (2001) pp. 137-151.

A cluster model $AS_v \rightarrow Ag_{12}-3O$ of the oxidized surface Ag(111) with a defect has been suggested. The defect is simulated by cationic vacancy V. Density functional theory (B3LYP/LANL1MB approximation) is used to calculate ethylene and oxygen adsorption on the regular (AS_r) and defect (AS_d) sites on the Ag(111). Oxygen interaction with site AS_r produces atomic oxygen species (AS_r-O). Oxygen adsorption on site AS_d is accompanied by its association with subsurface oxygen atoms to form a quasimolecular structure of metal ozonide type $-Ag-O-O_{ep}-O-Ag-$, containing electrophilic oxygen O_{ep} . Energies of atomic oxygen binding to the regular and defect surfaces are found to be approximately equal. On the

regular surface, ethylene forms a π -complex with binding energy $E_\pi (Ag-C_2H_4)=14.2$ kcal/mol. On the defect surface, ethylene produces a metal-ethylene-peroxide cycle such as $Ag-O-O-C_2H_4-Ag$. Determined are the frequencies of normal vibration for ethylene and oxygen species, adsorbed on the regular and defect surfaces. In the case of associative oxygen species and complete isotope replacement $^{16}O \rightarrow ^{18}O$, the main frequency at 1000 cm^{-1} shifts by $\Delta\nu=57-61\text{ cm}^{-1}$, but this shift decreases to $\Delta\nu=25-30\text{ cm}^{-1}$ for isotope mixtures $^{16}O/^{18}O$. For the adsorbed species of ethylene-oxygen mixtures, IR spectra show the frequencies within which $170-180\text{ cm}^{-1}$ are associated with stretching of bond Ag-C. Frequencies at $300-490\text{ cm}^{-1}$ are assigned to mode $\nu(Ag-O)$ of the functional group $Ag-O-O_{ep}-O-Ag$. The most intensive modes at 950 and 600 cm^{-1} are likely to stretching and bending of the functional groups containing the O-O-O and O-O-C bonds.

Monte-Carlo Simulations to Study Physico-Chemical Processes

MONTE CARLO MODEL OF OSCILLATORY CO OXIDATION HAVING REGARD TO THE CHANGE OF CATALYTIC PROPERTIES DUE TO THE ADSORBATE-INDUCED Pt(100) STRUCTURAL TRANSFORMATION

E.I. Latkin*, V.I. Elokhin, V.V. Gorodetskii

(*Novosibirsk State University, Novosibirsk, Russia)

J. Molec. Catal. A: Chemical, 166(1) (2001) pp. 23-30.

The statistical lattice model has been constructed for the oscillatory $(CO+O_2)/Pt(100)$ reaction. The model takes into account the change of surface properties due to the adsorbate-induced reversible surface transformation $hex \leftrightarrow 1 \times 1$. The Monte Carlo simulations reproduce the hysteresis and the synchronous oscillations of reaction rate, O_{ads} and CO_{ads} coverages and hex and 1×1 surface phases under the conditions close to the experimental ones. Self-oscillations of the reaction rate are accompanied by autowave processes on the model platinum surface. The existence of the reaction zone between the moving adsorbate islands has been shown.

MODELLING THE OXIDATION OF CO AT THE INTERFACE OF HETEROPHASE METAL CATALYSTS

N.I. Efremova, A.V. Kalinkin

React. Kinet. & Catal. Lett., 73(2) (2001) pp. 373-379.

CO oxidation on a surface composed of two types of patches was simulated by the Monte Carlo method. Each patch has kinetic properties close to those of Pt(100) and Rh(100). The reaction rate was shown to increase significantly at the interface, involving CO_{ads} on platinum and O_{ads} on rhodium, under particular conditions.

SIMULATION OF CO ADSORPTION AND OXIDATION ON Pt(110)

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

J. Chem. Phys., 114(12) (2001) pp. 5351-5357.

The clean Pt(110) surface exhibits missing-row (1×2) periodicity. CO adsorption on this surface may lift the (1×2) reconstruction. During CO oxidation, the interplay between the CO-induced surface restructuring and reaction steps may result in oscillations. The Monte Carlo simulations, executed with a qualitatively correct ratio of the rates of

elementary steps involved into the game, show that these phenomena can be described by using a lattice-gas model with Pt–Pt, Pt–CO, and CO–CO lateral interactions.

RAPID BISTABLE REACTIONS IN POROUS CATALYSTS

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

Catal. Lett., 72 (1-2) (2001) pp. 7-10.

The kinetics of rapid bistable reactions (e.g., CO or hydrogen oxidation on Pt) occurring on a nm catalyst particle located inside a mesoscopic pore have been analyzed. Limitations for reactant diffusion inside a single pore are shown to modify the dependence of the reaction rate on the reactant pressures outside the pore. In particular, the position of the maximum reaction rate is shifted to higher CO pressures (provided that the O₂ pressure is fixed). This effect is significant if a pore is not too short. Similar effects are possible during oscillations in CO oxidation on supported nm catalyst particles.

SURFACE RESTRUCTURING, KINETIC OSCILLATIONS, AND CHAOS IN HETEROGENEOUS CATALYTIC REACTIONS

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

J. Stat. Physics, 101(1-2) (2000) pp. 631-647.

Kinetic oscillations in catalytic reactions on single-crystal surfaces often result from the interplay of the purely chemical reaction steps and adsorbate-induced surface restructuring. A classical example is CO oxidation on Pt(100). The authors survey evolution of the models used to simulate this reaction and show how it can be described self-consistently by employing Monte Carlo simulations combined with the lattice-gas model, taking into account substrate-substrate, substrate-adsorbate and adsorbate-adsorbate lateral interactions. Under the reactive conditions, this approach predicts formation of mesoscopic restructured well ordered islands with atomically sharp boundaries.

OSTWALD RIPENING WITH KINETICALLY LIMITED BOND FORMATION

V.P. Zhdanov

European Physical J. B, 19(1) (2001) pp. 97-100.

The Monte Carlo simulations of the ripening of 2D islands in the case when the formation of the monomer-monomer bonds is kinetically limited is presented. The results obtained indicate that such limitations may modify the early stage of the kinetics. Asymptotically, the ripening is described by the Lifshitz-Slyozov law.

COUPLED CATALYTIC OSCILLATORS: BEYOND THE MASS-ACTION LAW

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

Chaos, 11(2) (2001) pp. 335-343.

Monte Carlo simulations of the reaction kinetics corresponding to two coupled catalytic oscillators in the case when oscillations result from the interplay between the reaction steps and adsorbate-induced surface restructuring are presented. The model used is aimed to mimic oscillations on a single nm catalyst particle with two kinds of facets or on two catalyst particles on a support. Specifically, the NO reduction has been treated by H₂ on a composite catalyst containing two catalytically active Pt(100) parts connected by an inactive link. The catalyst is represented by a rectangular fragment of a square lattice. The left- and right-hand parts of the lattice mimic Pt(100). With an appropriate choice of the model parameters, these sublattices play a role of catalytic oscillators. The central catalytically inactive sublattice is considered to be able only to adsorb NO reversibly and can be viewed as a Pt(111) facet or a support. The interplay of the reactions running on the catalytically active areas occurs via NO diffusion over the boundaries between the sublattices. Using this model, it has been shown that the coupling of the catalytically active sublattices may synchronize nearly harmonic oscillations observed on these sublattices and also may result in the appearance of aperiodic partly synchronized oscillations. The spatio-temporal patterns corresponding to these regimes are nontrivial. In particular, the model predicts that, due to phase separation, the reaction may be accompanied by the formation of narrow NO-covered zones on the left and right sublattices near the boundaries between these

sublattices and the central sublattice. Such patterns cannot be obtained by using the conventional mean-field reaction-diffusion equations based on the mass-action law. The experimental opportunities to observe the predicted phenomena are briefly discussed.

STANDING FRONTS IN OSCILLATORY REACTIONS ON COMPOSITE CATALYTIC SURFACES

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

Physica D: Nonlinear Phenomena,
151(1) (2001) pp. 73-81.

The Monte Carlo simulations of a standing reaction front formed during NO reduction by H₂ on a catalyst consisting of two metal strips is presented. One strip (to the right) is considered to be catalytically active. Specifically, the reaction is assumed to occur on Pt(100). The other strip (to the left) is catalytically inactive but can adsorb NO. The processes on the two strips are coupled via NO diffusion over their boundary. Kinetic oscillations result from NO-induced restructuring of the Pt(100) surface. The reaction fronts obtained for this model are quite unusual. For example, the NO coverage may be low on the left sublattice, high in a narrow zone on the right sublattice near the metal-metal boundary, and then again relatively low. These findings illustrate richness of spatio-temporal patterns which can be observed in heterogeneous catalytic reactions on the mesoscopic scale.

RATE-DETERMINING MOVES IN PROTEIN FOLDING

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

J. Chem. Phys., 115(6) (2001) pp. 2841-2845.

A lattice Monte Carlo simulations of protein folding for the three main types of 3-D native protein conformations, including globular structures, bundles of α helices, and β sheets are presented. Scrutinizing the relative role of the end, crankshaft, and corner monomer moves, it has been shown that the latter moves are rate-determining in all the cases.

SIMULATIONS OF OSCILLATORY GLYCOLYTIC PATTERNS IN CELLS

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

Phys. Chem. Chem. Phys., 3(17) (2001)
pp. 3786-3791.

Using the mean-field reaction-diffusion equations and Monte Carlo (MC) technique, the authors simulate oscillatory glycolytic kinetics in 3D spherical or 2D circular cells. The model employed takes into account the glucose supply to the cell *via* the cell membrane and a few elementary reaction steps running inside the cell. The model parameters are chosen so that the typical size of oscillatory patterns is comparable with the cell size. In the mean-field approximation, the oscillations are periodic and may occur with large amplitude. In contrast, the MC kinetics are appreciably irregular and the amplitude of oscillations is smaller in the latter case. Both these effects are connected with deviation of the metabolite distribution in the cell from the symmetrical one due to fluctuations. The spatiotemporal patterns obtained in our MC simulations are qualitatively similar to those observed recently in neutrophils.

CATALYTIC REACTIONS, SURFACE RESTRUCTURING, AND PATTERN FORMATION

V.P. Zhdanov

Surf. Sci., 486(3) (2001) L513-L518.

The Monte Carlo simulations of the island formation during heterogeneous catalytic AB \rightarrow C reaction occurring under the steady-state conditions via the Eley-Rideal mechanism in the case when adsorbed A particles are able to change the surface structure is presented. The island formation is demonstrated to be crucially dependent on the details of the mechanism of A diffusion. In the favourable situation, the dependence of the average linear island size on the rate of A diffusion is found to be logarithmic.

SIMULATION OF ENZYMATIC CELLULAR REACTIONS COMPLICATED BY PHASE SEPARATION

V.P. Zhdanov

Phys. Rev. E, 63(1) (2001) 011908 (6 pp.).

Two-dimensional Monte Carlo simulations of enzymatic cellular reaction occurring via the

Michaelis-Menten scheme in the case of attractive interactions between the reaction products are presented. The model employed predicts phase separation in the cell provided that the reaction is relatively fast. The shape of the corresponding patterns varies from a few separate islands to a large patch located in the center of the cell. The fluctuations of the reaction rate during such regimes are found to be much higher than those predicted by the Poissonian distribution.

SIMULATION OF TWO-DIMENSIONAL STREPTAVIDIN CRYSTALLIZATION

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

Proteins, 43(4) (2001) pp. 489-498.

The lattice Monte Carlo simulations of the growth of streptavidin islands at a biotinylated lipid layer is presented. The model employed takes into account attractive anisotropic lateral interactions between streptavidin tetramers. With a minimal set of interactions, the formation of rectangular islands experimentally observed at $\text{pH} \gtrsim 9.0$ is reproduced. Specifically, two scenarios of the island growth are analyzed. First, if streptavidin is rapidly adsorbed at $t=0$ (stepwise coverage change without ongoing adsorption), the average linear island size is found to grow according to the Lifshitz-Slyozov law, $R \propto t^{1/3}$. Second, if the island growth occurs in parallel with streptavidin adsorption limited by diffusion in the solution, the Lifshitz-Slyozov law is also applicable, but only at the late stage, when the streptavidin coverage is appreciable.

FOLDING OF BUNDLES OF α -HELICES IN SOLUTION, MEMBRANES, AND ADSORBED OVERLAYERS

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

Proteins, 42(4) (2001) pp. 481-494.

A coarse-grained lattice model for Monte Carlo simulations of folding of proteins consisting of several α -helices is proposed. A chain representing a protein is considered to contain A and B monomers forming

relatively stiff A subchains, mimicking helices, and flexible B links between these subchains, respectively. Using this model, (1) folding of four-helix proteins in solution; (2) folding of membrane proteins containing one, two, or four helices; and (3) refolding of four-helix proteins adsorbed at the liquid-solid interface are simulated. For these cases, typical scenarios of protein folding and refolding and study the dependence of the folding time on the chain length are shown. Combining the latter results with those already available in the literature, the relative rates of folding of proteins belonging to different classes are discussed.

DISAPPEARANCE OF OSCILLATIONS IN THE BRUSSELTATOR ON THE MESOSCOPIC SCALE

V.P. Zhdanov

Phys. Chem. Chem. Phys., 3(8) (2001) pp. 1432-1434.

The Brusselator is a classical model predicting kinetic oscillations in chemical reactions. Using a lattice version of this model, the authors show by employing Monte Carlo simulations how due to fluctuations the periodic oscillations may first become aperiodic and then disappear with decreasing system size.

ADSORPTION-DESORPTION KINETICS AND CHEMICAL POTENTIAL OF ADSORBED AND GAS-PHASE PARTICLES

V.P. Zhdanov

J. Chem. Phys., 114(10) (2001) pp. 4746-4748.

In the literature, one can find two alternative ways of using the chemical potential of adsorbed and gas-phase particles, μ_a and μ_g , for describing the adsorption-desorption kinetics. According to the first approach, the desorption rate depends only on μ_a . The second approach, proposed by Ward et al. in a series of papers published in the *Journal of Chemical Physics*, predicts that the desorption rate is proportional to $\exp[(\mu_a - \mu_g)/k_B T]$. Scrutinizing the formalism used by Ward et al., it has been shown that the latter dependence makes no sense because it contradicts the basic principles of the general theory of activated rate processes.

Development and Application of Physicochemical Methods for Catalysts Investigation

ABSOLUTE CALIBRATION OF X-RAY SEMICONDUCTOR DETECTORS IN THE 0.3-1.5 keV PHOTON ENERGY RANGE ON SYNCHROTRON RADIATION FROM VEPP-2M STORAGE RING

A.N. Subbotin*, V.A. Chernov, V.V. Gaganov*,
A.V. Kalutsky*, N.V. Kovalenko**,
A.K. Krasnov***, K.E. Kuper**,
A.G. Legkodymov**, A.D. Nikolenko**,
I.N. Nesterenko**, V.F. Pindyurin**,
V.N. Romaev* (*All-Russian Scientific Research
Institute of Experimental Physics, Sarov, Russia;
**G.I. Budker Institute of Nuclear Physics,
Novosibirsk, Russia; ***Research Institute of Pulse
Technique, Moscow, Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 452-458.

The paper presents the results of absolute spectral responsivity measurements for SPPD11 and SPPD11-04 pulse-type silicon detectors, carried out in the X-ray energy range from 0.3 to 1.5 keV with a relative uncertainty of about 8% (1σ). The measurements were performed using the detector exposure to a well-calculable synchrotron radiation through the selective filters with well-known transmittance. Synchrotron radiation from the VEPP-2M storage ring was utilized for these measurements. The spectral responsivity of the detectors was restored by solving the proper system of integral equation on the base of measurement data. For increasing the calibration accuracy, the X-ray transmittance near the L-absorption edges of the filters used and the angular spread in the positron beam of the storage ring were experimentally determined.

A SECONDARY X-RAY ANALYZER USING A FLAT RING-SHAPED RADially GRADED MULTILAYER

A.N. Buzykaeva*, V.A. Chernov, N.V. Kovalenko*,
S.V. Mytnichenko**
(*G.I. Budker Institute of Nuclear Physics,
Novosibirsk, Russia; **Institute of Solid State
Chemistry and Mechanochemistry, Novosibirsk,
Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 135-141.

A new type of efficient energy analyzer specialized for thin film studies is suggested. The key

feature of the analyzer is the use of a ring-shaped, flat multilayer with d -spacing linearly increasing with radius. At small angles of diffraction, a gradual extension of multilayer period ensures isochromatic Bragg reflection of divergent X-rays emitted by the sample. The main advantages of this kind of secondary analyzer are as follows: (1) a rather large acceptance angle (0.1-0.3sr); (2) good energy resolution (2-3%) and (3) easy tuning in a wide energy range. The instrument is particularly suited for grazing-exit fluorescence X-ray absorption fine structure (XAFS) and XMCD studies with spatial resolution. A prototype graded W/Si multilayer with a change of period of about 30% was fabricated and tested. Preliminary results taken with the K fluorescence emission of copper film are presented to demonstrate feasibility of the analyzer.

AN EXPERIMENTAL STUDY OF THE q_{\perp} -DEPENDENCE OF X-RAY RESONANT DIFFUSE SCATTERING FROM MULTILAYERS

V.A. Chernov, V.I. Kondratiev*, N.V. Kovalenko*,
S.V. Mytnichenko* (*G.I. Budker Institute of
Nuclear Physics, Novosibirsk, Russia; **Institute of
Solid State Chemistry and Mechanochemistry,
Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 145-154.

A study of X-ray resonant diffuse scattering from the W/Si multilayer was performed to examine its dependence on the momentum transfer normally to the specular diffraction plane, q_{\perp} . The data obtained show two evident disagreements with the present theoretical approximations. Firstly, when the incident angle was approximately equal to the Bragg angle, additional scattering concentrated in the specular diffraction plane was observed. Secondly, the q_{\perp} -dependence of the quasi-Bragg scattering intensity obtained from these experiments is not the same, at least at the small momentum transfer, as can be obtained from the scans in the specular diffraction plane, having tendency to accumulate near this plane. The possible reasons for these phenomena are discussed.

A HIGH-THROUGHPUT X-RAY ANALYZER USING A FLAT MULTILAYER MIRROR WITH RADIALLY INCREASING PERIOD

A.N. Buzykaeva*, N.V. Kovalenko*, S.V. Mytnichenko**, V.A. Chernov (*G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia; **Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 1 (2001) pp. 6-12.

A new energy-tunable multilayer analyzer with a usefully large solid angle is suggested. The key features of the analyzer are using radially-graded multilayer coating and a ring-like geometry of the flat multilayer mirror. The diffraction condition is satisfied without bending the multilayer, by grading the multilayer period instead. For a small Bragg angle, the grading ratio is a linear function of radius and has no energy dependence. A so-graded multilayer is suitable for the detection of different X-ray fluorescence requiring only the adjustment of the height between a point source and the mirror plane. The collection solid angle of the analyzer ranges from 0.1 to 0.3 sr depending on the energy range (1–10 keV). The energy resolution of the analyzer is about 2-3%. To test the validity of the analyzer concept, a graded W/Si multilayer has been prepared. A spectrum of copper K fluorescence with well-resolved K_{α} and K_{β} lines was obtained.

THE USE OF QUASI-BRAGG DIFFUSE SCATTERING FOR EXPRESS MEASUREMENT OF CHANGES IN MULTILAYER *d*-SPACING

V.A. Chernov, N.V. Kovalenko*, S.V. Mytnichenko** (*G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia; **Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 155-157.

The possibility of the use of quasi-Bragg diffuse scattering for express measurements of changes in multilayer *d*-spacing was studied. The error of this method was shown to be minimal, if the incident or scattered angles are sufficiently far from the critical total external reflection or Bragg angles. As an example, the measurements of the W/Si multilayer mirror with linearly varying *d*-spacing are presented.

AN X-RAY GRAZING INCIDENCE PHASE MULTILAYER GRATING

V.A. Chernov, N.V. Kovalenko*, S.V. Mytnichenko** (*G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia; **Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 158-161.

An X-ray grazing incidence phase multilayer grating, representing a thin grating placed on a multilayer mirror, is proposed. A high efficiency of grating diffraction can be obtained by the possibility of changing the phase shift of the wave diffracted from the multilayer under the Bragg and total external reflection conditions. A grazing incidence phase multilayer grating consisting of Pt grating stripes on a Ni/C multilayer and optimized for the hard X-ray range was fabricated. Its diffraction properties were studied at photon energies of 7 and 8 keV. The obtained maximum value of the diffraction efficiency of the +1 grating order was 9% at 7 keV and 6.5% at 8 keV. The data obtained are in a rather good accordance with the theory.

AN EXTENDED ANOMALOUS FINE STRUCTURE OF X-RAY QUASI-BRAGG DIFFUSE SCATTERING FROM MULTILAYERS

V.A. Chernov, N.V. Kovalenko*, S.V. Mytnichenko** (*G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia; **Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 210-214.

An X-ray quasi-Bragg diffuse scattering anomalous fine structure technique was probed near the absorption Ni K-edge to study the interfacial structure of the Ni/C multilayer deposited by the laser ablation. Like other combinations of the EXAFS and diffraction techniques, this method has a spatial selectivity and was shown qualitatively to provide atomic structural information from the mixed interfacial layers. The possibilities and advantages of this technique are discussed.

THE USING OF ION BEAMS FOR TREATMENT OF X-RAY OPTICAL SUBSTRATES

Yu.S. Sulyaev*, **N.V. Kovalenko***, **V.A. Chernov**
(*G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia)

Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 1 (2001) pp. 74-75.

X-ray optical substrates were treated by low-energy Ar⁺-ion beam under grazing-incidence conditions. X-ray angular specular reflectivity data were taken to measure substrate roughnesses before and after ion treatment. Results on fused silica substrates show substantial ion polishing effect.

EXAFS STUDY OF THE REACTION OF GRAPHITE-MeCl₂ (Me=Ni, Co) INTERCALATION COMPOUNDS WITH BROMINE FLUORIDES

A.M. Danilenko*, **V.A. Chernov**, **V.V. Kriventsov**
(*Institute of Inorganic Chemistry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 373-375.

The X-ray absorption spectroscopy (EXAFS) technique is used for studying the local environment of the metal in stage-2 graphite intercalation compounds (GICs)-MeCl₂ (Me=Ni, Co) and in the products of reaction of these compounds with bromine fluorides. The replacement of chloride ions in the environment of the metal ion by fluoride ions during the reaction is shown.

HIGH GAIN BEAM COMPRESSION IN NEW-GENERATION THIN-FILM X-RAY WAVEGUIDES

W. Jark*, **A. Cedola****, **S. Di Fonzo***, **M. Fiordelisi****, **S. Lagomarsino****, **N.V. Kovalenko*****, **V.A. Chernov** (*Sincrotrone Trieste, Basovizza, Italy; **Istituto Elettronica Stato Solido, Roma, Italy; ***G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia)

Appl. Phys. Lett., 78(9) (2002) pp. 1192-1194.

X-ray waveguides can compress an incident beam for microscopy applications above 8 keV photon energy to sizes smaller than 100 nm in one dimension, a range which is not routinely accessed with other X-ray optics (e.g., Fresnel zone plates). Beryllium, because of its low absorption, is expected to provide the highest intensity gain. Measured gains for a

beryllium waveguide of 74 nm thickness exceed values of 100 at 13 and 20 keV photon energy, which is an improvement by an order of magnitude compared to previously reported performances. The same object works also at 8 keV with gain 4.

PORTABLE HIGH PRECISION SMALL/WIDE ANGLE X-RAY SCATTERING DIFFRACTOMETER

Y.A. Gaponov*, **E.A. Dementyev****, **D.I. Kochubey**, **B.P. Tolochko*** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **G.I. Budker Institute of Nuclear Physics, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 467-468 (2001) pp. 1092-1096.

The portable high precision small/wide angle X-ray scattering diffractometer (modified Bonze-Hart optical scheme) was designed and developed for the investigation of structure rearrangement during liquid state-solid phase transformations (with reaction time of 10 h or more) for the investigation of the process of solid state phase formation. The FEM detectors are used as monitor and detector. The double crystal Si₁₁₁ analyzer (with changeable relative angle of second crystal) is used as analyzer. All controlling electronics are designed in CAMAC. The diffractometer is controlled by a Sun SPARCStation with SVIC/VCC modules under a Solaris 2.4 operating system, and allows one to obtain the SAXS curves with accuracies (on *s*-vector for photon energy 8 keV) of about $\delta s \sim 0.002 \text{ nm}^{-1}$, $s_{\min} \sim 0.005 \text{ nm}^{-1}$ (scattering centers with the size of about 200-500 nm may be observed) and $s_{\max} \sim 50 \text{ nm}^{-1}$ (scattering angle is about 80°).

ALTERATION OF EXAFS SPECTRUM STRUCTURE OF KBr CRYSTALS RESULTING FROM A CHANGE OF REGISTRATION METHOD

V.I. Kochubey*, **T.A. Bashkatova***, **D.I. Kochubey** (*Saratov State University, Saratov, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 323-326.

The influence of experimental technique and specimen nature on measurements of EXAFS spectra is revealed. For KBr crystals the dependence of the curve shape of radial distribution function on EXAFS spectrum registration methods is shown. The possible reasons are discussed.

INVESTIGATION OF STRUCTURE OF LUMINESCENCE CENTERS IN NaCl-Ni CRYSTALS

V.I. Kochubey*, Y.G. Konyukhova*,
T.A. Bashkatova*, K.E. Gyunsburg*,
N.P. Zvezdova*, D.I. Kochubey (*Saratov State
University, Saratov, Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 327-330.

When introduction of nickel activator into a NaCl crystal is performed by thermal diffusion in the near-surface area of the crystal, impurity clusters of various structures exist simultaneously in consequence of aggregate formation. The given paper shows the scope of application of the FLEXAFS method for examination of the spatial structure of impurity clusters in NaCl crystals with nickel impurity concentration of more than 12 ppm. Also, the possibility of investigation of time history of the cluster structure during synchrotron irradiation is demonstrated.

XAFS STUDY OF THE STRUCTURED MODIFIED OXIDES OF TITANIUM

V.V. Kriventsov, D.I. Kochubey, M.V. Tsodikov*,
J.A. Navio** (*A.V. Topchiev Institute of
Petrochemical Synthesis, Moscow, Russia; **Instituto
de Ciencia de Materiales de Sevilla, Universidad de
Sevilla, Sevilla, Spain)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 331-335.

The structured modified oxides of titanium produced by sol-gel alkoxo-method have been studied by XANES and EXAFS spectroscopy at Siberian Synchrotron Radiation Center (SSCR). Studies using XAFS method show that modification of TiO₂ by various types of modifiers leads to change of symmetry of the nearest oxygen arrangement of the titanium ions in the anatase lattice as compared with the non-modified TiO₂. It seems that modifier ions lead to changes of the tetragonal parameter in the (010) direction and that the degree of distortions is associated with the type of modifier. All the data obtained are in good agreement with the earlier XRD data.

STABILIZATION OF HEAVY METAL CATIONS IN THE FRAMEWORK OF ZIRCONIUM PHOSPHATES

V.V. Kriventsov, D.I. Kochubey, V.A. Sadykov,
S.N. Pavlova, G.V. Zabolotnaya

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 336-340.

Coordination forms of heavy metal cations (such as Pt, Mo and W) in the framework of zirconium phosphates and their influence on the matrix structure were studied by the EXAFS method. Additional stabilizing cations (La and Si in our case) are usually located in the structure of zirconium phosphates. It is shown that the basic sites of cation stabilization in the framework of zirconium phosphates are the positions of the second cations. Oxide particles MeO_x can grow at such sites if the sorption capacity of zirconium phosphates is not sufficient for stabilization of all introduced heavy metal cations.

STRUCTURAL DETERMINATION OF THE Fe-MODIFIED ZIRCONIUM OXIDE

V.V. Kriventsov, D.I. Kochubey, Y.V. Maksimov*,
I.P. Suzdalev*, M.V. Tsodikov**, J.A. Navio***,
M.C. Hidalgo***, G. Colon*** (*Institute of
Chemical Physics, Moscow, Russia;
**A.V. Topchiev Institute of Petrochemical Synthesis,
Moscow, Russia; ***Instituto de Ciencia de
Materiales de Sevilla, Universidad de Sevilla, Sevilla,
Spain)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 341-346.

Nanocomposite system Fe/ZrO₂ prepared by sol-gel synthesis was studied by the EXAFS, XRD and Mössbauer methods. According to the data of all the methods phase composition of the system depends on the percentage of Fe. Only the tetragonal ZrO₂ structure is found at high Fe concentration, but at low concentration up to 1 wt.% of Fe, the formed ZrO₂ is a mixture of monoclinic and tetragonal structures. It seems that for greater concentrations, the iron produces two-dimension layer structures. It was revealed that the iron is located on the external surface of the (111) plane of the ZrO₂ nanoparticles, namely as isolated ions at concentrations less than one monolayer.

XAFS STUDY OF TiO₂/SiO₂ SYSTEM PREPARED BY SOL-GEL FROM INORGANIC PRECURSORS

V.V. Kriventsov, D.I. Kochubey, M.V. Tsodikov*,
J.A. Navio**, G.M. Restrepo***, M. Macias**
(*A.V. Topchiev Institute of Petrochemical Synthesis,
Moscow, Russia; **Instituto de Ciencia de Materiales
de Sevilla, Universidad de Sevilla, Sevilla, Spain;
***Universidad de Antioquia, Medellin, Colombia)

Nuclear Instrum. & Methods Phys. Res. A,
470(1-2) (2001) pp. 347-352.

The samples of 5%TiO₂/SiO₂ prepared by sol-gel method from inorganic precursors calcinated at the various temperatures were studied by XAFS spectroscopy at Siberian Synchrotron Radiation Center. It was established that structural lability of this system and the change of symmetry of the oxygen coordination around the Ti(+4) ions depends on the calcinations temperature. It seems that the mechanism of dissolution of the Ti(4+) ions in SiO₂ depends on the calcinations temperature and consists in the formation of Wadsley defects following the incorporation of SiO₂ in TiO₂ particles.

EXAFS STUDY OF THE Fe_x/ZrO₂ COMPOSITE NANOMATERIALS OBTAINED BY SOL-GEL SYNTHESIS

V.V. Kriventsov, D.I. Kochubey, J.A. Navio*,
M.C. Hidalgo*, G. Colón*, M.V. Tsodikov**,
Y.V. Maksimov***, I.P. Suzdalev*** (*Instituto de
Ciencia de Materiales de Sevilla, Universidad de
Sevilla, Sevilla, Spain; **A.V. Topchiev Institute of
Petrochemical Synthesis, Moscow, Russia;
***Institute of Chemical Physics, Moscow, Russia)

J. Synchrotron Radiation, 8(2) (2001) pp. 528-530.

The local Zr and Fe arrangements in the nanocomposite system Fe_x/ZrO₂ (x=0-0.2) obtained by sol-gel method were studied by EXAFS. The phase composition was found to vary significantly on iron loading. For the samples calcined at 500 or 600°C, at x≤0.01, the formed ZrO₂ is a mixture of monoclinic and tetragonal structures. Only tetragonal structure is revealed at x≥0.05 with the exception of Fe_{0.2}/ZrO₂, calcined at 500°C, where new non-typically short Zr-Zr distances (3.29, 3.43Å) were observed. At low iron loading (less than one monolayer) Fe³⁺ ions were found to localize within the pre-surface layers of ZrO₂ nanoparticles showing property of isolated ions. For greater Fe loading, iron exhibits either two-dimensional layer structure or two-phase system.

X-RAY FILM INTERFEROMETER AS AN INSTRUMENT FOR SEMICONDUCTOR HETEROSTRUCTURE INVESTIGATION

A.P. Vasilenko*, A.V. Kolesnikov*,
S.G. Nikitenko, A.A. Fedorov*, L.V. Sokolov*,
A.I. Nikiforov*, E.M. Trukhanov* (*Institute of
Semiconductor Physics, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 110-113.

Translation Moiré pictures were first observed in interference topographs obtained using Synchrotron radiation. A film interferometer was prepared on the base of the GeSi heterosystem. Another film interferometer, which presents the heterosystem of *epitaxial Si/porous Si/substrate Si*, permitted to observe a decrease in the bending of the film atomic planes at annealing of the heterosystem. This bend smoothing was calculated with the sensitivity better than 1Å with the use of X-ray interference topographs. Contrast peculiarities in Moiré pictures are discussed for nondiffracting layers and crystal quantum wells.

INTERACTION OF HYDROGEN WITH COPPER-CONTAINING OXIDE CATALYSTS. 5. STRUCTURAL TRANSFORMATIONS IN COPPER CHROMITE DURING REDUCTION- REOXIDATION

L.M. Plyasova, I.Yu. Molina, T.A. Krieger,
L.P. Davydova, V.V. Malakhov, L.S. Dovlitova,
T.M. Yurieva

Kinetics & Catalysis, 42(1) (2001) pp. 126-131.

High-precision X-ray powder diffraction and differential dissolution methods are used to show that copper chromite with a structure of tetragonal spinel is recovered under certain conditions upon the reoxidation of the system of phases formed by the reduction of the initial copper chromite, cation-deficient spinel stabilized by hydrogen and Cu⁰ particles epitaxially bound to its surface at 250–350°C. However, because of destruction of the initial surface layer at the initial moment of reduction, equilibrium cannot be complete: reoxidized spinel is nonstoichiometric and contains some lattice oxygen-bound protons, and the copper oxide is formed on the surface in some amount. The difference in the phase transition of copper chromite during reduction–reoxidation from the reversible polymorphic transitions characteristic of copper chromite during temperature variations is analyzed.

X-RAY ABSORPTION AND PHOTOEMISSION STUDIES OF THE ACTIVE OXYGEN FOR ETHYLENE EPOXIDATION OVER SILVER

V.I. Bukhtiyarov, M. Hävecker*, V.V. Kaichev, A. Knop-Gericke*, R.W. Mayer*, R. Schlögl*
(*Fritz-Haber-Institut der MPG, Berlin, Germany)

Catal. Lett., 74(3-4) (2001) pp. 121-125.

Activation of clean polycrystalline silver by a $C_2H_4+O_2$ reaction mixture has been studied by XANES, XPS, and UPS. *In situ* monitoring of the O K-edge XAS spectrum of the pre-treated silver surface revealed a broad signal at 10-20 eV above the threshold. The comparison of the X-ray absorption spectra with O 1s and valence band photoemission data allowed us to attribute this XAS signal to "electrophilic" oxygen ($E_b(O\ 1s) = 530.4$ eV) which is known to be active in ethylene epoxidation. The complete absence of XAS features in photon energy range typical for π^* and σ^* transitions of molecular oxygen (530-535 eV) indicates both the atomic origin of the electrophilic oxygen and the absence of molecular species on the catalyst surface under the present reaction conditions.

COMBINED APPLICATION OF XANES AND XPS TO STUDY OXYGEN SPECIES ADSORBED ON Ag FOIL

V.I. Bukhtiyarov, M. Hävecker*, V.V. Kaichev, A. Knop-Gericke*, R.W. Mayer*, R. Schlögl*
(*Fritz-Haber-Institut der MPG, Berlin, Germany)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 302-305.

Adsorbed oxygen species realized in the course of ethylene epoxidation over polycrystalline silver have been characterized by X-ray absorption near the edge structure and X-ray photoelectron spectroscopy. Namely, the combined application of XANES and XPS in similar UHV conditions using the same sample allowed one to assign an XAS feature to the nucleophilic and electrophilic oxygen. This is of great significance, since these species are suggested to be included into the active center for ethylene epoxidation. The differences in the oxygen-silver bonding of these oxygen species are discussed.

EPR-SPECTROSCOPIC DETECTION AND CHARACTERIZATION OF A Cu^{II} COMPLEX WITH A PEROXYCARBOXIMIDIC ACID

E.P. Talsi, G.L. Elizarova, L.G. Matvienko, A.A. Shubin, V.N. Parmon

Mendeleev Commun., 11(6) (2001) pp. 206-207.

A copper(II) complex with peroxycarboximidic acid formed upon the interaction of alkaline hydrogen peroxide with acetonitrile was detected and characterized for the first time.

^{51}V AND ^{13}C NMR SPECTROSCOPIC STUDY OF THE PEROXOVANADIUM INTERMEDIATES IN VANADIUM CATALYZED ENANTIOSELECTIVE OXIDATION OF SULFIDES

K.P. Brylyakov, N.N. Karpyshev, S.A. Fominsky, A.G. Tolstikov, E.P. Talsi

J. Molec. Catal. A: Chemical, 171(1-2) (2001) pp. 73-80.

Using ^{13}C and $^{13}C\{^1H\}$ NMR spectroscopy, structure and reactivity of vanadium peroxo complexes formed in the catalytic system $[VO(Oi-Pr)_3]/Schiff$ base ligand/ H_2O_2 for enantioselective oxidation of sulfides were concerned. It was shown, that two types of monoperoxo vanadium(V) species bearing one Schiff base ligand per vanadium atom predominated in this catalytic system at low temperature. These complexes are unstable at room temperature and decompose with half-life time of 20 min. The rate of this decomposition markedly increases in the presence of methyl phenyl sulfide. Addition of a fresh portion of H_2O_2 restores partially the peroxo vanadium intermediates. These data suggest that the peroxo vanadium species observed could be the active intermediates in enantioselective oxidation of sulfides. Two types of peroxo complexes found, probably, differ in the mode of Schiff base ligand coordination.

NMR STUDY OF REACTIONS BETWEEN Pd, Ru, AND Rh NITRITE COMPLEXES WITH SULFAMIC ACID

A.V. Belyaev*, V.A. Emel'yanov*, S.P. Khranenko*, M.A. Fedotov (*Institute of Inorganic Chemistry, Novosibirsk, Russia)

Russ. J. Coord. Chem., 27(3) (2001) pp. 184-194.

Reactions of nitrite complexes of Pd, Ru, and Rh with sulfamic acid were studied by the $^{14,15}N$, and ^{17}O

NMR method. Chemical shifts were assigned, and the predominant forms of the complexes were established. The reaction products at room temperature are *cis*-nitroaqua complexes. Coordination of the sulfamate ion upon storage for a long time or on heating was detected.

FORMS OF Rh(III) IN NITRIC ACID SOLUTIONS

A.V. Belyaev*, **M.A. Fedotov**, **S.P. Khranenko***,
V.A. Emel'yanov* (*Institute of Inorganic
Chemistry, Novosibirsk, Russia)

Russ. J. Coord. Chem., 27(12) (2001) pp. 855-864.

The forms of Rh(III) in nitric acid solutions are studied by ^{14}N , ^{15}N , ^{17}O , and ^{103}Rh NMR and electronic absorption spectra. At HNO_3 concentrations below 5 mol/l, rhodium mainly exists as low-nuclear oligomers with a bridging fragment $\text{Rh}(\mu\text{-OH})$ ($\mu\text{-ONO}_2$)Rh; terminal positions of the central atoms are occupied by water molecules. It was found that the isotopic equilibrium $^{14}\text{NO}_3^- / ^{15}\text{NO}_3^-$ of the bridging ligand sets in at an abnormally high rate, at which the isotopic exchange $\text{H}_2^{17}\text{O} / \text{H}_2^{16}\text{O}$ of the terminal ligands also occurs in the dimers and trimers. The formation of low-nuclear oligomers is a common feature of Rh(III) complexes in aqueous solutions with ligand deficiency in the system. The possibility of isolating rhodium from nitric acid solutions using different methods is predicted.

^{51}V AND ^{31}P NMR STUDIES OF VO_x/TiO_2 CATALYSTS MODIFIED BY PHOSPHOROUS

O.B. Lapina, **D.F. Khabibulin**, **A.A. Shubin**,
V.M. Bondareva

J. Molec. Catal. A: Chemical, 162(1-2) (2000)
pp. 381-390.

Phosphorous doped VO_x/TiO_2 catalysts prepared by the spray-drying method and treated under catalytic reaction as well as individual phases (α_1 -, α_{II} -, β -) of VOPO_4 were studied using modern high-resolution solid-state NMR techniques, including fast MAS combined with the analysis of rotational satellites intensities by the SATRAS method; 2D triple-quantum, quintuple-quantum MAS NMR, and spin mapping echo experiments. The simultaneous determination of chemical shielding anisotropy and quadrupole tensor parameters as well as their distributions permits to draw a conclusion on the local

environment of vanadium sites in the catalysts. The formation of a triple V-P-Ti compound in phosphorous doped VO_x/TiO_2 catalysts has been revealed. Only one type of slightly distorted tetrahedral vanadium atoms bound via oxygen to phosphorus was found in this compound. The very large distribution of the quadrupole constant points to the irregular structure of this compound.

^{51}V NMR STUDY OF VOCl_3 IMMOBILIZED ON THE SiO_2 AND MgCl_2 SURFACE

O.B. Lapina, **M.A. Mats'ko***, **T.B. Mikenas**,
V.A. Zakharov, **E.A. Paukshtis**,
D.F. Khabibulin*, **A.P. Sobolev** (*Novosibirsk State
University, Novosibirsk, Russia)

Kinetics & Catalysis, 42(4) (2001) pp. 553-560.

The magnetic shielding tensor and quadrupole interaction parameters, as well as the mutual orientation of tensors for the $(\equiv\text{SiO})\text{VOCl}_2$ complex obtained by the immobilization of VOCl_3 on the SiO_2 surface are determined. The state of VOCl_3 on the surfaces of MgCl_2 and modified SiO_2 with all surface OH groups replaced by Cl atoms is studied. To prepare the modified SiO_2 , CCl_4 and SiCl_4 are used as chlorinating agents. The formation of structurally similar pentavalent vanadium complexes on the surface of these supports is shown. A model for the coordination environment of vanadium on the chlorine-containing supports is proposed. The vanadium atom exists in the distorted pentahedral environment and is bound to the support through either two chlorine atoms or chlorine and oxygen atoms. A correlation between the coordination of VOCl_3 and catalytic properties of $\text{VOCl}_3/\text{MgCl}_2$ is assumed.

n-PENTANE ISOMERIZATION OVER $\text{Pt}/\text{WO}_x/\text{ZrO}_2$ CATALYSTS: A ^1H AND ^{13}C NMR STUDY

S.V. Filimonova, **A.V. Nosov**, **M. Scheithauer***,
H. Knözinger* (*Universität München, München,
Germany)

J. Catal., 198 (1) (2001) pp. 89-96.

The skeletal isomerization of *n*-pentane over platinum-promoted tungstated zirconia has been studied by the ^1H and ^{13}C nuclear magnetic resonance technique. $\text{Pt}/\text{WO}_x/\text{ZrO}_2$ samples with varying Pt concentrations have been used as catalysts. ^{13}C -labeled *n*-pentane was used to analyze the isotopic label

distribution in the reaction products. A few aspects of the mechanism of *n*-pentane isomerization are discussed. Spectroscopic evidence was obtained indicating that initially *n*-pentane isomerization proceeds by a monomolecular pathway, most probably on Lewis acid sites, which permit hydride abstraction from *n*-alkane molecules. At higher conversion degrees, isopentane is produced both mono- and bimolecularly via oligomerization and β -fission of a chemisorbed C₁₀-carbenium ion.

***n*-PENTANE CONVERSION ON SULFATED ZIRCONIA IN THE ABSENCE AND PRESENCE OF CARBON MONOXIDE. EVIDENCE FOR MONOMOLECULAR MECHANISM OF ISOMERIZATION FROM THE ¹³C MAS NMR STUDY**

M.V. Luzgin, A.G. Stepanov, V.P. Shmachkova, N.S. Kotsarenko

J. Catal., 203(2) (2001) pp. 273-280.

In situ ¹³C MAS NMR analysis of hydrocarbon products formed from the selectively ¹³C-labeled *n*-pentane on sulfated zirconia in the absence and presence of carbon monoxide provide the evidence that *iso*-pentane forms by two parallel processes: isomerization and "conjunct polymerization". Peculiarities of the ¹³C label scrambling from *n*-pentane into *iso*-pentane provide unequivocal evidence for monomolecular mechanism of the alkane isomerization. Besides *iso*-pentane, conjunct polymerization affords also the products of *n*-pentane "disproportionation" butanes and hexanes and stable cyclopentenyl cations, the latter are in charge of deactivation of the catalyst. Carbon monoxide suppresses completely the process of conjunct polymerization, whereas the process of intramolecular isomerization does not. In the presence of carbon monoxide carbonylation of *n*-pentane occurs in parallel with its isomerization, giving rise to a mixture of aldehydes, ketones and carboxylic acids. Carbonylation of *n*-pentane with CO contributes to the earlier observed negative effect of CO on the alkane isomerization rate.

***n*-PENTANE CARBONYLATION WITH CO ON SULFATED ZIRCONIA: AN *IN SITU* SOLID-STATE ¹³C NMR STUDY**

M.V. Luzgin, A.G. Stepanov, V.P. Shmachkova, N.S. Kotsarenko

Mendeleev Commun., 11(1) (2001) pp. 23-25.

Using ¹³C CP/MAS NMR, the first evidence has been obtained for *n*-pentane carbonylation with carbon monoxide into C₆ aldehydes, ketones and carboxylic acids on a sulfated zirconia catalyst.

AN ION CYCLOTRON RESONANCE STUDY OF REACTIONS BETWEEN MOLYBDENUM OXIDE CLUSTER IONS AND METHANE AND CYCLOPROPANE IN THE GAS PHASE

V.B. Goncharov, E.F. Fialko

Russ. J. Phys. Chem., 75(5) (2001) pp. 760-765.

Reactions of molybdenum oxygen-containing clusters Mo_xO_y⁺ ($x=1-3$, $y=1-9$) with methane and cyclopropane were studied by ion cyclotron resonance. The formation of several organometallic ions, including molybdenum oxometallobenzenes Mo_xO_yCH₂⁺ ($x=1-3$, $y=2, 4, 5, 8$), was observed. The upper and lower bond energy limits were estimated: $111 > D^{\circ}(\text{Mo}_x\text{O}_y^+ - \text{CH}_2) > 82$ kcal/mol ($x=1-3$, $y=2, 5, 8$).

LIQUID AND GAS FLOW AND RELATED PHENOMENA IN MONOLITHIC CATALYSTS STUDIED BY ¹H NMR MICROIMAGING

I.V. Koptug*, L.Yu. Ilyina, A.V. Matveev*, R.Z. Sagdeev*, V.N. Parmon, S.A. Altobelli**
(*International Tomography Center, Novosibirsk, Russia; **New Mexico Resonance, Albuquerque, NM, USA)

Catal. Today, 69(1-4) (2001) pp. 385-392.

NMR is employed to study liquid and gas flow in a tube and in the channels of shaped catalysts, mass transport during drying of water saturated porous monoliths, and gas adsorption by porous alumina pellets. NMR flow imaging and pulsed field gradient NMR are shown to yield the same average propagators for liquid and gas flow in a straight circular tube. The complicated patterns of gas or liquid flow in shaped reactors are characterized successfully by NMR flow imaging through the detection of all three flow velocity components.

EVIDENCE FOR 9R-SiC?

U. Kaiser*, **A.L. Chuvilin**, **V.L. Kuznetsov**,
Yu.V. Butenko (*Friedrich-Schiller-Universität Jena,
Jena, Germany)

Microsc. & Microanal., 7(4) (2001) pp. 368-369.

Complementary to the first paper on the origin of threefold contrast on SiC high resolution transmission electron microscopy (HRTEM) images, it is now provided an example of threefold contrast produced by a stacking layer sequence which corresponds to one unit cell of the 9R polytype.

THE RELATIONSHIP BETWEEN THE STATE OF ACTIVE SPECIES IN A Ni/Al₂O₃ CATALYST AND THE MECHANISM OF GROWTH OF FILAMENTOUS CARBON

V.I. Zaikovskii, **V.V. Chesnokov**, **R.A. Buyanov**

Kinetics & Catalysis, 42(6) (2001) pp. 813-821.

The formation of active particles and their changes in the course of 1,3-butadiene decomposition on a Ni/Al₂O₃ catalyst at temperatures from 400 to 800°C were studied by high-resolution electron microscopy. It was found that carbon filaments of different types were formed at 400-800°C. The growth of thin filaments (20-30 nm in diameter) takes place at 400-600°C on a conical Ni particle located at the growing end of the filament, whereas disymmetrical filaments 50-100 nm in diameter grow on biconical metal particles. As the carbonization temperature was increased to 700-800°C, graphite nanotubes 5-20 nm in diameter were formed. It was found that the mechanism of formation and the structure of filaments are related to the state of catalytically active species, which consist of a solid solution of carbon in the metal. It is suggested that the metastable surface nickel carbide Ni₃C_{1-x} is an intermediate compound in the catalytic formation of graphite filaments from 1,3-butadiene. Upon termination of the reaction, the metastable Ni₃C_{1-x} microphase is decomposed with the formation of hexagonal nickel microinclusions. The role of epitaxy in the nucleation and growth of a graphite phase on the metal is discussed. Models are presented for the growth of structurally different carbon filaments depending on the formation of active metal species at various temperatures. Considerable changes in the structure of carbon and the formation of nanotubes at 700-800°C are related to the appearance of a viscous flow state of metal-carbon particles.

PROJECT OF ULTRAHIGH-VACUUM DOUBLE-CRYSTAL MONOCHROMATOR

A.I. Ancharov*, **N.G. Gavrillov****,
V.I. Kondrat'ev**, **I.V. Poletaev****,
M.A. Sheromov**, **A.N. Shmakov**,
B.P. Tolochko*, **V.M. Tsukanov****, **I.L. Zhogin***
(*Institute of Solid State Chemistry and
Mechanochemistry, Novosibirsk, Russia;
**G.I. Budker Institute of Nuclear Physics,
Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A,
470(1-2) (2001) pp. 128-130.

The project is aimed at the development of ultrahigh-vacuum mechanics and construction of devices with features allowing high-precision work in a warmed-up volume. The fundamental part of projected monochromator is a precise linear motion mechanism, linear stage, which can bear a warming-up in vacuum up to $t=400^{\circ}\text{C}$ without any change in its parameters. It is the tense friction wave transmission that serves to transfer the motion to the stage in the vacuum volume. The mechanism for precision tuning of the second crystal also has an original design and its compactness allows an easier solution of many design issues concerning the whole monochromator.

A MULTIPURPOSE UV-VISIBLE SPECTROSCOPIC SYSTEM

A.M. Sorokin, **V.V. Kaichev**, **A.I. Timoshin***,
O.V. Moskovkin**, **A.A. Rastorguev*****,
A.M. Badalyan*** (*Institute of Automation and
Electrometry, Novosibirsk, Russia; ** Institute for
Water and Environmental Problems, Barnaul, Russia;
*** Institute of Inorganic Chemistry, Novosibirsk,
Russia)

Instrum. & Exper. Techniques, 44(3) (2001)
pp. 375-380.

The complex is intended for recording the spectral responses of the UV-visible radiation in various analysis modes (absorption and emission spectrophotometry, spectrofluorometry, and Raman spectroscopy), as well as scanning modes (excitation and luminescence wavelengths, and synchronous one). The open architecture of the automation hardware and software allows one to flexibly change the complex configuration and operation mode and to expand the range and composition of spectral devices. The amplifier-converter with a low level of input current noise (1.5 fA in a range of 0-1 Hz) provides photocurrent recording in the 116-dB dynamic range.

NEUTRON DIFFRACTION, SYNCHROTRON RADIATION AND EXAFS SPECTROSCOPY STUDY OF CRYSTAL STRUCTURE PECULIARITIES OF THE LANTHANUM NICKELATES $\text{La}_{n+1}\text{Me}_n\text{O}_{3n+1}$ ($n=1,2,3$)

V.I. Voronin*, **I.F. Berger****, **V.A. Cherepanov*****, **L.Y. Gavrilova*****, **A.N. Petrov*****, **A.I. Ancharov******, **B.P. Tolochko******, **S.G. Nikitenko** (*Institute for Metal Physics, Yekaterinburg, Russia; **Institute of Solid State Chemistry, Yekaterinburg, Russia; ***Ural State University, Yekaterinburg, Russia; ****Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 202-209.

Complex oxides: La_2NiO_4 (I), $\text{La}_3\text{Ni}_2\text{O}_7$ (II) and $\text{La}_4\text{Ni}_3\text{O}_{10}$ (III), belonging to the homologous series $\text{La}_{n+1}\text{Me}_n\text{O}_{3n+1}$, were prepared by the traditional ceramic technique (I) and by that of citrate or nitrate precursors (II), (III). The crystal structure of all samples was determined by means of X-ray diffraction, neutron diffraction and synchrotron radiation spectroscopy. Data on nickel coordination were obtained by EXAFS spectroscopy. Phases (II) and (III) were used for structural investigation as prepared powders (quenched from 1100°C in air), phase (I) was pressed into rectangular bars (5x5x30 mm) and sintered at 1370°C for 5 h. Structural parameters of all phases were refined based on Cmc21 (I), Cmc21 (II) and Cmc21 (III) space group using the Rietveld analysis. Bond lengths in all compounds were calculated. Oxygen octahedrons centered by nickel ions were distorted in (I) and (II). (I) has two and (II) has four different Ni-O interatomic distances. Phase (III) has both ideal and distorted octahedrons in the structure and two types of nonequivalent Ni sites, as a result. The oxidation state of cations was estimated using the average cation-anion distance approach and the so-called bond valence approach. The results allowed the authors to suggest that Ni^{3+} preferably occupied the Ni1 sites, i.e. it is possible to assume some charge ordering inside the lattice.

ADSORPTION OF SMALL MOLECULES ON THE Pt(100) SINGLE CRYSTAL SURFACE STUDIED BY DISAPPEARANCE POTENTIAL SPECTROSCOPY

A.R. Cholach, V.M. Tapilin

Appl. Surf. Sci., 180(1-2) (2001) pp. 173-183.

Disappearance potential spectroscopy (DAPS) is used to elucidate the influence of H_2 , O_2 , NO, and CO

adsorption and $\text{NO}+\text{H}_{\text{ads}}$ interaction on the electronic structure of the Pt(100)-(1x1) single crystal surface. DAP spectra obtained after adsorption of different molecules reveal the similar features related to excitation of platinum core electrons. Besides, a set of the pronounced individual satellites originating from the adsorbed species are also exhibited in DAP spectra. The locations of these satellites with respect to the substrate Fermi level are found to be comparable with the ionization potentials of the given adsorbed particle. It evidences the conjugate pathway of the primary electron energy consumption, which includes an ordinary threshold excitation of the substrate core electron accompanied by ionization of the adsorbed species.

APPLICABILITY VERIFICATION FOR A NEW METHOD OF MEASURING THE COMPONENTS' SURFACE AREAS IN BICOMPONENT CATALYSTS AND ADSORBENTS

M.S. Mel'gunov, V.B. Felonov, R. Leboda*, **B. Charmas*** (*Maria Curie-Skladowska University, Lublin, Poland)

Colloids and Surfaces A: Physicochem. & Engin. Aspects, 186(3) (2001) pp. 203-209.

Efficiency of a new method of components' accessible surface areas (ASAs) measurement based on the analysis of unspecific adsorption interactions of some fluid with both components that exist on the surface of porous bicomponent solid is verified. For this purpose, adsorption studies of a model silica/alumina admix and a series of carbon-mineral adsorbents have been carried out. The obtained values of components' ASAs correlate well with the values measured by an alternative technique, regardless of the type of an adsorbate used, operational temperature, and examined component's type. It is discussed that the earlier proposed adsorption or chemisorption techniques, which are based on adsorbate interactions with only one component on the surface, can be considered as particular cases of the new method.

ON THE DEPENDENCE OF SURFACE TENSION OF LIQUIDS ON THE CURVATURE OF THE LIQUID-VAPOR INTERFACE

V.B. Fenelonov, G.G. Kodenev*,
V.G. Kostrovsky** (*Design and Technological
Institute of Instrument Engineering for Geophysics
and Ecology, Novosibirsk, Russia; **Institute of Solid
State Chemistry and Mechanochemistry, Novosibirsk,
Russia)

J. Phys. Chem. B, 105(5) (2001) pp. 1050-1055.

Conventional methods for measuring pore-size distribution (PSD), which are based on the capillary condensation (CC) and mercury intrusion porosimetry (MIP), are very sensitive to the numerical values of surface tension, σ , of the corresponding liquid phase. However, it is generally accepted that σ strongly depends on the curvature radius, r . Hence, PSD measuring seems unreliable if it does not involve the $\sigma(r)$ dependence. Experimental studies of the surface tension, σ , for nuclei of liquids formed in the vapor upon homogeneous nucleation support the idea of no significant dependence of σ on the curvature of the interface at the range of subnanometer radii.

THE CHARACTERIZATION OF THE STRUCTURE AND TEXTURE OF PILLARED INTERLAYER MATERIALS

V.B. Fenelonov, A.Yu. Derevyankin, V.A. Sadykov

Micropor. & Mesopor. Mater., 47(2-3) (2001)
pp. 359-368.

A method for the correct characterization of the structure and texture of pillared interlayered materials (PIM) is developed. This method is based upon the combined analysis of XRD and adsorption data within the frames of a geometrical PIM model. The application of this method is illustrated by analysis of the structure of pillared montmorillonite clays. Among the structural and textural parameters successfully estimated by this method are specific values of the accessible micropore surface A_m and volume V_m , a degree of the interlayer space filling by a guest (pillars), a degree of PIM ordering, the interpillar distance etc.

DEPENDENCE OF THE EFFICIENCY OF A MULTICAPILLARY COLUMN ON THE LIQUID PHASE LOADING METHOD

V.P. Zhdanov, V.N. Sidelnikov, A.A. Vlasov

J. Chromatography A, 928(2) (2001) pp. 201-207.

One of the main approaches employed to reach fast chromatographic separation is based on using columns containing up to 1000 capillaries with the diameter size down to 10–100 μm . The efficiency of such columns depends on the dispersion of the capillary radius and on the way of the liquid-film loading. The general equations describing these effects are presented. Specifically, it is shown theoretically and experimentally that the separation efficiency can be improved by using the loading methods specially designed in order to take into account correlation between the film thickness and capillary radius.

MECHANISM OF HEART VALVE MINERALIZATION

A.T. Titov*, P.M. Larionov**, V.S. Shchukin**,
V.I. Zaikovskii (*United Institute of Geology,
Geophysics and Mineralogy, Novosibirsk, Russia;
**Institute of Blood Circulation Pathology,
Novosibirsk, Russia)

*Surface Investigation: X-Ray, Synchrotron and
Neutron Techniques*, 3 (2001) pp. 74-79.

The structure, morphology and composition of calcsificates of heart valves with different degree of mineralization have been investigated by local methods of structural and chemical analysis – transmission electron microscopy, high resolution electron microscopy and X-ray microanalysis. The calcsificates consist of lamellar microcrystals of hydroxylapatite (HA) 0.005-5 microns in size with the most developed (1210) planes, that are not typical for macrocrystalline apatite, and (0001) planes. The HA particles, similar to those in fine fraction of calcsificate and in bones, were found in donors blood and blood of patients, having calcinosa of heart valve. The reason of heart calcsification may be the damage of endothelial lining capillaries and the other factors promoting penetration of HA microcrystals and calcium and phosphate ions to valve tissue. Valve heart system mineralization occurs as result of adhesion of active surface of HA on poly- and biopolymers.

Nature, Mechanism and Physicochemical Essence of the Low-Waste, Environmentally Friendly Methods of Preparation

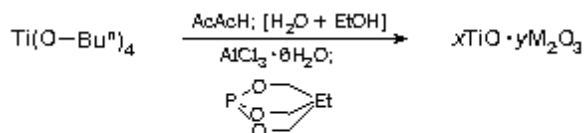
STRUCTURE AND ACID-BASIC PROPERTIES OF THE SURFACE OF TITANIUM OXIDES MODIFIED BY PHOSPHORUS AND ALUMINUM AND PREPARED BY THE ALKOXO METHOD.

1. STRUCTURAL ORGANIZATION OF MODIFIED TITANATE SYSTEMS

M.V. Tsodikov*, O.V. Bukhtenko*, E.V. Slivinskii*, L.N. Slastikhina*, A.M. Voloshchuk**, V.V. Kriventsov, L.E. Kitaev*** (*A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; **Physical-Chemistry Institute, Moscow, Russia; ***Moscow Lomonosov State University, Moscow, Russia)

Russ. Chem. Bull., 49(11) (2000) pp. 1803-1807.

An alkoxo method for the preparation of single-phase titanium oxides modified by phosphorus and aluminum is proposed and the mechanism of oxide formation is investigated. Structural studies showed that the sizes of the anatase microcrystallite grains and mesopores in the systems are characterized by a uniform distribution. The nature of the modifying agent and the conditions of synthesis influence the interatomic distances and the dimension of c , a tetragonal unit cell constant of anatase.



M = P, Al

STRUCTURE AND ACID-BASIC PROPERTIES OF THE SURFACE OF TITANIUM OXIDES MODIFIED BY PHOSPHORUS AND ALUMINUM AND PREPARED BY THE ALKOXO METHOD. 2. STUDY OF THE ACTIVE SURFACE OF TITANIUM OXIDES

M.V. Tsodikov*, E.V. Slivinskii*, V.V. Yushchenko**, L.E. Kitaev**, V.V. Kriventsov, D.I. Kochubey, A.T. Teleshev (*A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; **Moscow Lomonosov State University, Moscow, Russia)

Russ. Chem. Bull., 49(12) (2000) pp. 2003-2006.

The data of temperature-programmed desorption of ammonia from the surface of oxide systems and IR

spectroscopy were used to demonstrate that the strength of the surface acid sites in the titanium oxides prepared by the alkoxo method and modified by aluminum decreases with respect to that in the nonmodified titanium oxide. Modification of titanium oxide with P^{3+} ions from ethriol phosphite almost completely suppresses the acid properties. Modified oxides are able to chemisorb water. XANES data suggest that modification of titanium oxide with phosphorus ions increases the electron density on the titanium atoms and, correspondingly, the basicity of the materials.

STRUCTURE PECULIARITIES OF REDUCED VANADIUM-TITANIUM OXIDE CATALYSTS

G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya, V.F. Anufrienko, V.Yu. Gavrilov

Kinetics & Catalysis, 42(1) (2001) pp. 132-137.

The properties of vanadium–titanium oxide catalysts, which contain coherent phase boundaries formed by V_2O_5 and TiO_2 crystallites during reduction by hydrogen at 150–500°C, are examined. The phase boundary is preserved over the entire examined temperature range regardless of the structure of vanadium oxide, which is formed. The state of vanadium ions at the phase boundary is determined. The presence of a phase boundary in the catalyst is responsible for the $\text{V}_2\text{O}_5 \rightarrow \text{V}_2\text{O}_3$ transition without the formation of intermediate structures.

STRUCTURAL AND CATALYTIC PROPERTIES OF ULTRADISPERSED ENERGY SATURATED METALS

B.S. Bal'zhinimaev

J. Mendeleev Chem. Society, 45(3) (2001) pp. 59-65.

Ultra dispersed powders of various metals, synthesized by electric explosion in the inert atmosphere show unusual catalytic performance. At ethylene epoxidation by molecular oxygen over silver powder reaction selectivity towards ethylene oxide is close to 100%. Similar data were obtained over ultra dispersed platinum at partial oxidation of C-H bond in benzene and methane by molecular oxygen in hydrogen presence. At methane oxidation methanol and formaldehyde start to form selectively at room temperature. Specific non-equilibrium microstructures

are found on the metal surface. These species are formed in reaction course (Ag) or in the process of ultra disperse powder synthesis (Pt). Different acid-base or redox states of Ag or Pt, co-existing at the metal-microparticle interface, seem to be responsible for abnormally high selectivities discussed above.

COMPOSITE STEAM REFORMING CATALYSTS PREPARED FROM $\text{Al}_2\text{O}_3/\text{Al}$ MATRIX-PRECURSOR

S.F. Tikhov, V.A. Sadykov, I.I. Bobrova, Yu.V. Potapova, V.B. Fenelonov, S.V. Tsybulya, S.N. Pavlova, A.S. Ivanova, V.Yu. Kruglyakov, N.N. Bobrov

Stud. Surf. Sci. & Catal.,
Eds. I.I. Spivey, E. Iglesia, T. Fleisch,
Elsevier Sci., 136 (2001) pp. 105-110.

Several composite catalysts on the base of $\text{Al}_2\text{O}_3/\text{Al}$ matrix-precursor have been prepared and tested in the $\text{CH}_4/\text{H}_2\text{O}$ -reforming. The following sequence of the tested cermets activity ($\text{cm}^3 \text{CH}_4/\text{gCat bar s}$) was found: $6 > \text{Ni-Cr-La-Al-O} = \text{Ru-Sr-Zr-Al-O} > \text{Ni-La-Al-O} > \text{Co-La-Al-O} > \text{Rh-Sr-Zr-Al-O}$. The effect of the cermets properties on their activity have been discussed. The advantages of composite materials as coats on the tubes for the compact steam reformers were demonstrated.

PREPARATION OF $\text{Al}_2\text{O}_3/\text{Al}$ COMPOSITE THROUGH THE HYDROTHERMAL OXIDATION OF ALUMINUM FOIL

S.F. Tikhov, A.N. Salanov, Yu.V. Potapova, V.T. Yakushko, V.A. Sadykov, V.P. Ivanov, S.V. Tsybulya

Eurasian ChemTech J., 2 (2000) pp. 265-269.

The process of $\text{Al}_2\text{O}_3/\text{Al}$ composite preparation through aluminum foil hydrothermal oxidation at 150, 250°C with subsequent calcination at 540°C has been investigated. The evolution of micro- and microtexture had been studied. Nonuniformity of oxide relief has been discussed.

TEXTURE-STRENGTH PROPERTIES OF THE ALUMINA-MONTMORILLONITE COMPOSITE

V.A. Drozdov, V.P. Doronin, T.P. Sorokina, T.I. Gulyaeva, V.K. Duplyakin

Kinetics & Catalysis, 42(1) (2001) pp. 117-126.

The texture characteristics and strength properties of the molded alumina-montmorillonite composite are

studied. The mixture is obtained by mixing suspensions of activated clay and pseudoboehmite followed by drying (at 293 and 393 K) and calcination (at 873 K). It is a promising support for cracking and hydrotreating catalysts. The changes in the specific surface area; the volumes of micro-, meso-, macropore, and medium-size pores; and the strength of samples are studied by varying the montmorillonite concentration in the composite. The addition of 20–35 wt % clay largely results in a sharp in reduction of the macropore region and, correspondingly, provides the alumina oxide average strength of the extrudates of $\sim 10\text{--}12 \text{ MN/m}^2$, which is sufficient for industrial supports. This excludes the stage of standard acidic peptization from the technological scheme of alumina production. The complex study of the porous structure of the composite by adsorption and mercury porosimetry combined with elements of percolation theory makes it possible to predict the texture-strength properties of derivative materials.

KINETICS OF THE ALUMINUM POWDER OXIDATION BY WATER VAPOR AT MODERATE TEMPERATURES

Yu.V. Potapova, S.F. Tikhov, V.A. Sadykov, V.B. Fenelonov

React. Kinet. & Catal. Lett., 73(1) (2001)
pp. 55-61.

For the first time the detailed kinetics of aluminum oxidation by the water vapor at temperatures within 150–250°C range and steam pressure 500–5000 kPa was investigated. The "shrinking sphere" model was used for kinetics description. The effective kinetics parameters such as the apparent activation energy and the reaction order were estimated.

FINE α -ALUMINA WITH LOW ALKALI: NEW APPROACH FOR PREPARATION

V.I. Isupov*, L.A. Chupakhina*, G.N. Kryukova, S.V. Tsybulya (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Solid State Ionics, 141-142(1-4) (2001)
pp. 471-478.

Thermal decomposition of fine aluminium hydroxide, synthesized by intercalation-deintercalation of lithium salts into gibbsite, was studied. It is demonstrated that thermal decomposition of fine hydroxide at 1180–1200°C results in the formation of fine α -alumina ($10 \text{ m}^2/\text{g}$) with low alkali

content, forming pseudomorph with respect to the initial hydroxide. This allows to propose a new method to synthesize fine α -alumina, based on thermal decomposition of fine aluminium hydroxide obtained by intercalation–deintercalation of lithium salts into gibbsite. The major advantages of this method are the absence of wastes at the stage of the synthesis of fine hydroxide, relatively low temperature of α -alumina synthesis (1200°) at the absence of any fluorinating agents, and the absence of the necessity for thorough grinding of the synthesized α -alumina.

REAL STRUCTURE AND CATALYTIC ACTIVITY OF $\text{La}_{1-x}\text{Ca}_x\text{MnO}_{3+\delta}$ PEROVSKITES

L.A. Isupova, S.V. Tsybulya, G.N. Kryukova, G.M. Alikina, N.N. Boldyreva, I.S. Yakovleva, V.P. Ivanov, V.A. Sadykov

Solid State Ionics, 141-142(1-4) (2001) pp. 417-425.

Mechanoceramic and ceramic synthesis of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_{3+\delta}$ ($0 \leq x \leq 1$) perovskites were made using simple oxides as starting materials. Continuous solid solutions are formed during ceramic synthesis at 1100°C. Ca doping leads to formation of orthorhombic perovskites and to decreasing of their unit cell parameter. For $x=0.8$ a modulated perovskite structure was detected. For compositions with $0 \leq x \leq 0.4$ and $x=1$ calcination of activated oxides at 700-1100°C for 4 h leads to perovskite solid solutions formation. While the calcination temperature increases only the product content increases. For perovskites with $0.4 < x < 1$, after calcination at 700-900°C, very likely a composite is formed with a particles nucleus composed of phase with $x \leq 0.4$ and the surface layer enriched by CaMnO_3 and CaO . The interaction between composite layers at 1100°C leads to perovskite formation with $x=0.8$. Proposed composite model with the surface layer enriched by Ca cations (catalytic poison) does not conflict with a correlation between the catalytic activity in CO oxidation process and Ca content on the perovskite surface. In the absence of calcium in the surface layer of samples, catalytic activity increases when the interphase boundaries are present within particles of samples.

REAL STRUCTURE AND CATALYTIC ACTIVITY OF $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ PEROVSKITES

L.A. Isupova, G.M. Alikina, S.V. Tsybulya, N.N. Boldyreva, G.N. Kryukova, I.S. Yakovleva, V.A. Sadykov

Intern. J. Inorg. Mater., 3(6) (2001) pp. 559-562.

Mechanoceramic synthesis of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($0 \leq x \leq 1$) perovskites was made from simple oxides. Samples calcined at 900 and 1100°C for 4 h are nearly monophase and well crystallized. Sr adding was found to cause a structure rearrangements from the hexagonal (at $x \leq 0.4$) to the cubic one (at $0.8 > x > 0.4$) and back to the hexagonal at $x > 0.8$. There are 2 maxima of the catalytic activity versus chemical composition: at $x=0.3$ and at $x=0.8$. TEM data for these samples were obtained and disordered surface layers were detected. There is a correlation between the catalytic activity and surface layers microstructure.

CATALYSTS BASED ON FIBERGLASS SUPPORTS. 1. PHYSICO-CHEMICAL PROPERTIES OF SILICA FIBERGLASS SUPPORTS

L.G. Simonova, V.V. Barelko*, O.B. Lapina, E.A. Paukshtis, V.V. Terskikh, V.I. Zaikovskii, B.S. Bal'zhinimaev (*Institute of Problems of Chemical Physics, Chernogolovka, Russia)

Kinetics & Catalysis, 42(5) (2001) pp. 693-702.

The physicochemical properties and structure of supports prepared by leaching soda–silica fiberglass materials were studied using a set of physicochemical techniques (BET; IR spectroscopy; transmission electron microscopy; and ^{29}Si , ^{23}Na , ^{27}Al , ^{133}Cs , and ^{129}Xe (of adsorbed molecules) NMR spectroscopy). A matrix that corresponded in chemical composition to SiO_2 was formed at high degrees of leaching; however, it was considerably different from ordinary silica gels in properties. The structure and properties of this matrix are most adequately described by the model of a pseudolayer intercalation structure, which includes alternating layers of several silicon–oxygen tetrahedrons separated by narrow ($< 4 \text{ \AA}$) cavities. Considerable amounts of OH groups ($\sim 5000 \text{ \mu mol/g}$) are contained in these cavities, and these OH groups are different from the surface hydroxyl groups of ordinary globular silica. Although the interlayer spaces are small, comparatively bulky cations can be intercalated into them.

CATALYSTS BASED ON FIBERGLASS SUPPORTS. 2. PHYSICOCHEMICAL PROPERTIES OF ALUMINA BOROSILICATE FIBERGLASS SUPPORTS

L.G. Simonova, V.V. Barelko*, E.A. Paukshtis, O.B. Lapina, V.V. Terskikh, V.I. Zaikovskii, B.S. Bal'zhinimaev (*Institute of Problems of Chemical Physics, Chernogolovka, Russia)

Kinetics & Catalysis, 42(6) (2001) pp. 828-836.

The properties of borosilicate fiberglass supports were studied by various physicochemical techniques (BET, transmission electron microscopy and ^{11}B , ^{23}Na and ^{29}Si NMR spectroscopy). Unleached fiberglass was characterized by the presence of silicon primarily in the Q_2 form (two silicon atoms in the second coordination sphere of silicon-oxygen tetrahedrons) and by a comparatively homogeneous distribution of concomitant heteroatoms (B, Al and Na). Under the action of an acid, the extraction of nonsilica components and the rearrangement of a silicon-oxygen framework (the transition of Q_2 to $\text{Q}_3 + \text{Q}_4$) took place simultaneously. This was accompanied by the development of the surface and by the formation of channels with a wide range of sizes: from channels 1-50 Å in diameter (the adsorption properties of these channels are similar to those of mesopores in ordinary silica supports) to microchannels, which are typical pseudolayer intercalation structures described previously for leached soda-silica fiberglass.

CATALYSTS BASED ON FIBERGLASS SUPPORTS. 3. PROPERTIES OF SUPPORTED METALS (Pt, Pd) ACCORDING TO ELECTRON MICROSCOPY AND XPS DATA

L.G. Simonova, V.V. Barelko*, A.V. Toktarev, V.I. Zaikovskii, V.I. Bukhtiyarov, V.V. Kaichev, B.S. Bal'zhinimaev (*Institute of Problems of Chemical Physics, Chernogolovka, Russia)

Kinetics & Catalysis, 42(6) (2001) pp. 837-846.

Under varying preparation conditions metals supported on leached borosilicate and soda-silica fiberglasses form three types of particles. First, there are metallic particles with sizes from tens to hundreds of angstrom distributed over the outer surface of fibers. Second, in the presence of mesopores in fiberglass supports (borosilicate glasses), metallic particles of commensurable sizes (15-100 Å) are localized in the cavities. Third, dispersed (<10 Å) particles are intercalated into the bulk of leached fiberglasses as deep as several hundreds of angstrom. The amount of a metal

and the depth of penetration into the bulk of fiberglass can be controlled by preparation conditions and by the addition of cointercalates, which are responsible for pillaring effects.

SCIENTIFIC GROUNDS FOR THE APPLICATION OF MECHANOCHEMISTRY TO CATALYST PREPARATION

V.V. Molchanov, R.A. Buyanov

Kinetics & Catalysis, 42(3) (2001) pp. 366-374.

It is shown that mechanochemical activation is efficient in creating waste-free energy-saving methods for the preparation of hydride catalysts, heteropoly acid catalysts, and catalysts for hydrocarbon decomposition into hydrogen and carbon materials, as well for the synthesis of earlier unknown catalytic systems. The capabilities of the mechanochemical methods are demonstrated on modifying the catalytic properties of catalysts and supports: an increase in the strength and catalytic activity, sorption properties, etc. Adhesion theory applied to melts helps to describe the mechanism of mechanochemical synthesis of catalytic systems.

PHENOMENOLOGICAL MODEL OF MECHANOCHEMICAL ACTIVATION IN THE CATALYST TECHNOLOGY AND CATALYSIS

R.A. Buyanov, V.V. Molchanov

Chem. for Sustainable Devel., 9(3) (2001) pp. 369-377.

The phenomenological model of mechanochemical activation (MCA) has been suggested based on the conception of solution of defects of different types in crystal structure. The concentration of defects and the balance depend on the energy and dissipation. The Gibbs-Folmer conception of critical sizes and conditions of crystal grow are spread to the process of dispergation, defects reproduction and linear defects during MCA to linear and planar defects.

MECHANOCHEMICAL SYNTHESIS AND STRUCTURE OF NEW PHASES IN THE Pb-V-O SYSTEM

V.V. Zyryanov*, O.B. Lapina (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Inorg. Mater., 37(3) (2001) pp. 264-270.

The products of mechanochemical synthesis in the Pb-V-O system were characterized by X-ray

diffraction and magnetic resonance spectroscopy techniques. The mechanical processing was found to yield only new crystalline compounds, $Pb_{2.67}V_{1.33}O_{5.96}$ and $Pb_{3.5}V_{4.5}O_{14.75}$. Structural analysis of these phases revealed a low atomic density, mixed-valent states of the constituent cations, the presence of three of four types of vanadium polyhedra, and splitting of crystallographic sites, in line with the views on the mechanisms of mechanochemical reactions developed in the model for the reaction zone.

NANOCRYSTALLINE ULTRA HIGH SURFACE AREA MAGNESIUM OXIDE AS A SELECTIVE BASE CATALYST

R.M. Richards*, **R.S. Mulukutla***, **I.V. Mishakov**, **V.V. Chesnokov**, **A.M. Volodin**, **V.I. Zaikovskii**, **N. Sun***, **K.J. Klabunde*** (*Kansas State University, Manhattan, USA)

Scripta Mater., 44(8-9) (2001) pp. 1663-1666.

Nanocrystals of MgO having 4 nm average crystalline sizes with 450-550 m²/g surface area were prepared by the Aero-gel preparation method (AP-MgO). Dehydrohalogenation of 1-chlorobutane was performed using AP-MgO as a catalyst. 1-butene is the selective product formed even after several cycles of 1-chlorobutane injections. AP-MgO was allowed to react with Cl₂, which resulted in the formation of a highly reactive adduct which has a capability to selectively chlorinate propane.

CHANGES IN TEXTURE AND CATALYTIC ACTIVITY OF NANOCRYSTALLINE MgO DURING ITS TRANSFORMATION TO MgCl₂ IN THE REACTION WITH 1-CHLOROBUTANE

V.B. Fenelonov, **M.S. Mel'gunov**, **I.V. Mishakov**, **R.M. Richards***, **V.V. Chesnokov**, **A.M. Volodin**, **K.J. Klabunde*** (*Kansas State University, Manhattan, USA)

J. Phys. Chem. B, 105(18) (2001) pp. 3937-3941.

The interaction of 1-chlorobutane with nanocrystalline MgO at 200-350°C has been found to result in both stoichiometric and catalytic dehydrochlorination of 1-chlorobutane to isomers of butene and simultaneous topochemical conversion of MgO to MgCl₂. The obtained magnesium chloride appeared to be an active catalyst for the dehydrochlorination reaction, so the rate of 1-chlorobutane conversion grows significantly with time. Changes in the MgO texture during the

topochemical reaction are discussed and their effect on the catalytic activity is estimated.

REACTION OF POLYNUCLEAR PLATINUM CARBONYL WITH TIN(II) CHLORIDE

N.B. Shitova, **Yu.D. Perfil'ev***, **L.Ya. Al't**, **G.G. Savelieva** (*Moscow State University, Moscow, Russia)

Russ. J. Inorg. Chem., 46(3) (2001) pp. 376-381.

The H₂[Pt₃(CO)₆]₅+SnCl₂ reaction solutions and the precipitates isolated from these solutions were studied by IR and Mössbauer spectroscopy and NMR. At any initial reagent ratio in the range [Sn]:[Pt] = 1-5, the reaction yields a Pt-Sn-CO cluster with the atomic ratio Sn:Pt = 1:1. The adsorption properties of the platinum-tin-carbonyl cluster were examined. Strong adsorption of the cluster on ν -Al₂O₃ and its high stability in contact with the supporter allow to use it as a precursor of supported bimetallic Pt-Sn/ ν -Al₂O₃ catalysts and to prepare catalysts of the adsorption type of definite compositions.

Pd OXIDATION UNDER UHV IN A MODEL Pd/CERIA-ZIRCONIA CATALYST

M.Yu. Smirnov, **G.W. Graham*** (*Ford Research Laboratory, Dearborn, USA)

Catal. Lett., 72(1-2) (2001) pp. 39-44.

A model planar catalyst was prepared by depositing Pd onto a thick (few μ m) film of ceria-zirconia in ultrahigh vacuum (UHV), and the oxidation state of Pd and its support was determined by X-ray photoelectron spectroscopy, following thermal treatments in UHV, oxygen, or carbon monoxide. It was found that Pd could be oxidized simply by heating the catalyst in UHV, indicating that transfer of oxygen from the support to the metal is both thermodynamically favorable and facile.

PREPARATION OF CENOSPHERES OF STABILIZED COMPOSITIONS FROM VOLATILE SOLS AND THEIR PROPERTIES

T.A. Vereshchagina*, N.N. Anshits*, I.D. Zykova**, A.N. Salanov, A.A. Tretyakov***, A.G. Anshits* (*Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia; **Krasnoyarsk State Technical University, Krasnoyarsk, Russia; FGUP "Mining Enterprise", Zheleznogorsk, Russia)

Chem. for Sustainable Devel., 9(3) (2001) pp. 379-392.

Hollow aluminosilicate microspheres (cenospheres) of stabilized chemical and mineral phase compositions were isolated for the first time from volatile sols of combusted Kuznetsk coals through four-stage separation including magnetic separation, grain sizing, gravitational separation and isolation of perforated cenospheres. Scanning electron microscopy and inductively coupled plasma atomic emission analysis were used for studying morphology and composition of narrow fraction cenospheres. Viscosity and equilibrium mineral phase composition of oxide systems of the same composition as the narrow fraction cenospheres were calculated using a computing program for phase equilibria in magmatic systems. Correlations of the viscosity of aluminosilicate melts with concentrations of their silicon, aluminium and iron constituents, as well as with the decrystallization degree of the cenosphere glass were established. The quartz phase was shown dominating in all the products of cenosphere separation. Regarding the quartz content, the high-viscosity systems can be classified into two groups differing in the presence or absence of iron-containing phases. An extra phase of magnetite was detected in the low-viscosity melts (magnetic cenospheres). Potential expanding of the cenospheres application areas were discussed based on the microelemental composition data.

REDUCTION PROCESSES IN THE COURSE OF MECHANOCHEMICAL SYNTHESIS OF $\text{Li}_{1+x}\text{V}_3\text{O}_8$

N.V. Kosova*, S.V. Vosel**, V.F. Anufrienko, N.T. Vasenin*, E.T. Devyatkina* (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of Mineralogy and Petrography, Novosibirsk, Russia)

J. Solid State Chemistry, 160(2) (2001) pp. 444-449.

Mechanical activation (MA) of the $\text{LiOH}+\text{V}_2\text{O}_5$ and $\text{Li}_2\text{CO}_3+\text{V}_2\text{O}_5$ mixtures followed by brief heating at 673 K was used to prepare dispersed $\text{Li}_{1+x}\text{V}_3\text{O}_8$. It was shown that structural transformations during MA are accompanied by reduction processes. EPR spectra of $\text{Li}_{1+x}\text{V}_3\text{O}_8$ are attributed to vanadyl VO^{2+} ions with weak exchange interaction. The interaction of localized electrons (V^{4+} ions) with electron gas (delocalized electrons), which is exhibited through the dependence of EPR line width of vanadium ions versus measurement temperature (C-S-C relaxation), is revealed. It is shown that C-S-C relaxation is different for intermediate and final products. The properties of mechanochemically prepared $\text{Li}_{1+x}\text{V}_3\text{O}_8$ are compared with those of HT- $\text{Li}_{1+x}\text{V}_3\text{O}_8$, obtained by conventional solid state reaction. Mechanochemically prepared $\text{Li}_{1+x}\text{V}_3\text{O}_8$ is characterized by a similar amount of vanadium ions, producing electron gas, but a higher specific surface area.

SILICON CARBONITRIDE ALLOYS AS A NOVEL FUNCTIONAL MATERIAL OBTAINED BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION FROM DIMETHYL(2,2-HYDRAZINE)SYLANE

T.P. Smirnova*, A.M. Badalian*, L.V. Yakovkina*, V.V. Kaichev, V.I. Bukhtiyarov, A.N. Shmakov, V.I. Rachlin**, A.N. Fomina** (*Institute of Inorganic Chemistry, Novosibirsk, Russia; **Favorsky Institute of Chemistry, Irkutsk, Russia)

On-Line Journal "Investigated in Russia", 74 (2001) pp. 814-822.

Silicon carbonitride alloys were synthesised by RP CVD process using the novel single-source precursor $(\text{CH}_3)_2\text{HSiNH}(\text{CH}_3)_2$ that is derivative of 1,1-dimethylhydrazine (heptyl). The films were characterized by X-ray photoelectron (XPS), infrared (FTIR) and ultraviolet-visible (UV-vis) spectroscopy. The microstructure of the films was examined by scanning electron microscopy (SEM) and diffraction of synchrotron

radiation (DSR) methods. XPS and FTIR spectroscopy studies showed that the Si-C and Si-N are the main bonds in the deposited films. Concerning the C-N bonds, the results are less obvious: they are either negligible or not present at all. The films were found to be predominately amorphous with a number of crystallites within the amorphous matrix. The crystals appearance, their dimensions and crystal form did not depend on substrate temperature. It has been hypothesised that crystallisation could happen in the gas phase during deposition or nanocrystals were formed by the strain induced after a certain thickness of the amorphous film. The crystals were assigned to the structure closed to alfa-Si₃N₄ phase. According to FTIR and XPS data it is clear that the chemical bonding and the atomic local order in the amorphous matrix are much more complicated than those of Si₃N₄-SiC mixtures. It has been concluded that tetrahedral configurations of silicon carbide and silicon nitride units with mixed C/N environment are formed. The films are highly resistant to thermal degradation. It was also demonstrated that this new material has an optical band gap that was variable from 2.0 to 4.7 eV.

MECHANIC TREATMENT FOR SYNTHESIS OF LiCoO₂ – CATHODE MATERIAL FOR LITHIUM-IONIC ACCUMULATORS

N.V. Kosova*, **V.F. Anufrienko**, **T.V. Larina****, **E.T. Devyatkina*** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Institute of Inorganic Chemistry, Novosibirsk, Russia)

Chem. for Sustainable Devel., 9(3) (2001)

XRD, IR-spectroscopy and Electronic Diffuse Reflectance Spectroscopy were used for studying the phase composition and electron state of cobalt ions of

intermediate and final products formed in the course of mechanical treatment of LiOH/Co(OH)₂ and LiOH/CoOOH mixtures followed by heating at 400–800°C. Reduction processes were established in the activated LiOH/COOH mixture and oxidation processes in the activated LiOH/Co(OH)₂ mixture. Heating of the activated mixtures at 400, 600 and 800°C for 4 hours was shown to give rise to formation of a high-temperature modification of LiCoO₂, the constituting Co³⁺O₆ octahedra being less ideal than those in LiCoO₂ prepared by the ceramic method. Small amounts of [Co²⁺]_{Oh} ions were detected in the low-temperature samples and [Co²⁺]_{Td} ions in the high temperature ones.

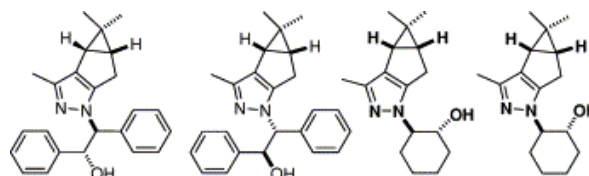
NOVEL OPTICALLY ACTIVE PYRAZOLE LIGANDS DERIVED FROM (+)-3-CARENE

S.A. Popov*, **Yu.V. Gatilov***, **T.V. Rybalova***, **O.A. Kholdeeva**, **A.V. Tkachev****

(*N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia; **Novosibirsk State University, Novosibirsk, Russia)

Tetrahedron: Asymmetry, 12(20) (2001) pp. 2875-2881.

Reactions of chiral β-diketone with racemic hydrazines as well as reaction of chiral pyrazole with cyclohexene epoxide and *trans*-stilbene epoxide have been examined as the routes to optically active pyrazolylethanols. Diastereomerically pure products have been isolated by crystallization or column chromatography in good yields.



Catalysis on Zeolites

THE SULPHUR AND WATER RESISTANCE OF MODIFIED WASHCOATED ZEOLITE-EXCHANGED MONOLITH CATALYSTS FOR SCR OF NO_x WITH PROPANE

Z.R. Ismagilov, **R.A. Shkrabina**, **L.T. Tsykoza**, **V.A. Sazonov**, **S.A. Yashnik**, **N.V. Shikina**, **H. Veringa*** (*Netherlands Energy Research Foundation, Petten, The Netherlands)

Topics in Catalysis, 16/17 (1-4) (2001) pp. 307-310.

The method of preparation of modified Cu-substituted zeolite DeNO_x catalysts washcoated on monolith ceramics has been developed. Non-modified

and modified monolith catalysts were tested in DeNO_x reaction with propane. It was shown that the catalyst modified by cerium and containing titania together with H-ZSM-5 and Al₂O₃ in the washcoating layer demonstrates high level of activity, and its resistance during multiple cycles of poisoning by sulfur compounds and water at 400 and 500°C is also high.

THE STABILITY OF MONOLITH CuZSM-5 CATALYSTS FOR THE SELECTIVE REDUCTION OF NITROGEN OXIDES WITH HYDROCARBONS: 1. SYNTHESIS AND CHARACTERIZATION OF BULK CuZSM-5 CATALYSTS

Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, S.A. Yashnik, V.A. Sazonov, V.V. Kuznetsov, M.V. Luzgin, A.V. Kalinkin, H. Veringa* (*Energy Research Foundation, Petten, The Netherlands)

Kinetics & Catalysis, 42(6) (2001) pp. 847-853.

The effects of ion-exchange conditions (the pH, the copper concentration in solution, and the solution-to-zeolite volume ratio) and the Si/Al atomic ratio of HZSM-5 zeolite on the concentration and state of copper in bulk CuZSM-5 catalysts and on the catalytic activity in the selective reduction of NO with propane were studied. It was found that the concentration and state of copper in the catalysts essentially depend on the pH of the solution used for ion exchange and on the copper concentration in this solution. An increase in the solution-to-zeolite volume ratio has almost no effect on the above characteristics. Regardless of the Si/Al atomic ratio of zeolite and of the pH of solution, a maximum activity (NO conversion) of the resulting catalyst is attained even at an exchange level (Cu/Al) close to 100% (80–140%). The absolute value of this catalytic activity depends only on the reaction temperature and is equal to 22–31% at 300°C or 85–97% at 400–500°C. The above exchange level is maximally attainable at pH~6 in the chosen range of copper acetate concentrations in solution (2–10 mg/ml accounted as CuO). An increase in the pH of ion exchange up to ~100% allows a wider variation in the exchange level and the state of copper in the zeolite with the same range of copper concentration in the solution. However, at Cu/Al >100% (up to ~430%), the catalyst activity is independent of the exchange level. The state of copper in freshly prepared samples affects the stability of the catalysts in storage. In turn, the state of copper depends on ion-exchange conditions and the Cu/Al ratio.

THE STABILITY OF MONOLITH CuZSM-5 CATALYSTS FOR THE SELECTIVE REDUCTION OF NITROGEN OXIDES WITH HYDROCARBONS. 2. SYNTHESIS AND CHARACTERIZATION OF BULK Cu(80% ZSM-5 + 20% Al₂O₃) CATALYSTS

Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, S.A. Yashnik, N.V. Shikina, V.A. Sazonov, H. Veringa* (*Energy Research Foundation, Petten, The Netherlands)

Kinetics & Catalysis, 42(6) (2001) pp. 854-857.

The effects of ion-exchange conditions and the zeolite Si/Al atomic ratio on the copper contents of Cu(80% ZSM-5 + 20%Al₂O₃) catalysts and on the catalytic activity in the selective reduction of NO with propane were studied. It was found that the synthesis of these catalysts exhibited the same behavior as in the case of bulk CuZSM-5 catalysts containing no Al₂O₃. The copper contents of the catalysts depend on the pH and concentration of copper solutions used for ion exchange, and the maximum activity (NO conversion) is attained even at an exchange level (Cu/Al) close to 100% regardless of pH and the zeolite Si/Al atomic ratio. At 300–400°C, the activity of the test catalysts is 10–20% lower than the activity of CuZSM-5 catalysts containing no Al₂O₃ at equal exchange levels. This difference in the activity almost disappeared as the reaction temperature was increased. It was also found that in the Cu(80% ZSM-5 + 20%Al₂O₃) catalysts, an exchange level close to that in CuZSM-5 catalysts is attained by ion exchange from more concentrated solutions. An increase in the exchange level to >100% (by an increase in the pH of a copper solution from ~6 to ~10, as in the case of CuZSM-5 catalysts), had no effect on the activity.

MECHANISM AND KINETICS OF THE SELECTIVE NO REDUCTION OVER Co-ZSM-5 STUDIED BY THE SSITKA TECHNIQUE. 1. NO_x ADSORBED SPECIES FORMATION

E.M. Sadovskaya, A.P. Suknev, L.G. Pinaeva, V.B. Goncharov, B.S. Bal'zhinimaev, C. Chupin*, C. Mirodatos* (*Institut de Recherches sur la Catalyse, Villeurbanne Cedex, France)

J. Catal., 201(2) (2001) pp. 159-168.

A steady-state isotopic transient analysis of NO adsorption over Co-ZSM-5 catalyst in the absence or in the presence of oxygen is reported by using doubly labeled nitric oxide. The kinetics and mechanism of

NO_x formation as well as the number of active sites for NO adsorption and their possible location on the catalyst surface are determined. The formation of NO₂^{δ+} species, active intermediates in DeNO_x chemistry in the presence of oxygen and hydrocarbons, is shown to proceed according two sequential steps: (i) molecular oxygen adsorption and (ii) NO reaction with oxidized surface sites. The frequency factor of that reaction is found to be two orders of magnitude higher than that of mononitrosyls formation via the adsorption of NO on cobalt sites. The oxygen exchange within NO₂^{δ+} is considerably slower than the formation of that intermediate species, indicating that its two oxygen atoms are nonequivalent. The concentration of active sites leading to NO₂^{δ+} formation is also estimated and related to the interface existing between cobalt oxide clusters and zeolite framework.

STOICHIOMETRY OF OXIDATION REACTIONS INVOLVING α-OXYGEN ON FeZSM-5 ZEOLITE

K.A. Dubkov, E.A. Paukshtis, G.I. Panov

Kinetics & Catalysis, 42(2) (2001) pp. 205-211.

The stoichiometry of the low-temperature reaction between surface α-oxygen formed by decomposing N₂O over Fe-containing ZSM-5 zeolite and methane, hydrogen stoichiometric ratios of 1:1.8 and 1:1.6, respectively. The observed stoichiometry is due to the mechanisms of the corresponding reactions. According to a mechanism proposed for the interaction of α-oxygen with methane and hydrogen, this reaction is accompanied by the dissociation of CH₄ and H₂ molecules. For hydrogen, such a mechanism is supported by IR spectroscopic studies of resulting surface compounds, namely, of new hydroxyl groups that were formed on the zeolite surface in the course of the reaction. α-Oxygen reacts with CO in the ratio of 1:1 to form CO₂ in amounts equal to those of α-oxygen on the surface.

IDENTIFICATION OF ACTIVE OXYGEN SPECIES OVER Fe COMPLEXES IN ZEOLITES

K.A. Dubkov, E.A. Paukshtis, G.I. Panov

"Catalysis by Unique Metal Ion Structures in Solid Materials", Eds. G. Centi et al., Kluwer Academic Publishers, 2001, pp. 149-163.

Using IRS, adsorption and isotope methods, the mechanism of α-oxygen insertion into methane and

benzene molecules at room temperature on zeolite FeZSM-5 (Si/Al= 72, C_{Fe}= 0.053 mass.%, Ca=2.0 10¹⁹ sites/g) has been studied. It has been shown that α-oxygen interaction with methane goes at a stoichiometry of 1:2, and is accompanied by methane dissociation yielding methoxyl and hydroxyl groups. Each group is bonded to O_α. A high value of kinetic isotope effect (K_H/K_D=3.2) indicates the cleavage of C-H bond in methane molecule to be reaction rate limiting stage. Alpha oxygen enters the composition of methanol, extracted from the zeolite surface. Alpha oxygen insertion into molecule C₆H₆ yielding phenol goes by the different mechanism most likely through benzene-oxide intermediate. Results obtained in the study reveal the mechanism of steady state catalytic process.

DIRECT ESR DETECTION OF STATES WITH S = 3/2 FOR NITROSYL COMPLEXES OF IRON IN FeZSM-5 ZEOLITES

A.M. Volodin, K.A. Dubkov, A. Lund* (Linköping University, Linköping, Sweden)

Chem. Phys. Lett., 333(1-2) (2001) pp. 41-44.

NO adsorption over FeZSM-5 zeolites results in the ESR signal with g=4.0 which can be reliably related to complexes of Fe²⁺ ions with NO with S=3/2. It is notable that such spectral characteristics are similar to those observed in enzymes while for oxide catalysts they were not known before. Nitrosyl complexes with these spectral characteristics are only one of the variety of forms known for biological systems. Still, the results presented in this paper indicate that such complexes can be observed by ESR in heterogeneous catalysts. NO is expected to be a very efficient spin probe for investigation of the state of Fe²⁺ ions in such systems.

THE Fe ACTIVE SITES IN FeZSM-5 CATALYST FOR SELECTIVE OXIDATION OF CH₄ TO CH₃OH AT ROOM TEMPERATURE

N.S. Ovanesyan*, K.A. Dubkov, A.A. Pyalling*, A.A. Shteinman* (*Institute of Problems of Chemical Physics, Chernogolovka, Russia)

J. Radioanalyt. & Nuclear Chem., 246(1) (2000) pp. 149-152.

It was shown recently that iron complexes formed during the thermal treatment of FeZSM-5 zeolite perform single-turnover cycles of methane oxidation to methanol at ambient conditions when nitrous oxide is used as a source of oxygen. The long-living active

intermediate is capable of transferring accepted O atom (called α -oxygen) into C-H bond of methane to produce methanol at 100% selectivity. The present work is aimed to the identification of iron active sites through a comparison of *in situ* ^{57}Fe Mössbauer spectra of FeZSM-5 after various thermal treatments and reaction stages. It is established that vacuum activation at 900°C accompanied by a manifold increase of α -centers leads to the transformation of inactive Fe^{3+} to the active, coordinatively unsaturated Fe^{2+} states. After α -oxygen loading, active Fe^{2+} states transform to a new Fe^{3+} states responsible for further methane oxidation. The latter reactions, as well as reaction with $^2\text{H}_2$, is not fully reversible: part of active Fe^{3+} transforms to other inactive Fe^{3+} form. On the contrary, reaction of α -oxygen with CO leads to a complete restoration of the initial, vacuum activated Fe^{2+} states. On the base of joint Mössbauer and catalytic data, the structure and composition of iron active centers are suggested.

NEW DATA ON THE POSSIBILITY OF CATALYTIC ABIOGENIC SYNTHESIS OF HYDROCARBONS IN THE EARTH'S CRUST

K.G. Ione, V.M. Mysov, V.G. Stepanov, V.N. Parmon

Petroleum Chemistry, 41(3) (2001) pp. 159-165.

The traditional models of the origin of hydrocarbon deposits in the earth's crust suggest the biogenic mechanism of the formation of oil and gas lenses. Nonetheless, a great deal of research on the catalytic synthesis of hydrocarbons from the gases CO, CO₂, and H₂ over bifunctional catalytic systems containing acid–base components of the clay or zeolite type together with oxidized metal particles has been carried out. The comparison of the composition of hydrocarbon mixtures that have been artificially prepared under different conditions over metal-containing catalysts and catalytic metal oxide systems

blended with clays, SiO₂, Al₂O₃, or zeolites with that of the naturally occurring oil-and-gas fields shows that the abiogenic inorganic synthesis of hydrocarbons can yield variations of hydrocarbon mixtures identical to the natural ones. The possibility of treating the processes of abiogenic hydrocarbon synthesis from the CO, CO₂, and H₂ gas mixture on inorganic catalysts as a model of macroscopic-scale processes that occurred in the earth's crust during different periods of the geochemical history of the earth is investigated.

CATALYTIC ABIOGENIC SYNTHESIS OF HYDROCARBONS IN THE EARTH'S CRUST

K.G. Ione, V.M. Mysov, V.G. Stepanov, V.N. Parmon

Chem. for Sustainable Devel., 9(1) (2001) pp. 129-143.

High thermodynamic probability has been shown for catalytic synthesis of hydrocarbon mixtures containing methane, n-alkanes, iso-alkanes and aromatic hydrocarbons identical to the naturally occurring oil and gas mixtures from the gases CO, CO₂, and H₂. These processes proceed with high exothermic effect.

Geochemical model of the earth evidences the existence of catalytically active areas – Fe, Ni, Mo, Co, Cu, Zn, Cr-containing ores with insertions of aluminosilicate or aluminophosphate components. Presence of hydrogen and carbon dioxide in gas emanations of the earth testifies high probability of generation of global areas of catalytic abiogenic synthesis of methane and high hydrocarbon mixtures from CO, CO₂, and H₂ gas mixtures. The comparison of the composition of hydrocarbon mixtures that have been artificially prepared from the CO, CO₂, and H₂ gas mixture on laboratory, pilot and commercial scales with natural ones have been made. The possibility of treating the processes of abiogenic hydrocarbon synthesis as a model of macroscopic-scale processes that occurred in the earth's crust during different periods of the geochemical history of the earth is discussed.

Studies on Zirconia-Based Materials

HIGHLY DISPERSED ZIRCONIUM-CONTAINING OXIDE SYSTEMS: SYNTHESIS, PROPERTIES, AND APPLICATIONS

A.S. Ivanova

Kinetics & Catalysis, 42(3) (2001) pp. 354-366.

The formation of the phase composition, dispersion, pore structure, and surface state of binary zirconium-

containing systems was examined depending on the nature and concentration of the second component, preparation conditions and procedures, and thermal treatment conditions. Various types of interactions were found, which are governed by the nature of the second component and the treatment temperature. The effects of surfactants on the physicochemical properties of precipitates depend on the conditions of synthesis: the

surfactant amount retained by a precipitate at pH 3–4 is greater than that at pH 9 by an order of magnitude. The thermolysis of samples synthesized at acidic pH, along with dehydration and dehydroxylation, is accompanied by the decomposition and degradation of surfactants. Because of this, certain compounds and their fragments capable of reducing corresponding phases are removed stepwise. Highly dispersed compositions were obtained at 110–400°C with a minimum particle size of 2.5–16 nm; at 700°C, the particle size was no higher than 20 nm. The ratio between the ionic radii of added and main components is a factor determining the dispersion of formed phases. In this case, changes in the nature of surfactants and in the conditions of a particular synthesis make it possible to prepare highly dispersed systems with monomesoporous structures. The total volume and the average diameter of pores can be controlled over wide limits.

SCIENTIFIC BASES FOR THE SYNTHESIS OF HIGHLY DISPERSED FRAMEWORK ZIRCONIUM PHOSPHATE CATALYSTS FOR PARAFFIN ISOMERIZATION AND SELECTIVE OXIDATION

V.A. Sadykov, S.N. Pavlova, G.V. Zabolotnaya, M.V. Chaikina*, R.I. Maksimovskaya, S.V. Tsybulya, E.B. Burgina, V.I. Zaikovskii, G.S. Litvak, Yu.V. Frolova, D.I. Kochubey, V.V. Kriventsov, E.A. Paukshtis, V.N. Kolomiichuk, V.V. Lunin**, N.N. Kuznetsova**, D. Agrawal***, R. Roy***
 (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Penn State University, PA, USA)

Kinetics & Catalysis, 42(3) (2001) pp. 390-398.

Results of the systematic study of the synthesis of highly dispersed framework zirconium phosphates stabilized by ammonium, lanthanum, aluminum, manganese, and cobalt cations are summarized. The synthesis involves the mechanochemical activation of a mixture of solid reactants (salts) or the sol–gel process each followed by the hydrothermal treatment (HTT) of obtained precursors in the presence of surfactants. The genesis of dispersed systems under investigation is studied by modern physical methods providing information on the state of the bulk and surface of the systems. It is found that the local structure of sol nanoparticles and zirconium phosphate crystalline nuclei arising from mechanochemical activation products depends on the nature of initial substances. This, in its

turn, makes different crystallization mechanisms possible during the HTT process: the dissolution/precipitation mechanism or the mechanism of oriented mating of primary particles. The crystallization mechanism in HTT and the reaction system composition influence the nature of resulting complex zirconium phosphate phases, their thermal stability, dispersity, and porous structure parameters. The relationship between the bulk structure parameters of framework zirconium phosphates, which are controlled by varying the chemical composition and conditions of synthesis, and the surface characteristics of the systems (the strength and concentration of different Lewis and Brønsted sites) is studied. It is shown that systems based on framework zirconium phosphates are promising catalysts for paraffin (pentane and hexane) isomerization, the selective oxidation of methane by oxygen into synthesis gas at short contact times, and the oxidative dehydrogenation of propane into propylene.

SUPPORTED CuO+Ag/PARTIALLY STABILIZED ZIRCONIA CATALYSTS FOR THE SELECTIVE CATALYTIC REDUCTION OF NO_x UNDER LEAN BURN CONDITIONS. 1. BULK AND SURFACE PROPERTIES OF THE CATALYSTS

V.A. Sadykov, R.V. Bunina, G.M. Alikina, S.A. Beloshapkin, A.S. Ivanova, D.I. Kochubey, B.N. Novgorodov, E.A. Paukshtis, V.B. Felonov, V.I. Zaikovskii, T.G. Kuznetsova, V.N. Kolomiichuk, E.M. Moroz, V.A. Matyshak*, G.A. Konin*, A.Ya. Rozovskii**, J.R.H. Ross***, J.P. Breen*** (*Semenov Institute of Chemical Physics, Moscow, Russia; **Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; ***University of Limerick, Limerick, Ireland)

J. Catal., 200(1) (2001) pp. 117-130.

Thermally stable cubic mesoporous zirconia samples stabilized by the alkaline-earth cations (Ca, Sr, Ba) were synthesized via the coprecipitation route followed by refluxing in the presence of surfactants. These systems were used as supports for copper cations and then modified by the addition of silver nanoparticles using impregnation or photoassisted deposition techniques. The structural, textural, and surface features of these nanosystems were studied by using TEM, X-ray diffraction, EXAFS, nitrogen adsorption isotherms, SAXS, FTIRS of adsorbed CO, and TPD of adsorbed NO_x species. Partially stabilized zirconia samples were found to possess a disordered cubic structure. A higher tendency of bulky Ba cation to segregate in the surface layer is reflected in a higher degree of surface

disordering, higher concentration of hydroxyls, and greater coordination unsaturation of isolated copper cations. In contrast to such traditional supports as γ -alumina, stabilized zirconia supports appear to favor formation of small reactive (probably, three-dimensional) clusters of copper cations possessing an increased reactivity and decreased strength of oxygen bonding with these cations. It is reflected in decreased thermal stability of surface nitrite and nitrate species located at these centers as compared with such species on the surface of CuO/alumina catalysts. This feature seems to be primarily determined by the specificity of the surface structure of fluorite-like supports (ceria, zirconia). Silver incorporation into copper oxidic clusters decreases the strength of copper-oxygen bonds as well as the thermal stability of adsorbed nitrite-nitrate species. For samples prepared via the photodeposition route, the clustering degree of copper cations is usually lower than in the case of samples obtained by traditional impregnation procedure.

SUPPORTED CuO+Ag/PARTIALLY STABILIZED ZIRCONIA CATALYSTS FOR THE SELECTIVE CATALYTIC REDUCTION OF NO_x UNDER LEAN BURN CONDITIONS. 2. CATALYTIC PROPERTIES

V.A. Sadykov, R.V. Bunina, G.M. Alikina, A.S. Ivanova, T.G. Kuznetsova, S.A. Beloshapkin, V.A. Matyshak*, G.A. Konin*, A.Ya. Rozovskii, V.F. Tretyakov**, T.N. Burdeynaya**, M.N. Davydova**, J.R.H. Ross***, J.P. Breen***** (*Semenov Institute of Chemical Physics, Moscow, Russia; **Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; ***University of Limerick, Limerick, Ireland)

J. Catal., 200(1) (2001) pp. 131-139.

The catalytic performances of copper oxidic species supported on mesoporous zirconia supports stabilized by alkaline earth cations were studied for the reactions of NO oxidation to NO₂ and the selective catalytic reduction (SCR) of NO_x in excess oxygen. Three different types of hydrocarbon reductants were studied, namely, propane, propylene and the long-chain hydrocarbon decane. For comparison, the performance of CuO and CuO+Ag supported on alumina for the SCR of NO_x by propane was also studied. This data was analyzed and discussed with reference to the information concerning the surface properties of these systems. In general, for the same system, the maximum level of NO_x conversion and temperature of maximum NO_x conversion is strongly

dependent upon the type of reducing agent. No universal relation was found between the surface density of coordinatively unsaturated cations able to activate hydrocarbons and the activity of the catalysts for the SCR reaction. In part, it can be explained by blocking the surface sites in reaction media either by strongly bound nitrate species or by coke. Addition of silver was found to be of significance only in the case of strong interaction between the metallic and oxidic components. Such a factor as the strength of oxygen and nitrate complexes bonding with the surface copper/copper-silver oxidic species depending upon the type of support and methods of samples synthesis appears to be the most important for performance of the systems studied in NO_x-selective reduction by hydrocarbons in the presence of excess oxygen.

Cu, Co, Ag-CONTAINING PILLARED CLAYS AS CATALYSTS FOR THE SELECTIVE REDUCTION OF NO_x BY HYDROCARBONS IN AN EXCESS OF OXYGEN

G.A. Konin*, A.N. Il'ichev*, V.A. Matyshak*, T.I. Khomenko*, V.V. Korchak*, V.A. Sadykov, V.P. Doronin, R.V. Bunina, G.M. Alikina, T.G. Kuznetsova, E.A. Paukshtis, V.B. Fenelonov, V.I. Zaikovskii, A.S. Ivanova, S.A. Beloshapkin, A.Ya. Rozovskii, V.F. Tretyakov**, J.R.H. Ross***, J.P. Breen***** (*Semenov Institute of Chemical Physics, Moscow, Russia; **Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; ***University of Limerick, Limerick, Ireland)

Topics in Catalysis, 16-17(1-4) (2001) pp. 193-197.

Thermally stable Al- and Zr-PILC loaded with copper and cobalt cations and silver nanoparticles were synthesized. The structural and surface features of these nanosystems were studied and compared with those of bulk analogs – partially stabilized ZrO₂ loaded with the same active components. Specificity of the catalytic properties of nanocomposites in SCR of NO_x by propane, propylene and decane in the excess of oxygen appears to be determined both by distribution of active components on the catalytic surface and degree of their interaction with supports. Formation of ads.-NO_x, nitroxyl-hydrocarbon C_xH_yNO₂ and isocyanate NCO intermediates was observed by ESR and IR spectroscopy *in situ*.

MECHANOCHEMICAL SYNTHESIS OF ZIRCONIUM PHOSPHATES

M.V. Chaikina*, V.A. Sadykov, S.N. Pavlova, G.N. Zabolotnaya, R.I. Maksimovskaya, V.V. Kriventsov, D.I. Kochubey, E.B. Burgina, R. Roy**, D.K. Agrawal** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Penn State University, USA)

J. Mater. Synth. & Processing, 8(5-6) (2000) pp. 279-286.

Cation- and anion-substituted zirconium-phosphates of $X_kZr_m(PO_4)_{n-y}Y$ composition, where $X = Na^+, La^{3+}, NH_4^+$, $Y = F^-, WO_4^{2-}$, $1/3 < k < 2$, $2 < m < 4$, $3 < n < 6$ were synthesized by the procedure including mechanical activation of the starting salts mixture followed by annealing at 300-900°C. The interaction between components was studied by XRD, EXAFS, FTIRS, ^{31}P MAS NMR. The possibility to synthesize non-stoichiometric compounds is demonstrated, and prospects for application of the mechanochemical method for synthesis of complex zirconium phosphates are outlined.

THE INFLUENCE OF SOLID PRECURSORS NATURE ON STRUCTURAL, TEXTURAL AND SURFACE PROPERTIES OF FRAMEWORK ZIRCONIUM PHOSPHATES SYNTHESIZED VIA MECHANOCHEMICAL ACTIVATION

S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, R.I. Maksimovskaya, V.I. Zaikovskii, S.V. Tsybulya, E.B. Burgina, M.V. Chaikina*, D. Agrawal**, R. Roy** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Penn State University, USA)

Solid State Ionics, 141-142(1-4) (2001) pp. 683-688.

The framework zirconium phosphates with incorporated La^{3+} and NH_4^+ cations were synthesized via mechanical activation of solids followed by the hydrothermal treatment. Their phase composition, local bulk structure, surface properties and microstructure appear to be defined both by the structure of amorphous zirconium phosphates formed via mechanical activation of solids depending on precursors acidity and reactivity and by the pH-dependent mechanism of subsequent crystallization during hydrothermal treatment.

THE NOVEL ACID CATALYSTS - FRAMEWORK ZIRCONIUM PHOSPHATES: THE BULK AND SURFACE STRUCTURE

S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, D.I. Kochubey, R.I. Maksimovskaya, V.I. Zaikovskii, V.V. Kriventsov, S.V. Tsybulya, E.B. Burgina, A.M. Volodin, M.V. Chaikina*, N.N. Kuznetsova**, V.V. Lunin**, D. Agrawal***, R. Roy*** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Penn State University, USA)

J. Molec. Catal. A: Chemical, 158(1) (2000) pp. 319-323.

Framework zirconium phosphates structural features and surface properties were studied and compared with catalytic performance in the reactions of hexane isomerization. Isomerization activity of cubic or rhombohedral zirconium phosphates samples correlates with the density of the strongest Lewis centers probed by TEMPO test molecule.

STRUCTURE OF ZIRCONIUM COMPLEXES IN AQUEOUS SOLUTIONS

V.V. Kanazhevskii*, B.N. Novgorodov, V.P. Shmachkova, N.S. Kotsarenko, V.V. Kriventsov, D.I. Kochubey (*Novosibirsk State University, Novosibirsk, Russia)

Mendeleev Commun., 11(6) (2001) pp. 211-212.

Two types of zirconium(IV) complexes with the different Zr-Zr distances were detected by EXAFS in the aqueous solutions of $ZrOCl_2 \cdot 8H_2O$, $ZrO(NO_3)_2 \cdot 2H_2O$ and $Zr(SO_4)_2 \cdot 4H_2O$ salts.

INTERACTION OF HYDROGEN AND n-PENTANE WITH SULFATED ZIRCONIA

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

Catal. Lett., 69(3-4) (2000) pp. 189-193.

Interaction of H_2 with sulfated zirconia catalysts was studied *in situ* at 473 K. Interaction of hydrogen with the sample evacuated at 673 K leads to the formation of new hydroxyl groups (wide bands near 3330 cm^{-1}) and water (1620 cm^{-1}). In the case of the sample evacuated at 887 K, SOH group (3660 cm^{-1}) and ZrH (1555 cm^{-1}). Adsorption of n-pentane in the range 253-383 K was studied. It was shown that hydrides and protonated cyclopentadienes form at low temperature.

Studies on Mesoporous Mesophase Materials

X-RAY STRUCTURAL MODELING OF SILICATE MESOPOROUS MESOPHASE MATERIAL

L.A. Solovyov*, S.D. Kirik*, A.N. Shmakov, V.N. Romannikov (*Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia)

Micropor. & Mesopor. Mater., 44-45(1-3) (2001) pp. 17-23.

Rietveld's technique in combination with a continuous electron density representation was applied to structural modeling of highly ordered pure siliceous mesoporous mesophase material $C_{16}\text{-SiO}_2\text{-MMM}$ of the MCM-41 type prepared by hydrothermal synthesis in the presence of $C_{16}H_{33}N(CH_3)_3Br$. Several important characteristics of the material in both as-synthesized and calcined forms were revealed. In particular, it was found that mesopores in the materials are of true hexagonal shape, and the wall electron density seems to be not continuous.

COMPARATIVE TEXTURAL STUDY OF HIGHLY ORDERED SILICATE AND ALUMINOSILICATE MESOPOROUS MESOPHASE MATERIALS HAVING DIFFERENT PORE SIZES

V.B. Fenelonov, A.Yu. Derevyankin, S.D. Kirik*, L.A. Solovyov*, A.N. Shmakov, J.-L. Bonardet**, A. Gedeon**, V.N. Romannikov (*Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia; **Université P. et M. Curie, Paris, France)

Micropor. & Mesopor. Mater., 44-45(1-3) (2001) pp. 33-40.

Honeycomb structure model was applied for describing surface properties in the MCM-41 and SBA-15 types of highly ordered silicas and aluminosilicates with different nominal mesopore diameters: about 4 nm and about 10 nm. As shown, calculations of internal specific surface area A_{me} require a heterogeneity of this surface to be taken into account, the latter being quantified by the roughness coefficient β . These calculations at the condition $\beta=1.0$ will allow to estimate the lower limit of specific surface area of the materials only, which will correspond to the perfectly smooth walls of mesopores. This description seems to be valid for the MCM-41 type systems, for which β is about 1.1–1.2. On the contrary, β is found to exceed 1.5 for the SBA-15 type materials. This fact is probably due to an essential non-smoothness of the mesopore surface in

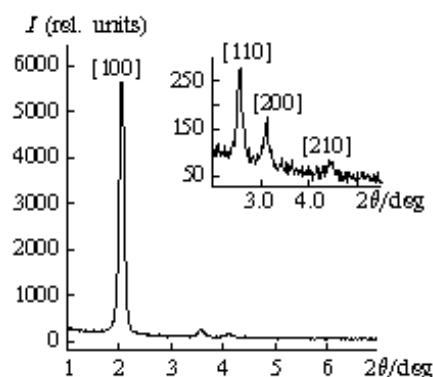
these systems and may be associated with their synthesis conditions.

PHYSICOCHEMICAL FEATURES OF THE FORMATION OF SILICEOUS POROUS MESOPHASES. 3. CONDITIONS OF FORMATION AND PROPERTIES OF MESOPOROUS SILICA

E.G. Kodenev, A.N. Shmakov, A.Yu. Derevyankin, A.V. Nosov, V.N. Romannikov

Russ. Chem. Bull., 49(10) (2000) pp. 1669-1675.

Data on the optimization of alkalinity of the reaction mixture and the reaction temperature in the formation of the siliceous porous mesophase material $C_{16}\text{-SiO}_2\text{-MMM}$ are presented. A criterion for the evaluation of the level of structure optimization for mesoporous mesophases is formulated. Measurements of the texture parameters of the materials treated in acidic media led to the assumption that the walls in the pure siliceous $C_{16}\text{-SiO}_2\text{-MMM}$ system consist of separate blocks, which, apparently, are not bound completely to one another by chemical interactions.



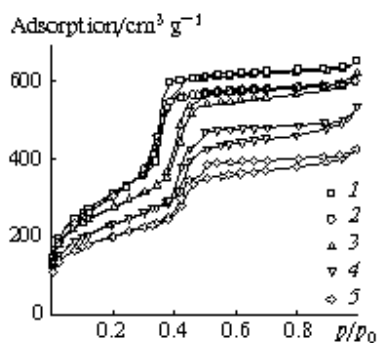
PHYSICOCHEMICAL FEATURES OF THE FORMATION OF SILICEOUS POROUS MESOPHASES. 4. EFFECT OF DURATION AND TEMPERATURE OF THE HYDROTHERMAL TREATMENT ON THE STRUCTURAL AND TEXTURAL PROPERTIES

A.Yu. Derevyankin, V.B. Fenelonov, A.N. Shmakov, V.N. Romannikov

Russ. Chem. Bull., 50(2) (2001) pp. 175-179.

The results of investigation of mesoporous mesophase materials $C_{12}\text{-SiO}_2\text{-MMM}$ and $C_{16}\text{-SiO}_2\text{-MMM}$ prepared at the optimized composition of the reaction mixture and different durations of hydrothermal treatment (HTT) at 120°C

and 140 °C are presented. Hydrothermal treatment at 120 °C influences slightly the specific surface area and the volume of the mesopores but gives a more ordered structure. Prolonged HTT at 140 °C results in irreversible structure degradation. The samples obtained with the optimal HTT duration are characterized by the minimum width of X-ray reflections, the maximum surface and volume of mesopores, and the minimum external surface.



PHYSICOCHEMICAL PROPERTIES OF MESOPOROUS MESOPHASE SILICATE MATERIALS FORMED VIA THE ELECTROSTATIC S⁺T MECHANISM

V.N. Romannikov, S.D. Kirik*, L.A. Solov'ev*, A.N. Shmakov, A.Yu. Derevyankin, V.B. Felonov, O.A. Kholdeeva, O.B. Lapina, E.A. Paukshtis (*Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia)

Kinetics & Catalysis, 42(6) (2001) pp. 857-866.

The formation of the structure of a highly organized silicate mesoporous mesophase material (MMM) with hexagonal packing via the S⁺T reaction pathway and MMM-based aluminosilicates (Al,Si)-MMM and titanosilicates (Ti,Si)-MMM with different concentrations of the elements are considered. The structural, textural, and catalytic properties of the materials are studied.

ALKENE AND THIOETHER OXIDATIONS WITH H₂O₂ OVER Ti- AND V-CONTAINING MESOPOROUS MESOPHASE CATALYSTS

N.N. Trukhan, A.Yu. Derevyankin, A.N. Shmakov, E.A. Paukshtis, O.A. Kholdeeva, V.N. Romannikov

Micropor. & Mesopor. Mater., 44-45 (1-3) (2001) pp. 603-608.

Well-organized Ti- and V-containing silicate mesoporous mesophase materials (MMM) were

synthesized using C₁₆H₃₃N(CH₃)₃Br and characterized by elemental analysis, IR, DRS-UV, XRD, and N₂ adsorption. Catalytic properties of these materials in alkene and thioether oxidations with aqueous H₂O₂ were examined. The structure-activity study was performed for the C₁₆-(Ti,Si)-MMM catalysts with the Si/Ti atomic ratio ranged from 19 to 166. The samples with the Si/Ti atomic ratio in the range of 49-124 showed the highest catalytic activities. Both structure perfection of the silicate matrix and degree of isolation of titanium ions in it appeared to be crucial factors determining catalytic activity of C₁₆-(Ti,Si)-MMM in alkene oxidation. For efficient oxidation of more nucleophilic substrates (thioethers) the structural perfection of the C₁₆-(Ti,Si)-MMM catalysts was less important. No titanium leaching occurred even in 1.1 M H₂O₂ solution at 353 K, whereas vanadium leaching was already pronounced at [H₂O₂]=0.05 M and room temperature. The oxidation processes proved to be true heterogeneous for C₁₆-(Ti,Si)-MMM and mostly homogeneous for C₁₆-(V,Si)-MMM.

OXIDATION OF 2,3,6-TRIMETHYLPHENOL OVER Ti- AND V-CONTAINING MESOPOROUS MESOPHASE CATALYSTS: STRUCTURE-ACTIVITY/SELECTIVITY CORRELATION

N.N. Trukhan, V.N. Romannikov, E.A. Paukshtis, A.N. Shmakov, O.A. Kholdeeva

J. Catal., 202(1) (2001) pp. 110-117.

The oxidation of 2,3,6-trimethylphenol (TMP) has been carried out over well-organized Ti- and V-containing mesoporous mesophase silicate catalysts (Ti- and V-MMM) using hydrogen peroxide and *tert*-butyl hydroperoxide (TBHP) as oxidants. Vanadium leaching was observed in the V-MMM/H₂O₂ and V-MMM/TBHP systems, whereas no titanium leaching occurred for Ti-MMM with both oxidants. TMP oxidation runs on a surface of Ti-MMM catalyst, producing 2,3,5-trimethyl-1,4-benzoquinone (TMBQ) with selectivity as high as 86% at 100% TMP conversion. Titanium content in Ti-MMM determines the state of the active catalytic site and influences the structure regularity, thus affecting the catalytic behavior. The catalysts with titanium loading in the 1.5-2 wt% range show the highest activity and selectivity. Some loss of catalytic properties observed after recycling may occur due to collapsing of the catalyst structure caused by water. The lower the water concentration in the reaction mixture, the more stable the catalyst.

Carbon and Carbon Containing Materials

SYNTHESIS OF CARBON FILMS WITH DIAMOND-LIKE STRUCTURE BY ELECTROCHEMICAL OXIDATION OF LITHIUM ACETYLIDE

E. Shevchenko*, E. Matiushenkov*, D.I. Kochubey, D.V. Sviridov*, A.I. Kokorin**, A.I. Kulak*** (*Belarus State University, Minsk, Belarus; **Semenov Institute of Chemical Physics, Moscow, Russia; ***Institute of General and Inorganic Chemistry, Minsk, Belarus)

Chem. Commun., 4 (2001) pp. 317-318.

Electrochemical oxidation of lithium acetylide in aprotic media affords carbon films containing a high fraction of sp³-type C bonds; the growth conditions and the photoelectrochemical behaviour of these films were investigated.

REHYBRIDIZATION OF THE ATOMIC ORBITALS AND THE FIELD ELECTRON EMISSION FROM NANOSTRUCTURED CARBON

A.N. Obratsov*, A.P. Volkov*, A.I. Boronin, S.V. Koshcheev (*Moscow State University, Moscow, Russia)

J. Experim. & Theoret. Physics, 93(4) (2001) pp. 846-853.

The field electron emission, structural features, and electronic properties of carbon films obtained by chemical vapor deposition were experimentally studied. It is shown that the field electron emission from the films composed of spatially oriented carbon nanotubes and platelike graphite nanocrystals is observed for the electric field strength lower by one to two orders of magnitude as compared to the values characteristic of the metal emitters. Experimental data reported for the first time are indicative of a local decrease in the electron work function in such carbon film materials as compared to that in graphite. A model of the emission center is proposed and a mechanism of the field electron emission from nanostructured carbon is described.

COKE DISPERSION IN CARBON-MINERAL POROUS ADSORBENTS

M.S. Mel'gunov, V.B. Fenelonov, R. Leboda*, B. Charnas* (*Maria Curie-Skłodowska University, Lublin, Poland)

Carbon, 39(3) (2001) pp. 357-366.

The morphology, dispersion and localization of coke in coked alumina and silica have been

investigated by a newly developed technique, which can be applied generally for studies of other systems of 'support+modifier' type. It is shown that, at the considered amounts of coke, deposited coke clusters partially cover the surface of silica leading to a mosaic-like structure of the resulting carbon-mineral material surface. These clusters are predominantly located in the pores of silica gel. Probably the pores filled with coke are formed by the tetrahedron packed SiO₂ globules. On the other hand, the intensity of coke formation on the alumina surface is considerably higher than on the silica surface, so coke formation is accompanied by the total surface coverage at low amounts of coke deposited. Possible reasons for these differences are considered.

CATALYTIC FILAMENTOUS CARBONS FOR IMMOBILIZATION OF BIOLOGICALLY ACTIVE SUBSTANCES AND NON-GROWING BACTERIAL CELLS

G.A. Kovalenko, E.V. Kuznetsova, Yu.I. Mogilnykh, I.S. Andreeva, D.G. Kuvshinov, N.A. Rudina

Carbon, 39(7) (2001) pp. 1033-1043.

Adsorption properties of supports based on catalytic filamentous carbon (CFC) have been studied with respect to different substances of biological origin — amino acid (*l-tyrosine*), protein (*bovine serum albumin*), enzyme (*glucoamylase*) and non-growing cells of microorganisms (*Eschericia coli*, *Bacillus subtilis*, *Rhodococcus* sp.). The factors influencing the adsorption efficiency have been investigated. In particular, the effect of surface chemical properties and textural parameters on the adsorption has been studied. Three independent methods have been suggested for determining accessible surface area for adsorbate molecules of different size.

REGULARITIES OF CATALYTIC FORMATION OF CARBON COMPOSITES FOR VARIOUS PURPOSES VIA DECOMPOSITION OF HYDROCARBONS ON IRON SUBGROUP METALS

R.A. Buyanov, V.V. Chesnokov

Eurasian ChemTech J., 2 (2000) pp. 223-230.

Scientific basis for preparation of new carbon-mineral adsorbents, supports, highly selective

catalysts, and composite materials synthesized by a carbide cycle mechanism on the finely disperse particles of the iron subgroup metals, their alloys with some other metals is discussed. It was found that the carbide cycle mechanism involves the chemical and physical steps. The regularities of the process performance on the both stages are considered. Graphite filaments may be formed of graphite layers with either coaxial-cylindrical, coaxial-conic or stack orientations in the filament body. A number of primary and secondary properties of the graphite aggregates is being discussed. The methods have been developed for control the synthesis of carbon-metal materials of the specified properties by varying the parameters of the metal particles, the nature of hydrocarbon decomposition, and the process mode.

KINETICS OF 2-PINANOL ISOMERIZATION TO LINALOOL ON THE MONOLITH CARBON-CONTAINING CATALYST

I.I. Il'ina, I.L. Simakova, V.A. Semikolenov

Kinetics & Catalysis, 42(5) (2001) pp. 686-692.

Isomerization of 2-pinanol into linalool is studied on a monolith carbon-containing catalyst at 733-893 K and a total pressure of 2-40 torr. The rate constants of *cis(trans)*-2-pinanol transformation into linalool and linalool cyclization are determined. Experimental data are described by the consecutive kinetic scheme. The mechanism of linalool formation is proposed according to which pinane ring opening occurs in an intramolecular reaction. A highly selective process of linalool synthesis by the thermal isomerization of 2-pinanol is shown to be possible.

IN SITU X-RAY DIFFRACTION STUDY OF SOLID STATE TRANSFORMATIONS DURING CATALYTIC GRAPHITISATION OF AMORPHOUS CARBON

O.P. Krivoruchko, A.N. Shmakov, V.I. Zaikovskii

Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 198-201.

The results of an *in situ* X-ray diffraction study of phase transformations during catalytic graphitisation of amorphous carbon are reported. It is demonstrated that there is unusual change of iron catalyst reflection intensity at low temperature ~640°C. This unusual intensity change may possibly be caused by the transition of some part of metal into liquid state at low temperature. It was also shown by electron

microscopy that although no graphite reflections were detected 80-90% of amorphous carbon becomes graphite after sample heating in a high temperature vacuum chamber.

ELECTRICAL RESISTIVITY OF GRAPHITIZED ULTRA-DISPERSE DIAMOND AND ONION-LIKE CARBON

V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, A.I. Romanenko, A.V. Okotrub* (*Institute of Inorganic Chemistry, Novosibirsk, Russia)

Chem. Phys. Lett., 336(5-6) (2001) pp. 397-404.

Here the results of measurements of electrical resistivity of ultra-disperse diamonds (UDD) with different graphitization degrees and onion-like carbon (OLC) prepared by vacuum annealing of UDD samples at various fixed temperatures are presented. Intermediate samples contain particles with a diamond core covered by closed curved graphitic shells. The temperature dependence of electrical resistivity $\rho(T)$ of these structures is characteristic for the systems with localized electrons and variable hopping-length hopping conductivity (VHLHC). The data on sample resistance are discussed in terms of the variation of dimensionality of conductivity and changing the number of defects in the system.

THERMODYNAMIC ANALYSIS OF NUCLEATION OF CARBON DEPOSITS ON METAL PARTICLES AND ITS IMPLICATIONS FOR THE GROWTH OF CARBON NANOTUBES

V.L. Kuznetsov, A.N. Usoltseva, A.L. Chuvilin, E.D. Obraztsova*, J.-M. Bonard** (*Natural Science Centre of Russian Academy of Sciences, Moscow, Russia; ** Institut de Physique Expérimentale, Lausanne EPFL, Switzerland)

Phys. Rev. B, 64 (23) (2001) 235401 (7 pp.).

By considering the catalytic mechanisms underlying the formation of various nanocarbon deposits on catalytic metal surfaces, the authors conclude that the majority of these mechanisms include some common steps. The most important of these is the nucleation of the carbon deposit on the metal surface. On the basis of experimental and literature data, it is proposed that the nucleus has the form of a flat saucer with its edges bonded to the metal surface. A thermodynamic analysis of the carbon nucleation on the metal surface is then performed to obtain an analytical equation for the dependence of the

critical radius of the nucleus on the reaction parameters. This equation demonstrates that a variation of the reaction parameters, such as the temperature and the nature of the metal catalyst and promoters, can lead to the formation of different carbon deposits, such as filamentous carbon, multiwall nanotubes or single-wall nanotubes (SWNTs). The performed analysis allows us to conclude that SWNT growth is likely to proceed on liquid metal particles.

MICRODESIGN OF NICKEL-COPPER ALLOY CATALYSTS FOR PRODUCTION OF NEW CARBON MATERIALS

T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, A.L. Chuvilin, V.A. Likholobov

Eurasian ChemTech J., 2 (2000) pp. 237-244.

The reaction of methane decomposition was investigated on the Ni-Cu-Al₂O₃ alloy catalysts at 625-675°C at a gas pressure of 1 bar to produce catalytic filamentous carbon (CFC) with a simultaneous formation of hydrogen. Using Ni-Cu alloy catalysts (8-15 wt. % Cu) at 625°C permits a CFC yield of 525 g/g_{cat} (700 g/g_{Ni}). According to the X-ray powder diffraction (XRD) and transmission electron microscopy (TEM) studies of Ni-Cu-Al₂O₃ catalysts, morphology of catalysts begins to change during 10 minutes after CH₄ decomposition by formation of “octopus” CFC structures. It should be noted, that copper additives substantially increase the thermal stability of Ni and modify the textural and structural properties of CFC.

DECOMPOSITION OF CHLORINATED HYDROCARBONS ON IRON-GROUP METALS

I.V. Mishakov, V.V. Chesnokov, R.A. Buyanov, N.A. Pakhomov

Kinetics & Catalysis, 42(4) (2001) pp. 543-548.

The decomposition of 1,2-dichloroethane and chlorobenzene on nickel–alumina, cobalt–alumina, and iron–alumina catalysts at 400–600°C was studied. Thermodynamic calculations demonstrated that the susceptibility of metals to chlorination under exposure to HCl increases in the order Ni<Co<Fe. The addition of hydrogen to the reaction mixture was found to dramatically decrease the rate of carbon deposition in the decomposition of 1,2-dichloroethane because of the intense hydrogenation of intermediates that are graphite precursors. Two fundamentally different reaction paths were found in the degradation of

1,2-dichloroethane: decomposition via a carbide-cycle mechanism with the formation of carbon as the main product (under conditions of a deficiency of hydrogen) and 1,2-dichloroethane hydrodechlorination accompanied by methanation of the formed carbon (under conditions of an excess of hydrogen). The degradation of chlorobenzene diluted with hydrogen in a molar ratio of 1:50 was not accompanied by carbon formation on the catalyst. A comparison between the selectivity for reaction products on nickel–alumina and cobalt–alumina catalysts indicated that the former catalyst is more active in the rupture of C–C bonds and in the methanation reaction of deposited carbon, whereas the latter is more favorable for hydrodechlorination. The optimum conditions and thermal regime for efficient and stable operation of the catalysts were found.

H₂S DECOMPOSITION ACTIVITY OF TS CARBON DERIVED FROM FURAN RESIN

J.-I. Ozaki*, Y. Yoshimoto*, A. Oya*, T. Takarada*, V.V. Kuznetsov, Z.R. Ismagilov
(*Gunma University, Gunma, Japan)

Carbon, 39(10) (2001) pp. 1611-1612.

The catalytic activity of a Fe-doped, thermally stable turbostratic (TS) C in the decomposition of H₂S into H₂ and S was studied in the temperature range 700°. The catalyst was prepared from a benzene solution of a furan resin precursor, which also contained 3 wt.% Fe as ferrocene and 10 wt.% of trichloroacetic acid. After removing benzene, the mixture was cured at 80° under N₂ and carbonized at 900° in a He flow. The activity of this catalyst shows a maximum at 300-400°, decreases as the temperature rises further, and increases again at >600°. After removing Fe by washing with HCl the activity maximum at 300-400° disappears, but the catalytic activity stays superior to that of a C sample prepared from the resin without additives (having a smaller BET surface, 39 vs. 159 m²/g). FTIR spectra of the catalyst after adsorption of CO indicated the presence of Fe(0) and Fe(III) species and Lewis acidic sites.

DECOMPOSITION OF METHANE OVER IRON CATALYSTS AT THE RANGE OF MODERATE TEMPERATURES: THE INFLUENCE OF STRUCTURE OF THE CATALYTIC SYSTEMS AND THE REACTION CONDITIONS ON THE YIELD OF CARBON AND MORPHOLOGY OF CARBON FILAMENTS

M.A. Ermakova, D.Yu. Ermakov, A.L. Chuvilin, G.G. Kuvshinov

J. Catal., 201(2) (2001) pp. 183-197.

Decomposition of high-purity methane in the presence of α -Fe-based catalysts to produce filamentous carbon was investigated. The reaction was studied in the temperature range of 650 to 800°C. Filamentous carbon was demonstrated to form at temperatures not lower than 680°C in the presence of both bare α -Fe and catalysts based thereon with admixtures of various hard-to-reduce oxides (SiO_2 , Al_2O_3 , ZrO_2 , and TiO_2). The maximal carbon yield, 45 g per g of iron, was obtained with the Fe/ SiO_2 catalyst comprising silica in amounts of 15 wt%. XRD and high-resolution electron microscopy were used for studying the carbon deposits. The data obtained allowed the conclusion on the essential influence of the chemical nature of the hard-to-reduce oxide admixture in

the iron catalyst on the microstructure and morphology of the carbon filaments. Depending on the admixture, specific shapes of filaments and nanotubes predominated. Carbon nanotubes with thin walls built up by coaxial cylindrical graphene layers were formed in large amount over the Fe/ Al_2O_3 catalyst. Centers of growth of *octopus*-like nanotubes were observed.

POROUS CARBON MATERIALS OF SIBUNIT TYPE

G.V. Plaksin

Chem. for Sustainable Devel., 9(5) (2001) pp. 609-620.

The structure and properties of new synthetic composite porous carbon materials of sibunit type are considered. The preparation procedure includes sequential stages of obtaining of formed porous matrixes of various size and shape from dispersed carbon, deposition of pyrolytic carbon on the matrix and partial selective composite gasification. The textural properties and composite characteristics dependence of the parameters of initial morphological units of dispersed carbon and conditions of composites preparation are established.

Studies on Metal Catalysts

CATALYTIC STEAM REFORMING OF METHANE: NEW DATA ON THE CONTRIBUTION OF HOMOGENEOUS RADICAL REACTIONS IN THE GAS PHASE. 2. A RUTHENIUM CATALYST

I.I. Bobrova, N.N. Bobrov, V.V. Chesnokov, V.N. Parmon

Kinetics & Catalysis, 42(6) (2001) pp. 805-812.

The kinetics of methane steam reforming and pyrolysis on Ru/ Al_2O_3 ($T=650-750^\circ\text{C}$, $P_{\text{CH}_4} = 0.001-0.030$ MPa) is studied. The values of the rates and activation energies are compared with the kinetic parameters for nickel catalysts. It was shown that steam reforming could occur on the ruthenium catalyst both heterogeneously and heterogeneously-homogeneously depending on the reaction conditions. Comparative activities of the Ru/ Al_2O_3 and Ni- Al_2O_3 catalysts are discussed under the conditions of purely heterogeneous and heterogeneous-homogeneous steam reforming.

FORMATION OF BIMETALLIC Pt-Rh SURFACE WITH NANOSIZE METAL DOMAINS

A.V. Kalinkin, A.V. Pashis, R.I. Kvon

React. Kinet. & Catal. Lett., 72(1) (2001) pp. 163-168.

An approach to produce a bimetallic Pt-Rh model catalyst has been developed. It includes vacuum deposition of platinum on a Rh_2O_3 film, followed by the oxide reduction with hydrogen. The thermal stability range of the resulting bimetallic structure has been determined.

HYDROGEN SPILLOVER IN H_2 OXIDATION ON Pd-Ti³⁺/TiO₂

V.V. Gorodetskii, A.V. Matveev

Stud. Surf. Sci. & Catal., 138 (2001) pp. 85-92.

A dual-site mechanism of H_2 dissociation on the Pd particles and then migration H_{ads} across the TiO_x surface to the active sites with the $\text{O}_2^{\delta_{\text{ads}}}$ species have been studied on the defects of $\text{Ti}^{3+}-\square_{\text{O}}/\text{TiO}_2$ and

Pd-Ti³⁺-□_o/TiO₂ types with XPS, UPS, TDS, mass-spectrometry and pre-adsorbed oxygen photodesorption techniques. The effect of spillover phenomena (H_{ads}/Pd → O_{2ads}/Ti³⁺/TiO₂) on the overall rate of H₂ oxidation have been studied as well. The role of defects (Ti³⁺ sites) in the adsorption centres formation, their stabilization by the palladium particles and then defects participation in H₂+O₂ reaction have been studied on the TiO_x surface. The results obtained with H₂+O_{ads} reaction over Pd (110) single crystal surface have been compared. A series of activity sets: Ti³⁺/TiO₂ << Pd ~ Pd-Ti³⁺/TiO₂ have been determined. Through the hydrogen spillover from Pd to Ti³⁺/TiO₂ H₂ oxidation proceeds on two sites of the Pd-model catalysts it can occur: on Pd particles and on the Ti³⁺/TiO₂ support.

STRUCTURE GAP IN HETEROGENEOUS CATALYSIS: KINETIC ASPECTS

V.P. Zhdanov

Phys. Rev. B, 64 (19) (2001) 193406 (4 pp.).

Analyzing the kinetics of C₃H₈ oxidation running on nanometer-sized supported Pt particles, the authors show that, due to the purely kinetic effects related to the interplay of the reaction kinetics on different facets, the activity of a catalyst particle may be appreciably higher than that calculated by using the conventional approximation based on the assumption that the facets operate independently.

HYDRODECHLORINATION OF POLYCHLORINATED BENZENES IN THE PRESENCE OF A BIMETALLIC CATALYST IN COMBINATION WITH A PHASE-TRANSFER CATALYST

V.I. Simagina, I.V. Stoyanova

Mendeleev Commun., 11(1) (2001) pp. 38-39.

Bimetallic supported catalysts (Pd-Ni/C and Ni-Cu/C) in combination with a phase-transfer catalyst were found efficient and selective in the

liquid-phase hydrodechlorination of polychlorinated benzenes under mild conditions

METALLIC NANOSYSTEMS IN CATALYSIS

V.I. Bukhtiyarov, M.G. Slin'ko* (*State Scientific Centre of the Russian Federation 'L.Ya. Karpov Institute of Physical Chemistry', Moscow, Russia)

Russ. Chem. Rev., 70(2) (2001) pp. 147-159.

The reactivities of metallic nanosystems in catalytic processes are considered. The activities of nanoparticles in catalysis are due to their unique microstructures, electronic properties and high specific surfaces of the active centres. The problems of increasing the selectivities of catalytic processes are discussed using several nanosystems as examples. The mutual effects of components of bimetallic nanoparticles are discussed. The prospects for theoretical and experimental investigations into catalytic nanosystems and the construction of industrial catalysts based on them are evaluated. The bibliography includes 207 references.

CATALYSTS AND PROCESSES FOR PARAFFIN AND OLEFIN DEHYDROGENATION

R.A. Buyanov, N.A. Pakhomov

Kinetics & Catalysis, 42(1) (2001) pp. 64-75.

General trends in the development of industrial processes and catalysts for the dehydrogenation of lower C₃-C₅ paraffins and olefins are considered. A brief review of studies on the improvement of commercial nickel-calcium phosphate and iron oxide catalysts for the dehydrogenation of olefins and ethylbenzene to dienes and styrene, respectively, performed in the Laboratory of Dehydrogenation at the Boreskov Institute of Catalysis in collaboration with OAO NPO Yarsintez is given. The results of studies on the development of new spinel-supported bimetallic Pt-Sn catalysts for the steam dehydrogenation of lower paraffins are presented.

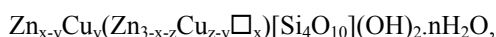
Copper-Containing Oxide Catalysts

NON-HYDROTHERMAL SYNTHESIS OF COPPER-, ZINC- AND COPPER-ZINC HYDROSILICATES

T.M. Yurieva, G.N. Kustova, T.P. Minyukova, E.K. Poels*, A. Bliet*, M.P. Demeshkina, L.M. Plyasova, T.A. Krieger, V.I. Zaikovskii
(*University of Amsterdam, Amsterdam, The Netherlands)

Mater. Res. Innov., 5(1) (2001) pp. 3-11.

Cu/SiO₂, Zn/SiO₂ and Cu-Zn/SiO₂ samples have been prepared by the homogeneous deposition-precipitation method. The samples were analyzed by thermal analysis, X-ray diffraction and infrared spectroscopy after various heat treatments and compared with data obtained for several minerals. It has been shown that interaction between the components occurs through formation of hydrosilicates. Copper-silica system at a Cu : Si ratio ≤ 1, gives rise to a hydrosilicate stable up to a calcination temperature of 930 K resembling the mineral Chrisocolla; at higher ratios a hydroxonitrate (gerhardite type) is also formed. Zinc-silica interaction produces two hydrosilicates such as a well crystallized Hemimorphite at Zn : Si = 2 and highly dispersed Zincsilite at Zn : Si ≤ 0.75, both stable up to 1073 K. The Zincsilite structure consists of three layered sheets (an octahedral layer sandwiched by two tetrahedral ones) like the Stevensite mineral group. For the copper-zinc-silica system no copper hydrosilicate is formed. Copper merely enters the Zincsilite structure independently of the applied (Cu+Zn) : Si ratio. Resulting layered copper-zinc hydrosilicate may be described by formula



where Zn_{3-x-z}Cu_{z-y}-ions are located in octahedral sites, Zn_{x-y}Cu_y-ions in the interlayer; □_x are vacancies in the layers. Copper and zinc in excess of the Zincsilite ratio of Me : Si = 0.75, gives rise to copper and copper-zinc hydroxonitrates.

COPPER IONS DISTRIBUTION IN SYNTHETIC COPPER-ZINC HYDROSILICATE

T.M. Yurieva, T.P. Minyukova, G.N. Kustova, L.M. Plyasova, T.A. Krieger, M.P. Demeshkina, V.I. Zaikovskii, V.V. Malakhov, L.S. Dovlitova

Mater. Res. Innov., 5(2) (2001) pp. 74-80.

Copper ions distribution in the structure of synthetic copper-zinc hydrosilicate of zincsilite

structure, obtained by non-hydrothermal synthesis have been studied. Zincsilite is referred to the layered silicates of smectite group and is described by the formula $\text{Zn}_x(\text{Zn}_{3-x}\square_x)[\text{Si}_4\text{O}_{10}](\text{OH})_2.n\text{H}_2\text{O}$, where Zn_{3-x} – are the ions located in the octahedral positions of layers, formed by two sheets of [Si₄O₁₀] tetrahedrons; Zn_x are zinc ions in the interlayer; □_x are the cation vacancies. Two types of copper ions were distinguished in accordance with the character of their interaction with hydrogen: (1) – substituting zinc ions in the octahedral positions of layers; (2) – substituting zinc ions in the interlayer. These two types of copper ions display the following properties when reacting with hydrogen: (1) – copper ions in octahedral positions start to be reduced at temperatures 553-573 K, and at 723 K reduction degree is 50%; (2) – copper ions from interlayer start to be reduced at 503-533 K with a constant energy of activation, and their reduction may be complete at this temperature.

METAL-SUPPORT INTERACTIONS IN COBALT-ALUMINUM Co-PRECIPIATED CATALYSTS: XPS AND CO ADSORPTION STUDIES

A.A. Khassin, T.M. Yurieva, V.V. Kaichev, V.I. Bukhtiyarov, A.A. Budneva, E.A. Paukshtis, V.N. Parmon

J. Molec. Catal. A: Chemical, 175(1-2) (2001) pp. 189-204.

Cobalt-aluminum catalysts were prepared using either the precipitation of Co²⁺ in the presence of freshly prepared Zn-Al hydrotalcite (the promoted sample) or the co-precipitation of Co²⁺ and Al³⁺ (the unpromoted samples). The evolution of the initial hydrotalcite-like structure was monitored during its calcination and the reductive treatment by means of XPS. It was shown that at 480°C the reduction of the calcined samples results in the formation of Co⁰ species, the further reduction at 650°C results in an increase of the amount of the Co⁰ species. The samples reduced at 650°C chemisorb readily carbon monoxide at 77 K, while the sample reduced at 480°C doesn't chemisorb CO at 77 K. At elevated temperatures, all reduced samples are found to be able to chemisorb CO. Terminal CO moieties as well as monodentate carbonates, formates and carboxyl

species were detected at the surface of the reduced samples at their exposure to the CO medium at the elevated temperature. The intensities of the IR absorption bands of chemisorbed CO are found proportional to the surface fraction of the Co^0 species, measured by XPS. The apparent red shift of the IR absorption bands is observed for CO adsorbed on the samples reduced at 480°C. The obtained data correlate with the catalytic properties of the Co-Al samples in hydrogenation reactions. The conclusion on the existence of a strong metal-support interaction in the samples under the study is made.

COBALT-ALUMINUM Co-PRECIPIATED CATALYSTS AND THEIR PERFORMANCE IN THE FISCHER-TROPSCH SYNTHESIS

A.A. Khassin, T.M. Yurieva, G.N. Kustova, I.Sh. Itenberg, M.P. Demeshkina, T.A. Krieger, L.M. Plyasova, G.K. Chermashentseva, V.N. Parmon

J. Molec. Catal. A: Chemical, 168(1-2) (2001) pp. 193-207.

Cobalt-aluminum catalysts were prepared using either Co^{2+} precipitation onto freshly prepared Mg-Al or Zn-Al hydrotalcite (promoted samples) or co-precipitation of Co^{2+} and Al^{3+} (non-promoted samples). The evolution of initial hydrotalcite structure was monitored during its calcination and reductive treatment. It has been shown that, at moderate temperatures, hydrotalcites results decomposition yields a Co oxide phase supported by a highly defective inverted spinel-like structure. Cations Co^{2+} enter the support structure, and occupy both tetrahedral and octahedral positions. Octahedron coordinated Co species are reduced at 580-620°C. After the reduction at 470-480°C catalyst phase composition shows Co^0 supported on inverted spinel-like structure, which contains Co^{2+} in the octahedral coordination. Further reduction at 600°C transforms the support to 'ideal' spinel, which contains no octahedron coordinated Co^{2+} . Chemical properties of the Co-Al catalysts, including their performance in the Fischer-Tropsch synthesis, were found to depend on the catalyst reduction temperature, and thus on the support structure. Metal-support interaction is supposed to explain the observed properties of metallic cobalt.

EVOLUTION OF THE STRUCTURE OF Co STEVENSITE DURING ITS TREATMENT IN THE AIR, INERT GAS FLOW AND FLOWING HYDROGEN

A.A. Khassin, T.M. Yurieva, G.N. Kustova, L.M. Plyasova, T.A. Krieger, I.Sh. Itenberg, M.P. Demeshkina, T.V. Larina, V.F. Anufrienko, V.N. Parmon

Mater. Res. Innov., 4(4) (2001) pp. 251-261.

Synthetic TOT (2 tetrahedron layers: 1 octahedron layer) trioctahedral hydrosilicates (stevensites) of Zn, Mg, Co and Co-Zn were prepared by the deposition-precipitation technique. The evolution of both the structure and spectral properties of the silicates were studied during their treatment in various media. The position of the $\nu(\text{OH})$ absorption band and the temperature of crystallization of the anhydrous silicate were found to be useful indicators of the cationic composition of stevensites. The data obtained are used to analyze and to review the earlier data on Co/ SiO_2 catalysts. It is concluded, that the formation of Co-stevensite occurs in the most cases, when the pH of the maternal solution during the preparation of a catalyst is above the value of 4.

COBALT-CONTAINING CATALYSTS SUPPORTED BY SYNTHETIC Zn- AND Mg- STEVENSITES AND THEIR PERFORMANCE IN THE FISCHER-TROPSCH SYNTHESIS

A.A. Khassin, T.M. Yurieva, G.N. Kustova, L.M. Plyasova, I.Sh. Itenberg, M.P. Demeshkina, G.K. Chermashentseva, V.F. Anufrienko, V.I. Zaikovskii, T.V. Larina, I.Yu. Molina, V.N. Parmon

J. Molec. Catal. A: Chemical, 168(1-2) (2001) pp. 209-224.

Co-containing catalysts supported onto the synthetic stevensites of Zn and Mg were prepared using various methods. The evolution of the catalyst structure was monitored during the calcination and a reductive treatment. During the calcination, Co^{2+} cations substitute the divalent cations of the support, that leads to the formation of the mixed Co-Me stevensite. These Co species cannot be reduced at temperatures below 700°C. The phase composition of the catalyst after the reduction at 500°C contains Co^0 particles supported by the Co-Me mixed stevensites. Unexpectedly, the performance of the Co/stevensite catalysts in the Fischer-Tropsch synthesis was much worse, than that of Co/MgO. The supposition on the metal-support interaction, which causes the low electron-donor capacity of the metallic Co may explain the experimental data.

Catalysis by Metal Complexes

COMPARATIVE STUDY OF AEROBIC ALKENE EPOXIDATIONS CATALYZED BY OPTICALLY ACTIVE MANGANESE (II) AND COBALT (II) SALEN COMPLEXES

O.A. Kholdeeva, M.P. Vanina

React. Kinet. & Catal. Lett., 73(1) (2001) pp. 83-89.

A comparative study of aerobic alkene epoxidations in the presence of pivalaldehyde catalysed by optically active Mn(III)Salen and Co(II)Salen complexes has been performed. The nature of asymmetric induction is discussed.

THE EFFECT OF Co AND IR ON THE ACTIVITY OF THE $K_2[Fe_2(CO)_8]$ - AND $K_2[Ru_4(CO)_{13}]$ -BASED SYSTEMS IN AMMONIA SYNTHESIS. THE SYNERGISTIC ACCELERATION OF THE AMMONIA SYNTHESIS OVER THE $K_2[Fe_2(CO)_8]+K$ CATALYSTS BY IRIIDIUM

S.M. Yunusov*, E.S. Kalyuzhnaya*, B.L. Moroz, S.N. Agafonova*, V.A. Likhobolov, V.B. Shur* (*A.N. Nesmeyanov Institute of Organoelement Compounds, Moscow, Russia)

J. Molec. Catal. A: Chemical, 165(1-2) (2001) pp. 141-147.

The effect of Co and Ir on the ammonia synthesis over the $K_2[Fe_2(CO)_8]+K$ and $K_2[Ru_4(CO)_{13}]+K$ catalysts on graphite-like active carbon "Sibunit" has been investigated. The catalysts were prepared by depositing $K_2[Fe_2(CO)_8]$ and $K_2[Ru_4(CO)_{13}]$ onto the "Sibunit" carbon-supported Co and Ir, followed by thermal decomposition of the deposited cluster and treatment of the resulting sample with metallic potassium. The catalysts containing no potassium metal have been studied as well. It has been found that the presence of Co in the Ru catalysts substantially decreases the ammonia synthesis rate. Similar results have been obtained on testing the Ru-Ir samples. By contrast, the introduction of Ir in the $K_2[Fe_2(CO)_8]+K$ catalysts leads to a synergistic acceleration of the process of the ammonia synthesis. The strongest accelerating effect of Ir is observed at 200°C. A rise in the reaction temperature to 250, 300 and then to 350°C results in a gradual weakening of the Fe-Ir synergism. An important feature of the Fe-Ir catalysts found is their increased activity in the ammonia synthesis at 150°C. The presence of Co in the iron catalysts little affects, in general, the ammonia

synthesis rate, although some acceleration of this process by Co at 350 and 400°C for the samples not treated with potassium metal can be noted.

THE SYNERGISTIC ACCELERATION OF THE AMMONIA SYNTHESIS OVER THE $K_2[Fe_2(CO)_8] + K$ CATALYSTS ON CARBON "SIBUNIT" BY RHODIUM

S.M. Yunusov*, E.S. Kalyuzhnaya*, B.L. Moroz, S.N. Agafonova*, V.A. Likhobolov, V.B. Shur* (*A.N. Nesmeyanov Institute of Organoelement Compounds, Moscow, Russia)

Appl. Catal., 218(1-2) (2001) pp. 251-256.

The effect of Rh on the ammonia synthesis over the $K_2[Fe_2(CO)_8]+K$ and $K_2[Ru_4(CO)_{13}]+K$ catalysts on the graphite-like active carbon "Sibunit" has been investigated. The catalysts were prepared by depositing $K_2[Fe_2(CO)_8]$ and $K_2[Ru_4(CO)_{13}]$, respectively, onto the "Sibunit" carbon-supported Rh, followed by thermal decomposition of the deposited cluster and treatment of the resulting sample with metallic potassium. The catalysts containing no potassium metal have been studied as well. It has been found that the presence of Rh in the Ru catalysts either little affects the ammonia synthesis rate or even somewhat decreases it. By contrast, the introduction of Rh in the $K_2[Fe_2(CO)_8]+K$ systems leads to a synergistic acceleration of the process of the ammonia synthesis. The strongest accelerating effects of Rh are observed at lowered temperatures. Thus, at 200°C, the Fe-Rh catalyst (Fe/carbon=5.6 wt.%, the Fe:Rh molar ratio is 1.6:1) proves to be 3.5 times more active than the corresponding Fe sample. A rise in the reaction temperature to 250, 300 and then to 350°C results in a gradual weakening of the Fe-Rh synergism. A remarkable feature of the Fe-Rh catalyst found is its increased activity in the ammonia formation at 150°C. The analogous Rh catalysts produce no ammonia at all at 150–200°C in the absence of Fe and their efficiency at 250–400°C is either equal to zero or very low.

PALLADIUM(II), COPPER(II), IRON(III), AND VANADIUM(V) COMPLEXES WITH HETEROPOLYANION $PW_9O_{34}^{9-}$: ^{31}P , ^{183}W , ^{51}V NMR AND IR SPECTROSCOPY STUDIES

L.G. Detusheva, L.I. Kuznetsova, M.A. Fedotov, V.A. Likholobov, L.S. Dovlitova, A.A. Vlasov, V.V. Malakhov

Russ. J. Coord. Chem., 27(12) (2001) pp. 838-845.

The formation of Pd(II)-containing and mixed Pd(II),Cu(II), Pd(II),Fe(III), and Pd(II),V(V) complexes with heteropolyanion $PW_9O_{34}^{9-}$ was studied using ^{31}P , ^{183}W , ^{51}V NMR, visible UV and IR spectroscopy, and the differentiating dissolution methods. In an aqueous solution and at optimal pH (3.7), the monometallic complexes $[Pd_3(PW_9O_{34})_2]^{12-}$ and $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{9-}$ ($n_{av} = 3$), the bimetallic complexes $[Pd_2Cu(PW_9O_{34})_2]^{12-}$, $[Pd_2Fe(PW_9O_{34})_2]^{11-}$, and $[PdFe_2(PW_9O_{34})_2]^{10-}$, and a mixture of the $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{9-}$ ($n_{av} \approx 10$) + $[(VO)_3(PW_9O_{34})_2]^{9-}$ complexes are formed. The title complexes were isolated from solution as CS^+ solid salts belonging to the same $[M_3(PW_9O_{34})_2]$ structural type.

AMINATION OF BENZENE AND TOLUENE WITH HYDROXYLAMINE IN THE PRESENCE OF TRANSITION METAL REDOX CATALYST

N.I. Kuznetsova, L.I. Kuznetsova, L.G. Detusheva, V.A. Likholobov, G.P. Pez*, H. Cheng* (*Air Products and Chemicals, Inc., Corporate Science and Technology Center, Allentown, USA)

J. Molec. Catal. A: Chemical, 161(1-2) (2000) pp. 1-9.

The amination of benzene and toluene to aniline and toluidines with hydroxylamine sulfate has been investigated in water-acetic acid and water-acetic acid-sulfuric acid media in the presence of transition metal compounds as catalysts. The process yields are strongly dependent on the temperature, added sulfuric acid and the composition of catalyst. For the amination of benzene, the soluble catalysts, $NaVO_3$ and Fe(III) salts produce high yields of aniline without addition of H_2SO_4 , whereas Na_2MoO_4 and $FeSO_4$ exhibit substantial activity only in 5 M H_2SO_4 . Amination is accompanied by a disproportionation of hydroxylamine catalyzed by the redox active transition metal ions. The favorable effect of H_2SO_4 on the amination is due mostly to the greater stability of hydroxylamine in the strongly acidic medium. Mixed oxides containing V(V) and Mo(VI) are active amination catalysts when suspended in 5 M solution of H_2SO_4 in acetic acid. Introduction of metallic Pd into these oxide catalysts improves performance increasing

the yield and selectivity of amination with respect to the aromatic substrate. Toluene exhibited a close to benzene reactivity in amination giving approximately equal yield of *o*-, *m*-, *p*-toluidines. Mechanistic considerations based on literature data and results of *ab initio* quantum mechanistic calculations suggest that the aminating species is the protonated amino radical $\cdot NH_3^+$, which in the rate-determining step reacts with benzene and toluene to yield the corresponding aminocyclohexadienyl radical intermediates. These are then oxidatively aromatized to give, respectively, aniline and non-regiospecific mixture of toluidines.

IR STUDY OF THE STRUCTURE OF PALLADIUM(II) ACETATE IN CHLOROFORM, ACETIC ACID, AND THEIR MIXTURES IN SOLUTION AND IN LIQUID-SOLID SUBSURFACE LAYERS

E.S. Stoyanov

J. Struct. Chem., 41(3) (2000) pp. 540-546.

It has been found that palladium acetate in chloroform solutions at the concentrations $1 \cdot 10^{-3}$ -0,7 M forms two molecular states: cyclic trimer I and linear dimer II. Mole fraction of dimer II increases upon the dilution. Upon the addition of acetic acid (HOAc) even in the small quantity an equilibrium $I \leftrightarrow II$ shifts to I because of the structure transformation of surface solvate shells. The concentration of II in 0,1M solution of $PdAc_2$ in 50 vol.% HOAc+ $CHCl_3$ is 10%. However, in thin subsurface layers of this solution the slow shift of equilibrium $I \leftrightarrow II$ to II up to concentrations 22 % after 60 min is observed on the interface CaF_2 – solution. The probable reason may be structuring of liquid phase in subsurface layers within the experimental time.

DERIVATIVES OF L-PIMARIC ACID IN THE SYNTHESIS OF CHIRAL ORGANOPHOSPHORUS LIGANDS FROM DECAHYDROPHENANTRENE SERIES

A.G. Tolstikov, N.N. Karpyshev, O.V. Tolstikova, T.B. Khlebnikova, G.E. Sal'nikov, V.I. Mamatyuk, Yu.V. Gatilov*, I.Yu. Bagryanskaya* (*N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia)

Russ. J. Organic Chem., 37(8) (2001) pp. 1134-1148.

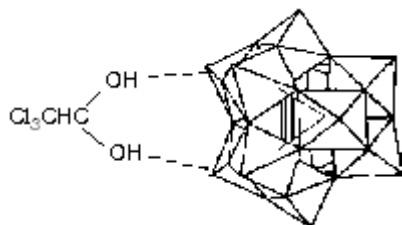
Starting with maleopimaric and fumaropimaric acids were prepared chiral organophosphorus ligands from dehydrophenanthrene series. Cationic complexes of Rh(I) prepared therefrom were tested for catalysts of asymmetric hydrogenation of unsaturated precursors of *N*-acetylphenylalanine and its derivatives.

Heteropolycompounds in Catalysis

A STUDY OF COMPLEXATION OF CHLORAL HYDRATE WITH HETEROPOLY ANIONS HAVING VARIOUS STRUCTURES

G.M. Maksimov, M.N. Timofeeva,
V.A. Likholobov

Russ. Chem. Bull., 50(9) (2001) pp. 1529-1532.



^1H NMR was applied to study the interaction of chloral hydrate in deuterionitrobenzene solution with tetrabutylammonium salts of the heteropoly acids (HPA) belonging to five structural types: Keggin ($\text{H}_3\text{PW}_{12}\text{O}_{40}$, $\text{H}_3\text{PMo}_{12}\text{O}_{40}$, $\text{H}_4\text{SiW}_{12}\text{O}_{40}$), Dawson ($\alpha\text{-H}_6\text{P}_2\text{W}_{18}\text{O}_{62}$, $\alpha\text{-H}_6\text{P}_2\text{Mo}_{18}\text{O}_{62}$, $\alpha\text{-H}_4\text{S}_2\text{Mo}_{18}\text{O}_{62}$), $\text{H}_6\text{P}_2\text{W}_{21}\text{O}_{71}(\text{H}_2\text{O})_3$, $\text{H}_6\text{As}_2\text{W}_{21}\text{O}_{71}(\text{H}_2\text{O})$, and $\text{H}_{21}\text{B}_3\text{W}_{39}\text{O}_{132}$. The surface of the HPA anions is nonuniform in acid-base properties. A general rule for all HPA was found, namely, that the HPA acidity increases with a decrease in the specific anion charge (per W or Mo).

ACIDITY OF SOLUTIONS OF HETEROPOLY ACIDS WITH VARIOUS STRUCTURES AND COMPOSITIONS

M.N. Timofeeva, G.M. Maksimov, V.A. Likholobov

Kinetics & Catalysis, 42(1) (2001) pp. 30-34.

Hammett acidity functions H_0 of solutions of heteropoly acids $\text{H}_3\text{PW}_{11}\text{XO}_{40}$ ($\text{X(IV)} = \text{Ti, Zr}$), $\text{H}_3\text{PW}_{12}\text{O}_{40}$, $\text{H}_4\text{SiW}_{12}\text{O}_{40}$, $\text{H}_6\text{P}_2\text{W}_{21}\text{O}_{71}$, and $\text{H}_{21}\text{B}_3\text{W}_{39}\text{O}_{132}$, as well as HClO_4 and $\text{CF}_3\text{SO}_3\text{H}$, in water and 90% aqueous acetone and acetonitrile, are measured at 20°C by the indicator method. In aqueous solutions all acids under study have the same strength, and in organic solvents their acidities differ. A correlation between the catalytic activity and acidity of the solution is found for the condensation of acetone to mesityl oxide.

ACIDITY OF HETEROPOLY ACIDS WITH VARIOUS STRUCTURES AND COMPOSITIONS STUDIED BY IR SPECTROSCOPY OF THE PYRIDINIUM SALTS

G.M. Maksimov, E.A. Paukshtis, A.A. Budneva,
R.I. Maksimovskaya, V.A. Likholobov

Russ. Chem. Bull., 50(4) (2001) pp. 587-590.

The acidity on the "proton affinity" scale was determined by IR spectroscopy of the pyridinium salts for nineteen heteropoly acids of nine structural types (including two with the previously unknown structure) and one isopoly acid. All heteropoly acids exhibited a high acidity at the level of $\text{CF}_3\text{SO}_3\text{H}$ and HClO_4 . $\text{H}_3\text{PW}_{12}\text{O}_{40}$ was the strongest acid.

A STUDY OF THE ACID PROPERTIES OF STRUCTURALLY AND COMPOSITIONALLY DIFFERENT HETEROPOLY ACIDS IN ACETIC ACID

M.N. Timofeeva, M.M. Matrosova*,
G.M. Maksimov, V.A. Likholobov (*Novosibirsk
State University, Novosibirsk, Russia)

Kinetics & Catalysis, 42(6) (2001) pp. 785-791.

The acid properties of heteropoly acids of the following three structure types were studied by conductometry in acetic acid: Keggin ($\text{H}_3\text{PW}_{12}\text{O}_{40}$, $\text{H}_3\text{PMo}_{12}\text{O}_{40}$, $\text{H}_4\text{SiW}_{12}\text{O}_{40}$, $\text{H}_3\text{PW}_{11}\text{ThO}_{39}$; and $\text{H}_5\text{PW}_{11}\text{XO}_{40}$, where $\text{X(IV)} = \text{Ti}$ or Zr), Dawson ($\alpha\text{-H}_6\text{P}_2\text{W}_{18}\text{O}_{62}$ and $\alpha\text{-H}_6\text{P}_2\text{Mo}_{18}\text{O}_{62}$), and $\text{H}_6\text{P}_2\text{W}_{21}\text{O}_{71}(\text{H}_2\text{O})_3$. These compounds are electrolytes that dissociate in only the first step of this solvent. The thermodynamic dissociation constants of the heteropoly acids were calculated by the Fuoss–Kraus method. The Hammett acidity functions H_0 of the solutions of $\text{H}_5\text{PW}_{11}\text{XO}_{40}$, $\text{H}_3\text{PW}_{12}\text{O}_{40}$, $\text{H}_4\text{SiW}_{12}\text{O}_{40}$, and $\text{H}_6\text{P}_2\text{W}_{21}\text{O}_{71}(\text{H}_2\text{O})_3$ in 85% acetic acid at 25°C were determined by the indicator method. All of the test heteropoly acids were found to be strong acids.

ESTERIFICATION OF *n*-BUTANOL WITH ACETIC ACID IN THE PRESENCE OF HETEROPOLY ACIDS WITH DIFFERENT STRUCTURES AND COMPOSITIONS

M.N. Timofeeva, M.M. Matrosova*, G.M. Maksimov, V.A. Likhobov, A.V. Golovin*, R.I. Maksimovskaya, E.A. Paukshtis (*Novosibirsk State University, Novosibirsk, Russia)

Kinetics & Catalysis, 42(6) (2001) pp. 791-796.

The esterification reaction of *n*-butanol with acetic acid ([BuOH] : [HOAc] = 1 : 15 mol/mol; 55°C, 5% H₂O) was studied in the presence of tungsten heteropoly acids of the Keggin (H₃PW₁₂O₄₀, H₄SiW₁₂O₄₀, H₅PW₁₁TiO₄₀, H₅PW₁₁ZrO₄₀, and H₃PW₁₁ThO₃₉) and Dawson structure (α-H₆P₂W₁₈O₆₂, H₆P₂W₂₁O₇₁(H₂O)₃, H₆As₂W₂₁O₆₉(H₂O), and H₂B₃W₃₉O₁₃₂). The reaction orders with respect to H₆P₂W₂₁O₇₁(H₂O)₃, H₃PW₁₂O₄₀, and H₆P₂W₁₈O₆₉ are equal to 0.78, 1.00, and 0.97, respectively. It was found that the reaction rate depends on the acidity, as well as on the structure and composition of heteropoly acids. The H₂B₃W₃₉O₁₃₂ heteropoly acid is most active, whereas the Keggin-structure heteropoly acids exhibit the lowest activities. Of the Keggin structure heteropoly acids, H₅PW₁₁ZrO₄₀ exhibits the highest activity because of the presence of a Lewis acid site in its structure.

ON SYNTHESIS OF SILICOALUMINOTUNGSTIC HETEROPOLY ACID

G.M. Maksimov, M.A. Fedotov

Russ. J. Inorg. Chem., 46(3) (2001) pp. 327-329.

The possibility of synthesizing heteropoly acid H₅SiW₁₁Al(H₂O)O₃₉ was studied with the use of ¹⁸³W and ²⁷Al NMR. A concentrated aqueous solution

containing the target acid (85% chemical purity) was obtained by electro dialysis. The attempts to obtain the acid in the solid state failed.

TITANIUM-SUBSTITUTED HETEROPOLYTUNGSTATES AS MODEL CATALYSTS FOR STUDYING THE MECHANISMS OF SELECTIVE OXIDATION BY HYDROGEN PEROXIDE

O.A. Kholdeeva, R.I. Maksimovskaya, G.M. Maksimov, L.A. Kovaleva

Kinetics & Catalysis, 42(2) (2001) pp. 217-222.

The ³¹P NMR method shows that four forms of titanium(IV)-monosubstituted Keggin-type heteropolytungstate (Ti-HPA) exist in MeCN: the dimer (Bu₄N)₇[{PTiW₁₁O₃₉}₂OH] (in the abbreviated form, (PW₁₁Ti)₂OH or H1), its conjugate base (PW₁₁Ti)₂O (1), and two monomers, PW₁₁TiO (2) and PW₁₁TiOH (H2). The ratio between the forms depends on the concentrations of H⁺ and H₂O. Dimer H1 is produced from 2 in MeCN when H⁺ (1.5 mol) is added, and monomer H2 is the key intermediate in this process. The catalytic activity of Ti-HPA in the oxidation of thioethers by H₂O₂ correlates with their activity in peroxo complex formation and decreases in the order H2 > H1 > 2. The reaction of 2 with H₂O₂ in MeCN occurs slowly to form the inactive peroxo complex PW₁₁TiO₂ (A). The addition of H₂O₂ to H1 and H2 most likely results in the formation of the active hydroperoxo complex PW₁₁TiOOH (B). Complexes A and B transform into each other when H⁺ or OH⁻ (1 mol) is added per 1 mol of A or B, respectively. The activity of B toward thioethers in the stoichiometric reaction is proven by ³¹P NMR and optical spectroscopy.

Studies on Selective Catalytic Oxidation

OSCILLATIONS DURING CATALYTIC OXIDATION OF PROPANE OVER A NICKEL WIRE

A.Yu. Gladky, V.K. Ermolaev, V.N. Parmon

Catal. Lett., 77(1-3) (2001) pp. 103-106.

Catalytic oxidation of propane with oxygen over a nickel wire at the temperature range 650-750°C and the reagent pressure *ca.* 1 Torr occurs in a self-oscillating mode. Periodic changes of the reagent concentration are found to be accompanied by significant synchronous changes of the catalyst temperature.

PREPARATION AND CATALYTIC STUDY OF METAL MODIFIED TS-1 IN THE OXIDATION OF BENZENE TO PHENOL BY N₂O

L.V. Piryutko, A.K. Uriarte*, V.S. Chernyavsky, A.S. Kharitonov, G.I. Panov (*Solutia Inc., Gonzales, USA)

Micropor. & Mesopor. Mater., 48(1-3) (2001) pp. 345-353.

The titanosilicalite TS-1 samples modified by Al, V, Cr, Fe, Co and Ru were synthesized, characterized and tested in the title reaction. As with the earlier studied zeolite systems, Fe introduction into the TS-1 matrix produces α-sites that can catalyze the oxidation of benzene to phenol with high activity and

selectivity. Other metals are shown to be inert. The quantitative dependencies of the catalytic activity on Fe content and on α -site concentration are discussed.

DEACTIVATION KINETICS OF V/Ti-OXIDE IN TOLUENE PARTIAL OXIDATION

D.A. Bulushev, S.I. Reshetnikov, L. Kiwi-Minsker*, A. Renken* (*Swiss Federal Institute of Technology, Lausanne, Switzerland)

Appl. Catal. A: General, 220(1-2) (2001) pp. 31-39.

Deactivation kinetics of a V/Ti-oxide catalyst was studied in partial oxidation of toluene to benzaldehyde (BA) and benzoic acid (BAc) at 523-573 K. The catalyst consisted of 0.37 monolayer of VO_x species and after oxidative pre-treatment contained isolated monomeric and polymeric metavanadate-like vanadia species under dehydrated conditions as was shown by FT-Raman spectroscopy. Under the reaction conditions via *in situ* DRIFTS fast formation of adsorbed carboxylate and benzoate species was observed accompanied by disappearance of the band of the monomeric species (2038 cm⁻¹) (polymeric species were not controlled). Slow accumulation of maleic anhydride, coupling products and/or BAc on the surface caused deactivation of the catalyst during the reaction. Temperature programmed oxidation after the reaction showed formation of high amounts of CO, CO₂ and water. Rate constants for the steps of the toluene oxidation were derived via mathematical modelling of reaction kinetics at low conversion and constant oxygen/toluene ratio of 20:1. The model allows predicting deactivation dynamics, steady state rates and selectivity. The highest rate constant was

found for the transformation of BA into BAc explaining a low BA yield in the reaction.

COPPER AND IRON HYDROXIDES AS NEW CATALYSTS FOR REDOX REACTIONS IN AQUEOUS SOLUTIONS

G.L. Elizarova, L.G. Matvienko, A.O. Kuzmin, E.R. Savinova, V.N. Parmon

Mendeleev Commun., 11(1) (2001) pp. 15-17.

The paper reports on the catechol oxidation to muconic acid derivative and benzene to phenol catalysed by supported or colloidal Cu(II) and Fe(III) hydroxides. The reactions proceed in aqueous hydrogen peroxide solutions at ambient temperature.

KINETICS OF PINANE OXIDATION TO PINANE HYDROPEROXIDE BY DIOXYGEN

I.I. Il'ina, I.L. Simakova, V.A. Semikolenov

Kinetics & Catalysis, 42(1) (2001) pp. 41-45.

The liquid-phase oxidation of pinane to pinane hydroperoxide (PHP) by dioxygen is studied at 353-373 K and under dioxygen pressures ranging from 2 to 4 atm. The rate of pinane oxidation is described by the equation $w = w_{O_2} + w_{PHP}$, where the term w_{O_2} is independent of the PHP concentration, w_{PHP} is a function of the concentration $[PHP]^n$, and n ranges from 0.5 at low $[PHP]$ to 1.0 at high $[PHP]$. The *cis*-isomer of 2-hydroperoxopinane generates free radicals during autooxidation. The ratio of the rate constants of *cis*- and *trans*-pinane oxidation is found ($k_{cis}/k_{trans} = 4.0$). The selectivity of the oxidation of pinane to PHP can reach 90-95%.

Studies on Electrocatalytic Processes

THE MORPHOLOGY, SURFACE COMPOSITION, AND CATALYTIC PROPERTIES OF SILVER CRYSTALS OBTAINED BY ELECTROLYSIS

V.N. Samoilenko*, L.A. Petrov, A.I. Boronin, K.T. Murzakhmetov, S.V. Koshchev, A.N. Salanov, V.T. Yakushko, S.L. Khokhlov**, L.N. Kurina***, O. V. Vodyankina***, I. G. Rozanov*, G. I. Murygin*, Yu. P. Zaikov*** (*Institute of High-Temperature Electrochemistry, Yekaterinburg, Russia; **Institute of Organic Synthesis, Yekaterinburg, Russia; ***Tomsk State University, Tomsk, Russia)

Russ. J. Physical Chem., 75(10) (2001) pp. 1607-1614.

The chemical composition and morphology of the surface of silver crystals used as catalysts of oxidative

dehydrogenation of ethylene glycol to glyoxal were studied. The crystals were prepared by electrolysis from solutions and by high-temperature electrodeposition from melts of silver nitrate and chloride. According to the scanning electron microscopy data, the surface of crystals obtained from solutions contained globular conglomerates, and crystals having the shape of branched dendrites were formed from melts. The subsurface silver layers were studied by X-ray photoelectron spectroscopy and found to contain carbon and oxygen as impurities. The suggestion was made that the high content of oxygen in the subsurface region of silver samples obtained from melts accelerated the transformation of ethylene glycol to glyoxal.

**EX SITU SCANNING TUNNELLING
MICROSCOPY STUDY OF UNDER-
POTENTIAL OXIDATION OF A Ag(111)
ELECTRODE IN AN ALKALINE
ELECTROLYTE**

**Sh.K. Shaikhutdinov*, E.R. Savinova,
A. Scheybal*, K. Doblhofer*, R. Schlögl*** (*Fritz-
Haber-Institut der Max-Planck-Gesellschaft, Berlin,
Germany)

J. Electroanal. Chem., 500(1-2) (2001)
pp. 208-212.

A Ag(111) single crystal electrode emerged from the NaF+NaOH electrolyte (pH 11) under potential control in the interval between -0.8V and +0.2 V vs Hg/HgO was studied by scanning tunneling microscopy (STM) in an inert atmosphere. The STM images show that the oxidation of the Ag(111) surface starts above the point of zero charge and exhibits a nucleation-growth mechanism. It starts at the steps and extends to the terraces as the electrode potential is scanned positive. The potential reversal restores the initial surface morphology. The reaction-induced features imaged in STM as dark spots are assigned to the islands of chemisorbed oxygen-containing species. The irregular shape of the islands points to the diffusion of the ad-species as the limiting step of the process.

**MODEL NANOSTRUCTURED
Pt ELECTRODES – AN APPROACH TO STUDY
SIZE/STRUCTURAL EFFECTS IN
ELECTROCATALYSIS**

**O.V. Sherstyuk, P.A. Simonov, A.L. Chuvilin,
E.R. Savinova**

*“The Global Climate Change: A Coordinated
Response by Electrochemistry and Solid-State Science
and Technology”*,

Eds. A. Wieckowski, E.W. Brooman, E.J. Rudd,
T.F. Fuller, J. Leddy,
The Electrochemical Society, INC., 2001, pp. 56-71.

Development of efficient anodes for fuel cells, e.g. DMFC, implies understanding effects of metal particle size and structure on their catalytic properties. The present paper demonstrates a possible approach to design model catalytic materials for studying size effects in electrocatalysis. Two types of materials are considered: (i) monoblock (single crystalline) Pt nanoparticles and (ii) Pt particles with nanocrystalline structure (that is, particles consisting of a number of nano-sized grains connected to each other via grain boundaries), in order to investigate the effect of grain boundaries on the adsorption and catalytic properties.

Carbon-supported nanostructured Pt electrodes were tested in a number of electrochemical reactions, relevant to low temperature fuel cells, including hydrogen and oxygen electrochemisorption, electrooxidation of adsorbed CO, and in ethyleneglycole oxidation. Remarkable effects of Pt particle size and nanostructure on the reaction overvoltages, adsorption properties, electrocatalytic activities and selectivities in model processes, as well as the tolerance to self-poisoning have been established. A variety of novel results has been observed and studied, which may be used to improve the operation of the direct fuel cell anodes (decrease overvoltage, increase tolerance to self-poisoning, etc.) via controlled synthesis of carbon supported Pt nanoparticles with desired size and nanostructure.

**PLATINUM ELECTRODEPOSITS ON GLASSY
CARBON: THE FORMATION MECHANISM,
MORPHOLOGY, AND ADSORPTION
PROPERTIES**

**O.V. Sherstyuk, S.N. Pron'kin*, A.L. Chuvilin,
A.N. Salanov, E.R. Savinova, G.A. Tsirlina*,
O.A. Petrii*** (*Moscow Lomonosov State University,
Moscow, Russia)

Russ. J. Electrochem., 36(7) (2000) pp. 741-751.

The deposition of platinum on glassy carbon (GC) is studied by chronoamperometry. Basic tendencies of the formation of aggregate platinum particles on the oxidized carbon surface are established. These include a primary instantaneous nucleation of platinum under diffusion control and the beginning of a secondary nucleation prior to filling primary active centers. The deposit morphology is examined by *ex situ* methods of scanning electron microscopy (SEM), transmission electron microscopy (TEM), and scanning tunneling microscopy (STM). A globular structure of platinum, formed by crystallites 3–5 nm in size, is revealed. A comparison of the STM, SEM, and TEM data demonstrates a high information value and accuracy of STM in studies of disperse materials in both nanometer and submicron ranges. Various coulometry techniques intended for the determination of the true surface area of deposited platinum are compared. The most informative techniques are the voltammetry of desorption of copper adatoms and chemisorbed carbon monoxide at, respectively, low and high platinum contents. Differences in the formation kinetics and properties of aggregate particles in Pt/GC and Pt/Pt are found, specifically, smaller Pt/GC crystallites and higher degrees of their conrescence (screening).

EFFECT OF LOW TEMPERATURE ADSORPTION OF N₂, O₂ AND Ar ON SUPERCONDUCTIVITY OF GdBa₂Cu₃O_{7-x} FILMS

L.L. Makarshin, D.V. Andreev, V.N. Parmon, O.M. Tukhto* (*Institute of Thermal Physics, Novosibirsk, Russia)

Mater. Res. Innov., 4(1) (2000) pp. 27-31.

By measuring the imaginary part of the magnetic susceptibility of a GdBa₂Cu₃O_{7-x} film, the authors found the effect of N₂, O₂ and Ar molecules low

temperature adsorption on the superconducting properties of the film. The low temperature adsorption of the gases affects the critical transport current and the transition temperature. In all cases, the transition region broadens, as the degree of coverage of the film with the gas molecules increases. By processing the experimental data, the authors found the critical current either growing linearly (for argon and nitrogen) or decreasing exponentially (for oxygen) with increasing surface coverage by the adsorbed gas molecules.

Photocatalytic and Related Processes

PHOTOCATALYTIC DESTRUCTION OF GASEOUS DIETHYL SULFIDE OVER TiO₂

A.V. Vorontsov, E.N. Savinov, L. Davydov*, P.G. Smirniotis* (*University of Cincinnati, Cincinnati, USA)

Appl. Catal. B: Environmental, 32(1-2) (2001) pp. 11-24.

Photooxidation of gaseous diethyl sulfide (DES) at a concentration in the order of hundreds of ppm was carried out in a flow reactor over four different samples of TiO₂ under ambient conditions. (C₂H₅)₂S₂, CH₃CHO, CH₃CH₂OH, C₂H₄, and CO₂ were detected as the major products in gaseous effluent of the reactor. The trace products in gas phase included CH₃COOH, C₂H₅SC(O)CH₃, and SO₂. All the catalysts studied showed deactivation with a characteristic temporal range of 100–300 min. The surface products extracted by isopropanol included (C₂H₅)₂S₂, (C₂H₅)₂S₃, (C₂H₅)₂SO, (C₂H₅)₂SO₂, and C₂H₅SCH₂CH₂OH. The residual activity was the highest for TiO₂ Hombikat UV 100. At relatively low light intensities (1.1 mW/cm²), the increase in humidity from less than 1% to ~20 and ~60% resulted in the increase of the quantities of diethyl sulfide converted. However, at relatively high light intensities (11mW/cm²) such an increase in humidity had an adverse effect on the conversions of diethyl sulfide. The quantities of (C₂H₅)₂S converted and the products formed correlate well with the specific surface area of the TiO₂ samples, thus indicating the importance of surface reactions in gas phase photooxidation of diethyl sulfide. Additions of H₂O₂ in the reactor feed stream increased the rate of diethyl sulfide destruction, but also altered the product distribution throughout the reaction time. Steps of the reaction mechanism are proposed to explain the formation of this set of

products and observed kinetic dependencies. The main routes of this mechanism are C-S bond cleavage, S-oxidation, and C-oxidation.

PHOTOCATALYSIS AND PHOTOSORPTION IN THE EARTH'S ATMOSPHERE

V.N. Parmon, V.S. Zakharenko

CATTECH, 5(2) (2001) pp. 96-115;
Chem. for Sustainable Devel., 9(3) (2001) pp. 461-483.

The troposphere of Earth is abundant in particles of solid and liquid aerosols which have a large specific surface area and can be activated by visible light and mild ultraviolet (UV) solar radiation with wavelengths $\lambda > 300$ nm for promoting different photocatalytic and photoadsorption processes. This paper discusses possible heterogeneous photocatalytic and photosorption phenomena on the surface of solid tropospheric aerosols. These phenomena can proceed in nature at ambient conditions and can make an important contribution to the global chemistry of the Earth's atmosphere. For example, the particles of semiconductor metal oxides like TiO₂, ZnO, and Fe₂O₃ are able to photocatalyze oxidation of organic compounds from the atmosphere by air oxygen and even mineralize them. For insulator metal oxides like SiO₂, Al₂O₃, MgO, and CaO, which are the main components of tropospheric solid aerosols, a substantial depletion of many halogen-containing organic compounds (freons) is possible via their destructive photoadsorption. All mentioned processes appear to be driven by mild solar UV radiation and can proceed in the troposphere, in contrast to direct photochemistry which can take place only in the upper layers of the atmosphere.

Catalysis for Synthesis Sulfur-Organic Compounds

CONVERSION OF DIMETHYL AND DIETHYL DISULFIDES INTO THIOLS IN THE PRESENCE OF SOLID CATALYSTS

A.V. Mashkina, V.N. Yakovleva,
L.G. Sakhaltueva, L.N. Khairulina

Petroleum Chemistry, 41(1) (2001) pp. 50-56.

The reaction of gas-phase conversion of dimethyl disulfide and diethyl disulfide in the presence of solid catalysts in different environments at atmospheric pressure and a temperature of 200–350°C was investigated. Over catalysts that contain Brønsted and Lewis acid sites on their surface, the disulfides decompose in a helium atmosphere to yield thiols by eliminating H₂S and ethylene; the reactions proceed via independent routes. A produced thiol disproportionates to form the sulfide and H₂S, this process is retarded in the presence of water. The addition of H₂S to helium increases the reaction rate. The yield of thiol in terms of the disulfide converted is 60–87 mol % at 90% disulfide conversion over catalysts containing weak Lewis acid sites, but increases to 92–98% over hydrogenating sulfide catalysts at $t = 200^\circ\text{C}$ in a hydrogen atmosphere.

CATALYTIC HYDROGENATION OF THIOPHENE TO THIOLANE IN GAS PHASE

A.V. Mashkina, L.G. Sakhaltueva

Chem. Heterocyclic Comp., 37(5) (2001) pp. 546-549.

The hydrogenation of thiophene in the gas phase in the presence of palladium-sulfide catalyst leads to

the production of thiolane and hydrogenolysis products (butane and hydrogen sulfide), which are formed during the decomposition of the thiophene and thiolane. The hydrogenation rate of thiophene increases with increase of its content in the reaction mixture and also with increase of the hydrogen pressure and is reduced by thiolane. The yield of thiolane calculated on the reacted thiophene is 70-90% with 30-60% conversion of the thiophene.

PERSPECTIVES OF ALKYL MERCAPTANES PROCESSING TO DIALKYL SULFIDES

A.V. Mashkina, V.N. Yakovleva

Chem. for Sustainable Devel., 9(1) (2001) pp. 269-275.

Regularities of catalytic transformation of alkylmercaptanes were studied at atmospheric pressure and moderate temperatures. Alkylmercaptanes are condensed on acid-base catalysts in an inert medium to form symmetrical dialkylsulfides; the latter interact with methanol to yield methylalkyl sulfides. Side reactions produce dimethylsulfide, hydrogen sulfide and alkenes. Aluminas are the most active and selective catalysts for formation of dialkylsulfides.

Heat Accumulation Processes

RETARDATION OF A HEAT FRONT IN A POROUS MEDIUM CONTAINING AN EVAPORATING LIQUID

Yu.Yu. Tanashev, V.N. Parmon, Yu.I. Aristov

J. Engin. Physics & Thermophysics, 74(5) (2001) pp. 1053-1058.

The heat transfer in a layer of silica gel impregnated with a liquid (water, aqueous solutions of calcium and magnesium chlorides, formic acid, and carbon tetrachloride) has been investigated. The layer was arranged on a substrate impenetrable for vapor and it was heated from above by a concentrated light flux. It has been found that the evaporation of the liquid contained in the pores of silica gel substantially slows down the propagation of the heat front into the

layer so that the effective thermal conductivity of the layer can be reduced to 0.01 W/(m·K); this value is approximately 4–20 times smaller than the values typical of the majority of standard heat-insulating materials. The time of the front lag depends on the layer thickness, density of the incident heat flux, amount of liquid in the pores, and evaporation heat of the liquid. The observed trends in the motion of the front have been described by a simple one-dimensional model that takes into account phase transition (liquid evaporation) in the interior of the porous matrix.

HEATS OF WATER SORPTION ON SILICA GEL CONTAINING CaCl₂ AND LiBr

Yu.D. Pankrat'ev, M.M. Tokarev, Yu.I. Aristov

Russ. J. Phys. Chem., 75(5) (2001) pp. 806-810.

The heats of sorption of water vapor on the calcium chloride (or lithium bromide)-porous matrix (KSK and KSM silica gels and MSM-41 sorbent) composite sorbents and on pure silica gels were measured by calorimetry. It was shown that samples based on KSK mesoporous silica gel can feature (a) adsorption on the surface of silica gel (pure or modified with salt ions) with a heat effect of $Q=76-84$ kJ/mol (at sorption values $w<1.0$ wt %), (b) formation of lower crystal hydrates of the salt with $Q=66-72$ kJ/mol (at $1 \text{ wt \%} < w < 9-14$ wt %), and (c) vapor absorption with $Q=50-54$ kJ/mol by a salt solution in pores (at $w>9-14$ wt %). Sorption mechanisms (a) and (c) were also observed for samples based on KSM microporous silica gel and MSM-41. The possibility of the formation of solid salt hydrates in micropores was discussed. It was revealed

that the heats of sorption measured in the regions of formation of hydrates and solutions are close to those obtained earlier by the sorption method. It was shown that the introduction of a hygroscopic salt into silica gel pores substantially increases the sorption capacity of the composite system compared to the initial host matrix.

SORPTION OF CO₂ FROM HUMID GASES ON POTASSIUM CARBONATE SUPPORTED BY POROUS MATRIX

V.E. Sharonov, E.A. Tyshchishchin, E.M. Moroz, A.G. Okunev, Yu.I. Aristov

Russ. J. Appl. Chem., 74(3) (2001) pp. 409-413.

Kinetics of sorption of carbon dioxide on potassium carbonate supported by different porous matrices was studied in a flow reactor at 40°C. The structural and chemical changes of potassium carbonate-aluminum oxide composite sorbents were studied by powder X-ray diffraction, thermogravimetry and low-temperature nitrogen sorption.

Biology Related Catalysis and Biotechnology

NEW ROUTE TO VICASOL, A WATER-SOLUBLE FORM OF VITAMIN K₃

K.I. Matveev, V.F. Odyakov, E.G. Zhizhina

Russ. J. Appl. Chem., 74(3) (2001) pp. 469-472.

A procedure was suggested for preparing vicasol in an approximately 85% yield in a two-phase system consisting of concentrated (5-6 M) aqueous solution of NaHSO₃ and a solution of 2-methyl-1,4-naphthoquinone in an incombustible organic solvent (e.g., chloroform or trichloroethylene).

CATALYTIC METHODS FOR SYNTHESIS OF CITRAL FROM PRODUCTS OF ORGANIC SYNTHESIS

V.F. Odyakov, K.I. Matveev

Chem. for Sustainable Devel., 9(4) (2001) pp. 503-517.

The review paper deals with criticism of two currently used ecologically friendly catalytic methods for synthesis of citral (C₁₀) via lengthening the carbon chain with either acetylene (C₂) and acetone (C₃) or side products of isoprene (C₅) synthesis used as feedstocks. The five-stage methylheptene method intermediated by 6-methylheptene-5-on-2 (C₈) is based on C₂- and

C₃-condensation, selective hydrogenation $C\equiv C- \rightarrow CH=CH-$ and rearrangement $>C(OH)C\equiv CH \rightarrow >C=CHCHO$. The recently developed isoprenoid method is based on C₅-condensation of prenal (3-methylbutene-2-al) with prenol (3-methylbutene-2-ol-1), which are produced by 2- or 3-stage methods. Catalysts, reactions and methods discussed in the review can be applied for synthesis of terpenoids C₂₀, among which are *isophytol* (a feedstock for synthesis of side branches of vitamins E and K₁) and *vitamin A* (bibliography 145 references)

LINALOOL SYNTHESIS FROM α -PINENE: KINETIC PECULIARITIES OF CATALYTIC STEPS

V.A. Semikolenov, I.I. Il'ina, I.L. Simakova

Appl. Catal. A: General, 211(1) (2001) pp. 91-107.

Synthesis of linalool from α -pinene which includes consecutively α -pinene hydrogenation to pinane on Pd/C catalyst, pinane oxidation to pinane-hydroperoxide by molecular oxygen and pinane-hydroperoxide hydrogenation to pinanol on Pd/C catalyst followed by its thermal isomerization to linalool is discussed. The effects of the reagent concentrations, temperature and catalyst content on

the reaction rate and selectivity are studied. The kinetic peculiarities and the mechanisms of reactions are presented. The synthetic conditions of high-selective linalool preparation are found.

CHEMICAL RIBONUCLEASES. 3. THE SYNTHESIS OF ORGANIC CATALYSTS FOR THE PHOSPHODIESTER BOND HYDROLYSIS ON THE BASIS OF QUATERNARY SALTS OF 1,4-DIAZABICYCLO[2.2.2]OCTANE

D.A. Konevets*, I.E. Beck, V.N. Sil'nikov*, M.A. Zenkova*, G.V. Shishkin (*Novosibirsk Institute of Bioorganic Chemistry, Novosibirsk, Russia)

Russ. J. Bioorganic Chem., 26(11) (2000) pp. 765-773.

A family of high performance catalysts for hydrolytic cleavage of phosphodiester bonds in

ribonucleic acids based on an imidazole residue and *bis*-quaternary salts of 1,4-diazobicyclo[2.2.2]octane has been synthesised (nDm series, where *n* is the number of positive charges in the molecule at neutral pH, *m* - the symbol of the catalytically active fragment: 1- histamine, 2 - methyl ester of histidine). A general-purpose technique permitting to vary as the number of positive charges in the RNA-binding domain of the chemical ribonuclease, as their catalytic centre has been proposed. The rate of the RNA hydrolysis by nDm conjugates has been shown to thirty fold grow at the increase of the number of positive charges from + 2 up to + 4 with the hydrolysis under physiological conditions of the *in vitro* transcript of tRNA^{Lys} from human mitochondria as an example.

Catalyst Deactivation

REVERSIBLE AND IRREVERSIBLE DEACTIVATION OF SUPPORTED BIMETALLIC CATALYSTS FOR THE DEHYDROGENATION OF LOWER PARAFFINS

N.A. Pakhomov

Kinetics & Catalysis, 42(3) (2001) pp. 334-343.

The reasons and nature of the deactivation of spinel-supported bimetallic Pt–Sn, Pt–In, and Pt–Cu catalysts in the steam dehydrogenation of C₄–C₅ paraffins are analyzed. The deactivation can be reversible and irreversible. Reversible deactivation is associated with the effects of the composition of reaction medium and gaseous medium for preliminary treatment on the surface composition of supported bimetallic alloys and with the coking of catalysts. Irreversible deactivation can result from the irreproducibility of the phase composition and dispersion of supported alloys in dehydrogenation–regeneration cycles and from the carbon erosion of catalysts. This erosion consists in the removal of active metal particles to the bulk of carbon deposits. The formation of carbon deposits on the surfaces of spinel supports and bimetallic catalysts is considered. Recommendations for optimizing the composition and the operating conditions of catalysts are given in order to reduce the effects of factors that result in reversible and irreversible deactivation.

REASONS FOR THE DEACTIVATION OF VANADIA-TITANIA CATALYSTS FOR PARTIAL DURENE OXIDATION DURING PROLONGED PERFORMANCE

B.I. Kutepov*, B.S. Bal'zhinimaev (*Institute of Petrochemistry and Catalysis, Ufa, Bashkortostan, Russia)

Kinetics & Catalysis, 42(3) (2001) pp. 291-300.

The catalytic properties of vanadia–titania catalysts and the reasons for their change in the course of durene oxidation to pyromellitic dianhydride are studied. The catalysts differ in preparation conditions and the composition of the active component film deposited on a nonporous support. The stability of the catalytic properties in the reaction medium of durene oxidation is mainly determined by the properties of titania precursors.

NEW MODELS OF CATALYST DEACTIVATION BY COKE. 1. MULTILAYER COKE FORMATION VIA THE CONSECUTIVE MECHANISM

N.M. Ostrovskii

Kinetics & Catalysis, 42(3) (2001) pp. 317-325.

The equations for deactivation during multilayer coke formation occurring via consecutive addition are derived. This mechanism is true for many oxide acid catalysts. The available linear and exponential relations between the activity and the coke

concentration are the specific cases of these equations. The models were experimentally supported for dehydrogenation, isomerization, and reforming.

NEW MODELS OF CATALYST DEACTIVATION BY COKE. 2. COKING OF SUPPORTED PLATINUM CATALYSTS

N.M. Ostrovskii

Kinetics & Catalysis, 42(3) (2001) pp. 326-333.

Metal and support deactivation upon the coking of supported metal catalysts occurs via different mechanisms. Several models of coking are presented. The most complete complex model is developed for supported platinum catalysts. It implies multilayer coke formation on support, the rapid formation of polymeric coke capable of self-regeneration by hydrogen directly in the course of reaction on platinum, and the slow conversion of this coke into graphite-like coke, which is removed only by

oxidative regeneration. The models are experimentally supported for cyclohexane dehydrogenation.

DEACTIVATION OF MANGANESE OXIDE-BASED HONEYCOMB MONOLITH CATALYST UNDER REACTION CONDITIONS OF AMMONIA DECOMPOSITION AT HIGH TEMPERATURE

**Z.R. Ismagilov, S.R. Khairulin, R.A. Shkrabina,
S.A. Yashnik, V.A. Ushakov, J.A. Moulijn*,
A.D. van Langeveld*** (*Delft University of
Technology, Delft, The Netherlands)

Catal. Today, 69(1-4) (2001) pp. 253-257.

The synthesis of manganese oxide-containing catalysts on honeycomb monolith support and their performance in reaction of ammonia decomposition are described. The catalytic activity of manganese oxide-containing catalysts drops within a temperature range 800-900°C due to a strong interaction of manganese species with the support. Ways of increasing of thermal stability and catalytic activity under elevated temperatures are described.

Catalysts for Detoxication

PURIFICATION OF WET WASTE GASES OF ISOPRENE PRODUCTION OVER OXIDE CATALYSTS

**E.V. Aleksandrovich*, V.A. Chumachenko*,
V.M. Bondareva, G.Ya. Popova,
T.V. Andrushkevich, G.Yu. Miloslavskii**,
Kh.V. Mustafin**, A.S. Noskov** (JSC "Katalizator"
Novosibirsk, Russia; JSC "Nizhnekamskneftekhim",
Nizhnekamsk, Russia)

Khimicheskaya Promyshlennost, 7 (2001) pp. 18-24.

The paper concerns the development and industrial implementation of catalytic gas purification on isoprene production. The results of laboratory tests of the process of toxic impurities (carbon oxide and formaldehyde) oxidation over oxide catalysts, estimation of basic technological parameters by method of mathematical modeling are given. The process of catalytic gas purification has been put into operation at the JSC "Nizhnekamskneftekhim".

KINETICS AND MECHANISM OF LOW- TEMPERATURE OXIDATION OF H₂S WITH OXYGEN IN THE GAS PHASE

O.N. Kovalenko, N.N. Kundo, P.N. Kalinkin

React. Kinet. & Catal. Lett., 72(1) (2001)
pp. 139-145.

The possibility of the formation of polysulfides during oxidation of H₂S with oxygen on oxide catalysts has been checked, and the sequence of the reaction stages at temperatures below the sulfur dew point determined. The amount of polysulfides formed during H₂S oxidation has been found to exceed significantly that obtained in the reaction of sulfur with H₂S. Polysulfides are concluded to be intermediates in H₂S oxidation to sulfur. The rate of formation of SO₂ from sulfur vapor is shown to be negligibly low at 100-200°C. A reaction scheme involving the formation of sulfur from polysulfides and the formation of sulfur dioxide by direct oxidation of H₂S is suggested.

NONSTATIONARY PHENOMENA IN THE LOW-TEMPERATURE GAS-PHASE CATALYTIC OXIDATION OF H₂S WITH OXYGEN

O.N. Kovalenko, N.N. Kundo, V.M. Novopashina, P.N. Kalinkin

Kinetics & Catalysis, 42(5) (2001) pp. 657-661.

The conditions of the existence were determined and reasons were revealed for the appearance of periodic oscillations of the SO₂ concentration in the reaction products and warming temperature in the catalyst bed in the oxidation of H₂S with oxygen at temperatures below the dew point of sulfur on the V–Al–Ti oxide catalyst. The formation of polysulfides during the reaction was experimentally found. It was proposed that the adsorption of sulfur and polysulfides on the catalyst surface is responsible for the observed oscillatory processes.

KINETIC PECULIARITIES IN THE LOW-TEMPERATURE OXIDATION OF H₂S ON VANADIUM CATALYSTS

P.N. Kalinkin, O.N. Kovalenko, N.N. Kundo

React. Kinet. & Catal. Lett., 74(1) (2001) pp. 177-184.

H₂S oxidation by oxygen on catalysts V₂O₅/Al₂O₃, V₂O₅/TiO₂, V₂O₅/Al₂O₃/TiO₂ was studied at temperatures below the sulfur dew point. High activity

and the oscillation character of the oxidation were demonstrated by catalysts with low contents of V₂O₅ (3–5 wt.%). The increase in the V₂O₅ concentration to 10–20 wt.% results in the reduction of the catalytic activity and oscillation ability. On a pure V₂O₅ catalyst, the oscillations were not detected. The difference between the catalysts with the high and low concentrations of V₂O₅ is explained in terms of the structures of the V⁵⁺ species formed in the catalysts.

SUPPORTED HONEYCOMB MONOLITH CATALYSTS FOR HIGH-TEMPERATURE AMMONIA DECOMPOSITION AND H₂S REMOVAL

Z.R. Ismagilov, R.A. Shkrabina, S.A. Yashnik, N.V. Shikina, I.P. Andrievskaya, S.R. Khairulin, V.A. Ushakov, J.A. Moulijn*, I.V. Babich* (*Delft University of Technology, Delft, The Netherlands)

Catal. Today, 69(1-4) (2001) pp. 351-356.

Catalysts that have potential in simultaneous removal of H₂S and NH₃ decomposition were developed. The monolith supports of high surface area and acceptable mechanical strength based on titania and silica-alumina precursors were prepared and tested. Preparation routine and composition of Mn, Fe and Cu oxides supported honeycomb catalysts have been optimized. Impregnated and washcoated monolith catalysts were tested in ammonia high temperature decomposition.

Catalytic Combustion

DEEP OXIDATION OF METHANE ON ALUMINA-MANGANESE AND Pt-CONTAINING CATALYSTS

P.G. Tsyrunnikov, V.S. Sal'nikov, V.A. Drozdov, A.S. Noskov, N.A. Chumakova, V.K. Ermolaev, I.V. Malakhova

J. Catal., 198 (2) (2001) pp. 164-171.

The kinetics of deep methane oxidation was studied over a manganese-alumina catalyst and a reference catalyst - a tableted mechanical mixture of 2% Pt+γ-Al₂O₃. The reaction temperature ranged from 400 to 800°C, the methane concentration was up to 4.5 vol%, and the oxygen content was up to stoichiometry. The higher the catalyst activity, the lower the probability for the homogeneous continuation of the catalytic reaction to proceed, even at 800°C with the stoichiometry gas mixture composition. The distance over which alkyl peroxide catalysts escape from the catalyst surface under reaction conditions was estimated.

NOVEL GLASS CRYSTAL CATALYSTS FOR THE PROCESSES OF METHANE OXIDATION

A.G. Anshits*, E.V. Kondratenko*, E.V. Fomenko**, A.M. Kovalev*, N.N. Anshits*, O.A. Bajukov***, E.V. Sokol****, A.N. Salanov (*Institute of Chemistry of Natural Organic Materials and Chemical Technology, Krasnoyarsk, Russia; **Krasnoyarsk State Technical University, Krasnoyarsk, Russia; ***Institute of Physics, Akademgorodok, Krasnoyarsk, Russia; ****Institute of Geology, Geophysics and Mineralogy, Novosibirsk, Russia)

Catal. Today, 64(1-2) (2001) pp. 59-67.

Novel catalysts were prepared from magnetic microspheres and cenospheres recovered from fuel ashes being formed in combustion of Irsha-Borodinskii lignite and Kuznetskii coal. The specific features of microsphere formation in the coal combustion were discussed. The morphology as well

as composition of different magnetic microspheres and cenospheres were studied by SEM, electron probe microanalysis and Mössbauer spectroscopy. The morphology of globules, crystallite size and defect structure of active phase was established to depend on the basicity of the glass phase. It was shown that

catalytic activity of magnetic microspheres and cenospheres in the reaction of deep oxidation of methane is determined by the spinel phase and depends on the extent of its accessibility and type of defect structure.

Polymerization Processes

COPOLYMERIZATION OF ETHYLENE WITH 1-HEXENE OVER SUPPORTED ZIRCONOCENE CATALYSTS

**L.G. Echevskaya, V.A. Zakharov,
N.V. Semikolenova, T.B. Mikenas**

Polimery, 46(1) (2001) pp. 40-43.

Two supported zirconocene catalysts were prepared: (I) $\text{SiO}_2/\text{MAO}/\text{Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2$ (0.1 wt. % Zr, 9.0 wt. % Al) and (II) $\text{MgCl}_2/\text{Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2$ (0.2 wt.% Zr, 1.6 wt.% Al). Ethylene was homopolymerized and copolymerized with 1-hexene (70-90°C, 6 bar, TIBA as cocatalyst) over (I) and (II). Catalyst (I) incorporated the comonomer as much as did the homogeneous catalyst in the same composition. MgCl_2 used as support resulted in reduced copolymerization reactivity of the catalyst. Copolymer crystallinity and catalyst activity were studied in relation to the concentration of 1-hexene.

POLYMERIZATION OF ETHYLENE USING SUPPORTED ZIRCONOCENE CATALYSTS

**L.G. Echevskaya, V.A. Zakharov,
N.V. Semikolenova, T.B. Mikenas, A.P. Sobolev**

Polymer Sci., ser. A, 43(3) (2001) pp. 220-227.

The polymerization of ethylene using supported zirconocene catalysts with varying support compositions $\text{SiO}_2\text{-MAO-Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2 + \text{TIBA}$ (catalyst I) and $\text{MgCl}_2\text{-Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2 + \text{TIBA}$ (catalyst II) (MAO is methylaluminumoxane, Ind is indenyl, and TIBA is triisobutylaluminum) was studied. The examined catalytic systems differ in their activity, ability to control the molecular mass of the resulting polymer, and kinetics of copolymerization with 1-hexene. The molecular structure of PE prepared with supported catalysts I and II and a homogeneous catalyst $\text{Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2 + \text{MAO}$ was studied by IR and ^{13}C NMR spectroscopy. As evidenced by ^{13}C NMR spectroscopy, PE samples synthesized with the homogeneous catalyst and catalyst I contain ethyl branches along with the end

methyl groups in the low-molecular-mass fractions. On the contrary, PE prepared with supported catalyst II is devoid of ethyl branches but contains vinyl groups as the basic type of unsaturation.

POLYMERIZATION OF ETHYLENE IN THE PRESENCE OF HYDROGEN OVER SUPPORTED VANADIUM-MAGNESIUM CATALYSTS

**T.B. Mikenas, V.A. Zakharov, L.G. Echevskaya,
M.A. Matsko**

Polimery, 45(5) (2000) pp. 349-352.

Catalyst activity was studied in a slurry polymerization of ethylene carried out over supported $\text{VCl}_4/\text{MgCl}_2$ and $\text{VOCl}_3/\text{MgCl}_2$ catalysts in relation to hydrogen concentration (0-40 mmols/L, *i.e.*, 0-2 bar) and to $\text{Al}(\text{i-Bu})_3$ and $\text{Al}(\text{i-Bu})_2\text{H}$, each used as cocatalyst. Hydrogen was found to reduce the activity of the catalyst by 2 to 6 times. The deactivation occurring in the presence of hydrogen was directly related to hydrogen pressure and found to be due to the hydride species of organoaluminum compounds forming in the side reaction of AlR_3 with the V-H bonds accompanied by adsorption of alkylaluminum hydride on active sites. A sequence of reactions is suggested to explain the deactivation and reactivation of the catalyst.

ETHYLENE POLYMERIZATION WITH SUPPORTED VANADIUM-MAGNESIUM CATALYST: HYDROGEN EFFECT

**T.B. Mikenas, V.A. Zakharov, L.G. Echevskaya,
M.A. Matsko**

Macromol. Chem. Phys., 202(4) (2001) pp. 475-481.

Ethylene polymerization on supported vanadium-magnesium catalysts with the composition $\text{VCl}_4/\text{MgCl}_2$ and $\text{VOCl}_3/\text{MgCl}_2$ was studied in the presence of hydrogen as the chain transfer agent. Vanadium-magnesium catalysts (VMC) are known to exhibit a high reactivity towards hydrogen. This reactivity is manifested

as a sharp decrease in polyethylene (PE) molecular weight accompanied by a dramatic (2-6-fold) loss of catalyst activity, when hydrogen is introduced. Catalyst deactivation in the presence of hydrogen is reversible. Catalyst activity is restored, when hydrogen is removed from the reaction medium. With this regard the effect of the concentration of hydrogen and of Al(i-Bu)₃ and Al(i-Bu)₂H, used as co-catalysts, on the activity of VMC has been studied. The reaction products formed after polymerization reaction in the presence of hydrogen have been also identified. Based on experimental data the reaction scheme leading to catalyst deactivation in the presence of hydrogen and its reactivation, when hydrogen is removed from the reaction medium, has been suggested. According to this scheme, catalyst deactivation is caused by dialkylaluminumhydride forming in the side reaction of AlR₃ co-catalyst with the V-H bonds and then being adsorbed onto the catalyst active sites. It is shown that the deactivation process may be diminished, if some modifiers able to bind with alkylaluminumhydride are introduced into the catalyst composition. Magnesium dichloride introduced into the catalytic system or aluminum trichloride introduced into the catalyst composition may be used for modification. Using this approach highly active supported VMC with an activity up to 50 kg/gV·h·bar C₂H₄ (80°C) at polymerization in the presence of hydrogen have been obtained.

ETHYLENE POLYMERIZATION WITH SUPPORTED VANADIUM-MAGNESIUM CATALYST: NUMBER OF ACTIVE CENTERS AND PROPAGATION RATE CONSTANT

M.A. Matsko, G.D. Bukatov, T.B. Mikenas, V.A. Zakharov

Macromol. Chem. & Phys., 202(8) (2001)
pp. 1435-1439.

The data on the number of active centers in the ethylene polymerization with highly active supported vanadium-magnesium catalyst (130 kg-PE/g·V·h·bar) were obtained by using ¹⁴CO as a radioactive inhibitor. The number of active centers was found to attain 0.06 mol/mol-V and the propagation rate constant equaled 2.2·10⁴ L/mol·s (80°C). The effect of reversible deactivation of the catalyst in ethylene polymerization in the presence of hydrogen was studied. It was found that a part of the active centers containing vanadium-polymer bonds transforms to a temporary inactive (dormant) state during the polymerization in presence of hydrogen that may explain the catalyst deactivation. As hydrogen is

removed from the reaction medium, these centers transform to the active state again.

STRUCTURE AND PERFORMANCE OF THE SOLID METHYLALUMOXANE AT TEMPERATURES 20-250°C: EXPERIMENTAL AND DFT CALCULATION STUDY

V.N. Panchenko, V.A. Zakharov, I.G. Danilova, E.A. Paukshtis, I.I. Zakharov, V.B. Goncharov, A.P. Suknev

J. Molec. Catal. A: Chemical, 174(1-2) (2001)
pp. 107-117.

The structure of solid methylalumoxane (MAO) and its behavior in the temperature interval from 20 to 250°C have been studied using IR spectroscopy in diffusion reflection mode (DRIFT) and mass-spectrometric methods. It has been shown that three-dimensional MAO molecule may entrap water molecule in its volume (a.b. 3550 cm⁻¹ in the IR-spectrum). Using a DFT quantum-chemical method, the three-dimensional molecular model of MAO with composition (-Al(CH₃)O)₁₂, comprising water molecule in its structure, has been calculated. The release of the water molecule from the structure of MAO is accompanied by the protolysis of Al-CH₃ bonds and methane evolving. This reaction seems to be responsible for the observed evolving of methane on the MAO aging. As the temperature of MAO heating increases from 20 to 250°C, the process of methane evolving intensifies.

The heating of the solid MAO samples is also accompanied by the release of trimethylaluminium (TMA) in significant amount (0.18 mole AlMe₃/mole Al_{MAO} at 100°C). Obviously, the released TMA was strongly associated with the MAO in the initial sample.

The data on the activity in the ethylene polymerization of catalyst Cp₂ZrCl₂/MAO prepared with the use of the MAO samples dried at temperatures 20 to 250°C are presented as well.

For the first time the statistical lattice models of adsorption and diffusion processes on the supported catalytically active metal particles has been elaborated which permit to take into account the dynamic change of the shape and surface morphology of the supported particle under the influence of the reaction media. The effect of the shape and of the surface morphology change induced by adsorption has been studied for the case of strong «metal-adsorbate» interaction.

**PROPYLENE ZIEGLER-NATTA
POLYMERIZATION: NUMBERS AND
PROPAGATION RATE CONSTANTS FOR
STEREOSPECIFIC AND NON-
STEREOSPECIFIC CENTERS**

G.D. Bukatov, V.A. Zakharov

Macromol. Chem. & Phys., 202(10) (2001)
pp. 2003-2009.

The data on the number of active centers (C_p) and values of propagation rate constants (K_p) have been obtained for stereospecific and non-stereospecific centers at propylene polymerization with catalytic systems of various composition: $TiCl_3-AlEt_3$ (I), $TiCl_4/D/MgCl_2-AlEt_3$ (II), $TiCl_4/D/MgCl_2-AlEt_3-TES$ (III), where D - dibutyl phthalate, TES - tetraethoxysilane. The C_p and K_p values were determined by ^{14}CO quenching method at the polymerization in the absence and the presence of hydrogen. The C_p and K_p values were determined for three PP fractions: boiling pentane soluble fraction (atactic PP), boiling heptane soluble fraction (stereoblock PP) and boiling heptane insoluble fraction (isotactic PP). The following results are obtained. (i) The K_p values increase in the following order: atactic centers < stereoblock centers < isotactic centers (from ≈ 200 to $\approx 3 \cdot 10^3$ l/mol·s, 70°C) for all catalysts studied. (ii) The respective K_p values do not differ essentially with the change of the catalyst composition (systems I, II, III). (iii) As the external donor is introduced in TMC (system III), the portion of stereospecific active centers increases (from 34 to 62%), but the total number of active centers changes insignificantly. Most likely the non-stereospecific active centers transform into stereospecific ones in the presence of silane.

**POLYMERIZATION OF ETHYLENE
CATALYZED BY IRON COMPLEX BEARING
2,6-BIS(IMINE)PYRIDYL LIGAND: 1H AND 2H
NMR MONITORING OF FERROUS SPECIES
FORMED VIA CATALYST ACTIVATION
WITH $AlMe_3$, MAO, $AlMe_3/B(C_6F_5)_3$ AND
 $AlMe_3/CPH_3(C_6F_5)_4$**

**E.P. Talsi, D.E. Babushkin, N.V. Semikolenova,
V.N. Zudin, V.N. Panchenko, V.A. Zakharov**

Macromol. Chem. & Phys., 202(10) (2001)
pp. 2046-2051.

1H and 2H NMR spectroscopic monitoring of ferrous species formed via interaction of 2,6-bis[1-(2,6-dimethylphenylimino)ethyl]pyridineiron(II)

chloride (**1**) with $AlMe_3$, MAO, $AlMe_3/B(C_6F_5)_3$ and $AlMe_3/CPH_3(C_6F_5)_4$ is reported. At interaction of **1** with MAO in toluene solution, the new stable heterodinuclear neutral complexes with proposed structures $LFe(II)(Cl)(\mu-Me)_2AlMe_2$ and $LFe(II)(Me)(\mu-Me)_2AlMe_2$ are formed (L is initial tridentate ligand). Complex $LFe(II)(Cl)(\mu-Me)_2AlMe_2$ predominates at low Al/Fe ratios (less than 50), while $LFe(II)(Me)(\mu-Me)_2AlMe_2$ at high Al/Fe ratios (more than 500). Complex assigned to $LFe(II)(Me)(\mu-Me)_2AlMe_2$ can be prepared via interaction of **1** with $AlMe_3$. Activation of $LFe(II)(Me)(\mu-Me)_2AlMe_2$ by $B(C_6F_5)_3$ and $CPH_3B(C_6F_5)_4$ gives rise to formation of new complexes with proposed structures $[LFe(\mu-Me)_2AlMe_2]^+[MeB(C_6F_5)_3]^-$ and $[LFe(\mu-Me)_2AlMe_2]^+[B(C_6F_5)_4]^-$. Unexpectedly, the activity at ethylene polymerization was even higher for **1**/ $AlMe_3$ than for **1**/MAO catalytic system. The co-catalytic activity of MAO towards **1** dramatically decreased with the diminishing of $AlMe_3$ content in the composition of MAO. Activity of the catalyst **1**/ $AlMe_3$ and the molecular structure of polyethylene produced do not change noticeably at the addition of $B(C_6F_5)_3$ to **1**/ $AlMe_3$. These data allow to suggest, that active species of **1**/ $AlMe_3$ and **1**/MAO systems are neutral methylated ferrous complexes but not cationic intermediates. Probably, complex $LFe(II)(Me)(\mu-Me)_2AlMe_2$ is the closest precursor of these active species.

**ETHYLENE POLYMERIZATION IN THE
PRESENCE OF
IRON(II) 2,6-BIS(IMINE)PYRIDINE COMPLEX:
STRUCTURES OF KEY INTERMEDIATES**

**E.P. Talsi, D.E. Babushkin, N.V. Semikolenova,
V.N. Zudin, V.A. Zakharov**

Kinetics & Catalysis, 42(2) (2001) pp. 147-153.

The structures of intermediates generated by the activation of 2,6-bis[1-(2,6-dimethylphenylimino)ethyl]pyridineiron(II) chloride (**1**) with various cocatalysts, methylalumoxane (MAO), trimethylaluminum (TMA), and TMA in combination with $B(C_6F_5)_3$ and $Ph_3CB(C_6F_5)_4$, is studied by 1H and 2H NMR spectroscopy. The **1**/ $AlMe_3$ system exhibits a higher catalytic activity in ethylene polymerization than the **1**/MAO system. The activity of the latter decreases sharply with a decrease in the amount of $AlMe_3$ in MAO. Neutral Fe(II) complexes rather than cationic intermediates are

suggested to be active components in both catalytic systems.

HOLLOW-PARTICLE LATEXES: PREPARATION AND PROPERTIES

V.N. Pavlyuchenko, O.V. Sorochinskaya, S.S. Ivanchev, V.V. Klubin, G.S. Kreichman, V.P. Budtov, M. Skrifvars*, E. Halme*, J. Koskinen* (*Neste Chemicals OY, Porvoo, Finland)

J. Polymer Sci., Part A - Polymer Chemistry, 39(9) (2001) pp. 1435-1449.

Hollow-particle latexes were prepared according to the following stages: (1) the preparation of the methyl methacrylate-methacrylic acid (MAA)-ethylene glycol dimethacrylate copolymer (**I**) latex, (2) the preparation of a shell (**II**) based on polystyrene or styrene-acrylonitrile-divinyl benzene copolymer polymerized onto copolymer (**I**) particles, and (3) the neutralization of the core (**I**) carboxyl groups with a base (NH₄OH or NaOH) at temperatures close to the glass-transition temperature of the polymer (**II**). The neutralization resulted in the expansion of the particles and formed water-filled hollow particles. The microspheres had an overall diameter of 460-650 nm and a hollow diameter of 300-450 nm. Rheological studies and particle size measurements by transmission electron microscopy and dynamic light scattering of the copolymer (**I**) latex indicate that the maximum particle swelling occurred at an approximately equimolar MAA/base ratio. It was found that even without the neutralization of the MAA units, a small hollow formation in the latex particles occurred during stage 2 because one volume of the copolymer (**I**) retained about 8 volume parts of water. It was also discovered that the final hollow-particle geometry after neutralization depends on the shell copolymer thickness and type as well as on the conditions during stage 3, that is, the time, temperature, base type, and concentration. The opacifying ability of the synthesized hollow particles was investigated in latex coatings. The opacifying ability values were generally in agreement with the hollow-particle geometry. The only exception was related to the copolymer (**I**)/copolymer (**II**) ratio. The maximum hollow volume was obtained at this value equal to 1/8, whereas the highest opacifying ability was observed at 1/10.

SEGREGATION OF POLYMERS IN THE COURSE OF FILM FORMATION FROM A MIXTURE OF LATEXES

V.N. Pavlyuchenko, O.N. Primachenko, S.Ya. Khaikin, S.S. Ivanchev, M.E. Jones* (*Dow Chemical, USA)

Russ. J. Appl. Chem., 74(7) (2001) pp. 1173-1177.

Film formation from binary mixtures of latexes of thermodynamically incompatible polymers was studied. Partial segregation of the polymers in the course of latex film formation, causing asymmetry of the resulting films, was proved by FTIR spectroscopy. The influence of various factors on the segregation of polymers was examined.

WATER-RESISTANT FILMS AND COATINGS BASED ON CROSS-LINKING STYRENE- ACRYLATE LATEX COPOLYMERS

S.S. Ivanchev, V.N. Pavlyuchenko, N.A. Byrdina, M. Skrifars*, J. Koskinen* (*Neste Chemicals Oy, Porvoo, Finland)

Russ. J. Appl. Chem., 74(2) (2001) pp. 309-315.

Water-resistant films and coatings were prepared from latexes of copolymers of styrene, n-butyl acrylate, 2-hydroxyethyl methacrylate, glycidyl methacrylate, and methacrylic acid. The degree of cross-linking of the copolymers in the course of film formation and the water resistance of the films and coatings, associated with this parameter and evaluated by the water absorption and mechanical properties of wet films, were studied in relation to the gross composition of the latex copolymer, conditions of its synthesis, distribution of functional groups responsible for cross-linking in a latex particle, and temperature of film formation.

POLYMERIZATION AND COPOLYMERIZATION OF ETHYLENE WITH HIGHER α -OLEFINS USING IRON CHLORIDE 2,6-BIS(IMINO)PYRIDYL DERIVATIVES - METHYLALUMINOXANE CATALYTIC SYSTEMS

S.S. Ivanchev, G.A. Tolstikov*, V.K. Badaev, N.I. Ivancheva, I.I. Oleinik*, M.I. Serushkin, L.V. Oleinik* (*Institute of Organic Chemistry, Novosibirsk, Russia)

Polymer Sci., ser. A, 43(12) (2001) pp. 1189-1192.

The kinetics of polymerization of ethylene and its copolymerization with 1-octene and 4-methyl-1-

pentene catalyzed by four new 2,6-bis(imino)pyridyl iron complexes containing bulky substituents in the *ortho* position of the aryl ring ($R^2 =$ cyclopentyl, $R^3 =$ H, Me, cyclopentyl, $R^4 =$ H, Me) combined with methylaluminumoxane were studied at various temperatures and ethylene pressures. The polymerizing activity of the synthesized complexes was measured in the temperature range 50–80°C and at pressures varying from 0.1 to 0.55MPa. Using the DSC method, the thermal properties of the samples of PE were determined and their molecular characteristics estimated. A complex with two *ortho* cyclopentyl substituents was found to exhibit high thermal stability. The produced polymer samples possess high density (965–972 kg/m³), thus indicating the absence of branching in the macromolecules. The examined catalysts proved to be inactive in the copolymerization of ethylene with 1-octene and 4-methyl-1-pentene.

RADIATION CROSSLINKING OF POLYPROPYLENE IN THE PRESENCE OF MONOMERS INCAPABLE OF HOMOPOLYMERIZATION

S.S. Ivanchev, M. Ratzsch*, A.M. Mesh, S.Ya. Khaikin, H. Bucka*, A. Hesse*, N. Reichelt*, M.E. Moiseeva (*Borealis AG, Linz, Austria)

Polymer Sci., ser. B, 43(3-4) (2001) pp. 85-90.

The process of the radiation crosslinking of PP which makes it possible to achieve gelation at a low irradiation dose was studied. An efficient crosslinking is ensured if a pair of monomers (vinylalkoxysilane and maleic anhydride) incapable of homopolymerization is used as a crosslinking additive. The mechanism of the crosslinking process was examined. It was shown that γ -irradiation of PP carried out in the presence of the above compounds leads to the grafting of each monomer onto PP as single units and to the chemical interaction between the functional groups of the grafted fragments to yield crosslinks between the macrochains of PP.

GRAFTING POLYMERIZATION OF VINYL MONOMERS ONTO POLYPROPYLENE IN THE PRESENCE OF ACETYLACETONATES OF VARYING VALENCE METALS

A.M. Mesh, S.S. Ivanchev, M. Ratzsch*, S.Ya. Khaikin, N. Reichelt*, N.K. Fedorova (*Borealis AG, Linz, Austria)

Polymer Sci., ser. B, 43(9) (2001) pp. 272-275.

It was shown that acetylacetonates of variable valence metals absorbed together with vinyl monomers in a PP matrix efficiently initiate the polymerization of these monomers. The process proceeds at a high rate even at room temperature if the aging degree of the PP matrix is characterized by insignificant degree of aging. The polymerization of styrene in the matrix yields up to ~50% grafted macromolecules. It is suggested that a partially oxidized PP matrix exerts a promoting effect on the process of polymerization initiation due to the incorporation of oxygen-containing functional groups into the PP matrix.

SYNTHESIS OF POLYMER METHACRYLATE MICROSPHERES IN THE PRESENCE OF DEXTRAN AND ITS DERIVATIVES

A.Yu. Men'shikova*, T.G. Evseeva*, N.A. Chekina*, S.S. Ivanchev(*Institute of Macromolecular Compounds, St. Petersburg, Russia)

Russ. J. Appl. Chem., 74(3) (2001) pp. 489-493.

Emulsion polymerization of methyl methacrylate initiated by a carboxyl-containing azo initiator in the presence of polymeric stabilizer (dextran or its functionalized derivatives) was studied with the aim to prepare monodisperse microspheres of polymer methacrylate with surface carboxy, amido, and aldehyde groups. The optimal conditions for the formation of monodisperse microspheres were found allowing control of their diameter in the submicrometer range and of the nature and content of surface functional groups.

EMULSIFIER-FREE POLYMERIZATION OF METHYL METHACRYLATE WITH A CARBOXYL-CONTAINING INITIATOR

A.Yu. Men'shikova*, **T.G. Evseeva***,
M.V. Peretolchin*, **N.A. Chekina***, **S.S. Ivanchev**
(*Institute of Macromolecular Compounds,
St. Petersburg, Russia)

Polymer Sci., ser. A, 43(4) (2001) pp. 366-374.

It was shown that the emulsifier-free polymerization of methyl methacrylate initiated by 4,4'-azobis(4-cyanovaleric acid) at high initial pH values differs from the polymerization of styrene carried out under analogous conditions. It was demonstrated that the hydrolysis of the monomer in an alkaline medium with the formation of methacrylic acid leads to a decrease in the rate of polymerization and to a reduction in the diameter of microspheres; nevertheless, the extent of carboxylation of the particle surface drops as pH increases. Varying the initial pH value enables one to control the diameter of the monodisperse microspheres of PMAA in a submicron range.

RADIATION GRAFTING OF VINYLALKOXYSILANES ONTO POLYPROPYLENE

S.S. Ivanchev, **M. Ratzsch***, **A.M. Mesh**,
S.Ya. Khaikin, **H. Bucka***, **A. Hesse**** (*Agrolinz
Melamin GmbH, Linz, Austria, ** Borealis AG, Linz,
Austria)

Polymer Sci., ser. A, 43(4) (2001) pp. 490-494.

The process of radiation grafting of vinylalkoxysilanes, monomers inactive in free-radical polymerization, onto PP was studied. The effects of the chemical structure of vinylalkoxysilanes and their sorption-diffusion characteristics, as well as irradiation parameters on the efficiency of radiation grafting were assessed. Based on the data obtained, the experimental conditions which make it possible to exclude the diffusion control of the process were

determined. It was shown that the hydrolysis of alkoxy groups of vinylsilanes radiation-grafted onto PP provides a means of obtaining structured PP with a desired content of gel fraction.

POLYTETRAFLUORINETHYLENE REACTION WITH OXIDES AND HYDROXIDES OF ALKALINE-EARTH METALS

Zh.A. Vnitskikh*, **A.A. Fedorov***,
Yu.S. Chekryshkin*, **E.A. Zhilkina***,
Z.R. Ismagilov, **M.A. Kerzhentsev** (*Ural Institute
of Technical Chemistry, Perm', Russia)

Chem. for Sustainable Devel., 9(6) (2001)
pp. 715-722.

Polytetrafluorinethylene reaction with magnesium and calcium oxides and hydroxides has been studied in isothermal and non-isothermal conditions. The kinetic parameters of dehydration of magnesium and calcium hydroxides were estimated. The kinetic data obtained for the polymer breakdown were compared to those of hydroxides dehydration and formation of fluorides and carbonates of alkaline-earth metals.

THERMAL-OXIDATIVE BREAKDOWN OF POLYTETRAFLUORINETHYLENE

Zh.A. Vnitskikh*, **A.A. Fedorov***,
Yu.S. Chekryshkin*, **Z.R. Ismagilov**,
M.A. Kerzhentsev (*Ural Institute of Technical
Chemistry, Perm', Russia)

Chem. for Sustainable Devel., 9(5) (2001)
pp. 621-623.

Thermal-oxidative breakdown of polytetrafluorinethylene has been studied in isothermal and non-isothermal conditions. Several stages of the process of polymer breakdown have been revealed. The activation energies and specific rates of the reaction of polytetrafluorinethylene breakdown have been determined.

Aerosol Nucleation Processes

EXPERIMENTAL DETERMINATION OF THE SURFACE ENERGY OF CRITICAL NUCLEI DURING THE NUCLEATION OF SUPERSATURATED VAPOR

M.P. Anisimov, A.G. Nasibulin*,
S.D. Shandakov*, I.N. Shaimordanov (*Kemerovo State University and Kemerovo Scientific Center, Kemerovo, Russia)

Colloid J., 63(2) (2001) pp. 131-136.

Theoretical substantiation of the empirical method for determining the surface (or excess) energy of critical nuclei was performed within the framework of thermodynamic approach. Characteristics of critical nuclei were determined based on the studies of the nucleation of supersaturated vapors of glycerol in the vicinity of its melting point and the critical temperature of carrier gas. The effect of the specific features of physicochemical parameters of the studied substance and carrier gas on the parameters of critical nuclei was revealed. Experimental values of the surface energy of critical nuclei were compared with those calculated by the droplet model. The necessity for the allowance for the temperature dependence of the surface energy of critical nuclei was demonstrated. It was noted that the largest deviation from the predictions of droplet model arises at small (about 10) numbers of molecules in a critical nucleus; as the size of a nucleus increases, the surface energy, in the limiting case, tends to physically correct value.

EXPERIMENTAL DETERMINATION OF THE SURFACE ENERGY OF CRITICAL NUCLEI DURING THE NUCLEATION

M.P. Anisimov, S.D. Shandakov*,
I.N. Shaimordanov, A.S. Berezina,
Yu.I. Polygalov, S.A. Timoshenko* (*Kemerovo State University, Kemerovo, Russia)

J. Mendeleev Chem. Society, 45(3) (2001) pp. 38-44.

Theoretical substantiation of the empiric method for determining of the critical nuclei surface (or excess) energy was performed within the framework of thermodynamic approach. Characteristics of critical nuclei were determined based on the studies of the nucleation of supersaturated vapors of glycerol in the vicinity of its melting temperature and critical temperature of gas-carrier. The effect of the specific features of physicochemical parameters of the studied

substance and gas-carrier on the characteristics of critical nuclei was revealed. The experimental values of the critical nuclei surface energy were compared with those calculated by the droplet model. The necessity to take into account the temperature dependence of the critical nuclei surface energy was shown. It was noted the largest discrepancy from the droplet model arises at small (about 10) numbers of molecules in a critical nucleus; as the nucleus size increases, the surface energy, in the limiting case, tends to physically correct value following from the droplet model. The interpretation of the nucleation in the vapor-gas system in the binary approach is presented as the more reasonable. The development of experimental methods for determining of multi-channel nucleation and the separating of total nucleation rate to ones for each channel becomes actual.

TRANSPORT IN THE STATIC DIFFUSION CLOUD CHAMBER REVISITED

M.P. Anisimov, S.D. Shandakov*,
Yu.I. Polygalov, R.H. Heist** (*Kemerovo State University, Kemerovo, Russia; **Manhattan College, New York, USA)

J. Chem. Phys., 114(2) (2001) pp. 899-906.

The static diffusion chamber (SDC) allows the measurement of critical supersaturation and of nucleation rates and it is a powerful instrument for the vapor nucleation study. Earlier, within the scope of the International Nucleation Workshop Group, nucleation rates of the n-Pentanol–helium system have been measured using different experimental techniques. Disagreement of experimental data obtained using the static diffusion chamber and data obtained using other methods, particularly the laminar flow diffusion chamber, can be explained by re-examining the mass and energy transport analysis used to describe static diffusion chamber operation. In the present research the mass and energy transport is described in the SDC modeled as an effectively open system with mass and energy transport in one direction with a nonzero diffusion flux at the system boundaries. Calculated values for vapor supersaturation are compared with the n-pentanol nucleation rate experimental results of the American–Czech group and with a nucleation rate Reference Equation obtained from an earlier

investigation involving the n-pentanol–helium system. One can see that there is a significant difference in the calculated supersaturation for all of the data. The magnitude of this difference is quite large even for the relatively small vapor mass fractions at a nucleation temperature of 260 K. It is also noted that the calculated nucleation temperatures from analysis are slightly larger than those reported in the work of Rudek et al. The calculations were performed with and without the thermal diffusion term. The effect of thermal diffusion on the transport process is relatively small and is not particularly essential to include in the comparison the effects of the different flux boundary conditions.

BINARY *n*-OCTANOL - SULFUR HEXAFLUORIDE NUCLEATION

M.P. Anisimov, P.K. Hopke*, I.N. Shaimordanov, S.D. Shandakov, L.-E. Magnusson***** (*Clarkson University, Potsdam, USA; **Kemerovo State University, Kemerovo, Russia; ***Southern Illinois University, Carbonale, USA)

J. Chem. Phys., 115(2) (2001) pp. 810-816.

Recently the accuracy of vapor nucleation rate measurements has vastly increased. However, when experimental conditions become close to the values to the critical parameters of investigated systems, significant discrepancies were found between experimental results and predictions of the theory. Some researchers have found the agreement between experimental results and theory only within a narrow range of nucleation conditions. Therefore, it is an appropriate time to investigate the nucleation of new systems to obtain new ideas to guide nucleation theory development. Alcohols are the most studied class of chemical compounds, but up to now, there are no experimental data on n-octanol vapor nucleation. The present study is devoted to the investigations of the homogeneous nucleation of the n-octanol in sulfur hexafluoride. Comparison of the critical pressures for binary mixture with the Laplace pressure calculated in droplet approximation using bulk liquid surface tension shows that the carrier gas has a more active role in the nucleation than assumed by classical theory. The exceedingly high critical embryo Laplace pressure calculated in droplet approximation as compared to the highest possible critical pressure for

binary system under investigation illustrates the problem of critical embryo excess energy calculations when using the bulk liquid surface tension. Disagreement of the experimental results and predictions of the classical nucleation theory as well as the Dillmann-Meier theory or any other theories have the same basic problem. At least two incorrect points of view are reasonable to change now: vapor – gas nucleation as well as a size and temperature dependence for the critical embryo excess energy should be considered in binary approximation instead of single component consideration. Theories for single component vapor nucleation should be compared with the really single component vapor nucleation experimental results.

TWO CHANNEL VAPOR NUCLEATION IN THE VICINITY OF THE TRIPLE POINT

L.M. Anisimova, P.K. Hopke*, J. Terry** (*Clarkson University, Potsdam, USA; **University of Maryland, Maryland, USA)

J. Chem. Phys., 114(22) (2001) pp. 9852-9855.

Considering the topology of semiempirical nucleation rate surfaces originate from lines describing the appropriate phase equilibria, there will be two nucleation rate surfaces that exist for the different physical states of the critical embryo phases that are formed near the triple point. Each rate surface is independently related to a nucleation channel and is described by individual equations for nucleation rates. Because of the differences in the sticking probability of vapor molecules when they collide with a physical surface (in this case, with the surface of the nucleation embryos) in the different phases, the growth rates of the different phase clusters will be different. As a result of this difference, one expects to find different sized particles for two cluster phases in the vicinity of the triple point for first order phase transitions. In the present study, particle size distributions were measured near glycerin triple point. A clearly bimodal size distribution was observed. This result suggests that there are two independent nucleation channels that exist near the triple point. This experimental system has the ability to discern particles produced through the two separate nucleation channels so that the nucleation rates can be measured for each channel.

Mathematical Simulation of Chemical Processes and Reactors.

Chemical Engineering

MATHEMATICAL MODEL OF A CATALYTIC PROCESS ON A POROUS GRAIN IN A GAS-LIQUID-SOLID THREE-PHASE SYSTEM

M.G. Slin'ko*, **V.A. Kirillov**, **I.A. Mikhailova**, **S.I. Fadeev**** (*SSC RF "Karpov Institute of Physical Chemistry", Moscow, Russia; **Sobolev Institute of Mathematics, Novosibirsk, Russia)

Doklady Chemistry, 376(1-3) (2001) pp. 42-46.

Mathematical model of a catalytic steady-state process on a porous grain in the gas-liquid-solid three-phase system is proposed based on physical and physico-chemical regularities, and numerical experiments have been carried out.

NONEQUILIBRIUM THERMODYNAMICS OF AUTOWAVES OF LAMINAR COMBUSTION

A.P. Gerasev

Combustion, Explosion and Shock Waves, 37(6) (2001) pp. 13-21.

Within the framework of the Zel'dovich–Frank–Kamenetskii theory of thermal propagation of flame, thermodynamic properties of an open nonlinear system are considered, and nonequilibrium entropy of a steady combustion wave is constructed. The nonequilibrium dynamic system is analyzed qualitatively and quantitatively, and the distribution functions of local entropy production in terms of the spatial variable are constructed. It is shown that total entropy production in the system is a functional on integral curves that possess extreme properties, and its minimum corresponds to a unique physically sustainable solution of the problem. The procedure of "cutting" (vanishing) of the reaction rate is justified by methods of nonequilibrium thermodynamics. A variational formulation of the problem is presented for calculation of a steady combustion wave.

PHASE TRANSITIONS IN THE BED OF VANADIUM CATALYST FOR SULFURIC ACID PRODUCTION: EXPERIMENT AND MODELING

B.S. Bal'zhinimaev, **N.P. Belyaeva**, **S.I. Reshetnikov**, **E.S. Yudina**, **A.A. Ivanov**

Chem. Eng. J., 84(1) (2000) pp. 31-41.

Sulfur dioxide oxidation on vanadium catalysts in sulfuric acid production may cause phase transitions

in the catalyst active component. These phase transitions involve crystallization of vanadium(IV), and thus may influence catalyst activity. In the present study it has been shown that reaction mixture flow through the fixed catalyst bed is accompanied by the moving front of crystal phase, which decreases SO₂ conversion at reactor outlet. Front profile and its movement velocity depend on the chemical composition of active component, support porous structure, catalyst grain size, and other parameters. A simplified mathematical model, which (qualitatively and quantitatively) describes experimentally observed dynamics of front generation and movement, and related changes in the bed activity has been suggested basing on the Gibbs-Folmer theory. Model allows to predict catalyst behavior in industrial scale reactor, and to optimize catalyst properties.

CHEMICAL EQUILIBRIUM CALCULATIONS FOR A MULTICOMPONENT MIXTURE TAKING INTO ACCOUNT ITS NONIDEALITY

A. Yermakova, **S.I. Fadeev***, **V.I. Anikeev** (*Sobolev Institute of Mathematics, Novosibirsk, Russia)

Russ. J. Phys. Chem., 75(8) (2001) pp. 1266-1273.

An effective algorithm for calculating the equilibrium composition of a multicomponent mixture when the reacting system is described by deterministic chemical reactions is suggested based on the known method of solution continuation over a parameter. Nonideality corrections were calculated by the Redlich–Kwong–Soave equation of state. Examples of equilibrium calculations for the syntheses of ammonia, methanol, etc. are given. The calculation results are compared with the experimental data.

ANALYSIS OF A TWO-PHASE PERFECTLY MIXED REACTOR UNDER THE CONDITION OF A PHASE EQUILIBRIUM

A. Yermakova, **M.V. Gudkov**, **V.I. Anikeev**

Theor. Found. of Chem. Engin., 35(5) (2001) pp. 486-493.

A mathematical model is formulated for a gas-liquid perfectly mixed flow reactor under the condition that the two-phase flow at the reactor outlet is at thermodynamic equilibrium. The phase

equilibrium is calculated using the Redlich–Kwong–Soave equation of state. The set of nonlinear algebraic equations of the model is numerically solved by the efficient algorithm of the homotopy method. The steady-state modes of reactor operation are analyzed for liquid-phase benzene hydrogenation. It is shown that, under isothermal isobaric conditions, there can be a multiplicity of steady-state solutions, which is, on the one hand, due to the nonlinearity of the kinetic law and, on the other, due to the deviation of the properties of the reaction mixture from the properties of an ideal system. The stability of the steady-state solutions is analyzed, and the causes of the multiplicity and instability are explained.

“SUPERCRITICAL WATER” DENSITY EFFECTS ON THE RATE OF ISOPROPANOL DEHYDRATION

V.I. Anikeev, D. Menion*, A. Yermakova
(*National Institute of Standards and Technologies, Gaithersburg, Maryland, USA)

Russ. J. Phys. Chem., 75(8) (2001) pp. 1259-1265.

A new experimental procedure for studying the kinetics and thermodynamics of chemical reactions in supercritical fluids-solvents was suggested. The kinetics and mechanism of the dehydration of 2-propanol in supercritical water in a closed reactor were studied. It was found that, first, the dehydration mechanism significantly differed from that observed in the presence of a homogeneous acid catalyst and, secondly, the rate of the reaction substantially depended on the density of supercritical water. A general mechanism of the dehydration of 2-propanol in supercritical water was suggested based on experimental studies of the hydration and hydrogenation reactions of some desired reaction products. The experimental data were well described by first-order kinetic equations. The kinetics of the reaction was studied and its rate constants determined. The density of supercritical water can be used as a parameter for controlling the kinetics and selectivity of the reaction.

MATHEMATICAL MODELING OF NITROGEN DESORPTION FROM AN IRIDIUM SURFACE: A STUDY OF THE EFFECTS OF SURFACE STRUCTURE AND SUBSURFACE OXYGEN

E.S. Kurkina*, N.L. Semendyaeva*, A.I. Boronin
(*Moscow Lomonosov State University, Moscow, Russia)

Kinetics & Catalysis, 42(5) (2001) pp. 703-717.

Thermal recombination of atomic nitrogen on iridium surfaces is studied by X-ray photoelectron spectroscopy and thermal desorption. Based on experimental data, new mathematical models are proposed and studied for nitrogen desorption from the surfaces of Ir(111), Ir(110), and iridium foil in the presence of adsorbed oxygen. The models take into account the specific features of the catalytic surface, the effect of oxygen, and the morphology of the adsorbed layer. The conditions for the appearance of an additional desorption maximum of N₂ are determined. Computational studies are carried out in the framework of point deterministic and stochastic models.

ON A GLOBAL ERROR ESTIMATE IN LONG-TERM NUMERICAL INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS

G.A. Chumakov*, N.A. Chumakova (*Institute of Mathematics, Novosibirsk, Russia)

Selcuk J. Appl. Mathem., 2(1) (2001) pp. 27-46.

An effective computational procedure of obtaining estimate for the global error in the long-term numerical integration with one-step embedded explicit Runge-Kutta methods applied to an ODE system is described. The paper relies on the existence of an asymptotic expansion for the global error. An example is given using a particular ODE system modeling the behavior of a heterogeneous catalytic reaction with complex dynamics.

HEAT DISSIPATION IN EXOTHERMIC REACTIONS ON NON-TRADITIONAL SUPPORTED CATALYSTS

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

Catal. Lett., 75(1-2) (2001) pp. 61-64.

Employing modern fabrication technologies, one can prepare catalysts consisting of nm metal crystallites deposited on μm oxide particles located on a planar oxide or metal support. The general equations

for estimation of the time scales characterizing dissipation of heat released in exothermic reactions occurring on such catalysts have been derived. Using the results obtained, the authors show that in such systems overheating of oxide particles is usually negligible.

THERMODYNAMICS OF ISOMERIZATION OF BUTYLENES: EQUILIBRIUM COMPOSITIONS

A.V. Lavrenov, N.M. Ostrovskii, Yu. K. Demanov

Petroleum Chemistry, 41(2) (2001) pp. 126-130.

The disagreement in the literature data on equilibrium concentrations in the mixture of butylenes was demonstrated, and their correct values were calculated. The temperature dependence for the equilibrium constant of the isomerization of *n*-butylenes into isobutylene was derived. It was shown that the product compositions achieved in the manufacture of isobutylene by the skeleton isomerization of *n*-butylenes could be close to the equilibrium ratios. The experimental results obtained on F/Al₂O₃ and Nb₂O₅/Al₂O₃ catalysts are given.

A CATALYTIC HEAT-EXCHANGING TUBULAR REACTOR FOR COMBINING OF HIGH TEMPERATURE EXOTHERMIC AND ENDOTHERMIC REACTIONS

Z.R. Ismagilov, V.V. Pushkarev, O.Yu. Podyacheva, N.A. Koryabkina, H. Veringa*
(*ECN, Pettem, The Netherlands)

Chem. Eng. J., 82(1-3) (2001) pp. 355-360.

A multifunctional catalytic heat-exchanging (HEX) tubular reactor for combining exothermic and endothermic reactions has been developed and tested for catalytic methane oxidation and methane steam reforming. The methane combustion and steam reforming catalysts were synthesized on the heat-conducting metal foam support materials by application of preliminary plasma spraying of alumina in order to increase adhesive properties of the active layer. The HEX reactor with perovskite-supported catalyst on Ni-Cr foam material on the external surface of the HEX tube and with Ni containing reforming catalyst on the internal Ni foam was successfully tested in methane combustion reaction combined with methane steam reforming.

PRODUCTION OF HYDROGEN FROM DIMETHYL ETHER

V.V. Galvita, G.L. Semin, V.D. Belyaev, T.M. Yurieva, V.A. Sobyenin

Appl. Catal. A: General, 216(1-2) (2001) pp. 85-90.

Catalytic reaction of steam reforming of dimethyl ether (DME) to hydrogen-rich gas was studied in a fixed-bed continuous-flow reactor at a temperature of 200–360°C under atmospheric pressure over a mechanical mixture of catalysts for DME hydration and for methanol steam reforming. It was found that the mechanical mixture of 12-tungstosilicoheteropolyacid deposited on γ -Al₂O₃ (DME hydration catalyst) and copper deposited on SiO₂ (methanol steam reforming catalyst) provided a 100% DME conversion and hydrogen outlet concentration of ~71 vol.% at 290°C and GHSV ~1200 h⁻¹.

SYNTHESIS GAS PRODUCTION BY STEAM REFORMING OF ETHANOL

V.V. Galvita, G.L. Semin, V.D. Belyaev, V.A. Semikolenov, P. Tsiakaras*, V.A. Sobyenin
(*University of Thessaly, Pedion Areos, Volos, Greece)

Appl. Catal. A: General, 220(1-2) (2001) pp. 123-127.

A two-layer fixed-bed catalytic reactor for syngas production by steam reforming of ethanol has been proposed. In the reactor, ethanol is first converted to a mixture of methane, carbon oxides and hydrogen over a Pd-based catalyst and then this mixture is converted to syngas over a Ni-based catalyst for methane steam reforming. It has been shown that the use of the two-layer fixed-bed reactor prevents coke formation and provides the syngas yield closed to equilibrium.

EXPERIMENTAL STUDY OF VAPORIZATION EFFECT ON STEADY STATE AND DYNAMIC BEHAVIOR OF CATALYTIC PELLETS

A.V. Kulikov, N.A. Kuzin, A.B. Shigarov, V.A. Kirillov, A.E. Kronberg*, K.R. Westerterp*
(*Twente University, Enschede, The Netherlands)

Catal. Today, 66(2-4) (2001) pp. 255-262.

The impact of the combined evaporation of the liquid phase and reaction on single catalyst pellet performance has been studied experimentally. The exothermic, catalyzed hydrogenation of α -methylstyrene (AMS) to cumene has been

employed as a model reaction. Steady state and dynamic experiments have been performed in a single catalytic pellet reactor using five catalytic pellets of different porous structures, thermal conductivity, apparent catalytic activity and distribution of catalyst in the pellet. Gas-phase temperature, concentration of AMS in the gas phase and the liquid flow rates have been varied. The measured center and surface temperatures of each pellet reveal the existence of two significantly different steady states in the range of liquid flow rate. The range of the liquid flow rate over which the two steady states were observed, the pellet temperature and the pellet dynamics depend strongly on the amount of AMS vapor in the gas phase and the catalyst properties. The obtained experimental data are helpful to elucidate the mechanism of hot-spot formation and runaway in multiphase fixed-bed reactors.

AN ENVIRONMENTALLY CLEAN CATALYTIC WATER BOILER FOR COMBUSTION OF NATURAL GAS

V.A. Kirillov, N.A. Kuzin, I.A. Onufriev*, I.V. Khlystov** (*Plant "Izmeritel", Smolensk, Russia), **State Enterprise "Kometa", Novosibirsk, Russia)

Chem. Ingenieur Technik, 73(6) (2001) 665
(Published Online)

A reinforced metal porous catalyst, a catalytic heat generating element and a prototype of the water boiler based on the principle of catalytic combustion of natural gas have been designed, and manufactured and tested.

NONLINEAR PHENOMENA IN A DOWNWARD GAS-LIQUID FLOW THROUGH A FIXED GRANULAR CATALYST BED

M.G. Slin'ko*, V.A. Kirillov, N.A. Kuzin, A.B. Shigarov (*SSC RF "Karpov Institute of Physical Chemistry", Moscow, Russia)

Doklady Chemistry, 380(1) (2001) pp. 271-274.

Steady state experiments have been performed in a reactor with descending gas and liquid currents. Hydrogenation of α -methylstyrene has been employed as a model reaction.

The obtained results elucidated the strong influence of vaporization and vapor phase reaction on the generation of such nonlinear phenomena as hysteresis, runaway and phase non-equilibrium.

THE USE OF CATALYTIC OXIDATION OF HYDROCARBON GASES FOR HEAT GENERATION IN HOUSEHOLD THERMAL ENGINEERING

V.A. Kirillov, N.A. Kuzin, A.V. Kulikov

Thermal Engineering, 47(1) (2000) pp. 18-23.

The prospects and the current state of the art of implementing catalytic heating elements for heat generation in the oxidation of hydrocarbon gases are considered. Various technical solutions are presented, and experimental data is obtained from the tests of heaters with concurrent or separate supply of the reactants.

CATALYTIC HEATING ELEMENTS FOR AUTONOMOUS DOMESTIC HEATING SYSTEMS

B.N. Luk'yanov, N.A. Kuzin, V.A. Kirillov, A.V. Kulikov, A.B. Shigarov, M.M. Danilova

Chem. for Sustainable Devel., 9(5) (2001)
pp. 667-677.

New heat-conducting metal porous reinforced catalysts were developed to manufacture a catalytic heat generating element (CHGE) of 25 kW power. The element was subjected to thermophysical, hydraulic and ecological testing. A prototype of the catalytic water boiler supplied with a CHGE of 25 kW power was manufactured and tested. Local temperature and gas flow rates were determined in different places of the outer catalytic bed surface. The boiler provides below yield of toxic waste: CO 5–10 ppm, NO_x traces, CH₄ 10-20 ppm, CO₂ 10 vol.%, the other gases 89.5 vol.%. CHGE is promising as a device for ecologically safe heat production for household appliances.

FLUIDIZED CATALYST BED COMBUSTION OF FUELS FOR LOCAL HEAT SUPPLY

A.D. Simonov, N.A. Yazykov, P.I. Vedyakin, G.A. Lavrov, V.N. Parmon

Chem. for Sustainable Devel., 9(1) (2001)
pp. 97-104.

Technical data and description are given for heating units based on combustion of liquid fuels in the fluidized catalyst bed. The results of many year operation of catalytic heating units KTU-02 are discussed. The units of 230 kWt capacity were manufactured by Arsenal-2 Company (Novosibirsk) based on BIC's research advances in the field of fuel oxidation in a fluidized catalyst bed. The data on combustion of fuels of different metamorphism degree are discussed. It is shown that the

higher is the metamorphism degree, the lower is the degree of the fuel catalytic burning. Results of start-and-adjustment testing are presented for a demonstration heating unit (230 kWt capacity) based on catalytic combustion of solid fuels.

ADSORPTION-CONTACT DRYING OF DEFORMABLE MATERIALS

A.D. Simonov, N.A. Yazykov, V.N. Parmon

Chem. for Sustainable Devel., 9(5) (2001) pp. 685-694.

The transfer of moisture in the process of adsorption-contact drying of deformable materials

such as hydrogel of aluminum hydroxide has been studied. Two specific fields of liquid-phase moisture transfer conditioned by rheological properties of dryable material have been established. Taking into account these properties allows to calculate exactly the kinetics of moisture removal. The parameters of adsorption-contact drying of freshly formed pellets of aluminum hydroxide have been optimized. The results obtained have been proved by the experiments in semi-commercial installation.

SCIENTIFIC PUBLICATIONS

JOURNAL PUBLICATIONS AND MONOGRAPHS

1. **(E.V. Aleksandrovich, V.A. Chumachenko), V.M. Bondareva, G.Ya. Popova, T.V. Andrushkevich, (G.Yu. Miloslavskii, Kh.F. Mustafin), A.S. Noskov,** Purification of Wet Waste Gases of Isoprene Production over Oxide Catalysts, *Khimicheskaya Promyshlennost*, 7 (2001) pp. 18-24 (in Russian).
2. **(A.I. Ancharov, N.G. Gavrillov, V.I. Kondrat'ev, I.V. Poletaev, M.A. Sheromov), A.N. Shmakov, (B.P. Tolochko, V.M. Tsukanov, I.L. Zhogin),** Project of Ultrahigh-Vacuum Double-Crystal Monochromator, *Nuclear Instrum. & Methods in Phys. Res. A*, 470(1-2) (2001) pp. 128-130.
3. **V.I. Anikeev, (D. Menion), A. Yermakova,** "Supercritical Water" Density Effects on the Rate of Isopropanol Dehydration, *Russ. J. Phys. Chem.*, 75(8) (2001) pp. 1259-1265 (English language translation).
4. **M.P. Anisimov, (A.G. Nasibulin, S.D. Shandakov), I.N. Shaimordanov,** Experimental Determination of the Surface Energy of Critical Nuclei During the Nucleation of Supersaturated Vapor, *Colloid J.*, 63(2) (2001) pp. 131-136 (English language translation).
5. **M.P. Anisimov, (S.D. Shandakov), Yu.I. Polygalov, (R.H. Heist),** Transport in the Static Diffusion Cloud Chamber Revisited, *J. Chem. Phys.*, 114(2) (2001) pp. 899-906.
6. **M.P. Anisimov, (S.D. Shandakov), I.N. Shaimordanov, A.S. Berezina, Yu.I. Polygalov, (S.A. Timoshenko),** Experimental Determination of the Surface Energy of Critical Nuclei During the Nucleation, *J. Mendeleev Chem. Society*, 45(3) (2001) pp. 38-44 (in Russian).
7. **M.P. Anisimov, (P. Hopke), I.N. Shaimordanov, (S.D. Shandakov, L.-E. Magnusson),** Binary *n*-Octanol – Sulfur Hexafluoride Nucleation, *J. Chem. Phys.*, 115(2) (2001) pp. 810-816.
8. **L.M. Anisimova, (P. Hopke, J. Terry),** Two Channel Vapor Nucleation in the Vicinity of the Triple Point, *J. Chem. Phys.*, 114(22) (2001) pp. 9852-9855.
9. **(A.G. Anshits, E.V. Kondratenko, E.V. Fomenko, A.M. Kovalev, N.N. Anshits, O.A. Bajukov, E.V. Sokol), A.N. Salanov,** Novel Glass Crystal Catalysts for the Processes of Methane Oxidation, *Catal. Today*, 64(1-2) (2001) pp. 59-67.
10. **Yu.I. Aristov, N.N. Bukhavtsova, N.V. Vernikovskaya, (V.P. Voloshin, V.N. Glaznev), L.Yu. Ilyina, (I.V. Koptuyug, Yu.G. Korobeinikov, I.N. Korotkikh, V.A. Luchnikov, N.N. Medvedev), N.M. Ostrovskii, V.N. Parmon, A.D. Simonov, M.M. Tokarev, V.B. Fenelonov, (V.M. Fomin), N.A. Chumakova, N.A. Yazykov,** "Modern Approach to Studying and Description of Porous Solids Drying", Ed. V.N. Parmon, Novosibirsk, SB RAS, 300 pp. (in Russian).
11. **V.I. Avdeev, G.M. Zhidomirov,** Ethylene and Oxygen Species Adsorbed on a Defect Oxidized Surface Ag(111): Theoretical Analysis by DFT Method, *Surf. Sci.*, 492(1-2) (2001) pp. 137-151.
12. **B.S. Bal'zhinimaev,** Structural and Catalytic Properties of Ultradispersed Energy Saturated Metals, *J. Mendeleev Chem. Society*, 45(3) (2001) pp. 59-65 (in Russian).

13. **B.S. Bal'zhinimaev, N.P. Belyaeva, S.I. Reshetnikov, E.S. Yudina, A.A. Ivanov,**
Phase Transitions in the Bed of Vanadium Catalyst for Sulfuric Acid Production: Experiment and Modeling,
Chem. Eng. J., 84(1) (2001) pp. 31-41.
14. **(L.A.M.M. Barbosa), G.M. Zhidomirov, (R.A. van Santen),**
Theoretical Study of Methane Adsorption on Zn(II) Zeolites,
Phys. Chem. Chem. Phys., 2(17) (2000) pp. 3909-3918.
15. **(L.A.M.M. Barbosa), G.M. Zhidomirov, (R.A. van Santen),**
Theoretical Study of the Molecular Hydrogen Adsorption and Dissociation on Different Zn(II) Active Sites of Zeolites,
Catal. Lett., 77(1-3) (2001) pp. 55-62.
16. **(A.V. Belyaev, V.A. Emel'yanov, S.P. Khramenko), M.A. Fedotov,**
NMR Study of Reactions Between Pd, Ru, and Rh Nitrite Complexes with Sulfamic Acid,
Russ. J. Coord. Chem., 27(3) (2001) pp. 184-194 (English language translation).
17. **(A.V. Belyaev), M.A. Fedotov, (S.P. Khramenko, V.A. Emel'yanov),**
Forms of Rh(III) in Nitric Acid Solutions,
Russ. J. Coord. Chem., 27(12) (2001) pp. 855-864 (English language translation).
18. **I.I. Bobrova, N.N. Bobrov, V.V. Chesnokov, V.N. Parmon,**
Catalytic Steam Reforming of Methane: New Data on the Contribution of Homogeneous Radical Reactions in the Gas Phase. 2. A Ruthenium Catalyst,
Kinetics & Catalysis, 42(6) (2001) pp. 805-812 (English language translation).
19. **V.F. Borbat, O.A. Golovanova, P.A. Kachesova, A.I. Nizovskii, A.V. Bubnov, M.V. Trenikhin, A.N. Vichkanov,**
Peculiarities of Mineralization of Stones in Urinary System for Inhabitants of Omsk Region,
Ural Geological J., 6 (2000) pp. 173-175 (in Russian).
20. **V.F. Borbat, O.A. Golovanova, P.A. Kachesova, A.I. Nizovskii, A.V. Bubnov, M.V. Trenikhin, A.N. Vichkanov,**
Physical Methods for Diagnostics, Prognostication of Recurrences and Principals of Treatment of Urino-Stone Diseases,
Omsk Scientific Bull., 14 (2001) pp. 152-155 (in Russian).
21. **K.P. Brylyakov, N.N. Karpyshev, S.A. Fominsky, A.G. Tolstikov, E.P. Talsi,**
⁵¹V and ¹³C NMR Spectroscopic Study of the Peroxovanadium Intermediates in Vanadium Catalyzed Enantioselective Oxidation of Sulfides,
J. Molec. Catal. A: Chemical, 171(1-2) (2001) pp. 73-80.
22. **G.D. Bukatov, V.A. Zakharov,**
Propylene Ziegler-Natta Polymerization: Numbers and Propagation Rate Constants for Stereospecific and Non-Stereospecific Centers,
Macromol. Chem. & Phys., 202(10) (2001) pp. 2003-2009.
23. **V.I. Bukhtiyarov, (M. Hävecker), V.V. Kaichev, (A. Knop-Gericke, R.W. Mayer, R. Schlögl),**
Combined Application of XANES and XPS to Study Oxygen Species Adsorbed on Ag Foil,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 302-305.
24. **V.I. Bukhtiyarov, (M. Hävecker), V.V. Kaichev, (A. Knop-Gericke, R.W. Mayer, R. Schlögl),**
X-Ray Absorption and Photoemission Studies of the Active Oxygen for Ethylene Epoxidation Over Silver,
Catal. Lett., 74(3-4) (2001) pp. 121-125.
25. **V.I. Bukhtiyarov, (M.G. Slin'ko),**
Metallic Nanosystems in Catalysis,
Russ. Chem. Rev., 70(2) (2001) pp. 147-159 (English language translation).

26. **D.A. Bulushev, S.I. Reshetnikov, (L. Kiwi-Minsker, A. Renken),**
Deactivation Kinetics of V/Ti-Oxide in Toluene Partial Oxidation,
Appl. Catal. A: General, 220(1-2) (2001) pp. 31-39.
27. **(A.N. Buzykaeva), V.A. Chernov, (N.V. Kovalenko, S.V. Mytnichenko),**
A Secondary X-Ray Analyzer Using a Flat Ring-Shaped Radially Graded Multilayer,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 135-141.
28. **(A.N. Buzykaeva, N.V. Kovalenko, S.V. Mytnichenko), V.A. Chernov,**
A High-Throughput X-Ray Analyzer Using a Flat Multilayer Mirror with Radially Increasing Period,
Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 1 (2001) pp. 6-12 (in Russian).
29. **R.A. Buyanov, V.V. Chesnokov,**
Regularities of Catalytic Formation of Carbon Composites for Various Purposes via Decomposition
of Hydrocarbons on Iron Subgroup Metals,
Eurasian ChemTech. J., 2(3-4) (2000) pp. 223-230.
30. **R.A. Buyanov, V.V. Molchanov,**
Endothermic Chemical Reactor with Gas-Dynamic Control,
Pre-print of the Institute of Theoretical and Applied Mathematics, №5, 2001, pp. 1-24 (in Russian).
31. **R.A. Buyanov, V.V. Molchanov,**
Phenomenological Model of Mechanochemical Activation in the Catalyst Technology and Catalysis,
Chem. for Sustainable Devel., 9(3) (2001) pp. 369-378 (in Russian).
32. **R.A. Buyanov, N.A. Pakhomov,**
Catalysts and Processes for Paraffin and Olefin Dehydrogenation,
Kinetics & Catalysis, 42(1) (2001) pp. 64-75 (English language translation).
33. **(M.V. Chaikina), V.A. Sadykov, S.N. Pavlova, G.N. Zabolotnaya, R.I. Maksimovskaya,**
V.V. Kriventsov, D.I. Kochubey, E.B. Burgina, (R. Roy, D.K. Agrawal),
Mechanochemical Synthesis of Zirconium Phosphates,
J. Mater. Synth. & Processing, 8(5-6) (2000) pp. 279-286.
34. **(E.A. Cherezov), V.I. Elokhin, (A.V. Myshlyavtsev),**
Adsorption on the Surface of Body-Centered Kossel Crystal: Simulation Modeling,
Proceedings of the Tuvian Institute for Exploration of Natural Resources SB RAS, 2001,
pp. 100-107 (in Russian).
35. **V.A. Chernov, (V.I. Kondratiev, N.V. Kovalenko, S.V. Mytnichenko),**
An Experimental Study of the q_{\perp} -Dependence of X-Ray Resonant Diffuse Scattering from
Multilayers,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 145-154.
36. **V.A. Chernov, (N.V. Kovalenko, S.V. Mytnichenko),**
The Use of Quasi-Bragg Diffuse Scattering for Express Measurement of Changes in Multilayer
 d -Spacing,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 155-157.
37. **V.A. Chernov, (N.V. Kovalenko, S.V. Mytnichenko),**
An X-Ray Grazing Incidence Phase Multilayer Grating,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 158-161.
38. **V.A. Chernov, (N.V. Kovalenko, S.V. Mytnichenko),**
An Extended Anomalous Fine Structure of X-Ray Quasi-Bragg Diffuse Scattering from Multilayers,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 210-214.

39. **A.R. Cholach, V.M. Tapilin,**
Adsorption of Small Molecules on the Pt(100) Single Crystal Surface Studied by Disappearance Potential Spectroscopy,
Appl. Surf. Sci., 180(1-2) (2001) pp. 173-183.
40. **(G.A. Chumakov), N.A. Chumakova,**
On a Global Error Estimate in Long-Term Numerical Integration of Ordinary Differential Equations,
Selcuk J. Appl. Mathematics, 2(1) (2001) pp. 27-46.
41. **N.A. Chumakova, N.V. Vernikovskaya, M.M. Tokarev, (I.V. Koptuyug), L.Yu. Ilyina, Yu.I. Aristov,**
Water Vapor Sorption-Desorption in Fixed Bed of Composite Sorbent: The Refinement of Transfer Parameters and Sorption Kinetics,
Chem. Ingenieur Tech., 73(6) (2001) 776 (On-line publication).
42. **(A.M. Danilenko), V.A. Chernov, V.V. Kriventsov,**
EXAFS Study of the Reaction of Graphite-MeCl₂ (Me = Ni, Co) Intercalation Compounds with Bromine Fluorides,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 373-375.
43. **A.Yu. Derevyankin, V.B. Fenelonov, A.N. Shmakov, V.N. Romannikov,**
Physicochemical Features of the Formation of Siliceous Porous Mesophases. 4. Effect of Duration and Temperature of the Hydrothermal Treatment on the Structural and Textural Properties,
Russ. Chem. Bull., 50(2) (2001) pp. 175-179 (English language translation).
44. **L.G. Detusheva, L.I. Kuznetsova, M.A. Fedotov, V.A. Likhobov, L.S. Dovlitova, A.A. Vlasov, V.V. Malakhov,**
Palladium(II), Copper(II), Iron(III), and Vanadium(V) Complexes with Heteropolyanion PW₉O₃₄⁹⁻. ³¹P, ¹⁸³W, ⁵¹V NMR and IR Spectroscopy Studies,
Russ. J. Coord. Chem., 27(12) (2001) pp. 838-845 (English language translation).
45. **(K. Dimitrievski, B. Kasemo), V.P. Zhdanov,**
Rate-Determining Moves in Protein Folding,
J. Chem. Phys., 115(6) (2001) pp. 2841-2845.
46. **V.A. Drozdov, V.P. Doronin, T.P. Sorokina, T.I. Gulyaeva, V.K. Duplyakin,**
Texture-Strength Properties of the Alumina-Montmorillonite Composite,
Kinetics & Catalysis, 42(1) (2001) pp. 117-126 (English language translation).
47. **K.A. Dubkov, E.A. Paukshtis, G.I. Panov,**
Stoichiometry of Oxidation Reactions Involving α -Oxygen on FeZSM-5 Zeolite,
Kinetics & Catalysis, 42(2) (2001) pp. 205-211 (English language translation).
48. **K.A. Dubkov, E.A. Paukshtis, G.I. Panov,**
Identification of Active Oxygen Species over Fe Complexes in Zeolites,
Catalysis by Unique Metal Ion Structures in Solid Materials, Eds. G. Centi et al., Kluwer Academic Publishers, 2001, pp. 149-163.
49. **L.G. Echevskaya, V.A. Zakharov, N.V. Semikolenova, T.B. Mikenas, A.P. Sobolev,**
Polymerization of Ethylene Using Supported Zirconocene Catalysts,
Polymer Sci., ser. A, 43(3) (2001) pp. 220-227 (English language translation).
50. **L.G. Echevskaya, V.A. Zakharov, N.V. Semikolenova, T.B. Mikenas,**
Copolymerization of Ethylene with 1-Hexene over Supported Zirconocene Catalysts,
Polimery, 46(1) (2001) pp. 40-43.
51. **N.I. Efremova, A.V. Kalinkin,**
Modelling the Oxidation of CO at the Interface of Heterophase Metal Catalysts,
React. Kinet. & Catal. Lett., 73(2) (2001) pp. 373-379.

52. **G.L. Elizarova, L.G. Matvienko, A.O. Kuzmin, E.R. Savinova, V.N. Parmon,**
Copper and Iron Hydroxides as New Catalysts for Redox Reactions in Aqueous Solutions,
Mendeleev Commun., 11(1) (2001) pp. 15-17.
53. **M.A. Ermakova, D.Yu. Ermakov, A.L. Chuvilin, G.G. Kuvshinov,**
Decomposition of Methane over Iron Catalysts at the Range of Moderate Temperatures: The
Influence of Structure of the Catalytic Systems and the Reaction Conditions on the Yield of Carbon
and Morphology of Carbon Filaments,
J. Catal., 201(2) (2001) pp. 183-197.
54. **V.K. Ermolaev, (P.P. Rodionov, V.A. Burmistrov, A.M. Gnetnev, E.M. Blagitko),**
ESR-Studying of Antibacterial Silver Preparations and Drugs on its Base. Possibility of
Antibacterial Silver Action by Complexing with Air Oxygen,
Collected Articles "Gel of Polyethylene Oxide-1500 "Geko" in Medicine and Cosmetology",
Novosibirsk-Saratov-Pyatigorsk, 2001, pp. 93-99 (in Russian).
55. **V.B. Fenelonov,**
MMM Without Illusions or Innovations in Biomimetic Synthesis,
Chemistry and Life, 11 (2001) pp. 8-11 (in Russian).
56. **V.B. Fenelonov, A.Yu. Derevyankin, (S.D. Kirik, L.A. Solovyov), A.N. Shmakov,**
(J.-L. Bonarder, A. Gedeon), V.N. Romannikov,
Comparative Textural Study of Highly Ordered Silicate and Aluminosilicate Mesoporous
Mesophase Materials Having Different Pore Sizes,
Micropor. & Mesopor. Mater., 44-45(1-3) (2001) pp. 33-40.
57. **V.B. Fenelonov, A.Yu. Derevyankin, V.A. Sadykov,**
The Characterization of the Structure and Texture of Pillared Interlayer Materials,
Micropor. & Mesopor. Mater., 47(2-3) (2001) pp. 359-368.
58. **V.B. Fenelonov, (G.G. Kodenev, V.G. Kostrovsky),**
On the Dependence of Surface Tension of Liquids on the Curvature of the Liquid-Vapor Interface,
J. Phys. Chem. B, 105(5) (2001) pp. 1050-1055.
59. **V.B. Fenelonov, M.S. Mel'gunov, I.V. Mishakov, (R.M. Richards), V.V. Chesnokov,**
A.M. Volodin, (K.J. Klabunde),
Changes in Texture and Catalytic Activity of Nanocrystalline MgO During its Transformation to
MgCl₂ in the Reaction with 1-Chlorobutane,
J. Phys. Chem. B, 105(18) (2001) pp. 3937-3941.
60. **S.V. Filimonova, A.V. Nosov, (M. Scheithauer, H. Knözinger),**
n-Pentane Isomerization over Pt/WO₃/ZrO₂ Catalysts: A ¹H and ¹³C NMR Study,
J. Catal., 198(1) (2001) pp. 89-96.
61. **V.V. Galvita, G.L. Semin, V.D. Belyaev, T.M. Yurieva, V.A. Sobyenin,**
Production of Hydrogen from Dimethyl Ether,
Appl. Catal. A: General, 216(1-2) (2001) pp. 85-90.
62. **V.V. Galvita, G.L. Semin, V.D. Belyaev, V.A. Semikolenov, (P. Tsiakaras), V.A. Sobyenin,**
Synthesis Gas Production by Steam Reforming of Ethanol,
Appl. Catal. A: General, 220(1-2) (2001) pp. 123-127.
63. **(Y.A. Gaponov, E.A. Dementyev), D.I. Kochubey, (B.P. Tolochko),**
Portable High Precision Small/Wide Angle X-Ray Scattering Diffractometer,
Nuclear Instrum. & Methods in Phys. Res. A, 467-468 (2001) pp. 1092-1096.
64. **A.P. Gerasev,**
Non-Equilibrium Thermodynamics of Autowaves of Laminar Combustion,
Combustion, Explosion and Shock Waves, 37(6) (2001) pp. 13-21 (English language translation).

65. **(P. Gisdakis), I.V. Yudanov, (N. Roesch),**
Olefin Epoxidation by Molybdenum and Rhenium Peroxo and Hydroperoxo Compounds.
A Density Functional Study of Energetics and Mechanisms,
Inorg. Chem., 40(15) (2001) pp. 3755-3765.
66. **A.Yu. Gladky, V.K. Ermolaev, V.N. Parmon,**
Oscillations During Catalytic Oxidation of Propane over a Nickel Wire,
Catal. Lett., 77(1-3) (2001) pp. 103-106.
67. **V.B. Goncharov, E.F. Fialko,**
An Ion Cyclotron Resonance Study of Reactions between Molybdenum Oxide Cluster Ions and
Methane and Cyclopropane in the Gas Phase,
Russ. J. Phys. Chem., 75(5) (2001) pp. 760-765 (English language translation).
68. **V.V. Gorodetskii, A.V. Matveev,**
Hydrogen Spillover in H₂ Oxidation on Pd-Ti³⁺/TiO₂,
Stud. Surf. Sci. & Catal., 138 (2001) pp. 85-92.
69. **I.I. Il'ina, I.L. Simakova, V.A. Semikolenov,**
Kinetics of Pinane Oxidation to Pinane Hydroperoxide by Dioxygen,
Kinetics & Catalysis, 42(1) (2001) pp. 41-45 (English language translation).
70. **I.I. Il'ina, I.L. Simakova, V.A. Semikolenov,**
Kinetics of 2-Pinanol Isomerization to Linalool on the Monolith Carbon-Containing Catalyst,
Kinetics & Catalysis, 42(5) (2001) pp. 686-692 (English language translation).
71. **K.G. Ione, V.M. Mysov, V.G. Stepanov, V.N. Parmon,**
New Data on the Possibility of the Abiogenic Synthesis of Hydrocarbons in the Earth's Crust,
Petroleum Chemistry, 41(3) (2001) pp. 159-165 (English language translation).
72. **K.G. Ione, V.M. Mysov, V.G. Stepanov, V.N. Parmon,**
Catalytic Phenomena in Abiogenic Synthesis of Hydrocarbons in the Earth's Crust,
Chem. for Sustainable Devel., 9(1) (2001) pp. 129-144 (in Russian).
73. **Z.R. Ismagilov, S.R. Khairulin, R.A. Shkrabina, S.A. Yashnik, V.A. Ushakov,**
(J.A. Moulijn, A.D. van Langeveld),
Deactivation of Manganese Oxide Based Honeycomb Monolith Catalyst under Reaction Conditions
of Ammonia Decomposition at High Temperature,
Catal. Today, 69(1-4) (2001) pp. 253-257.
74. **Z.R. Ismagilov, V.V. Pushkarev, O.Yu. Podyacheva, N.A. Koryabkina, (H. Veringa),**
A Catalytic Heat-Exchanging Tubular Reactor for Combining of High Temperature Exothermic and
Endothermic Reactions,
Chem. Eng. J., 82(1-3) (2001) pp. 355-360.
75. **Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, S.A. Yashnik, V.A. Sazonov, V.V. Kuznetsov,**
M.V. Luzgin, A.V. Kalinkin, (H. Veringa),
The Stability of Monolith CuZSM-5 Catalysts for the Selective Reduction of Nitrogen Oxides with
Hydrocarbons. 1. Synthesis and Characterization of Bulk CuZSM-5 Catalysts,
Kinetics & Catalysis, 42(6) (2001) pp. 847-853 (English language translation).
76. **Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, S.A. Yashnik, N.V. Shikina, V.A. Sazonov,**
(H. Veringa),
The Stability of Monolith CuZSM-5 Catalysts for the Selective Reduction of Nitrogen Oxides with
Hydrocarbons. 2. Synthesis and Characterization of Bulk Cu(80% ZSM-5 + 20% Al₂O₃) Catalysts,
Kinetics & Catalysis, 42(6) (2001) pp. 854-857 (English language translation).

77. **Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, V.A. Sazonov, S.A. Yashnik, N.V. Shikina, (H. Veringa),**
The Sulphur and Water Resistance of Modified Washcoated Zeolite-Exchanged Monolith Catalysts for SCR of NO_x with Propane,
Topics in Catalysis, 16-17(1-4) (2001) pp. 307-310.
78. **Z.R. Ismagilov, R.A. Shkrabina, S.A. Yashnik, N.V. Shikina, I.P. Andrievskaya, S.R. Khairulin, V.A. Ushakov, (J.A. Moulijn, I.V. Babich),**
Supported Honeycomb Monolith Catalysts for High-Temperature Ammonia Decomposition and H₂S Removal,
Catal. Today, 69(1-4) (2001) pp. 351-356.
79. **(V.I. Isupov, L.A. Chupakhina), S.V. Tsybulya, G.N. Kryukova,**
Fine α -Alumina with Low Alkali: New Approach for Preparation,
Solid State Ionics, 141-142(1-4) (2001) pp. 471-478.
80. **L.A. Isupova, S.V. Tsybulya, G.N. Kryukova, G.M. Alikina, N.N. Boldyreva, I.S. Yakovleva, V.P. Ivanov, V.A. Sadykov,**
Real Structure and Catalytic Activity of La_{1-x}Ca_xMnO_{3+ δ} Perovskites,
Solid State Ionics, 141-142(1-4) (2001) pp. 417-425.
81. **L.A. Isupova, G.M. Alikina, S.V. Tsybulya, N.N. Boldyreva, G.N. Kryukova, I.S. Yakovleva, V.A. Sadykov,**
Real Structure and Catalytic Activity of La_{1-x}Sr_xCoO₃ Perovskites,
Intern. J. Inorg. Materials, 3(6) (2001) pp. 559-562.
82. **S.S. Ivanchev, V.N. Pavlyuchenko, N.A. Byrdina, (M. Skrifars, J. Koskinen),**
Water-Resistant Films and Coatings Based on Cross-Linking Styrene-Acrylate Latex Copolymers,
Russ. J. Appl. Chem., 74(2) (2001) pp. 309-315 (English language translation).
83. **S.S. Ivanchev, (M. Ratzsch), A.M. Mesh, S.Ya. Khaikin, (H. Bucka, A. Hesse),**
Radiation Grafting of Vinylalkoxysilanes onto Polypropylene,
Polymer Sci., ser. A, 43(5) (2001) pp. 490-494 (English language translation).
84. **S.S. Ivanchev, (M. Ratzsch), A.M. Mesh, S.Ya. Khaikin, (H. Bucka, A. Hesse, N. Reichelt), M.E. Moiseeva,**
Radiation Crosslinking of Polypropylene in the Presence of Monomers Incapable of Homopolymerization,
Polymer Sci., ser. B, 43(3-4) (2001) pp. 85-90 (English language translation).
85. **S.S. Ivanchev, (G.A. Tolstikov), V.K. Badaev, N.I. Ivancheva, (I.I. Oleinik), M.I. Serushkin, L.V. Oleinik,**
Polymerization and Copolymerization of Ethylene with Higher α -Olefins Using Iron Chloride 2,6-bis(Imino)pyridyl Derivatives - Methylaluminoxane Catalytic Systems,
Polymer Sci., ser. A, 43(12) (2001) pp. 1189-1192 (English language translation).
86. **A.S. Ivanova,**
Highly Dispersed Zirconium-Containing Oxide Systems: Synthesis, Properties, and Applications,
Kinetics & Catalysis, 42(3) (2001) pp. 354-366 (English language translation).
87. **(W. Jark, A. Cedola, S. Di Fonzo, M. Fiordelisi, S. Lagomarsino, N.V. Kovalenko), V.A. Chernov,**
High Gain Beam Compression in New-Generation Thin-Film X-Ray Waveguides,
Appl. Phys. Lett., 78(9) (2001) pp. 1192-1194.
88. **(U. Kaiser), A.L. Chuvilin, V.L. Kuznetsov, Yu.V. Butenko,**
Evidence for 9R-SiC?,
Microscopy & Microanalysis, 7(4) (2001) pp. 368-369.

89. **A.V. Kalinkin, A.V. Pashis, R.I. Kvon,**
Formation of Bimetallic Pt-Rh Surface with Nanosize Metal Domains,
React. Kinet. & Catal. Lett., 72(1) (2001) pp. 163-168.
90. **P.N. Kalinkin, O.N. Kovalenko, N.N. Kundo,**
Kinetic Peculiarities in the Low-Temperature Oxidation of H₂S on Vanadium Catalysts,
React. Kinet. & Catal. Lett., 74(1) (2001) pp. 177-184.
91. **(V.V. Kanazhevskii), B.N. Novgorodov, V.P. Shmachkova, N.S. Kotsarenko, V.V. Kriventsov, D.I. Kochubey,**
Structure of Zirconium Complexes in Aqueous Solutions,
Mendeleev Commun., 11(6) (2001) pp. 211-212.
92. **A.A. Khassin, T.M. Yurieva, G.N. Kustova, I.Sh. Itenberg, M.P. Demeshkina, T.A. Krieger, L.M. Plyasova, G.K. Chermashentseva, V.N. Parmon,**
Cobalt-Aluminum Co-Precipitated Catalysts and their Performance in the Fischer-Tropsch Synthesis,
J. Molec. Catal. A: Chemical, 168(1-2) (2001) pp. 193-207.
93. **A.A. Khassin, T.M. Yurieva, V.V. Kaichev, V.I. Bukhtiyarov, A.A. Budneva, E.A. Paukshtis, V.N. Parmon,**
Metal-Support Interactions in Cobalt-Aluminum Co-Precipitated Catalysts: XPS and CO Adsorption Studies,
J. Molec. Catal. A: Chemical, 175(1-2) (2001) pp. 189-204.
94. **A.A. Khassin, T.M. Yurieva, G.N. Kustova, L.M. Plyasova, I.Sh. Itenberg, M.P. Demeshkina, G.K. Chermashentseva, V.F. Anufrienko, V.I. Zaikovskii, T.V. Larina, I.Yu. Molina, V.N. Parmon,**
Cobalt-Containing Catalysts Supported by Synthetic Zn- and Mg-Stevensites and their Performance in the Fischer-Tropsch Synthesis,
J. Molec. Catal. A: Chem., 168(1-2) (2001) pp. 209-224.
95. **A.A. Khassin, T.M. Yurieva, G.N. Kustova, L.M. Plyasova, T.A. Krieger, I.Sh. Itenberg, M.P. Demeshkina, T.V. Larina, V.F. Anufrienko, V.N. Parmon,**
Evolution of the Structure of Co Stevensite During its Treatment in the Air, Inert Gas Flow and Flowing Hydrogen,
Mater. Res. Innov., 4(4) (2001) pp. 251-261.
96. **O.A. Kholdeeva, R.I. Maksimovskaya, G.M. Maksimov, L.A. Kovaleva,**
Titanium-Substituted Heteropolytungstates as Model Catalysts for Studying the Mechanisms of Selective Oxidation by Hydrogen Peroxide,
Kinetics & Catalysis, 42(2) (2001) pp. 217-222 (English language translation).
97. **O.A. Kholdeeva, M.P. Vanina,**
Comparative Study of Aerobic Alkene Epoxidations Catalyzed by Optically Active Manganese (II) and Cobalt (II) Salen Complexes,
React. Kinet. & Catal. Lett., 73(1) (2001) pp. 83-89.
98. **V.A. Kirillov, N.A. Kuzin, A.V. Kulikov,**
The Use of Catalytic Oxidation of Hydrocarbon Gases for Heat Generation in Household Thermal Engineering,
Thermal Engineering, 47(1) (2000) pp. 18-23 (English language translation).
99. **V.A. Kirillov, N.A. Kuzin, (I.A. Onufriev, I.V. Khlystov),**
An Environmentally Clean Catalytic Water Boiler for Combustion of Natural Gas,
Chem. Ingenieur Tech., 73(6) (2001) 665 (On-line publication).

100. **(V.I. Kochubey, T.A. Bashkatova), D.I. Kochubey,**
Alteration of EXAFS Spectrum Structure of KBr Crystals Resulting from a Change of Registration Method,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 323-326.
101. **(V.I. Kochubey, Y.G. Konyukhova, T.A. Bashkatova, K.E. Gyunsburg, N.P. Zvezdova), D.I. Kochubey,**
Investigation of Structure of Luminescence Centers in NaCl-Ni Crystals,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 327-330.
102. **E.G. Kodenev, A.N. Shmakov, A.Yu. Derevyankin, A.V. Nosov, V.N. Romannikov,**
Physicochemical Features of the Formation of Siliceous Porous Mesophases. 3. Conditions of Formation and Properties of Mesoporous Silica,
Russ. Chem. Bull., 49(10) (2000) pp. 1669-1675 ((English language translation).
103. **(D.A. Konevets), I.E. Beck, (V.N. Sil'nikov, M.A. Zenkova, G.V. Shishkin),**
Chemical Ribonucleases. 3. The Synthesis of Organic Catalysts for the Phosphodiester Bond Hydrolysis on the Basis of Quaternary Salts of 1,4-Diazabicyclo[2.2.2]octane,
Russ. J. Bioorganic Chem., 26(11) (2000) pp. 765-773 (English language translation).
104. **(G.A. Konin, A.N. Il'ichev, V.A. Matyshak, T.I. Khomenko, V.N. Korchak), V.A. Sadykov, V.P. Doronin, R.V. Bunina, G.M. Alikina, T.G. Kuznetsova, E.A. Paukshtis, V.B. Fenelonov, V.I. Zaikovskii, A.S. Ivanova, S.A. Beloshapkin, (A.Ya. Rozovskii, V.F. Tretyakov, J.R.H. Ross, J.P. Breen),**
Cu, Co, Ag-Containing Pillared Clays as Catalysts for the Selective Reduction of NO_x by Hydrocarbons in an Excess of Oxygen,
Topics in Catal., 16-17(1-4) (2001) pp. 193-197.
105. **(I.V. Koptug), L.Yu. Ilyina, A.V. Matveev, (R.Z. Sagdeev), V.N. Parmon, (S.A. Altobelli),**
Liquid and Gas Flow and Related Phenomena in Monolithic Catalysts Studied by ¹H NMR Microimaging,
Catal. Today, 69(1-4) (2001) pp. 385-392.
106. **(I.V. Koptug), L.Yu. Ilyina, V.B. Fenelonov, A.Yu. Derevyankin, (R.Z. Sagdeev), V.N. Parmon,**
Application of ¹H NMR Microimaging to the *in situ* Investigation of Liquid Evaporation from the Object Modelling Porous Solids,
Doklady Chemistry, 376(6) (2001) pp. 777-781 (in Russian).
107. **(N.V. Kosova, S.V. Vosel), V.F. Anufrienko, (N.T. Vasenin, E.T. Devyatkina),**
Reduction Processes in the Course of Mechanochemical Synthesis of Li_{1+x}V₃O₈,
J. Solid State Chem., 160(2) (2001) pp. 444-449.
108. **(N.V. Kosova), V.F. Anufrienko, (T.V. Larina, E.T. Devyatkina),**
Mechanic Treatment for Synthesis of LiCoO₂ – Cathode Material for Lithium-Ionic Accumulators,
Chem. for Sustainable Devel., 9(2) (2001) pp. 235-242 (in Russian).
109. **O.N. Kovalenko, N.N. Kundo, P.N. Kalinkin,**
Kinetics and Mechanism of Low-Temperature Oxidation of H₂S with Oxygen in the Gas Phase,
React. Kinet. & Catal. Lett., 72(1) (2001) pp. 139-145.
110. **O.N. Kovalenko, N.N. Kundo, V.M. Novopashina, P.N. Kalinkin,**
Nonstationary Phenomena in the Low-Temperature Gas-Phase Catalytic Oxidation of H₂S with Oxygen,
Kinetics & Catalysis, 42(5) (2001) pp. 657-661 (English language translation).
111. **G.A. Kovalenko, E.V. Kuznetsova, Yu.I. Mogilnykh, I.S. Andreeva, D.G. Kuvshinov, N.A. Rudina,**
Catalytic Filamentous Carbons for Immobilization of Biologically Active Substances and Non-Growing Bacterial Cells,
Carbon, 39(7) (2001) pp. 1033-1043.

112. **V.V. Kriventsov, D.I. Kochubey, V.A. Sadykov, S.N. Pavlova, G.V. Zabolotnaya,**
Stabilization of Heavy Metal Cations in the Framework of Zirconium Phosphates,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 336-340.
113. **V.V. Kriventsov, D.I. Kochubey, (Y.V. Maksimov, I.P. Suzdalev, M.V. Tsodikov, J.A. Navio, M.C. Hidalgo, G. Colon),**
Structural Determination of the Fe-Modified Zirconium Oxide,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 341-346.
114. **V.V. Kriventsov, D.I. Kochubey, (J.A. Navio, M.C. Hidalgo, G. Colon, M.V. Tsodikov, Y.V. Maksimov, I.P. Suzdalev),**
EXAFS Study of the Fe_x/ZrO₂ Composite Nanomaterials Obtained by Sol-Gel Synthesis,
J. Synchrotron Radiation, 8(2) (2001) pp. 528-530.
115. **V.V. Kriventsov, D.I. Kochubey, (M.V. Tsodikov, J.A. Navio),**
XAFS Study of the Structured Modified Oxides of Titanium,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 331-335.
116. **V.V. Kriventsov, D.I. Kochubey, (M.V. Tsodikov, J.A. Navio, G.M. Restrepo, M. Macias),**
XAFS Study of TiO₂/SiO₂ System Prepared by Sol-Gel from Inorganic Precursors,
Nuclear Instrum. & Methods Phys. Res. A, 470(1-2) (2001) pp. 347-352.
117. **O.P. Krivoruchko, A.N. Shmakov, V.I. Zaikovskii,**
In situ X-ray Diffraction Study of Solid State Transformations during Catalytic Graphitisation of Amorphous Carbon,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 198-201.
118. **A.V. Kulikov, N.A. Kuzin, A.B. Shigarov, V.A. Kirillov, (A.E. Kronberg, K.R. Westerterp),**
Experimental Study of Vaporization Effect on Steady State and Dynamic Behavior of Catalytic Pellets,
Catal. Today, 66(2-4) (2001) pp. 255-262.
119. **(E.S. Kurkina, N.L. Semendyaeva), A.I. Boronin,**
Mathematical Modeling of Nitrogen Desorption from an Iridium Surface: A Study of the Effects of Surface Structure and Subsurface Oxygen,
Kinetics & Catalysis, 42(5) (2001) pp. 703-717 (English language translation).
120. **(B.I. Kutepov), B.S. Bal'zhinimaev,**
Reasons for the Deactivation of Vanadia-Titania Catalysts for Partial Durene Oxidation During Prolonged Performance,
Kinetics & Catalysis, 42(3) (2001) pp. 291-300 (English language translation).
121. **(B.N. Kuznetsov, A.V. Rudkovsky, M.L. Shchipko, J.M. Guet, N. Cohaut), V.K. Duplyakin, T.I. Gulyaeva,**
The Influence of Conditions of Water-Steam Activation on Microtexture and Sorption Properties of Active Carbons,
Chem. for Sustainable Devel., 8(6) (2000) pp. 809-814.
122. **V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, A.I. Romanenko, (A.V. Okotrub),**
Electrical Resistivity of Graphitized Ultra-Disperse Diamond and Onion-Like Carbon,
Chem. Phys. Lett., 336(5-6) (2001) pp. 397-404.
123. **V.L. Kuznetsov, A.N. Usoltseva, A.L. Chuvilin, (E.D. Obratsova, J.-M. Bonard),**
Thermodynamic Analysis of Nucleation of Carbon Deposits on Metal Particles and its Implications for the Growth of Carbon Nanotubes,
Phys. Rev. B, 64(23) (2001) 235401, 7 pages.
124. **N.I. Kuznetsova, L.I. Kuznetsova, L.G. Detusheva, V.A. Likholobov, (G.P. Pez, H. Cheng),**
Amination of Benzene and Toluene with Hydroxylamine in the Presence of Transition Metal Redox Catalyst,
J. Molec. Catal. A: Chemical, 161(1-2) (2000) pp. 1-9.

125. **O.B. Lapina, (D.F. Khabibulin), A.A. Shubin, V.M. Bondareva,**
⁵¹V and ³¹P NMR Studies of VO_x/TiO₂ Catalysts Modified by Phosphorous,
J. Molec. Catal. A: Chemical, 162(1-2) (2000) pp. 381-390.
126. **O.B. Lapina, M.A. Matsko, T.B. Mikenas, V.A. Zakharov, E.A. Paukshtis, (D.F. Khabibulin), A.P. Sobolev,**
⁵¹V NMR Study of VOCl₃ Immobilized on the SiO₂ and MgCl₂ Surface,
Kinetics & Catalysis, 42(4) (2001) pp. 553-560 (English language translation).
127. **(E.I. Latkin), V.I. Elokhin, V.V. Gorodetskii,**
Monte Carlo Model of Oscillatory Co Oxidation Having Regard to the Change of Catalytic Properties Due to the Adsorbate-Induced Pt(100) Structural Transformation,
J. Molec. Catal. A: Chemical, 166(1) (2001) pp. 23-30.
128. **A.V. Lavrenov, N.M. Ostrovskii, Yu.K. Demanov,**
Thermodynamics of Isomerization of Butylene. Equilibrium Composition,
Petroleum Chemistry, 41(2) (2001) pp. 126-130 (English language translation).
129. **B.N. Luk'yanov, N.A. Kuzin, V.A. Kirillov, A.V. Kulikov, A.B. Shigarov, M.M. Danilova,**
Catalytic Heating Elements for Autonomous Domestic Heating Systems,
Chem. for Sustainable Devel., 9(5) (2001) 667-677 (in Russian).
130. **M.V. Luzgin, A.G. Stepanov, V.P. Shmachkova, N.S. Kotsarenko,**
n-Pentane Carbonylation with CO on Sulfated Zirconia: an *in-situ* Solid-State ¹³C NMR Study,
Mendeleev Commun., 11(1) (2001) pp. 23-25.
131. **M.V. Luzgin, A.G. Stepanov, V.P. Shmachkova, N.S. Kotsarenko,**
n-Pentane Conversion on Sulfated Zirconia in the Absence and Presence of Carbon Monoxide. Evidence for Monomolecular Mechanism of Isomerization from the ¹³C MAS NMR Study,
J. Catal., 203(2) (2001) pp. 273-280.
132. **L.L. Makarshin, D.V. Andreev, V.N. Parmon, (O.M. Tukhto),**
Effect of Low Temperature Adsorption of N₂, O₂ and Ar on Superconductivity of GdBa₂Cu₃O_{7-x} Films,
Mater. Res. Innov., 4(1) (2000) pp. 27-31.
133. **G.M. Maksimov, M.A. Fedotov,**
On Synthesis of Silicoaluminotungstic Heteropoly Acid,
Russ. J. Inorg. Chem., 46(3) (2001) pp. 327-329 (English language translation).
134. **G.M. Maksimov, E.A. Paukshtis, A.A. Budneva, R.I. Maksimovskaya, V.A. Likhobolov,**
Acidity of Heteropoly Acids with Various Structures and Compositions Studied by IR Spectroscopy of the Pyridinium Salts,
Russ. Chem. Bull., 50(4) (2001) pp. 587-590 (English language translation).
135. **G.M. Maksimov, M.N. Timofeeva, V.A. Likhobolov,**
A Study of Complexation of Chloral Hydrate with Heteropoly Anions Having Various Structures,
Russ. Chem. Bull., 50(9) (2001) pp. 1529-1532 (English language translation).
136. **R.I. Maksimovskaya, G.M. Maksimov,**
NMR Studies of Heteropolyanion [P₂W₂₀O₇₀(H₂O)₂] Complexes with Metal Cations,
Inorg. Chem., 46(3) (2001) pp. 1284-1290.
137. **A.V. Mashkina, V.N. Yakovleva, L.G. Sakhaltueva, L.N. Khairulina,**
Conversion of Dimethyl and Diethyl Disulfides into Thiols in the Presence of Solid Catalysts,
Petroleum Chemistry, 41(1) (2001) pp. 50-56 (English language translation).
138. **A.V. Mashkina, L.G. Sakhaltueva,**
Catalytic Hydrogenation of Thiophene to Thiolane in Gas Phase,
Chem. of Heterocyclic Comp., 37(5) (2001) pp. 546-549 (English language translation).

139. **A.V. Mashkina, V.N. Yakovleva,**
Perspectives of Alkylmercaptanes Processing to Dialkyl Sulfides,
Chem. for Sustainable Devel., 9(2) (2001) pp. 269-276 (in Russian).
140. **M.A. Matsko, G.D. Bukatov, T.B. Mikenas, V.A. Zakharov,**
Ethylene Polymerization with Supported Vanadium-Magnesium Catalyst: Number of Active Centers and Propagation Rate Constant,
Macromol. Chem. & Phys., 202(8) (2001) pp. 1435-1439.
141. **K.I. Matveev, V.F. Odyakov, E.G. Zhizhina,**
New Route to Vicasol, a Water-Soluble Form of Vitamin K₃,
Russ. J. Appl. Chem., 74(3) (2001) pp. 469-472 (English language translation).
142. **(V.E. Medvedev), V.V. Malakhov, A.A. Vlasov, I.L. Kraevskaya, (L.P. Kundo, V.A. Kramintsev), I.A. Ovsyannikova,**
Chemical Composition of Korsak Bronzes,
Archaeological and Ethnographic Studies in Siberia and Far East during 1994-1996 Years,
Eds. A.P. Derevyanko, E.V. Laricheva, Novosibirsk, Institute of Archaeology and Ethnography, 2000, pp. 166-189.
143. **M.S. Mel'gunov, V.B. Fenelonov, (R. Leboda, B. Charmas),**
Coke Dispersion in Carbon–Mineral Porous Adsorbents,
Carbon, 39(3) (2001) pp. 357-366.
144. **M.S. Mel'gunov, V.B. Fenelonov, (R. Leboda, B. Charmas),**
Applicability Verification for a New Method of Measuring the Components' Surface Areas in Bicomponent Catalysts and Adsorbents,
Colloids and Surfaces A: Physicochem. & Engin. Aspects, 186(3) (2001) pp. 203-209.
145. **(A.Yu. Men'shikova, T.G. Evseeva, M.V. Peretolchin, N.A. Chekina), S.S. Ivanchev,**
Emulsifier-Free Polymerization of Methyl Methacrylate with a Carboxyl-Containing Initiator,
Polymer Sci., ser. A, 43(4) (2001) pp. 366-374 (English language translation).
146. **(A.Yu. Men'shikova, T.G. Evseeva, N.A. Chekina), S.S. Ivanchev,**
Synthesis of Polymer Methacrylate Microspheres in the Presence of Dextran and its Derivatives,
Russ. J. Appl. Chem., 74(3) (2001) pp. 489-493 (English language translation).
147. **A.M. Mesh, S.S. Ivanchev, (M. Ratzsch), S.Ya. Khaikin, (N. Reichelt), N.K. Fedorova,**
Grafting Polymerization of Vinyl Monomers onto Polypropylene in the Presence of Acetylacetonates of Varying Valence Metals,
Polymer Sci., ser. B, 43(9-10) (2001) pp. 273-275 (English language translation).
148. **T.B. Mikenas, V.A. Zakharov, L.G. Echevskaya, M.A. Matsko,**
Ethylene Polymerization with Supported Vanadium-Magnesium Catalyst: Hydrogen Effect,
Macromol. Chem. Phys., 202(4) (2001) pp. 475-481.
149. **T.B. Mikenas, V.A. Zakharov, L.G. Echevskaya, M.A. Matsko,**
Polymerization of Ethylene in the Presence of Hydrogen over Supported Vanadium-Magnesium Catalysts,
Polimery, 45(5) (2000) pp. 349-352.
150. **I.V. Mishakov, V.V. Chesnokov, R.A. Buyanov, N.A. Pakhomov,**
Decomposition of Chlorinated Hydrocarbons on Iron-Group Metals,
Kinetics & Catalysis, 42(4) (2001) pp. 543-548 (English language translation).
151. **V.V. Molchanov, R.A. Buyanov,**
Scientific Grounds for the Application of Mechanochemistry to Catalyst Preparation,
Kinetics & Catalysis, 42(3) (2001) pp. 366-374 (English language translation).

152. **A.S. Noskov**,
International Conference “Chemreactor-15”,
Catalysis in Industry, 2 (2001) pp. 61-63 (in Russian).
153. **A.S. Noskov, V.N. Parmon**,
Basic Researches in Catalysis and Heterogeneous Chemical Reactions and Prospects of their Using
(Analysis of RFBR Grants of 1994-1999 Years),
RFBR Bulletin, 2(24) (2001) pp. 5-16 (in Russian).
154. (**A.N. Obraztsov, A.P. Volkov**), **A.I. Boronin, S.V. Koshcheev**,
Rehybridization of the Atomic Orbitals and the Field Electron Emission from Nanostructured
Carbon,
J. Exper. & Theoret. Physics, 93(4) (2001) pp. 846-853 (English language translation).
155. **V.F. Odyakov, K.I. Matveev**,
Catalytic Methods for Synthesis of Citral From Products of Organic Synthesis,
Chem. for Sustainable Devel., 9(4) (2001) pp. 503-517 (in Russian).
156. (**A.V. Okotrub, L.G. Bulusheva**), **V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, (M.I. Heggie)**,
X-Ray Emission Studies of the Valence Band of Nanodiamonds Annealed at Different
Temperatures,
J. Phys. Chem. A, 105 (2001) pp. 9781-9787.
157. (**A.V. Okotrub, L.G. Bulusheva**), **A.I. Romanenko, A.L. Chuvilin, N.A. Rudina,**
(Y.V. Shubin, N.F. Yudanov, A.V. Gusel'nikov),
Anisotropic Properties of Carbonaceous Material Produced in Arc Discharge,
Appl. Phys. A, 72(4) (2001) pp. 481-486.
158. **N.M. Ostrovskii**,
“*Kinetics of Catalysts Deactivation*”, Ed. V.N. Parmon, “Nauka”, 2001, 335 pp. (in Russian).
159. **N.M. Ostrovskii**,
New Models of Catalyst Deactivation by Coke. 1. Multilayer Coke Formation via the Consecutive
Mechanism,
Kinetics & Catalysis, 42(3) (2001) pp. 317-325 (English language translation).
160. **N.M. Ostrovskii**,
New Models of Catalyst Deactivation by Coke. 2. Coking of Supported Platinum Catalysts,
Kinetics & Catalysis, 42(3) (2001) pp. 326-333 (English language translation).
161. (**N.S. Ovanesyan**), **K.A. Dubkov, (A.A. Pyalling, A.A. Shteinman)**,
The Fe Active Sites in FeZSM-5 Catalyst for Selective Oxidation of CH₄ to CH₃OH at Room
Temperature,
J. Radioanalyt. & Nuclear Chem., 246(1) (2000) pp. 149-152.
162. (**J.-I. Ozaki, Y. Yoshimoto, A. Oya, T. Takarada**), **V.V. Kuznetsov, Z.R. Ismagilov**,
H₂S Decomposition Activity of TS Carbon Derived from Furan Resin,
Carbon, 39(10) (2001) pp. 1611-1612.
163. **N.A. Pakhomov**,
Reversible and Irreversible Deactivation of Supported Bimetallic Catalysts for the Dehydrogenation
of Lower Paraffins,
Kinetics & Catalysis, 42(3) (2001) pp. 334-343 (English language translation).
164. **V.N. Panchenko, V.A. Zakharov, I.G. Danilova, E.A. Paukshtis, I.I. Zakharov,**
V.B. Goncharov, A.P. Suknev,
Structure and Performance of the Solid Methylalumoxane at Temperatures 20-250°C: Experimental
and DFT Calculation Study,
J. Molec. Catal. A: Chemical, 174(1-2) (2001) pp. 107-117.

165. **Yu.D. Pankrat'ev, M.M. Tokarev, Yu.I. Aristov,**
Heats of Water Sorption on Silica Gel Containing CaCl₂ and LiBr,
Russ. J. Phys. Chem., 75(5) (2001) pp. 806-810 (English language translation).
166. **V.N. Parmon,**
Natural Selection in a Homogeneous System with Noninteracting Autocatalyst "Populations",
Doklady Physical Chem., 377(4-6) (2001) pp. 91-95 (in Russian).
167. **V.N. Parmon, A.S. Noskov,**
Domestic Catalysts and New Resources-Economy Catalytic Processes in Present-Day Russia,
Catalysis in Industry, 1 (2001) pp. 6-17 (in Russian).
168. **V.N. Parmon, V.S. Zakharenko,**
Photocatalysis and Photosorption in the Earth's Atmosphere,
CATTECH, 5(2) (2001) pp. 96-115.
169. **V.N. Parmon, V.S. Zakharenko,**
Photocatalysis and Photosorption in the Earth's Atmosphere,
Chem. for Sustainable Devel., 9(3) (2001) pp. 461-483 (in Russian).
170. **E.A. Paukshtis, N.S. Kotsarenko, V.P. Shmachkova,**
Interaction of Hydrogen and *n*-Pentane with Sulfated Zirconia,
Catal. Lett., 69(3-4) (2000) pp. 189-193.
171. **S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, D.I. Kochubey, R.I. Maksimovskaya, V.I. Zaikovskii, V.V. Kriventsov, S.V. Tsybulya, E.B. Burgina, A.M. Volodin, (M.V. Chaikina, N.N. Kuznetsova, V.V. Lunin, D. Agrawal, R. Roy),**
The Novel Acid Catalysts - Framework Zirconium Phosphates: The Bulk and Surface Structure,
J. Molec. Catal. A: Chemical, 158(1) (2000) pp. 319-323.
172. **S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, R.I. Maksimovskaya, V.I. Zaikovskii, S.V. Tsybulya, E.B. Burgina, (M.V. Chaikina, D. Agrawal, R. Roy),**
The Influence of Solid Precursors Nature on Structural, Textural and Surface Properties of Framework Zirconium Phosphates Synthesized via Mechanochemical Activation,
Solid State Ionics, 141-142(1-4) (2001) pp. 683-688.
173. **V.N. Pavlyuchenko, O.N. Primachenko, S.Ya. Khaikin, S.S. Ivanchev, (M.E. Jones),**
Segregation of Polymers in the Course of Film Formation from a Mixture of Latexes,
Russ. J. Appl. Chem., 74(7) (2001) pp. 1173-1177 (English language translation).
174. **V.N. Pavlyuchenko, O.V. Sorochinskaya, S.S. Ivanchev, V.V. Klubin, G.S. Kreichman, V.P. Budtov, (M. Skrifvars, E. Halme, J. Koskinen),**
Hollow-Particle Latexes: Preparation and Properties,
J. Polymer Sci., Part A – Polymer Chemistry, 39(9) (2001) pp. 1435-1449.
175. **L.V. Piryutko, (A.K. Uriarte), V.S. Chernyavsky, A.S. Kharitonov, G.I. Panov,**
Preparation and Catalytic Study of Metal Modified TS-1 in the Oxidation of Benzene to Phenol by N₂O,
Micropor. & Mesopor. Mater., 48(1-3) (2001) pp. 345-353.
176. **B.N. Plakhutin, (R. Carbo-Dorca),**
Erratum to "Icosahedral Symmetry Structures with Open-Shell Electronic Configuration h^{N₂}" [Phys. Lett. A, 267 (2000) pp. 370-378],
Phys. Lett. A., 279(1-2) (2001) pp. 102-103.
177. **G.V. Plaksin,**
Porous Carbon Materials of Sibunit Type,
Chem. for Sustainable Devel., 9(5) (2001) pp. 609-620 (in Russian).

178. **G.V. Plaksin, O.N. Baklanova, V.K. Duplyakin, V.A. Drozdov,**
Nanosorbents Produced by Pyrolysis and Gasification of Hydrolytic Lignin,
“*Progress in Thermochemical Biomass Conversion*”, Ed. A. Bridgwater, Blackwell Science, 2001,
1744 p.
179. **L.M. Plyasova, I.Yu. Molina, T.A. Krieger, L.P. Davydova, V.V. Malakhov, L.S. Dovitova,
T.M. Yurieva,**
Interaction of Hydrogen with Copper-Containing Oxide Catalysts. 5. Structural Transformations in
Copper Chromite during Reduction-Reoxidation,
Kinetics & Catalysis, 42(1) (2001) pp. 126-131 (English language translation).
180. **(S.A. Popov, Yu.V. Gatilov, T.V. Rybalova), O.A. Kholdeeva, A.V. Tkachev,**
Novel Optically Active Pyrazole Ligands Derived from (+)-3-Carene,
Tetrahedron: Asymmetry, 12(20) (2001) pp. 2875-2881.
181. **Yu.V. Potapova, S.F. Tikhov, V.A. Sadykov, V.B. Fenelonov,**
Kinetics of Aluminium Powder Oxidation by Water Vapor at Moderate Temperature,
React. Kinet. & Catal. Lett., 73(1) (2001) pp. 55-61.
182. **(R. Richards, R.S. Mulukutla), I.V. Mishakov, V.V. Chesnokov, A.M. Volodin, V.I. Zaikovskii,
(N. Sun, K.J. Klabunde),**
Nanocrystalline Ultra High Surface Area Magnesium Oxide as a Selective Base Catalyst,
Scripta Materialia, 44(8-9) (2001) pp. 1663-1666.
183. **T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, A.L. Chuvilin, V.A. Likholobov,**
Microdesign of Nickel-Copper Alloy Catalysts for Production of New Carbon Materials,
Eurasian ChemTech J., 2 (2000) pp. 237-244.
184. **V.N. Romannikov, (S.D. Kirik, L.A. Soloviev), A.N. Shmakov, A.Yu. Derevyankin,
V.B. Fenelonov, O.A. Kholdeeva, O.B. Lapina, E.A. Paukshtis,**
Physicochemical Properties of Mesoporous Mesophase Silicate Materials Formed via the
Electrostatic S⁺T Mechanism,
Kinetics & Catalysis, 42(6) (2001) pp. 857-866 (English language translation).
185. **(N. Roesch, P. Gisdakis), I.V. Yudanov, (C. Di Valentin),**
Mechanistic Aspects of Transition Metal Catalyzed Olefin Epoxidation from Density Functional
Studies,
“*Peroxide Chemistry: Mechanistic and Preparative Aspects of Oxygen Transfer*”; Ed. W. Adam,
Wiley-VCH, Weinheim, 2000, pp. 601-619.
186. **E.M. Sadvskaya, A.P. Suknev, L.G. Pinaeva, V.B. Goncharov, B.S. Bal'zhinimaev,
(C. Chupin, C. Mirodatos),**
Mechanism and Kinetics of the Selective NO Reduction over Co-ZSM-5 Studied by the SSITKA
Technique. 1. NO_x Adsorbed Species Formation,
J. Catal., 201(2) (2001) pp. 159-168.
187. **V.A. Sadykov, R.V. Bunina, G.M. Alikina, A.S. Ivanova, D.I. Kochubey, B.N. Novgorodov,
E.A. Paukshtis, V.B. Fenelonov, V.I. Zaikovskii, T.G. Kuznetsova, (S.A. Beloshapkin),
V.N. Kolomiichuk, E.M. Moroz, (V.A. Matyshak, G.A. Konin, A.Ya. Rozovskii, J.R.H. Ross,
J.P. Breen),**
Supported CuO+Ag/Partially Stabilized Zirconia Catalysts for the Selective Catalytic Reduction of
NO_x under Lean Burn Conditions. 1. Bulk and Surface Properties of the Catalysts,
J. Catal., 200(1) (2001) pp. 117-130.

188. **V.A. Sadykov, R.V. Bunina, G.M. Alikina, A.S. Ivanova, T.G. Kuznetsova, S.A. Beloshapkin, (V.A. Matyshak, G.A. Konin, A.Ya. Rozovskii, V.F. Tretyakov, T.N. Burdeynaya, M.N. Davydova, J.R.H. Ross, J.P. Breen),**
Supported CuO+Ag/Partially Stabilized Zirconia Catalysts for the Selective Catalytic Reduction of NO_x under Lean Burn Conditions. 2. Catalytic Properties,
J. Catal., 200(1) (2001) pp. 131-139.
189. **V.A. Sadykov, S.N. Pavlova, G.V. Zabolotnaya, (M.V. Chaikina), R.I. Maksimovskaya, S.V. Tsybulya, E.B. Burgina, V.I. Zaikovskii, G.S. Litvak, (Yu.V. Frolova), D.I. Kochubey, V.V. Kriventsov, E.A. Paukshtis, V.N. Kolomiichuk, (V.V. Lunin, N.N. Kuznetsova, D. Agrawal, R. Roy),**
Scientific Bases for the Synthesis of Highly Dispersed Framework Zirconium Phosphate Catalysts for Paraffin Isomerization and Selective Oxidation,
Kinetics & Catalysis, 42(3) (2001) pp. 390-398 (English language translation).
190. **(V.N. Samoilenko, L.A. Petrov), A.I. Boronin, K.T. Murzakhmetov, S.V. Koshcheev, A.N. Salanov, V.T. Yakushko, (S.L. Khokhlov, L.N. Kurina, O.V. Vodyankina, I.G. Rozanov, G.I. Murygin, Yu. P. Zaikov),**
The Morphology, Surface Composition, and Catalytic Properties of Silver Crystals Obtained by Electrolysis,
Russ. J. Phys. Chem., 75(10) (2001) pp. 1607-1614 (English language translation).
191. **(R.A. van Santen), G.M. Zhidomirov, A.A. Shubin, A.L. Yakovlev, (L.A.M.M. Barbosa),**
Reactivity Theory of Zinc Cation Species in Zeolites,
“*Catalysis by Unique Metal Ion Structures in Solid Matrices. From Science to Application*”,
Eds. G. Centi et al., NATO ASI Series book, 2001, pp. 187-204.
192. **V.A. Semikolenov, I.I. Il'ina, I.L. Simakova,**
Linalool Synthesis from α -Pinene: Kinetic Peculiarities of Catalytic Steps,
Appl. Catal. A: General, 211(1) (2001) pp. 91-107.
193. **(Sh.K. Shaikhutdinov), E.R. Savinova, (A. Scheybal, K. Doblhofer, R. Schlögl),**
Ex situ Scanning Tunneling Microscopy Study of Under-Potential Oxidation of a Ag(111) Electrode in an Alkaline Electrolyte,
J. Electroanal. Chem., 500(1-2) (2001) pp. 208–212.
194. **V.E. Sharonov, E.A. Tyshchishchin, E.M. Moroz, A.G. Okunev, Yu.I. Aristov,**
Sorption of CO₂ from Humid Gases on Potassium Carbonate Supported by Porous Matrix,
Russ. J. Appl. Chem., 74(3) (2001) pp. 409-413 (English language translation).
195. **V.E. Sharonov, A.G. Okunev, E.M. Moroz, I.G. Danilova, T.A. Krieger, Yu.I. Aristov,**
Sorption of the Carbon Dioxide from Wet Gases by K₂CO₃ in Porous Matrix: Influence of the Matrix Nature,
Chem. Ing. Tech., 73(6) (2001) 736 (On-line publication).
196. **O.V. Sherstyuk, (S.N. Pron'kin), A.L. Chuvilin, A.N. Salanov, E.R. Savinova, (G.A. Tsirlina, O.A. Petrii),**
Platinum Electrodeposits on Glassy Carbon: The Formation Mechanism, Morphology and Adsorptive Properties,
Russ. J. Electrochem., 36(7) (2000) pp. 741-751 (English language translation).
197. **O.V. Sherstyuk, P.A. Simonov, A.L. Chuvilin, E.R. Savinova,**
Model Nanostructured Pt Electrodes – an Approach to Study Size/Structural Effects in Electrocatalysis,
“*The Global Climate Change: a Coordinated Response by Electrochemistry and Solid-State Science and Technology*”, Eds. A. Wieckowski, E.W. Brooman, E.J. Rudd, T.F. Fuller, J. Leddy,
The Electrochemical Society, INC., 2001, pp. 56-71.

198. **(E. Shevchenko, E. Matiushenkov), D.I. Kochubey, (D.V. Sviridov, A.I. Kokorin, A.I. Kulak),**
Synthesis of Carbon Films with Diamond-Like Structure by Electrochemical Oxidation of Lithium
Acetylide,
Chem. Commun., 4 (2001) pp. 317-318.
199. **N.B. Shitova, (Yu.D. Perfil'ev), L.Ya. Al't, G.G. Savelieva,**
Reaction of Polynuclear Platinum Carbonyl with Tin(II) Chloride,
Russ. J. Inorg. Chem., 46(3) (2001) pp. 376-381 (English language translation).
200. **A.A. Shubin, G.M. Zhidomirov, (A.L. Yakovlev, R.A. van Santen),**
Comparative Quantum Chemical Study of Stabilization Energies of Zn^{2+} Ions in Different Zeolite
Structures,
J. Phys. Chem. B, 105(21) (2001) pp. 4928-4935.
201. **V.I. Simagina, I.V. Stoyanova,**
Hydrodechlorination of Polychlorinated Benzenes in the Presence of a Bimetallic Catalyst in
Combination with a Phase-Transfer Catalyst,
Mendeleev Commun., 11(1) (2001) pp. 38-39.
202. **A.D. Simonov, N.A. Yazykov, V.N. Parmon,**
Adsorption-Contact Drying of Deformable Materials,
Chem. for Sustainable Devel., 9(5) (2001) pp. 685-694 (in Russian).
203. **A.D. Simonov, N.A. Yazykov, P.I. Vedyakin, G.A. Lavrov, V.N. Parmon,**
Fluidized Catalyst Bed Combustion of Fuels for Local Heat Supply,
Chem. for Sustainable Devel., 9(1) (2001) pp. 97-104 (in Russian).
204. **L.G. Simonova, (V.V. Barelko), O.B. Lapina, E.A. Paukshtis, V.V. Terskikh, V.I. Zaikovskii,
B.S. Bal'zhinimaev,**
Catalysts Based on Fiberglass Supports. 1. Physicochemical Properties of Silica Fiberglass Supports,
Kinetics & Catalysis, 42(5) (2001) pp. 693-702 (English language translation).
205. **L.G. Simonova, (V.V. Barelko), E.A. Paukshtis, O.B. Lapina, V.V. Terskikh, V.I. Zaikovskii,
B.S. Bal'zhinimaev,**
Catalysts Based on Fiberglass Supports. 2. Physicochemical Properties of Alumina Borosilicate
Fiberglass Supports,
Kinetics & Catalysis, 42(6) (2001) pp. 828-836 (English language translation).
206. **L.G. Simonova, (V.V. Barelko), A.V. Toktarev, V.I. Zaikovskii, V.I. Bukhtiyarov,
V.V. Kaichev, B.S. Bal'zhinimaev,**
Catalysts Based on Fiberglass Supports. 3. Properties of Supported Metals (Pt, Pd) According to
Electron Microscopy and XPS Data,
Kinetics & Catalysis, 42(6) (2001) pp. 837-846 (English language translation).
207. **(M.G. Slin'ko), V.A. Kirillov, I.A. Mikhailova, (S.I. Fadeev),**
Mathematical Model of a Catalytic Process on a Porous Grain in a Gas-Liquid-Solid Three-Phase
System,
Doklady Chemistry, 376(1-3) (2001) pp. 42-46 (English language translation).
208. **(M.G. Slin'ko), V.A. Kirillov, N.A. Kuzin, A.B. Shigarov,**
Nonlinear Phenomena in a Downward Gas-Liquid Flow through a Fixed Granular Catalyst Bed,
Doklady Chemistry, 380(1) (2001) pp. 271-274 (English language translation).
209. **M.Yu. Smirnov, (G.W. Graham),**
Pd Oxidation under UHV in a Model Pd/Ceria-Zirconia Catalyst,
Catal. Lett., 72(1-2) (2001) pp. 39-44.

210. **(T.P. Smirnova, A.M. Badalian, L.V. Yakovkina), V.V. Kaichev, V.I. Bukhtiyarov, A.N. Shmakov, (V.I. Rachlin, A.N. Fomina),**
Silicon Carbonitride Alloys as a Novel Functional Material Obtained by Plasma Enhanced Chemical Vapor Deposition from Dimethyl(2,2-hydrazine)sylane,
On-Line J. "Investigated in Russia", 74 (2001) pp. 814-822.
211. **V.N. Snytnikov, E.M. Yurchenko,**
Splitting Scheme for Gas Filtration Problems with Chemical Reactions,
J. "Computational Technologies", 6(5) (2001) pp. 95-105 (in Russian).
212. **(L.A. Solovyov, S.D. Kirik), A.N. Shmakov, V.N. Romannikov,**
X-Ray Structural Modeling of Silicate Mesoporous Mesophase Materials,
Micropor. & Mesopor. Mater., 44-45(1-3) (2001) pp. 17-23.
213. **A.M. Sorokin, V.V. Kaichev, (A.I. Timoshin, O.V. Moskovkin, A.A. Rastorguev, A.M. Badalyan),**
A Multipurpose UV-Visible Spectroscopic System,
Instrum. & Exper. Techniques, 44(3) (2001) pp. 375-380 (English language translation).
214. **E.S. Stoyanov,**
IR Study of the Structure of Palladium(II) Acetate in Chloroform, Acetic Acid, and their Mixtures in Solution and in Liquid-Solid Subsurface Layers,
J. Struct. Chem., 41(3) (2000) pp. 540-546 (in Russian).
215. **(A.N. Subbotin), V.A. Chernov, (V.V. Gaganov, A.V. Kalutsky, N.V. Kovalenko, A.K. Krasnov, K.E. Kuper, A.G. Legkodymov, A.D. Nikolenko, I.N. Nesterenko, V.F. Pindyurin, V.N. Romaev),**
Absolute Calibration of X-Ray Semiconductor Detectors in the 0.3-1.5 keV Photon Energy Range on Synchrotron Radiation from VEPP-2M Storage Ring,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 452-458.
216. **(Yu.S. Sulyaev, N.V. Kovalenko), V.A. Chernov,**
The Using of Ion Beams for Treatment of X-Ray Optical Substrates,
Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 1 (2001) pp. 74-75 (in Russian).
217. **E.P. Talsi, D.E. Babushkin, N.V. Semikolenova, V.N. Zudin, V.N. Panchenko, V.A. Zakharov,**
Polymerization of Ethylene Catalyzed by Iron Complex Bearing 2,6-Bis(imine)pyridyl Ligand: ^1H and ^2H NMR Monitoring of Ferrous Species Formed via Catalyst Activation with AlMe_3 , MAO, $\text{AlMe}_3/\text{B}(\text{C}_6\text{F}_5)_3$ and $\text{AlMe}_3/\text{CPh}_3\text{B}(\text{C}_6\text{F}_5)_4$,
Macromol. Chem. & Phys., 202(10) (2001) pp. 2046-2051.
218. **E.P. Talsi, D.E. Babushkin, N.V. Semikolenova, V.N. Zudin, V.A. Zakharov,**
Ethylene Polymerization in the Presence of Iron(II) 2,6-Bis(imine)pyridine Complex: Structures of Key Intermediates,
Kinetics & Catalysis, 42(2) (2001) pp. 147-153 (English language translation).
219. **E.P. Talsi, G.L. Elizarova, L.G. Matvienko, A.A. Shubin, V.N. Parmon,**
EPR-Spectroscopic Detection and Characterization of a Cu^{II} Complex with a Peroxycarboximidic Acid,
Mendeleev Commun., 11(6) (2001) pp. 206-207.
220. **Yu.Yu. Tanashev, V.N. Parmon, Yu.I. Aristov,**
Retardation of a Heat Front in a Porous Medium Containing an Evaporating Liquid,
J. Engin. Physics & Thermophysics, 74(5)(2001) pp. 1053-1058 (English language translation).
221. **V.M. Tapilin,**
Basis Functions with Polynomial Tails for Band Structure Calculations,
J. Struct. Chem., 42(3) (2001) pp. 411-417 (in Russian).

222. **S.F. Tikhov, V.A. Sadykov, I.I. Bobrova, Yu.V. Potapova, V.B. Fenelonov, S.V. Tsybulya, S.N. Pavlova, A.S. Ivanova, V.Yu. Kruglyakov, N.N. Bobrov,**
Composite Steam Reforming Catalysts Prepared from Al₂O₃/Al Matrix Precursor,
Stud. Surf. Sci. & Catal., Eds. I.I. Spivey, E. Iglesia, T. Fleisch, Elsevier Sci., 136 (2001) pp. 105-110.
223. **S.F. Tikhov, A.N. Salanov, Yu.V. Potapova, V.T. Yakushko, V.A. Sadykov, V.P. Ivanov, S.V. Tsybulya,**
Preparation of Al₂O₃/Al Composite through the Hydrothermal Oxidation of Aluminum Foil,
Eurasian ChemTech J., 2 (2000) pp. 265-269.
224. **M.N. Timofeeva, G.M. Maksimov, V.A. Likholobov,**
Acidity of Solutions of Heteropoly Acids with Various Structures and Compositions,
Kinetics & Catalysis, 42(1) (2001) pp. 30-34 (English language translation).
225. **M.N. Timofeeva, (M.M. Matrosova), G.M. Maksimov, V.A. Likholobov,**
A Study of the Acid Properties of Structurally and Compositionally Different Heteropoly Acids in Acetic Acid,
Kinetics & Catalysis, 42(6) (2001) pp. 758-791 (English language translation).
226. **M.N. Timofeeva, (M.M. Matrosova), G.M. Maksimov, V.A. Likholobov, A.V. Golovin, R.I. Maksimovskaya, E.A. Paukshtis,**
Esterification of *n*-Butanol with Acetic Acid in the Presence of Heteropoly Acids with Different Structures and Compositions,
Kinetics & Catalysis, 42(6) (2001) pp. 791-796 (English language translation).
227. **(A.T. Titov, P.M. Larionov, V.S. Shchukin), V.I. Zaikovskii,**
Mechanism of Heart Valve Mineralization,
Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 3 (2001) pp. 74-79 (in Russian).
228. **A.G. Tolstikov, N.N. Karpyshev, O.V. Tolstikova, T.B. Khlebnikova, G.E. Sal'nikov, V.I. Mamatyuk, (Yu.V. Gatilov, I.Yu. Bagryanskaya),**
Derivatives of L-Pimaric Acid in the Synthesis of Chiral Organophosphorus Ligands from Decahydrophenantrene Series,
Russ. J. Organic Chem., 37(8) (2001) pp. 1134-1148 (English language translation).
229. **N.N. Trukhan, V.N. Romannikov, E.A. Paukshtis, A.N. Shmakov, O.A. Kholdeeva,**
Oxidation of 2,3,6-Trimethylphenol over Ti- and V-Containing Mesoporous Mesophase Catalysts: Structure-Activity/Selectivity Correlation,
J. Catal., 202(1) (2001) pp. 110-117.
230. **N.N. Trukhan, A.Yu. Derevyankin, A.N. Shmakov, E.A. Paukshtis, O.A. Kholdeeva, V.N. Romannikov,**
Alkene and Thioether Oxidations with H₂O₂ over Ti- and V-Containing Mesoporous Mesophase Catalysts,
Micropor. & Mesopor. Mater., 44-45(1-3) (2001) pp. 603-608.
231. **(M.V. Tsodikov, O.V. Bukhtenko, E.V. Slivinskii, L.N. Slastikhina, A.M. Voloshchuk), V.V. Kriventsov, (L.E. Kitaev),**
Structure and Acid-Basic Properties of the Surface of Titanium Oxides Modified by Phosphorus and Aluminum and Prepared by the Alkoxo Method. 1. Structural Organization of Modified Titanate Systems,
Russ. Chem. Bull., 49(11) (2000) pp. 1803-1807 (English language translation).
232. **(M.V. Tsodikov, E.V. Slivinskii, V.V. Yushchenko, L.E. Kitaev), V.V. Kriventsov, D.I. Kochubey, (A.T. Teleshev),**
Structure and Acid-Basic Properties of the Surface of Titanium Oxides Modified by Phosphorus and Aluminum and Prepared by the Alkoxo Method. 2. Study of the Active Surface of Titanium Oxides,
Russ. Chem. Bull., 49(12) (2000) pp. 2003-2006 (English language translation).

233. **P.G. Tsyrl'nikov, V.S. Sal'nikov, V.A. Drozdov, A.S. Noskov, N.A. Chumakova, V.K. Ermolaev, I.V. Malakhova,**
Deep Oxidation of Methane on Alumina-Manganese and Pt-Containing Catalysts,
J. Catal., 198(2) (2001) pp. 164-171.
234. **(A.P. Vasilenko, A.V. Kolesnikov), S.G. Nikitenko, (A.A. Fedorov, L.V. Sokolov, A.I. Nikiforov, E.M. Trukhanov),**
X-Ray Film Interferometer as an Instrument for Semiconductor Heterostructure Investigation,
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 110-113.
235. **(T.A. Vereshchagina, N.N. Anshits, I.D. Zykova), A.N. Salanov, (A.A. Tretyakov, A.G. Anshits),**
Preparation of Cenospheres of Stabilized Compositions from Volatile Sols and their Properties,
Chem. for Sustainable Devel., 9(3) (2001) pp. 379-392 (in Russian).
236. **(Zh.A. Vnutskikh, A.A. Fedorov, Yu.S. Chekryshkin), Z.R. Ismagilov, M.A. Kerzhentsev,**
Thermal-Oxidative Breakdown of Polytetrafluorinethylene,
Chem. for Sustainable Devel., 9(5) (2001) pp. 621-623 (in Russian).
237. **(Zh.A. Vnutskikh, A.A. Fedorov, Yu.S. Chekryshkin, E.A. Zhilkina), Z.R. Ismagilov, M.A. Kerzhentsev,**
Polytetrafluorinethylene Reaction with Oxides and Hydroxides of Alkaline-Earth Metals,
Chem. for Sustainable Devel., 9(6) (2001) pp. 715-722 (in Russian).
238. **A.M. Volodin, K.A. Dubkov, (A. Lund),**
Direct ESR Detection of $S = 3/2$ States for Nitrosyl Iron Complexes of Iron in FeZSM-5 Zeolites,
Chem. Phys. Lett., 333(1-2) (2001) pp. 41-44.
239. **(V.I. Voronin, I.F. Berger, V.A. Cherepanov, L.Y. Gavrilova, A.N. Petrov, A.I. Ancharov, B.P. Tolochko), S.G. Nikitenko,**
Neutron Diffraction, Synchrotron Radiation and EXAFS Spectroscopy Study of Crystal Structure Peculiarities of the Lanthanum Nickelates $La_{n+1}Me_nO_{3n+1}$ ($n=1,2,3$),
Nuclear Instrum. & Methods in Phys. Res. A, 470(1-2) (2001) pp. 202-209.
240. **A.V. Vorontsov, E.N. Savinov, (L. Davydov, P.G. Smirniotis),**
Photocatalytic Destruction of Gaseous Diethyl Sulfide over TiO_2 ,
Appl. Catal. B: Environmental, 32(1-2) (2001) pp. 11-24.
241. **(A.L. Yakovlev), A.A. Shubin, G.M. Zhidomirov, (R.A. van Santen),**
DFT Study of Oxygen-Bridged Zn^{2+} Ion Pairs in Zn/ZSM-5 Zeolites,
Catal. Lett., 70(3-4) (2000) pp. 175-181.
242. **(A.L. Yakovlev), G.M. Zhidomirov, (R.A. van Santen),**
 N_2O Decomposition Catalysed by Transition Metal Ions,
Catal. Lett., 75(1-2) (2001) pp. 45-48.
243. **A. Yermakova, (S.I. Fadeev), V.I. Anikeev,**
Chemical Equilibrium Calculations for a Multicomponent Mixture Taking into Account its Nonideality,
Russ. J. Phys. Chem., 75(8) (2001) pp. 1266-1273 (English language translation).
244. **A. Yermakova, M.V. Gudkov, V.I. Anikeev,**
Analysis of a Two-Phase Perfectly Mixed Reactor under the Condition of a Phase Equilibrium,
Theor. Found. of Chem. Engin., 35(5) (2001) pp. 486-493 (English language translation).
245. **(S.M. Yunusov, E.S. Kalyuzhnaya), B.L. Moroz, (S.N. Agafonova), V.A. Likhoboy, (V.B. Shur),**
The Effect of Co and Ir on the Activity of the $K_2[Fe_2(CO)_8]$ - and $K_2[Ru_4(CO)_{13}]$ -Based Systems in Ammonia Synthesis. The Synergistic Acceleration of the Ammonia Synthesis over the $K_2[Fe_2(CO)_8]+K$ Catalysts by Iridium,
J. Molec. Catal. A: Chemical, 165(1-2) (2001) pp. 141-147.

246. **(S.M. Yunusov, E.S. Kalyuzhnaya), B.L. Moroz, (S.N. Agafonova), V.A. Likhobolov, (V.B. Shur),**
The Synergistic Acceleration of the Ammonia Synthesis over the $K_2[Fe_2(Co)_8] + K$ Catalysts on
Carbon "Sibunit" by Rhodium,
Appl. Catal. A: Chemical, 218(1-2) (2001) pp. 251-256.
247. **T.M. Yurieva, G.N. Kustova, T.P. Minyukova, (E.K. Poels, A. Bliet), M.P. Demeshkina,
L.M. Plyasova, T.A. Krieger, V.I. Zaikovskii,**
Non-Hydrothermal Synthesis of Copper-, Zinc- and Copper-Zinc Hydrosilicates,
Mater. Res. Innov. 5(1) (2001) pp. 3-11.
248. **T.M. Yurieva, T.P. Minyukova, G.N. Kustova, L.M. Plyasova, T.A. Krieger, M.P. Demeshkina,
V.I. Zaikovskii, V.V. Malakhov, L.S. Dovlitova,**
Copper Ions Distribution in Synthetic Copper-Zinc Hydrosilicate,
Mat. Res. Innovat., 5(2) (2001) pp. 74-80.
249. **V.I. Zaikovskii, V.V. Chesnokov, R.A. Buyanov,**
The Relationship between the State of Active Species in a Ni/Al_2O_3 Catalyst and the Mechanism of
Growth of Filamentous Carbon,
Kinetics & Catalysis, 42(6) (2001) pp. 813-821 (English language translation).
250. **I.I. Zakharov, V.A. Zakharov,**
A Density Functional Theory (DFT) Quantum-Chemical Approach to the Real Structure of
Polymethylalumoxane,
Macromol. Theory & Simul., 10 (2001) pp. 108-116.
251. **V.A. Zakharov, I.I. Zakharov, V.N. Panchenko,**
Structures of MAO: Experimental Study of Solid MAO and Molecular Models According to DFT
Quantum Chemical Simulations,
"Organometallic Catalysts and Olefin Polymerization", Eds. R. Blom, A. Follestad, E. Rytter,
M. Tilset, M. Ystenes, Springer-Verlag, Berlin, 2001, pp. 63-71.
252. **G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya, V.F. Anufrienko, V.Yu. Gavrilov,**
Structure Peculiarities of Reduced Vanadium-Titanium Oxide Catalysts,
Kinetics & Catalysis, 42(1) (2001) pp. 132-137 (English language translation).
253. **V.P. Zhdanov,**
Ostwald Ripening with Kinetically Limited Bond Formation,
European Physical J. B, 19(1) (2001) pp. 97-100.
254. **V.P. Zhdanov,**
Pattern Formation in Catalytic Reactions due to Lateral Adsorbate-Adsorbate Interactions,
Langmuir, 17 (2001) pp. 1793-1799.
255. **V.P. Zhdanov,**
Disappearance of Oscillations in the Brusselator on the Mesoscopic Scale,
Phys. Chem. Chem. Phys., 3(8) (2001) pp. 1432-1434.
256. **V.P. Zhdanov,**
Oscillations in Heterogeneous Catalytic Reactions: Carbon Model with Adsorbate-Adsorbate Lateral
Interactions,
Rev. Lett., 8 (2001) pp. 51-59.
257. **V.P. Zhdanov,**
Simulation of Enzymatic Cellular Reactions Complicated by Phase Separation,
Phys. Rev. E, 63(1) (2001) 011908 (6 pages).
258. **V.P. Zhdanov,**
Catalytic Reactions, Surface Restructuring, and Pattern Formation,
Surf. Sci., 486(3) (2001) L513-L518.

259. **V.P. Zhdanov**,
Adsorption-Desorption Kinetics and Chemical Potential of Adsorbed and Gas-Phase Particles,
J. Chem. Phys., 114(10) (2001) pp. 4746-4748.
260. **V.P. Zhdanov**,
Structure Gap in Heterogeneous Catalysis: Kinetic Aspects,
Phys. Rev. B, 64(19) (2001) 193406 (4 pages).
261. **V.P. Zhdanov, (F. Höök, B. Kasemo)**,
Simulation of Two-Dimensional Streptavidin Crystallization,
Proteins, 43(4) (2001) pp. 489-498.
262. **V.P. Zhdanov, (B. Kasemo)**,
Coupled Catalytic Oscillators: Beyond the Mass-Action Law,
Chaos, 11(2) (2001) pp. 335-343.
263. **V.P. Zhdanov, (B. Kasemo)**,
Surface Restructuring, Kinetic Oscillations, and Chaos in Heterogeneous Catalytic Reactions,
J. Stat. Physics, 101(1-2) (2000) pp. 631-647.
264. **V.P. Zhdanov, (B. Kasemo)**,
Rapid Bistable Reactions in Porous Catalysts,
Catal. Lett., 72(1-2) (2001) pp. 7-10.
265. **V.P. Zhdanov, (B. Kasemo)**,
Heat Dissipation in Exothermic Reactions on Non-Traditional Supported Catalysts,
Catal. Lett., 75(1-2) (2001) pp. 61-64.
266. **V.P. Zhdanov, (B. Kasemo)**,
Folding of Bundles of α -Helices in Solution, Membranes, and Adsorbed Overlayers,
Proteins, 42(4) (2001) pp. 481-494.
267. **V.P. Zhdanov, (B. Kasemo)**,
Simulations of Oscillatory Glycolytic Patterns in Cells,
Phys. Chem. Chem. Phys., 3(17) (2001) pp. 3786-3791.
268. **V.P. Zhdanov, (B. Kasemo)**,
Van der Waals Interaction During Protein Adsorption on a Solid Covered by a Thin Film,
Langmuir, 17 (2001) pp. 5407-5409.
269. **V.P. Zhdanov, (B. Kasemo)**,
Standing Fronts in Oscillatory Reactions on Composite Catalytic Surfaces,
Physica D, 151(1) (2001) pp. 73-81.
270. **V.P. Zhdanov, (B. Kasemo)**,
Comments on Rupture of Adsorbed Vesicles,
Langmuir, 17 (2001) pp. 3518-3521.
271. **V.P. Zhdanov, (B. Kasemo)**,
Simulation of CO Adsorption and Oxidation on Pt(110),
J. Chem. Phys., 114(12) (2001) pp. 5351-5357.
272. **V.P. Zhdanov, V.N. Sidelnikov, A.A. Vlasov**,
Dependence of the Efficiency of a Multicapillary Column on the Liquid-Phase Loading Method,
J. Chromatogr. A, 928(2) (2001) pp. 201-207.
273. **(V.V. Zyryanov), O.B. Lapina**,
Mechanochemical Synthesis and Structure of New Phases in the Pb-V-O System,
Inorg. Mater., 37(3) (2001) pp. 264-270 (English language translation).

ABSTRACTS, PROCEEDINGS

1. **(G.N. Abramov, M.N. Achasov, V.M. Aulchenko, K.I. Beloborodov, A.V. Berdyugin, A.G. Bogdanchikov, A.V. Bozhenok, D.A. Bukin, M.A. Bukin, S.V. Burdin), A.F. Danilyuk, (T.V. Dimova, A.A. Drozdetsky, V.P. Druzhinin, V.B. Golubev, V.N. Ivanchenko, P.M. Ivanov, A.A. Korol, S.V. Koshuba, E.A. Kravchenko, L.V. Maksimov, A.E. Obrazovsky, A.P. Onuchin, A.V. Ovchar, E.V. Pakhtusova, M.A. Peshkov, V.M. Popov, E.E. Pyata, A.A. Salnikov, S.I. Serednyakov, V.V. Shary, Yu.M. Shatunov, Z.K. Silagadze, A.A. Sirotkin, A.G. Skripkin, Yu.V. Usov, A.V. Vasiljev, Yu.S. Velikzhanin),**
SND Upgrade,
e+ e-Physics at Intermediate Energies, SLAC, Stanford, California, 30 April- 2 May, Published in eConf C010430: e-Print Archive: hep-ex/0105093.
2. **(M.G. Adamson, V.G. Balakhonov, Yu.S. Chekryshkin, A.C. Heywood), Z.R. Ismagilov, M.A. Kerzhentsev, (E.N. Malyi, V.A. Matyukha),**
Study of Treatment of Mixed Organic Radioactive Wastes in Catalytically Active Molten Salts, *International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial Complex of Western Ural"*, 17-23 June, Perm, Russia. Abstracts, pp. 3-4.
3. **D.G. Aksenov, A.N. Startsev,**
A Comparison of Oxide and Sulfide Forms of the Sibunit Supported Catalysts in a Model Reaction of C-O-Bond Hydrogenolysis,
2nd International Symposium "Molecular Aspects of Catalysis by Sulfides", 14-18 May, Porquerolles, France. Abstracts, P 7.
4. **(E.V. Aleksandrovich, V.A. Chumachenko), T.V. Andrushkevich, V.M. Bondareva, G.Ya. Popova,**
Catalytic Detoxification of Wet Gas Emissions over Oxide Catalysts in Isoprene Production,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 211-215.
5. **(N. Alonso-Vante), I.V. Malakhov, S.G. Nikitenko, E.R. Savinova, D.I. Kochubey,**
In situ Probing Centers of Ru Chalcogenide Electrocatalysis during Oxygen Reduction Using EXAFS Spectroscopy,
200th ECS & 52nd ISE Meeting, 2-7 September, San Francisco, CA. Abstracts, No. 1066.
6. **V.I. Anikeev, (J. Manion), A. Yermakova,**
Kinetics and Thermodynamics of 2-Propanol Dehydration Reaction in Supercritical Water,
International Workshop "Supercritical Fluids as Active Media: Fundamentals and Applications", Valladolid, Spain. Proceedings, pp. 83-94.
7. **V.I. Anikeev, A. Yermakova,**
Chemical Reactions in Supercritical Solvents. Fundamentals and Applications,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 157-158.
8. **V.I. Anikeev, A. Yermakova,**
Thermodynamics of Subcritical and Supercritical Fluids,
6th Conference on Supercritical Fluids and Their Applications, 9-12 September, Maiori, Italy. Proceedings, pp. 381-382.
9. **V.I. Anikeev, A. Yermakova,**
Thermodynamics and Kinetics of Chemical Reactions in Supercritical Fluids,
International Workshop "Supercritical Fluids as Active Media: Fundamentals and Applications", Valladolid, Spain. Proceedings, pp. 27-39.

10. **M.P. Anisimov, (P.K. Hopke), I.N. Shaimordanov, Yu.I. Polygalov,**
Carrier Gas Effects on Vapor Nucleation Rates,
Annual AAAR Conference, 15-19 October, Portland, Oregon, USA. Abstracts, p. 132.
11. **M.P. Anisimov, (P.K. Hopke, S.D. Shandakov), P. Serafimov,**
Estimation of Binary Intermolecular Interaction for Water-Alcohol Systems,
Annual AAAR Conference, 15-19 October, Portland, Oregon, USA. Abstracts, p. 133.
12. **M.P. Anisimov, (P.K. Hopke, S.D. Shandakov, V.A. Pinaev), A.S. Berezina,**
Numerical 2-D Solution of the Flow Diffusion Chamber Heat Mass Transfer Problem,
Annual AAAR Conference, 15-19 October, Portland, Oregon, USA. Abstracts, p. 137.
13. **L.M. Anisimova, (P. L. Hopke, J. Terry),**
Bimodal Size Distribution of Vapor Nucleated Aerosol,
Annual AAAR Conference, 15-19 October, Portland, Oregon, USA. Abstracts, p. 131.
14. **Yu.I. Aristov, (I.V. Koptug), L.Yu. Ilyina, L.G. Gordeeva,**
NMR-Imaging for Analysis of Mass Transfer in Adsorption Heat Pumps,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 70.
15. **Yu.I. Aristov, M.M. Tokarev, L.G. Gordeeva, V.N. Parmon,**
Selective Water Sorbents: New Composite Materials for Accumulation of Low-Potential Heat,
7th International Conference "Hydrogen Materials Science and Chemistry of Metal Hydrides", "ICHMS'01", 16-22 September, Alushta, Crimea. Abstracts, pp. 740-741.
16. **A.B. Ayupov, G.V. Echevsky, E.A. Paukshtis, (D.J. O'Rear, C.L. Kibby),**
External Surface Acidity of Modified Zeolites: ESR via Adsorption of Stable Nitroxyl Radicals and IR Spectroscopy,
13th International Zeolite Conference, 8-13 July, Montpellier, France. Abstracts, 8 pp.
17. **D.E. Babushkin, V.N. Parmon,**
NMR Spectroscopic Characterization of Stabilized Colloids of Copper and Iron Hydroxides by Probe Molecules Relaxation Measurements,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, pp. 72-73.
18. **B.S. Bal'zhinimaev, L.G. Simonova, (V.V. Barelko), A.V. Toktarev, V.I. Zaikovskii, (V.V. Chumachenko),**
The Pt, Pd-Containing Catalysts on a Base of Fiber Glass Woven Supports: A New Alternative for Traditional Vanadium Catalysts in SO₂-Oxidation Process,
5th Italian Conference on Chemical and Process Engineering, "ICheaP-5", 20-23 May, Florence, Italy.
19. **B.S. Bal'zhinimaev, L.G. Simonova, (V.V. Barelko), A.V. Toktarev, (V.V. Chumachenko),**
The Pt, Pd-Containing Catalysts on a Base of Fiber Glass Woven Supports - a New Alternative for Traditional Vanadium Catalysts in SO₂-Oxidizing Process,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 177.
20. **(M.Yu. Barnyakov, V.S. Bobrovnikov, A.R. Buzykaev, G.M. Kolachev, S.A. Kononov, E.A. Kravchenko, G.D. Minakov, A.P. Onuchin), A.F. Danilyuk, (F.F. Guber, A.B. Kurepin, V.A. Krasnov),**
Proposal for the Aerogel Cherenkov Counters for the Pep-N Detector,
e+ e- Physics at Intermediate Energies, SLAC, 30 April-2 May, Stanford, California. Published in eConf C010430. e-Print Archive: hep-ex/0106016.

21. **L.V. Barysheva, E.S. Borisova, V.M. Khanaev,**
Movement of Finely Dispersed Heat Carrier through the Fixed Catalyst Bed,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 180-181.
22. **L.V. Barysheva, V.M. Khanaev, E.S. Borisova,**
Movement of Finely Dispersed Heat Carrier through the Fixed Catalyst Bed,
*Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the
70th Anniversary of the Birthday of Prof. V.A. Koptug*, 13-15 June, Omsk, Russia. Abstracts,
pp. 148-150.
23. **M.V. Batygina, N.M. Dobrynkin, M.D. Marunyak, A.S. Noskov,**
Catalytic Liquid-Phase Oxidation of Chloroform and Dichloroethane by Oxygen,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 8-P-22.
24. **D.V. Bavykin, E.N. Savinov, V.N. Parmon,**
The Study of the Heterojunction Formation in CdS/Me_xS_y (Me=Cu, Ag, Bi, Hg) Nanocolloids,
15th International Conference on Photochemistry, "ICP-XX", 31 July-3 August, Moscow, Russia.
Abstracts, pp. 184-185.
25. **(A.V. Belyaev), M.A. Fedotov, (S.P. Khramenko, V.A. Emel'yanov),**
State of Rhodium in Nitrate Solutions,
XVII International Chernyaev Meeting on Chemistry, Analysis and Technology of Platinum Metals,
17-19 April, Moscow, Russia. Abstracts, p. 13.
26. **A.S. Belyi, V.K. Duplyakin, G.V. Echevsky, V.A. Likhonobov, B.S. Bal'zhinimaev, V.N. Parmon,**
New Catalytic Process of the Liquid Hydrocarbons Production via Direct Inclusion of Light
Paraffins into Target Products,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts, p. 14.
27. **A.S. Belyi, V.K. Duplyakin, V.A. Likhonobov, V.N. Parmon,**
New Catalytic Process of the Liquid Hydrocarbons Production via Direct Inclusion of Light
Paraffins into Target Products,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 10-O-03.
28. **A.S. Bobrin, N.N. Bobrov,**
Application of Gradientless Reactors with Outside Mixing Devices to Studying Kinetics of Catalytic
Processes,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 328-331.
29. **N.N. Bobrov,**
Intensification of Kinetic Experiments with Heterogeneous Catalysts: Potentialities of a
Two-Reactor Flow-Recycling System for Combinatorial Catalysis,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 12-O-09.
30. **N.N. Bobrov,**
Experimental Methods for Catalyst Testing,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September,
Novosibirsk, Russia.
31. **I.I. Bobrova, N.N. Bobrov, V.N. Parmon,**
Partial Oxidation of Methane to Formaldehyde: the Catalysts Testing by an Improved
Flow-Recycling Method,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 10-P-10.

32. **(S. Boghosian), B.S. Bal'zhinimaev, (M. Eriksen, R. Fehrmann, V. Parvulescu, J. Winnick), A.N. Zagoruiko, Y.N. Zhukov,**
Catalytic and Electrochemical Processes for SO₂ and NO_x Emission Abatement: Part 1,
221st ACS Meeting, 1-5 April, San Diego, USA.
33. **V.F. Borbat, O.A. Golovanova, P.A. Kachesova, A.I. Nizovskii, A.V. Bubnov, M.V. Trenikhin, A.N. Vichkanov,**
X-Ray Analysis to Study Pathogenic Biominerals in Human Organism,
International Conference "Crystallogenesi s and Mineralogy", 17-21 September, St. Petersburg, Russia. Abstracts, pp. 54-55.
34. **A.I. Boronin, E.M. Pazhetnov, S.V. Koshcheev,**
XPS and XAES Study of Carbon States on the Surface of Pt(111),
13th International Conference on Vacuum Ultraviolet Radiation, 23 July, Trieste, Italy. Abstracts, ABS1316.
35. **K.P. Brylyakov, N.V. Semikolenova, V.A. Zakharov, E.P. Talsi,**
¹³C NMR Study of Ti(IV) Species Formed via Activation of Cp*TiCl₃ with Methylaluminoxane (MAO),
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 80.
36. **G.D. Bukatov, V.A. Zakharov,**
Effect of Donors on the Number and Propagation Rate Constants for Stereospecific and Non-Stereospecific Centers at Propylene Polymerization with Supported Ziegler-Natta Catalysts,
International Symposium on Future Technology for Polyolefin and Olefin Polymerization Catalysts, March, Tokyo, Japan.
37. **V.I. Bukhtiyarov,**
Atomic Oxygen Species Adsorbed on Silver. Consideration of the "Pressure and Material Gap" Problems in Ethylene Epoxidation,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 19-O-03.
38. **V.I. Bukhtiyarov, I.P. Prosvirin,**
In-situ XPS Study of Oxygen Active in Selective Oxidation of Methanol over Copper,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 21-P-21.
39. **G.A. Bukhtiyarova, V.A. Varnek, V.V. Kaichev, N.S. Sakaeva, I.V. Delii, V.I. Bukhtiyarov,**
A Comparative Study of Alumina- and Silica-Supported Iron-Containing Catalysts Prepared with FeSO₄ as Precursor,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 8-P-56.
40. **L.G. Bulusheva, (A.V. Okotrub), V.L. Kuznetsov, Yu.V. Butenko,**
Topology and Electronic Structure of Caged Carbon,
5th Biennial International Workshop "Fullerenes and Atomic Clusters", "IWFAC'2001", 2-6 July, St. Petersburg, Russia. Abstracts, p. 75.
41. **L.G. Bulusheva, (A.V. Okotrub), V.L. Kuznetsov, A.L. Chuvilin, Yu.V. Butenko, (M.I. Heggie),**
Topology and Electronic Structure of Onion-Like Carbon and Graphite/Diamond Nanocomposites,
Material Research Society Fall Meeting, 26-30 November, Boston, Massachusetts, USA.
42. **L.G. Bulusheva, (A.V. Okotrub), V.L. Kuznetsov, Yu.V. Butenko, (M.I. Heggie),**
An Influence of Defect Structure of Fullerene-Like Carbon on the X-Ray Emission Band,
3rd International Conference on Nanotechnology in Carbon and Related Materials, 29 August – 1 September, Brighton, UK. Abstracts, p. 41.

43. **Yu.V. Butenko, V.L. Kuznetsov, P.A. Simonov, A.L. Chuvilin,**
Structural, Chemical and Optical Properties of the Onion-Like Carbon (OLC) Prepared by Vacuum Annealing of Nanodiamonds,
5th Biennial International Workshop "Fullerenes and Atomic Clusters", "IWFAC'2001", 2-6 July, St. Petersburg, Russia. Abstracts, p. 79.
44. **(Yu.S. Chekryshkin, A.A. Fyodorov), Z.R. Ismagilov, M.A. Kerzhentsev, (T.A. Rozdialovskaya, O.A. Tetenova),**
Deep Catalytic Oxidation of Halogenated Hydrocarbons in Molten Catalysts,
International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial Complex of Western Ural", 17-23 June, Perm, Russia. Abstracts, pp. 25-26.
45. **(Ts.Ts. Cherninov, V.V. Shevlyuk, B.I. Sokolov), G.V. Echevsky, A.S. Noskov, V.N. Parmon,**
A New One-Step CH₄ and C₃-C₄ Paraffins Co-Processing into Aromatic Hydrocarbons,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 202-203.
46. **O.V. Cherstyuk, P.A. Simonov, A.L. Chuvilin, E.R. Savinova,**
Oxidation of CO Monolayer on Nanosized Pt Particles Supported on Glassy Carbon,
200th ECS & 52nd ISE Meeting, 2-7 September, San Francisco, CA. Abstracts, No. 31.
47. **V.V. Chesnokov, R.A. Buyanov,**
Mechanism of Catalytic Filamentous Carbon Formation from Hydrocarbons over the Fe Group Metals and their Alloys with Some other Metals,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, p. 68.
48. **A.R. Cholach, V.M. Tapilin,**
An Electronic Fingerprint of the Adsorbed Species Revealed by Substrate Core Level Excitation,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 21-P-70.
49. **(G.A. Chumakov), N.A. Chumakova,**
Relaxation Oscillations in Catalytic Hydrogen Oxidation Including a Chase on French Ducks,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 75-78.
50. **D.P. Chzsu, E.N. Kudrya, G.G. Savelieva, M.D. Smolikov, V.F. Borbat, A.V. Bubnov,**
Thermoactivation Phenomena in the Supported Catalysts Pt/MeO_x (MeO_x – Al₂O₃, CeO₂, La₂O₃, ZrO₂) for Combustion,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptyug, 13-15 June, Omsk, Russia. Abstracts, pp. 190-192.
51. **(P. Ciambelli), L.A. Isupova, (V. Palma), V.A. Sadykov, V.P. Ivanov, (D. Sannino),**
Monolith Perovskite for Catalytic Combustion of Methane,
3rd European Workshop on Environmental Catalysis "Environmental Catalysis. A Step Forward", "ENVICAT'2001", 2-5 May, Maiori, Italy. Abstracts, pp. 209-210.
52. **A.K. Demin, (P.E. Tsiakaras), V.A. Sobyenin, S.Yu. Hramova,**
Thermodynamic Analysis of a Methane Fed Solid Oxide Fuel Cell System Based on a Proton Conductor,
International Conference on Solid State Ionics, 8-13 July, Cairns, Australia. Extended abstracts, p. 151.
53. **N.M. Dobrynkin, M.V. Batygina, A.S. Noskov,**
Catalytic Oxidation of Pollutants in Industrial Waste Waters,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 226-229.

54. **N.M. Dobrynkin, M.V. Batygina, A.S. Noskov,**
Wet Air Catalytic Oxidation of Industrial Effluents and Waste Waters,
Conference "Ecology and Rational Natural Use", 15-16 October, St. Petersburg, Russia. Abstracts.
55. **N.M. Dobrynkin, A.S. Noskov, M.V. Batygina,**
Wet Air Oxidation of Waste Water and Technological Solutions in the Presence of Solid Catalyst,
International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial Complex of Western Ural", 17-23 June, Perm, Russia. Abstracts, p. 17.
56. **N.M. Dobrynkin, A.S. Noskov, M.V. Batygina,**
Wet Air Oxidation of Waste Water and Technological Solutions in the Presence of Solid Catalyst,
Seminar "New Challenges in Catalysis – III", 29-30 October, Belgrade, Yugoslavia.
57. **N.M. Dobrynkin, P.G. Tsyrunnikov, N.B. Shitova, A.S. Noskov, D.I. Kochubey, V.V. Malakhov, V.I. Bukhtiyarov, I.P. Prosvirin, L.S. Dovlitova, V.I. Zaikovskii, D.A. Shlyapin,**
Supported Ru-Carbon Catalysts for Ammonia Synthesis,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 1-O-23.
58. **N.M. Dobrynkin, P.G. Tsyrunnikov, N.B. Shitova, A.S. Noskov, D.I. Kochubey, V.V. Malakhov, V.I. Bukhtiyarov, I.P. Prosvirin, L.S. Dovlitova, V.I. Zaikovskii, D.A. Shlyapin,**
Study of Carbon Catalysts in Liquid-Phase Oxidation of Heteroatomic Molecules by Oxygen,
15th National Symposium on Catalysis and 2nd Conference of Indo-Pacific Catalysis Association, "CATSYMP-15 & IPCAT-2", 23-25 January, Pune, India. Abstracts, v.1.
59. **V.P. Doronin,**
Modern Trends in Development of Catalytic Petroleum Refining,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.
60. **V.A. Drozdov, V.P. Doronin, T.P. Sorokina, T.I. Gulyaeva,**
Formation of the Texture of Industrial Cracking Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 13-P-24.
61. **S.V. Dudarev, A.V. Toktarev, G.V. Echevsky, (C.L. Kibby, D.J. O'Rear),**
Some Aspects of NU-86 Zeolite Crystallization,
13th International Zeolite Conference, 8-13 July, Montpellier, France. Abstracts, 8 pp.
62. **G.V. Echevsky,**
Application of Zeolite Catalysis for Petroleum Chemistry and Petroleum Refining,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.
63. **G.V. Echevsky, A.B. Ayupov, E.A. Paukshtis, (D.J. O'Rear, C.L. Kibby),**
Coke Deactivation of Acid Sites on ZSM-5 Zeolite,
9th International Symposium on Catalyst Deactivation, 7-10 October, Lexington, Kentucky, USA.
Abstracts, 8 pp.
64. **G.V. Echevsky, O.V. Kikhtyanin, O.V. Klimov, S.V. Dudarev, E.G. Kodenev, S.P. Kildyashev, A.S. Noskov, V.N. Parmon, (Ts.Ts. Cherninov, V.V. Shevlyuk, B.I. Sokolov),**
A New One-Step CH₄ and C₃-C₄ Paraffins Co-Processing into Aromatic Hydrocarbons,
International Gas Research Conference, "IGRC2001", 5-8 November, Amsterdam, The Netherlands. Abstracts, 10 pp.
65. **G.V. Echevsky, O.V. Kikhtyanin, O.V. Klimov, S.V. Dudarev, E.G. Kodenev, S.P. Kildyashev, A.S. Noskov, V.N. Parmon, (Ts.Ts. Cherninov, V.V. Shevlyuk, B.I. Sokolov),**
A New One-Step CH₄ and C₃-C₄ Paraffins Processing into Aromatic Hydrocarbons,
2nd Scientific Applied Conference "Petroleum and Gas Production, Pretreatment and Transportation", 24-27 September, Tomsk, Russia. Abstracts, pp. 36-38.

66. **V.I. Elokhin, E.V. Kovalyov, E.D. Resnyanskii, B.S. Bal'zhinimaev, (A.V. Myshlyavtsev),**
Novel Statistical Lattice Model of the Adsorption and Reaction Processes Performance on the Supported Nanometer-Sized Catalyst Taking into Account the Change of the Shape and of the Surface Morphology of the Catalyst Particle,
222nd ACS National Meeting, 26-30 August, Chicago, Illinois, USA. Abstracts, No 234.
67. **V.I. Elokhin, (E.I. Latkin), V.V. Gorodetskii,**
Mechanisms of Oscillatory and Autowave Behavior During Carbon Monoxide Oxidation over Pt and Pd: Monte Carlo Models,
222nd ACS National Meeting, 26-30 August, Chicago, Illinois, USA. Abstracts, No 94.
68. **(V.A. Emelyanov, A.V. Belyaev), M.A. Fedotov, (S.P. Khrenenko),**
Formation and Transformation of Ruthenium(III) Nitroso-Chloride Complexes in Aqueous Solutions,
XVII International Chernyaev Meeting on Chemistry, Analysis and Technology of Platinum Metals, 17-19 April, Moscow, Russia. Abstracts, p. 49.
69. **(V.A. Emelyanov), M.A. Fedotov, (A.V. Belyaev),**
Studies on Interaction of Ruthenium Nitroso Complexes with Denitrating Reagents,
XVII International Chernyaev Meeting on Chemistry, Analysis and Technology of Platinum Metals, 17-19 April, Moscow, Russia. Abstracts, p. 48.
70. **M.A. Ermakova, D.Yu. Ermakov, G.G. Kuvshinov,**
Production of Hydrogen and Filamentous Carbon by Direct Cracking of Methane over Nickel and Iron Catalysts,
17th North American Catalysis Society Meeting, "17th NACS-2001", 3-8 June, Toronto, Canada. Abstracts, p. 124.
71. **M.A. Ermakova, D.Yu. Ermakov, G.G. Kuvshinov,**
Synthesis of Catalytic Systems with Use of Heterophase Sol-Gel Technology,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, Limerick, Ireland. Abstracts, 1-P-79.
72. **M.A. Ermakova, D.Yu. Ermakov, G.G. Kuvshinov,**
Design of Structure of Dispersed Catalytic Systems Based on Heterophase Sol-Gel Synthesis,
17th North American Catalysis Society Meeting, "17th NACS-2001", 3-8 June, Toronto, Canada. Abstracts, p. 52.
73. **M.A. Ermakova, D.Yu. Ermakov, M.Yu. Lebedev, G.G. Kuvshinov,**
Filamentous Carbon Templated SiO₂ Aerogel: Structure and Catalytic Properties,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-P-78.
74. **M.A. Fedotov,**
NMR Tools for Detecting of Colloids and Polynuclear Species,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 88.
75. **(R. Fehrmann), B.S. Bal'zhinimaev, (S. Boghosian, M. Eriksen, V. Parvulescu, J. Winnick), A.N. Zagoruiko, (Y.N. Zhukov),**
Catalytic and Electrochemical Processes for SO₂ and NO_x Emission Abatement: Part II,
221st ACS National Meeting, 1-5 April, San Diego, USA.
76. **V.B. Fenelonov,**
Fundamentals of Adsorption and Theory of Catalysts Texture Control,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.

77. **(F. Frusteri, L. Spadaro, A. Mezzapica), A.L. Chuvilin,**
Carbon Deposited in CO₂ Reforming of CH₄ over Ni/MgO Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
Limerick, Ireland. Abstracts, 6-P-44.
78. **V.V. Galvita, V.D. Belyaev, G.L. Semin, V.A. Sobyenin,**
Hydrogen Production by Steam Reforming of Ethanol or Dimethyl Ether: Fuel Cell Application,
6th Italian Seminar on Catalysis, Fundamentals and Application to Environmental Problems,
18-24 June, Grado, Italy. Abstracts, p. 1.
79. **V.V. Galvita, V.D. Belyaev, (P. Tsiakaras), V.A. Sobyenin,**
Eastern Mediterranean Ethanol Decomposition over Pd-Based Catalyst in Steam Presence,
Chemical Engineering Conference for Collaborative Research, Ankara, Turkey. Abstracts,
pp. 155-156.
80. **A.P. Gerasev,**
Thermodynamic Theory of Autowave Processes in Fixed Catalyst Bed,
4th All-Russian Seminar "Modelling of Non-Equilibrium Systems - 2001", October, Krasnoyarsk,
Russia. Abstracts, pp. 30-31.
81. **(A.Sh. Gladkaya, I.F. Golovaneva, O.N. Evstafieva), M.A. Fedotov, (G.G. Aleksandrov),**
Pt(IV) Complexes with N-Nitrozoamidated Polyamines: Structure and Properties,
XVII International Chernyaev Meeting on Chemistry, Analysis and Technology of Platinum Metals,
17-19 April, Moscow, Russia. Abstracts, p. 37.
82. **V.V. Goidin, A.V. Tkachev, V.V. Molchanov,**
Mechanochemical Transformation of Betulin and Ursolic Acid,
International Conference "Fundamental Bases of Mechanochemical Technologies", 16-18 August,
Novosibirsk, Russia. Abstracts, p. 102.
83. **V.V. Gorodetskii, V.I. Elokhin, (S.I. Fadeev, G.A. Chumakov, M.M. Slin'ko, A.A. Ukharskii,**
M.A. Vasylyev, A.G. Blaschuk, B.N. Nieuwenhuys, N.I. Jaeger, R. Imbihl),
Experimental and Theoretical Studies of Temporal and Spatial Self-Organization Processes in
Oxidative Reactions over Platinum Group Metals: An Approach to Bridge the Gap between Single
Crystals and Nano-Sized Supported Catalyst Particles,
*4th INTAS Interdisciplinary Symposium on Physical and Chemical Methods in Biology, Medicine
and Environment (Grant Monitoring Conference)*, 30 May-3 June, Moscow, Russia. Proceedings,
pp. 73-74.
84. **V.V. Gorodetskii, (S. Wehner, F. Zaera),**
Isothermal Study of CO+O₂ and NH₃+O₂ Reactions on Rh(111) Using a Molecular Collimated
Beam Doser,
4th World Congress on Oxidation Catalysis, 16-21 September, Berlin, Germany. Abstracts, v. II,
pp. 277-278.
85. **(N.V. Gretshman), N.I. Kuznetsova, L.I. Kuznetsova, V.A. Likholobov,**
Reductive Activation of Dioxygen in Pt-HPC Catalytic Systems: Oxidation of Hydrocarbons,
Bangkok International Conference on Heterogeneous Catalysis, 7-9 January, Bangkok, Thailand.
Abstracts, p. 33.
86. **(A.C. Heywood), Z.R. Ismagilov, S.R. Khairulin, (V.F. Komarov, G.V. Kutsenko, L.N. Rolin,**
G.V. Sakovich, V.A. Shandakov),
Development of the Technology for Utilization of the Large-Scale Composite Solid Rocket
Propellant Charges,
*International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial
Complex of Western Ural"*, 17-23 June, Perm, Russia. Abstracts, p. 49.

87. **(R. Hubaut), O.B. Lapina, D. Khabibulin, (A. Rives, C.E. Scott),**
Synergy Phenomenon in Bulk Ruthenium-Vanadium Mixed Sulfides: ^{51}V NMR and ESR Studies, *NATO ARW "Magnetic Resonance in Colloid and Interface Science"*, 26-30 June, St. Petersburg, Russia. Abstracts, p. 102.
88. **K.G. Ione,**
Preparation of Precursors and Monomers for Organic Synthesis over Solid Catalysts, *"Contemporary Problems of Organic Chemistry"*, *The Scientific Conference Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptuyug*, 17-21 September, Novosibirsk, Russia. Abstracts.
89. **K.G. Ione,**
Studies on Catalytic Properties of Fe-Containing Catalysts (Ores) in Abiogenic Synthesis of Hydrocarbons from $\text{CO}+\text{CO}_2+\text{H}_2$ Mixtures, *International Scientific-Applied Conference "Forecast of Oil-Gas Bearing of the New and Old Platforms. New Ideas of the 21st Century"*, 4-8 June, Kazan, Russia. Abstracts.
90. **K.G. Ione,**
Catalytic Phenomena in Abiogenous Origin of the Hydrocarbon Masses, *5th European Congress on Catalysis, "EUROPACAT-V"*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 14-P-01.
91. **K.G. Ione,**
Novel Technologies of Motor Fuels Synthesis at Small Refineries as a Method to Improve Economical Efficiency of their Production, *5th Annual Roundtable "Refining and Petrochemicals in Russia and the CIS Republics"*, 13 December, Vienna, Austria.
92. **K.G. Ione, V.M. Mysov,**
Integration of the Results of Pilot Testing of Catalytic CO , CO_2 and H_2 -Containing Gases Conversion to Motor Fuels, *Russian Conference "Actual Problems of Petrochemistry"*, 17-22 April, Moscow, Russia. Abstracts, p. 34.
93. **K.G. Ione, V.M. Mysov,**
Novel Technologies for Production of Motor Fuels and Valuable Organic Products from Coals and Natural Gas, *Conference "Low Tonnage Oil and Gas Processing in Republic Sakha (Yakutia)"*, 26-27 July, Yakutsk, Russia. Abstracts, pp. 88-92.
94. **K.G. Ione, V.M. Mysov, V.G. Stepanov,**
New Approach to Catalytic Abiogenic Hydrocarbon Synthesis in the Earth's Crust, *Russian Conference "Actual Problems of Petrochemistry"*, 17-22 April, Moscow, Russia. Abstracts, p. 326.
95. **Z.R. Ismagilov,**
Progress Trends in Development of Catalytic Processes for Environmental Protection, *Extension Courses in the Field of Catalysts and Catalytic Processes*, 24-29 September, Novosibirsk, Russia.
96. **I.Z. Ismagilov, Z.R. Ismagilov, M.A. Kerzhentsev, (Yu.V. Ostrovsky), V.N. Parmon, (N.V. Pestereva, L.N. Rolin, G.V. Sakovich), V.A. Sazonov, (V.N. Yeryomin, Yu.L. Zuev),**
Environmentally Safe Catalytic Technology for the Utilization of Liquid Rocket Fuel UDMH and Wastes, Containing UDMH, *International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial Complex of Western Ural"*, 17-23 June, Perm, Russia. Abstracts, pp. 52-53.

97. **I.Z. Ismagilov, M.A. Kerzhentsev, Z.R. Ismagilov, (V.A. Shandakov, F. Garin, H.J. Veringa),**
Oxidation of 1,1-Dimethylhydrazine over Heterogeneous Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 7-P-03.
98. **I.Z. Ismagilov, M.A. Kerzhentsev, V.A. Rogov, (V.A. Shandakov),**
Regularities of Intermediate Products Generation upon Catalytic Destruction of 1,1-Dimethylhydrazine,
*All-Russian Scientific-Applied Conference "Utilization of Rockets Using Solid Fuel. Problems and
Methodology of Mix Solid Rocket Fuels, Wastes and Liquid Rocket Fuels Residues Utilization in the
Rocket-Space Technique"*, 25-28 September, Byisk, Russia.
99. **Z.R. Ismagilov, M.A. Kerzhentsev, I.Z. Ismagilov, V.A. Sazonov, V.N. Parmon,
G.L. Elizarova, O.P. Pestunova, (V.A. Shandakov, Yu.L. Zuev, L.N. Rolin, V.N. Eryomin,
N.V. Pestereva),**
Catalytic Combustion of Liquid Rocket Fuel 1,1-Dimethylhydrazine,
32nd International ICT-Conference "Energetic Materials - Ignition, Combustion and Detonation",
3-6 July, Karlsruhe, Germany.
100. **Z.R. Ismagilov, M.A. Kerzhentsev, I.Z. Ismagilov, V.A. Sazonov, V.N. Parmon,
G.L. Elizarova, O.P. Pestunova, (V.A. Shandakov, Yu.L. Zuev, L.N. Rolin, V.N. Eryomin,
N.V. Pestereva, F. Garin, H.J. Veringa),**
Oxidation of Unsymmetrical Dimethylhydrazine over Oxide and Noble Metal Catalysts. Solution of
Environmental Problems of Production, Storage and Disposal of Highly Toxic Rocket Fuel,
3rd European Workshop on Environmental Catalysis "Environmental Catalysis. A Step Forward",
"ENVICAT'2001", 2-5 May, Maiori, Italy. Abstracts, p. 97.
101. **Z.R. Ismagilov, M.A. Kerzhentsev, (Yu.V. Ostrovsky, B.I. Lunyushkin),**
Ecologically Safe Destruction of Liquid Organic Radioactive Wastes,
4th International Conference "Radiation Safety: Ecology – Nuclear Energy", 24-28 September,
St. Petersburg, Russia. Abstracts, v.3, p. 219-220.
102. **Z.R. Ismagilov, M.A. Kerzhentsev, V.A. Sazonov, I.Z. Ismagilov, V.N. Parmon, G.L. Elizarova,
O.P. Pestunova, (Yu.V. Ostrovsky, Yu.L. Zuev, V.N. Eryomin, N.V. Pestereva, L.N. Rolin,
V.A. Shandakov),**
Development of Multi-Reactor Process for Catalytic Destruction of Highly Toxic Rocket Fuel
1,1-Dimethylhydrazine,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 207-210.
103. **Z.R. Ismagilov, R.A. Shkrabina, L.T. Tsykoza, S.A. Yashnik, N.V. Shikina, V.A. Sazonov,
(H.J. Veringa),**
Supported Honeycomb Monolith DeNO_x Catalysts Performance in Presence of H₂S and H₂O,
1st International Conference on Structured Catalysts and Reactors, "ICOSCAR-1", 21-24 October,
Delft, The Netherlands.
104. **Z.R. Ismagilov, R.A. Shkrabina, S.A. Yashnik, N.V. Shikina, I.P. Andrievskaya,
S.R. Khairulin, V.A. Ushakov, (J.A. Moulijn, I.V. Babich),**
Supported Honeycomb Monolith Catalysts for High-Temperature Ammonia Decomposition and H₂S
Removal,
1st International Conference on Structured Catalysts and Reactors, "ICOSCAR-1", 21-24 October,
Delft, The Netherlands.
105. **Z.R. Ismagilov, (V.G. Vasiliev, A.A. Kachesov, A.I. Falchevsky, V.N. Antsiferov,
Yu.V. Danchenko), S.E. Glaznev, S.A. Yashnik,**
Environmentally Friendly Catalytic Water-Heating Boiler,
*International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial
Complex of Western Ural"*, 17-23 June, Perm, Russia. Abstracts, p. 14.

106. **Z.R. Ismagilov, S.A. Yashnik, S.R. Khairulin, R.A. Shkrabina, N.V. Shikina, (I.V. Babich, J.A. Moulijn),**
Ammonia Decomposition and Hydrogen Sulfide Adsorption on Monolithic Supported Mn-Containing Catalysts,
3rd European Workshop on Environmental Catalysis “Environmental Catalysis. A Step Forward”, “ENVICAT’2001”, 2-5 May, Maiori, Italy. Abstracts, p. 253.
107. **Z.R. Ismagilov, S.A. Yashnik, R.A. Shkrabina, S.R. Khairulin, V.A. Ushakov, (J.A. Moulijn, A.D. van Langeveld),**
Deactivation of Manganese Oxide Based Honeycomb Monolith Catalyst under Reaction Conditions of Ammonia Decomposition at High Temperature,
1st International Conference on Structured Catalysts and Reactors, “ICOSCAR-1”, 21-24 October, Delft, The Netherlands.
108. **L.A. Isupova, G.M. Alikina, S.V. Tsybulya, A.N. Salanov, N.N. Boldyreva, E.S. Rusina, I.A. Ovsyannikova, V.A. Rogov, R.V. Bunina, V.A. Sadykov,**
Honeycomb Supported Perovskite Catalysts for High-Temperature Processes,
3rd European Workshop on Environmental Catalysis “Environmental Catalysis. A Step Forward”, “ENVICAT’2001”, 2-5 May, Maiori, Italy. Abstracts, pp. 59-60.
109. **L.A. Isupova, V.A. Sadykov,**
Mechanochemical Synthesis and Catalytic Activity of $\text{LaMe}^1\text{Me}^2\text{O}_3$ Perovskite Oxides,
8th European Conference on Solid State Chemistry, “ECSSC’2001”, 4-7 July, Oslo, Norway.
110. **L.A. Isupova, S.V. Tsybulya, G.N. Kryukova, V.A. Sadykov,**
Mechanical Activation in $\text{A}^1\text{A}^2\text{BO}_3$ Perovskite Synthesis for Oxidation Catalytic Processes,
4th World Congress on Oxidation Catalysis, “4WCOC”, 16-21 September, Berlin/Potsdam, Germany. Extended abstracts, v.1, pp. 37-41.
111. **L.A. Isupova, I.S. Yakovleva, V.A. Sadykov,**
Mechanical Activation in $\text{A}^1\text{A}^2\text{BO}_3$ Perovskite Synthesis for Oxidation Catalytic Processes,
International Conference “Fundamental Bases of Mechanochemical Technologies”, 16-18 August, Novosibirsk, Russia. Abstracts, p. 74.
112. **S.S. Ivanchev,**
Polyolefins – the Present and Future,
Ukrainian-Russian Symposium on High-Molecular Compounds, 28-30 October, Donetsk, Ukraine. Abstracts, p. 15.
113. **S.S. Ivanchev,**
New Catalysts for Ethylene Polymerization and Copolymerization with α -Olefins,
European Polymer Federation Congress, 15-20 July, Eindhoven, The Netherlands. Abstracts, p. 12.
114. **E.A. Ivanov, S.I. Reshetnikov, A.N. Startsev,**
Modeling in the Periodic Operation of Benzene Hydrogenation over the Sulfide Catalysts,
2nd International Symposium “Molecular Aspects of Catalysis by Sulfides”, 14-18 May, Porquerolles, France. Abstracts, P 6.
115. **(T.I. Izaak), A.N. Salanov, (G.M. Mokrousov, O.V. Babkina),**
Metal-Polymer Composites Obtained from Macroporous Polymer Networks,
European Polymer Federation Congress, 15-20 July, Eindhoven, The Netherlands.
116. **(T.I. Izaak), A.N. Salanov, (G.M. Mokrousov, O.V. Babkina),**
Phase Separation in the Polyacrylic Gels and Structure of the Porous Networks Obtained on their Base,
European Polymer Federation Congress, 15-20 July, Eindhoven, The Netherlands.

117. **V.V. Kanazhevskii, B.N. Novgorodov, V.P. Shmachkova, N.S. Kotsarenko, D.I. Kochubey**, EXAFS Studies of the Structure of Zr(IV) Complexes in Aqueous Salt Solutions, *III All-Russian Conference on Clusters Chemistry "Polynuclear Systems and CO₂ Activation"*, 20-25 August, Kazan-Cheboksary, Russia. Abstracts, p. 57.
118. **V.N. Kashkin, V.S. Lakhmostov, I.A. Zolotariskii, A.S. Noskov, (J.J. Zhou)**, Studies on the Onset Velocity of Turbulent Fluidization for Alpha-Alumina Particles, *15th International Conference on Chemical Reactors, "CHEMREACTOR-15"*, 5-8 June, Helsinki, Finland. Abstracts, pp. 126-128.
119. **V.N. Kashkin, M.S. Mel'gunov, A.I. Madyarov, S.A. Pokrovskaya, N.A. Chumakova, I.A. Zolotariskii, V.B. Fenelonov**, Separation of Methane-Ethane Gas Mixtures on Carbon Microporous Adsorbents by Pressure Swing Adsorption, *15th International Conference on Chemical Reactors, "CHEMREACTOR-15"*, 5-8 June, Helsinki, Finland. Abstracts, pp. 321-323.
120. **D.V. Kazachkin, D.G. Aksenov, V.B. Goncharov, E.A. Paukshtis, A.N. Startsev**, *In situ* FTIR Investigation of the Donor Molecule Adsorption over the Sulfide HDS Catalysts, *2nd International Symposium "Molecular Aspects of Catalysis by Sulfides"*, 14-18 May, Porquerolles, France. Abstracts, P 15.
121. **(E. Kemnitz), V.A. Sadykov, T.G. Kuznetsova, A.V. Simakov, N.N. Sazonova, N.N. Bulgakov, E.B. Burgina, E.M. Moroz, V.I. Zaikovskii, E.A. Paukshtis, V.P. Ivanov, S.N. Trukhan, S.A. Beloshapkin, (V.V. Lunin, A. Aboukais)**, Effect of Cation and Anion Modification of Lanthanum Manganite on its Bulk and Surface Oxygen Properties as Related to Catalysis of Propane Deep and Selective Oxidation, *4th World Congress on Oxidation Catalysis, "4WCOC"*, 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.1, pp. 249-252.
122. **(E. Kemnitz), V.A. Sadykov, T.G. Kuznetsova, A.V. Simakov, N.N. Sazonova, N.N. Bulgakov, E.B. Burgina, E.M. Moroz, V.I. Zaikovskii, E.A. Paukshtis, V.P. Ivanov, S.N. Trukhan, (V.V. Lunin, A. Aboukais)**, Fluorine Modified Lanthanum Manganite: Bulk and Surface Oxygen Mobility as Related to Catalysis of Propane Oxidative Dehydrogenation, *5th European Congress on Catalysis, "EUROPACAT-V"*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 5-O-26.
123. **D.F. Khabibulin, A.A. Shubin, O.B. Lapina, (K.M. Eriksen, R. Fehrmann)**, ⁵¹V NMR Spectra of the M₆(VO)₄(SO₄)₈ Compounds Containing Mixed-Valent Vanadium(IV)-Vanadium(V), *NATO ARW "Magnetic Resonance in Colloid and Interface Science"*, 26-30 June, St. Petersburg, Russia. Abstracts, p. 107.
124. **D.F. Khabibulin, A.A. Shubin, O.B. Lapina**, Correlation of ⁵¹V NMR Parameters with Local Environment of Vanadia Sites, *NATO ARW, 9th International Symposium on Magnetic Resonance in Colloid and Interface Science*, 26-30 June, St. Petersburg, Russia. Abstracts, p. 108.
125. **S.R. Khairulin, Z.R. Ismagilov**, Direct Catalytic Oxidation of Hydrogen Sulfide. A New Advanced Technology for Oil and Gas Processing Industries, *International Symposium "Combustion and Plasmochemistry"*, 9-11 October, Almaty, Kazakh Republic. Abstracts, pp. 68-69.

126. **A.A. Khassin, V.V. Molchanov, T.M. Yurieva, I.Sh. Itenberg, V.N. Parmon,**
 Selective Hydrogenation of Acetylene to Ethylene Using the Cobalt Containing Catalyst,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
 University of Limerick, Limerick, Ireland. Abstracts, 1-P-36.
127. **A.A. Khassin, T.M. Yurieva, I.Sh. Itenberg, G.N. Kustova, E.A. Paukshtis, V.V. Kaichev,
 V.I. Bukhtiyarov, V.F. Anufrienko, V.N. Parmon,**
 Cobalt-Containing Catalysts Derived from Hydrotalcites: A Strong Metal-Support Interaction?,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
 University of Limerick, Limerick, Ireland. Abstracts, 6-P-70.
128. **O.A. Kholdeeva, G.M. Maksimov, R.I. Maksimovskaya, L.A. Kovaleva, M.A. Fedotov,
 (V.A. Grigoriev, C.L. Hill),**
 Titanium-Containing Heteropolytungstates: Synthesis, Characterization and Use as Homogeneous
 Models for Studying Mechanisms of H₂O₂-Based Selective Oxidations,
NATO ASI Polyoxometalate Molecular Science, 25 August-5 September, Tenerife, Spain. Abstracts.
129. **O.A. Kholdeeva, S.N. Stasko, (S.A. Popov, A.V. Tkachev),**
 Oxidation of Thioethers and Allylic Alcohols Catalyzed by Vanadium Complexes with New Chiral
 Terpenoid-Based Ligands,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
 University of Limerick, Limerick, Ireland. Abstracts, 16-P-09.
130. **O.A. Kholdeeva, N.N. Trukhan, V.N. Romannikov, V.N. Parmon, (J. Mrowiec-Bialoń,
 A.B. Jarzębski),**
 A New Environmentally Friendly Method for the Production of 2,3,5-Trimethylbenzoquinone,
*3rd European Workshop on Environmental Catalysis "Environmental Catalysis. A Step Forward",
 "ENVICAT'2001"*, 2-5 May, Maiori, Italy. Abstracts, pp. 133-134.
131. **V.A. Kirillov, N.A. Kuzin, (I.A. Onufriev, I.V. Khlystov),**
 An Environmentally Clean Catalytic Water Boiler for Combustion of Natural Gas,
3rd European Congress on Chemical Engineering, "ECCE-3", 26-28 June, Nuerenberg, Germany.
 Abstracts.
132. **N.V. Kirillova, N.I. Kuznetsova, L.I. Kuznetsova, V.A. Likholobov,**
 Heteropolyacid Catalysts Prepared from Platinum Salts of H₃PMO₁₂O₄₀ for O₂/H₂ Oxidation,
*10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis,
 "SHHC-10"*, 2-6 July, Lyon, France. Abstracts, p. 63.
133. **V.A. Kirillov, I.A. Mikhailova, (S.I. Fadeev, M.G. Slin'ko),**
 The Exothermic Catalytic Reaction in a Single Partially-Wetted Porous Catalyst Particle,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
 Finland. Abstracts, pp. 129-132.
134. **D.I. Kochubey,**
 Catalysis and Physicochemical Methods,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk,
 Russia.
135. **E.G. Kodenev, G.V. Echevsky,**
 Study of the Effect of Ratio Between Hydro/Dehydrating and Acid Functions of Zeolite Catalysts
 on their Efficiency in Light Paraffins Aromatization,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts.
136. **O.V. Komova, A.V. Simakov, V.A. Rogov, D.I. Kochubey, G.V. Odegova, V.V. Kriventsov,
 E.A. Paukshtis, V.A. Ushakov, N.N. Sazonova, T.A. Nikoro,**
 Investigation of the State of Copper in Supported Copper-Titanium Oxide Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
 University of Limerick, Limerick, Ireland. Abstracts, 6-P-84.

137. **(D.A. Konevets), I.E. Beck, (V.N. Sil'nikov, G.V. Shishkin),**
Design and Synthesis of 1,4-Diazabicyclo[2.2.2]Octane / Imidazole Conjugates as RNA Phosphodiester Bonds Cleaving Agents,
International Conference "RNA as Therapeutic and Genomic Target", 30 August-2 September, Novosibirsk, Russia. Ed. V. Koval, "In-Quarto" Print House, p. 68.
138. **(G.A. Konin, A.N. Il'ichev, V.A. Matyshak, T.I. Khomenko, V.N. Korchak, D.M. Papakhin, D.Yu. Kuritsyn), A.S. Ivanova, V.A. Sadykov, (A.Ya. Rozovskii, J.R.H. Ross),**
The Mechanism of NO_x SCR by Propylene in the Excess of O₂ on ZrO₂,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 21-O-10.
139. **(I.V. Koptug), L.Yu. Ilyina, Yu.I. Aristov, M.M. Tokarev, (R.Z. Sagdeev), V.N. Parmon,**
Application of ¹H NMR Microimaging to Study Water Vapor Sorption by Composite Selective Sorbents of Water,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 115.
140. **(I.V. Koptug), L.Yu. Ilyina, (R.Z. Sagdeev), V.N. Parmon,**
NMR Imaging of Mass Transport and Related Phenomena in Porous Catalysts and Sorbents,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 30.
141. **N.A. Koryabkina, V.A. Ushakov, Z.R. Ismagilov, V.A. Rogov, N.A. Rudina,**
Nickel Supported Mixed Oxide Catalysts for Dry Reforming of Methane,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 5-P-13.
142. **(O.S. Koscheeva, O.V. Shuvaeva), L.I. Kuznetsova,**
The Use of Heteropoly Complexes for the Arsenic Speciation in Environmental Analysis,
NATO ASI Polyoxometalate Molecular Science, 25 August-5 September, Tenerife, Spain. Abstracts.
143. **G.A. Kovalenko, O.V. Komova, A.V. Simakov, V.V. Khomov, N.A. Rudina,**
Glucoamylase Immobilized on Carbonized Ceramics as a Heterogeneous Biocatalyst for Starch Hydrolysis,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 17-O-03.
144. **G.A. Kovalenko, O.V. Komova, A.V. Simakov, V.V. Khomov, N.A. Rudina,**
Immobilization of Glucoamylase on Carbonized Ceramics to Develop Heterogeneous Biocatalyst for Continuous Starch Hydrolysis,
10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, "SHHC-10", 2-6 July, Lyon, France.
145. **O.P. Krivoruchko,**
Reactor for Catalysts' Synthesis by Precipitation as a Complicated Hierarchical System with Interactive Levels,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 324-327.
146. **G.N. Kryukova, G.A. Zenkovets, S.V. Tsybulya, V.N. Parmon,**
Structural Genesis of the Nanostructured Molybdenum Doped Vanadia-Based Catalysts,
4th World Congress on Oxidation Catalysis, "4WCOC", 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.1, pp. 59-60.
147. **(E.S. Kurkina, N.L. Semendyaeva), A.I. Boronin,**
The Mechanism of the Low Temperature Nitrogen Desorption from Iridium Surface,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 249-252.

148. **D.G. Kuvshinov, A.M. Glushenkov,**
Technological Peculiarities of the Process of Filamentous Carbon Production from Hydrocarbons Containing Inert Admixtures,
III Scientific Technical Conference "Novel Chemical Technologies: Production and Application,
August, Penza, Russia.
149. **D.G. Kuvshinov, G.G. Kuvshinov,**
Effect of Inert Admixtures on the Process of Utilization of Hydrocarbon Gases to Produce Filamentous Carbon,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 5-P-32.
150. **V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, (B. Segall),**
Low Temperature Diamond Graphitization,
12th European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, Nitrides and Silicon Carbide, 2-7 September, Budapest, Hungary. Abstracts, 5.3.16.
151. **V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, (E.D. Obratsova, A.V. Okotrub), L.G. Bulusheva, A.I. Romanenko,**
Synthesis and Properties of Onion-Like Carbon Prepared by the Annealing of Nanodiamond,
5th Biennial International Workshop "Fullerenes and Atomic Clusters", "IWFAC'2001", 2-6 July, St. Petersburg, Russia. Abstracts, p. 110.
152. **V.L. Kuznetsov, A.N. Usoltseva, A.L. Chuvilin, (E.D. Obratsova, J.-M. Bonard),**
Thermodynamic Analysis of Carbon Nucleation on the Metal Surface,
5th Biennial International Workshop "Fullerenes and Atomic Clusters", "IWFAC'2001", 2-6 July, St. Petersburg, Russia. Abstracts, p. 24.
153. **V.L. Kuznetsov, A.N. Usoltseva, A.L. Chuvilin, (E.D. Obratsova, J.-M. Bonard),**
Thermodynamic Analysis of Carbon Nucleation on the Metal Surface,
Material Research Society Fall Meeting, 26-30 November, Boston, Massachusetts, USA.
154. **E.V. Kuznetsova, G.L. Elizarova, E.N. Savinov,**
Development of Photocatalysts for Oxidation Reactions Under Visible Light,
15th International Conference on Photochemistry, "ICP-XX", 31 July-3 August, Moscow, Russia. Abstracts, p. 338.
155. **N.I. Kuznetsova, L.I. Kuznetsova, N.V. Kirillova, V.A. Likholobov,**
Novel Catalytic Systems for Producing Alcohols and Ketones via O₂/H₂ Oxidation of Hydrocarbons,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 182-184.
156. **A.O. Kuzmin, G.L. Elizarova, L.G. Matvienko, A.A. Lysova, E.R. Savinova, V.N. Parmon,**
Cu- and Fe-Hydroxides as Novel Efficient Catalysts for the Partial Oxidation of Hydrocarbons in Water-Organic Systems,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 10-P-02.
157. **O.B. Lapina,**
⁵¹V NMR Studies of Vanadia Based Catalysts,
14th Conference of the International Society of Magnetic Resonance, "ISMAR-2001", 19-23 August, Rhodes, Greece. Abstracts, p. 60.
158. **O.B. Lapina, (P.R. Bodart, J.-P. Amoureux),**
⁵¹V 3QMAS NMR and its Application for the Studies of Vanadia Based Catalysts,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 50.

159. **E.I. Latkin, V.I. Elokhin, V.V. Gorodetskii,**
Spiral Waves in the Monte Carlo Model of CO Oxidation over Pd(110) Caused by Synchronization via CO_{ads} Diffusion Between Different Sections of Catalytic Surface,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 59-62.
160. **A.V. Lavrenov, V.P. Finevich, E.A. Paukshtis, V.K. Duplyakin, B.S. Bal'zhinimaev,**
Alkylation of Isobutane with Butenes over Zirconium-Sulfate Catalysts,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptug, 13-15 June, Omsk, Russia. Abstracts, pp. 172-174.
161. **M.Yu. Lebedev, D.G. Kuvshinov, V.V. Shinkarev, G.G. Kuvshinov,**
Peculiarities of Direct Oxidation of Hydrogen Sulfide into Sulfur in Oxygen Excess on the Filamentous Carbon,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-O-20.
162. **V.A. Likholobov,**
Catalysis. Introduction and Main Conceptions,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.
163. **E.A. Lobytsev, V.S. Sal'nikov, P.G. Tsyrunnikov,**
Comparable Tests of Supported Palladium and Oxide Catalysts for Methane Oxidation,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, p. 186.
164. **S.V. Lopatkin, V.G. Stepanov, K.G. Ione,**
The Effect of the Reaction Mixture Composition on the Transformation of C₆-C₈ Hydrocarbons over a Fe-Containing Zeolite HZSM-5,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 10-O-04.
165. **S.V. Lopatkin, V.G. Stepanov, K.G. Ione,**
Hydrocarbons Transformation over the Catalysts, Containing Zeolites with Various Structure,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts, p. 156.
166. **(A.I. Lukashovich), V.V. Goidin, R.A. Buyanov, (G.A. Tolstikov), V.V. Molchanov,**
Application of Mechanochemistry in Hydroalumination Reactions,
International Conference "Fundamental Bases of Mechanochemical Technologies", 16-18 August, Novosibirsk, Russia. Abstracts, p. 1.
167. **B.N. Luk'yanov, V.A. Kirillov, N.A. Kuzin, M.M. Danilova, A.V. Kulikov, A.B. Shigarov,**
Catalytic Heating Elements for Autonomous Domestic Heating Systems,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 174-176.
168. **M.V. Luzgin, A.G. Stepanov,**
Carbonylation of Hydrocarbons on Solid Acid Catalysts. *In situ* Solid-State NMR Study,
1st EFCATS School on Catalysis "New Trends in Catalysis Research and Application", 28 March-1 April, Prague, Czech Republic. Materials, p. 17.
169. **M.V. Luzgin, A.G. Stepanov, V.P. Shmachkova, N.S. Kotsarenko,**
n-Pentane Conversion on Sulfated Zirconia in the Absence and Presence of Carbon Monoxide. Evidence for Monomolecular Mechanism of Isomerization from the ¹³C MAS NMR Study,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 21-P-14.

170. **A.A. Lysova, A.O. Kuzmin, G.L. Elizarova, E.R. Savinova, V.N. Parmon,**
Kinetic Studies on the Mechanism of Gaseous Hydrocarbons Oxidation with Hydrogen Peroxide in Presence of Iron and Copper Hydroxides in Aqueous Solutions,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 5-P-08.
171. **A.A. Lysova, A.O. Kuzmin, G.L. Elizarova, E.R. Savinova, V.N. Parmon,**
Kinetic Studies on the Mechanism of Gaseous Hydrocarbons Oxidation with Hydrogen Peroxide in Presence of Iron and Copper Hydroxides in Aqueous Solutions,
4th World Congress on Oxidation Catalysis, "4WCOC", 16-21 September, Berlin/Potsdam,
Germany. Abstracts, v. II, p. 67.
172. **A.I. Madyarov, N.A. Chumakova,**
Parametric Sensitivity of the Methanol Oxidation Process as a Solution of a Boundary Value Problem with a Parameter,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 107-110.
173. **R.I. Maksimovskaya, V.M. Bondareva, G.M. Maksimov,**
Studies of the Products and Mechanism of Thermolysis of P-Containing Heteropoly Acids with Application of ³¹P NMR in Solution and Solid State,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg,
Russia. Abstracts, p. 124.
174. **A.V. Mashkina, L.N. Khairulina,**
Catalytic Hydrogenation of Diethyldisulfide to Ethylmercaptane,
All-Russian Symposium on Chemistry of Silicon and Sulfur Organic Compounds,
2-7 December, Irkutsk, Russia. Abstracts.
175. **A.V. Matveev,**
Critical Phenomena on the Pd(110) Plane: Surface Phase Transformations, Chemical Waves and Self-Oscillations,
XXXIX International Scientific Student Conference "Students and Scientific and Technological Advance. Physics", 9-13 April, Novosibirsk, Russia. Abstracts, p. 99.
176. **A.V. Matveev,**
Critical Phenomena on the Pd(110) Plane: Surface Phase Transformations, Chemical Waves and Self-Oscillations,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptyug, 13-15 June, Omsk, Russia. Abstracts,
pp. 174-176.
177. **I.V. Mishakov, V.V. Chesnokov, R.A. Buyanov,**
Regularities of Chlorohydrocarbons Conversion over Ni- and Co-Containing Catalysts,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia.
Abstracts, pp. 87-88.
178. **I.V. Mishakov, V.V. Chesnokov, R.A. Buyanov,**
Chlorohydrocarbons Utilization by "Carbide Cycle" Mechanism over Ni- and Co-Containing Catalysts,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptyug, 13-15 June, Omsk, Russia. Abstracts, p. 47.
179. **V.V. Molchanov, V.V. Goidin, R.A. Buyanov, (A.V. Tkachov, A.I. Lukashevich),**
Mechanochemical Reactions under High-Pressure Gas Phase,
International Conference "Fundamental Bases of Mechanochemical Technologies", 16-18 August,
Novosibirsk, Russia. Abstracts, p. 28.

180. **V.V. Molchanov, M.G. Zuev, S.V. Bogdanov,**
Mechanochemical Synthesis of Tantalates of Rare-Earth Metals,
International Conference "Fundamental Bases of Mechanochemical Technologies", 16-18 August,
Novosibirsk, Russia. Abstracts, p. 114.
181. **A.N. Moseichuk, A.V. Maltsev, V.S. Zakharenko,**
Photoadsorption of Oxygen and Nitrogen Oxides on Air Exposed Alumina and Silica,
1st International Conference on Semiconductor Photochemistry, "SP-1", 23-25 July, Glasgow, UK.
Abstracts, p. 98.
182. **A.S. Noskov,**
Catalytic Methods to Purify Gas Exhausts and Waste Waters,
International Conference on Heterogeneous Catalysis, 7-9 January, Bangkok, Thailand.
183. **A.S. Noskov,**
Catalytic Technologies for Secondary Primary Goods Processing and Environment Protection,
II Congress on Chemical Technologies, 30-31 October, St. Petersburg, Russia. Abstracts. p.13.
184. **A.S. Noskov, I.A. Zolotarskii, S.A. Pokrovskaya, V.N. Korotkikh, V.N. Kashkin,
V.V. Mokrinskii, E.M. Slavinskaya,**
Simulation of Tubular Reactor for Nitrous Oxide Production,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 161-164.
185. **(A.V. Okotrub), L.G. Bulusheva, V.L. Kuznetsov, Yu.V. Butenko, (M.I. Heggie),**
Probing the Electronic Structure of Onion-Like Carbon by X-Ray Emission Spectroscopy,
15th International Winterschool on Electronic Properties of Novel Materials, 3-10 March,
Kirchberg/Tirol, Austria. Abstracts, p. 75.
186. **A.G. Okunev, Yu.I. Aristov,**
Macrokinetic Regularities of Dissolution of Highly Dispersed Silicas in Aqueous Alkali Solutions,
XIX All-Russian School-Symposium of Young Scientists on Chemical Kinetics, 12-16 February,
Klyaz'ma, Russia. Abstracts, p. 52.
187. **A.G. Okunev, V.E. Sharonov, A.V. Gubar, T.A. Krieger, I.G. Danilova, E.M. Moroz,
V.N. Parmon, Yu.I. Aristov,**
Composite Sorbents of Carbon Dioxide: K₂CO₃-in-Porous Alumina,
III All-Russian Conference on Cluster Chemistry, 20-25 August, Cheboksary, Russia. Abstracts, p. 30.
188. **A.G. Okunev, V.E. Sharonov, E.M. Moroz, I.G. Danilova, T.A. Krieger, Yu.I. Aristov,**
Sorption of the Carbon Dioxide from Wet Gases by K₂CO₃-in-Porous Matrix: Influence of the
Matrix Nature,
3rd European Conference of Chemical Engineering, 24-26 June, Nuerenberg, Germany.
189. **A.G. Okunev, V.E. Sharonov, V.N. Parmon, Yu.I. Aristov,**
Composite Sorbents of Carbon Dioxide for Environmentally Sound Catalytic Processes,
3rd International Workshop on Environmental Catalysis, 2-4 May, Maiory, Italy. Abstracts, pp. 269-270.
190. **A.I. Oruzhenikov, A.I. Nizovskii, M.V. Trenikhin, A.V. Bubnov, A.N. Salanov,**
Investigation of the Process of Separation and Physico-Chemical Characteristics of Magnetic
Fraction of Ashes Produced Upon Combustion of Ekibastuz Coals,
3rd Scientific Applied Conference "Fuel Mineral Component, Slag Formation, Boilers Cleaning",
19-21 June, Chelyabinsk, Russia. Abstracts.
191. **N.M. Ostrovskii,**
Catalyst Deactivation Models Based on Stage Mechanisms,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki,
Finland. Abstracts, pp. 153-156.

192. **(Yu.V. Ostrovsky, B.I. Lunyushkin, G.M. Zabortsev), Z.R. Ismagilov, M.A. Kerzhentsev, (E.N. Malyi, V.A. Matyukha, V.G. Balakhonov),**
New Technologies for Destruction of Liquid and Solid Radioactive Wastes,
International Scientific Seminar "Innovation Technologies – 2001", 20-22 June, Krasnoyarsk, Russia. Abstracts, v.2, pp. 128-132.
193. **(Yu.V. Ostrovsky, G.M. Zabortsev), Z.R. Ismagilov, M.A. Kerzhentsev,**
Pyrolysis of Lean Extraction Mixtures in Fluid Bed,
4th International Conference "Radiation Safety: Ecology – Nuclear Energy", 24-28 September, St. Petersburg, Russia. Abstracts, v.3, p. 225-226.
194. **Z.P. Pai,**
Catalytic Liquid-Phase Technologies for Purification of Waste Gases from Toxic Emissions (SO₂, NO_x, As₂O₃, H₂S, COS, HCN),
International Seminar "Scientific-Technical Potential for Conversion in the Military-Industrial Complex of Western Ural", 17-23 June, Perm, Russia. Abstracts, pp. 78-79.
195. **Z.P. Pai,**
SLP-As Technology for Purification of Waste Gases and Waters from Sulfur and Arsenic Compounds,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 218-221.
196. **N.A. Pakhomov,**
Scientific Bases for Catalysts Preparation. Catalysts Supports,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.
197. **G.I. Panov, K.A. Dubkov, E.V. Starokon, E.A. Paukshtis, A.M. Volodin,**
Mechanism of Selective Oxidation by α -Oxygen over Fe-ZSM-5 Zeolites,
4th World Congress on Oxidation Catalysis, 16-20 September, Berlin-Potsdam, Germany. Extended Abstracts, v.2, pp. 147-148.
198. **G.I. Panov, (A. Uriarte), L.V. Piryutko, V.S. Chernyavsky, A.S. Kharitonov,**
New Catalytic Systems for Hydroxylation of Benzene to Phenol by Nitrous Oxide,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-O-07.
199. **V.N. Parmon,**
Catalysis in Nontraditional and Renewable Energetics,
Bangkok International Conference on Heterogeneous Catalysis, 7-9 January, Bangkok, Thailand. Abstracts, pp. 104-106.
200. **V.N. Parmon, Z.R. Ismagilov, V.A. Kirillov, A.D. Simonov,**
Catalytic Combustion to Solve Ecological and Energetics Problems,
All-Russian Conference "Energetics of Russia in XXI Century: Problems and Scientific Bases of Stable and Safety Development", 14-17 September, 2000, Irkutsk, Russia. Proceedings, pp. 162-180.
201. **V.N. Parmon, Z.R. Ismagilov, V.A. Kirillov, A.D. Simonov,**
Catalytic Combustion to Solve Ecological and Energetics Problems,
6th Session of International School on Executive Training in the Field of Engineering Chemistry, 5-9 February, Moscow, Russia. Proceedings, v.2, pp. 50-72.
202. **V.N. Parmon, Z.R. Ismagilov, V.A. Kirillov, A.D. Simonov,**
Catalytic Combustion in Solving the Environmental and Energy Problems,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, p. 7.

203. **V.N. Parmon, (J.T. Gleaves), V.N. Snytnikov, (G.I. Dudnikova, S.A. Nikitin, V.O. Stoyanovsky, V.A. Vshivkov, G.S. Yablonsky), V.S. Zakharenko,**
Protoplanetary Disk as Space Chemical Reactor,
1st Annual JURRISS Conference, 16-18 July, Washington D.C., USA. Abstracts, pp. 27-28.
204. **V.N. Parmon, V.A. Sobyenin,**
Developments of the United Institute of Catalysis in the Field of New Catalysts and Catalytic Technologies,
International Symposium "Adaptation and Transfer of Advanced Technologies in Asia", 21-23 August, Novosibirsk, Russia. Abstracts, p. 49.
205. **S.N. Pavlova, L.I. Kuznetsova, M.N. Bredikhin,**
Supported Catalysts Based on Pd and P-Mo-V Heteropolycomplexes for Low-Temperature CO Oxidation: *In situ* IR Study,
4th World Congress on Oxidation Catalysis, "4WCOC", 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.2, pp. 287-290.
206. **S.N. Pavlova, V.A. Sadykov, V.N. Parmon, I.I. Bobrova, I.A. Zolotarskii, V.A. Kuzmin, A.N. Salanov, R.V. Bunina, N.F. Saputina, O.I. Snegurenko, Z.Yu. Vostrikov,**
Partial Oxidation of Methane to Synthesis Gas at Short Contact Times over Pt-Promoted Ceria-Zirconia Solid Solutions Supported onto Corundum Monoliths,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 5-O-04.
207. **S.N. Pavlova, V.A. Sadykov, Yu.V. Frolova, N.F. Saputina, P.M. Vedenikin, I.A. Zolotarskii, V.A. Kuzmin,**
The Effect of the Catalytic Layer Design on Oxidative Dehydrogenation of Propane over Monoliths at Short Contact Times,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 274-277.
208. **V.N. Pavlyuchenko, O.V. Sorochinskaya, S.S. Ivanchev, (M. Skrifvars, G.S. Kreichman, V.V. Klubin),**
Hollow-Particle Latexes: Physicochemical Aspects of Preparation,
Nordiska Polymerdagarna (Nordic Polymer Days), June, Stockholm, Sweden. Abstracts, p. 147.
209. **V.N. Pavlyuchenko, O.N. Primachenko, S.S. Ivanchev, S.Ya. Khaikin,**
Latex Self-Organized Groups,
3rd International Conference "Chemistry of Highly-Ordered Substances and Scientific Bases of Nanotechnology", 26-29 June, St.-Petersburg, Russia. Abstracts, pp. 68-70.
210. **O.P. Pestunova, G.L. Elizarova, Z.R. Ismagilov, M.A. Kerzhentsev, V.N. Parmon,**
Detoxication of Water Containing 1,1-Dimethylhydrazine by Catalytic Oxidation with Dioxygen and Hydrogen Peroxide over Cu- and Fe-Containing Catalysts,
3rd European Workshop on Environmental Catalysis "Environmental Catalysis. A Step Forward", "ENVICAT'2001", 2-5 May, Maiori, Italy. Abstracts, p. 137.
211. **O.P. Pestunova, G.L. Elizarova, Z.R. Ismagilov, M.A. Kerzhentsev, V.N. Parmon,**
Catalytic Oxidation of UDMH for Solution of Environmental Problems of Missilery,
32nd International ICT-Conference "Energetic Materials - Ignition, Combustion and Detonation", 3-6 July, Karlsruhe, Germany.
212. **O.P. Pestunova, G.L. Elizarova, V.N. Parmon,**
Detoxication of 1,1-Dimethylhydrazine Water Containing by Catalytic Oxidation with Dioxygen and Hydrogen Peroxide over Fe-Hydroxides,
4th World Congress on Oxidation Catalysis, 16-21 September, Berlin/Potsdam, Germany. Abstracts.

213. **O.P. Pestunova, O.L. Ogorodnikova, G.L. Elizarova, E.N. Savinov, V.N. Parmon,**
Photocatalytic Oxidation of 1,1-dimethylhydrazine in Aqueous Solution with TiO₂ and FeO(OH) as Photocatalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 8-P-29.
214. **L.M. Plyasova, T.A. Krieger, A.A. Khasin, V.N. Parmon,**
Separate Determination of Temperature of the Active Component and its Support for an Operating Ni/MgO Catalyst via a High-Temperature *in situ* XRD Technique,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 6-P-33.
215. **O.Yu. Podyacheva, Z.R. Ismagilov, N.V. Shikina, S.A. Yashnik, V.V. Kuznetsov, V.A. Ushakov, V.A. Rogov, (H.J.Veringa),**
Synthesis of High Temperature Combustion Catalysts on Metal Foams for Catalytic Heat Exchanger Application,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 8-P-28.
216. **G.Ya. Popova, T.V. Andrushkevich, I.I. Zakharov, Y.A. Chesalov, E.S. Stoyanov,**
Mechanism of the Selective Oxidation of Formaldehyde on V-Ti-O Catalyst,
4th World Congress on Oxidation Catalysis, "4WCOC", 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.1, pp. 399-400.
217. **T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, A.L. Chuvilin, V.A. Likholobov,**
Stable Carbon Growth from Methane over Modified Ni-Al₂O₃ Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September,
University of Limerick, Limerick, Ireland. Abstracts, 5-P-01.
218. **T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, V.A. Likholobov,**
Modifying of Ni and Fe Catalysts to Increase the Efficiency of Methane Decomposition,
2nd Regional Conference "Chemistry of Oil and Gas – 2001", 24-25 October, Tomsk, Russia. Abstracts.
219. **S.I. Reshetnikov, N.M. Ostrovskii, G.S. Litvak, V.A. Sobyenin, N.A. Davydov, A.N. Ilyin,**
Mathematical Modeling of Regeneration of the Catalyst for Tetrafluoroethane and Pentafluoroethane Production,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 259-261.
220. **A.I. Romanenko, (O.B. Anikeeva, A.V. Okotrub), V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, (C. Dong, Y. Ni),**
Temperature Dependence of Electroresistivity, Negative and Positive Magnetoresistivity of Carbon Nanoparticles,
5th Biennial International Workshop "Fullerenes and Atomic Clusters", "IWFAC'2001", 2-6 July, St. Petersburg, Russia. Abstracts, p. 54.
221. **A.I. Romanenko, (O.B. Anikeeva, A.V. Okotrub), V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, (C. Dong, Y. Ni),**
Temperature Dependence of Electroresistivity, Negative and Positive Magnetoresistivity of Carbon Nanoparticles,
Material Research Society Fall Meeting, 26-30 November, Boston, Massachusetts, USA.
222. **V.A. Sadykov,**
Oxide Catalysts,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.

223. V.A. Sadykov, V.P. Doronin, T.P. Sorokina, T.G. Kuznetsova, G.M. Alikina, R.V. Bunina, D.I. Kochubey, B.N. Novgorodov, E.A. Paukshtis, V.B. Fenelonov, A.Yu. Derevyankin, V.I. Zaikovskii, L.M. Plyasova, A.S. Ivanova, S.A. Beloshapkin, V.F. Anufrienko, N.T. Vasenin, (A.Ya. Rozovskii, V.F. Tretyakov, T.N. Burdeynaya, M.N. Davydova, V.A. Matyshak, G.A. Konin, J.R.H. Ross, J. P. Breen), Nanostructured Catalysts of NO_x Selective Reduction by Hydrocarbons Based upon Zirconia-Pillared Clays, *3rd European Workshop on Environmental Catalysis “Environmental Catalysis. A Step Forward”*, “ENVICAT’2001”, 2-5 May, Maiori, Italy. Abstracts, pp. 171-172.
224. V.A. Sadykov, V.P. Doronin, T.P. Sorokina, T.G. Kuznetsova, G.M. Alikina, R.V. Bunina, D.I. Kochubey, B.N. Novgorodov, E.A. Paukshtis, V.B. Fenelonov, A.Yu. Derevyankin, V.I. Zaikovskii, L.M. Plyasova, S.A. Beloshapkin, V.N. Kolomiichuk, V.F. Anufrienko, N.T. Vasenin, (A.Ya. Rozovskii, V.F. Tretyakov, T.N. Burdeynaya, M.N. Davydova, V.A. Matyshak, G.A. Konin, J. R. H. Ross, J.P. Breen), Thermally Stable Zirconia-Pillared Clays with Supported Copper and Cobalt Oxides as Nanostructured Catalysts of NO_x Selective Reduction by Hydrocarbons: Synthesis and Properties, *5th European Congress on Catalysis, “EUROPACAT-V”*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-O-19.
225. V.A. Sadykov, A.S. Ivanova, R.V. Bunina, G.M. Alikina, T.G. Kuznetsova, E.A. Paukshtis, V.I. Zaikovskii, E.M. Moroz, V.F. Anufrienko, S.A. Beloshapkin, (V.A. Matyshak, G.A. Konin, A.Ya. Rozovskii, V.F. Tretyakov, T.N. Burdeynaya, M.N. Davydova, J.R.H. Ross, J.P. Breen), Transition Metal Oxide Supported Low Temperature Cubic Zirconia Catalysts for Selective Catalytic Reduction of NO_x Under Lean-Burn Conditions, *5th European Congress on Catalysis, “EUROPACAT-V”*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 7-P-22.
226. V.A. Sadykov, T.G. Kuznetsova, G.M. Alikina, V.P. Doronin, T.P. Sorokina, R.V. Bunina, D.I. Kochubey, B.N. Novgorodov, E.A. Paukshtis, V.B. Fenelonov, A.Yu. Derevyankin, V.I. Zaikovskii, S.A. Beloshapkin, V.N. Kolomiichuk, V.F. Anufrienko, N.T. Vasenin, (A.Ya. Rozovskii, V.F. Tretyakov, T.N. Burdeynaya, M.N. Davydova, V.A. Matyshak, G.A. Konin, J.R.H. Ross, J.P. Breen), Precious Metals Effect on Performance of Cu - and Co-Loaded Zirconia-Pillared Clays in NO_x Selective Reduction by Hydrocarbons, *5th European Congress on Catalysis, “EUROPACAT-V”*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 7-O-03.
227. V.A. Sadykov, S.N. Pavlova, R.V. Bunina, T.G. Kuznetsova, I.A. Zolotarskii, V.A. Kuzmin, A.V. Simakov, N.N. Sazonova, S.A. Veniaminov, V.N. Parmon, E.A. Paukshtis, V.A. Rogov, I.I. Bobrova, N.N. Bulgakov, (Z.Yu. Vostrikov), Methane Selective Oxidation into Syngas at Short Contact Times: Design of Monolith Catalysts and their Performance, *12th CRC International Symposium on Advanced Chemical Conversion of Methane*, 18-20 November, Hokkaido University, Sapporo, Japan. Abstracts, pp. 11-12.
228. V.A. Sadykov, S.N. Pavlova, M.V. Chaikina, G.V. Zabolotnaya, R.I. Maksimovskaya, S.V. Tsybulya, E.B. Burgina, V.I. Zaikovskii, G.S. Litvak, Yu.V. Frolova, D.I. Kochubey, V.V. Kriventsov, E.A. Paukshtis, V.N. Kolomiichuk, V.P. Ivanov, V.F. Anufrienko, N.N. Boldyreva, (N.N. Kuznetsova, V.V. Lunin, D. Agrawal, R. Roy), Synthesis of Framework Complex Zirconium Phosphates via Mechanochemical Activation of Mixed Solid Salts, *International Conference “Fundamental Bases of Mechanochemical Technologies”*, 16-18 August, Novosibirsk, Russia. Abstracts, p. 10.

229. **V.A. Sadykov, S.N. Pavlova, Yu.V. Frolova, N.F. Saputina, A.V. Simakov, N.N. Sazonova, I.A. Zolotariskii, V.A. Kuzmin, D.I. Kochubey, V.V. Kriventsov, E.A. Paukshtis, P.M. Vedenikin, V.I. Zaikovskii, V.P. Ivanov, V.F. Anufrienko, (R. Roy, D.K. Agrawal),** Oxidative Dehydrogenation of Propane over Monoliths at Short Contact Times: Effect of the Catalyst Composition and Gas-Phase Reactions, *4th World Congress on Oxidation Catalysis, "4WCOC"*, 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.1, pp. 151-154.
230. **V.A. Sadykov, S.A. Veniaminov, D.I. Kochubey, B.N. Novgorodov, T.G. Kuznetsova, E.B. Burgina, E.M. Moroz, E.A. Paukshtis, V.P. Ivanov, S.N. Trukhan, S.A. Beloshapkin, Yu.V. Potapova, (V.V. Lunin, A. Aboukais, E. Kemnit),** Cation/Anion Modified Ceria-Zirconia Solid Solutions Promoted by Pt as Catalysts of Methane Oxidation into Syngas by Water in Reversible Redox Cycles, *5th European Congress on Catalysis, "EUROPACAT-V"*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 5-O-08.
231. **V.A. Sadykov, I.A. Zolotariskii, S.N. Pavlova, R.V. Bunina, V.A. Kuz'min, A.V. Simakov, N.F. Saputina, V.A. Chumachenko, L.L. Gogin, O.I. Snegurenko, Z.Yu. Vostrikov, L.N. Bobrova,** Catalytic Conversion of Natural Gas to Reduce Harmful Emissions of Gas-Turbine Engines, *Russian Scientific-Applied Conference "Thermophysics of Combustion and Environmental Protection"*, 13-15 October, Rybinsk, Russia.
232. **A.N. Salanov, V.N. Bibin, A.I. Titkov,** Oscillation in CO Oxidation on Pd(110) and Structural Transformation in Overlayers, *5th European Congress on Catalysis, "EUROPACAT-V"*, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 21-O-02.
233. **(R.I. Samoilova, S.A. Dikanov, E. Lisenkin), V.F. Anufrienko, N.S. Kotsarenko, (E. Zinger, J. Hüttermann),** Reversible Nitrosyl Adduct Formation on the Sulfated Zirconium and Aluminium Oxide Surface), *NATO ARW "Magnetic Resonance in Colloid and Interface Science"*, 26-30 June, St. Petersburg, Russia. Abstracts, pp. 138-139.
234. **E.N. Savinov, A.N. Pershin,** Photocatalytic Purification of Air from Organic Admixtures: Advantages and Problems, *1st International Conference on Semiconductor Photochemistry, "SP-1"*, 23-25 July, Glasgow, Scotland. Abstracts, p. 50.
235. **E.R. Savinova, O.V. Cherstyuk, P.A. Simonov, A.L. Chuvilin,** Electrocatalysis at Pt Nanoparticle Surfaces, *Fundamental Problems of Electrochemistry: Electrocatalysis & Heterogeneous Catalysis*, 11-13 May, Pommersfelden, Germany.
236. **(W. Schmidt), A.V. Toktarev, (F. Schüth), K.G. Ione, (K. Unger),** The Influence of Different Silica Sources on the Crystallization Kinetics of Zeolite Beta, *13th International Zeolite Conference*, 8-13 July Montpellier, France. Abstracts, 8 pp.
237. **N.V. Selivanova, M.N. Timofeeva, K.P. Brylyakov, Z.P. Pai,** Selective Oxidation of Cyclic Olefins by Hydrogen Peroxide Catalyzed with Peroxopolymetallates, *Youth Scientific School-Conference "Actual Problems of Organic Chemistry"*, 2-6 April, Ekaterinburg, Russia. Abstracts, p. 223.
238. **V.A. Semikolenov,** Supported Metal Catalysts, *Extension Courses in the Field of Catalysts and Catalytic Processes*, 24-29 September, Novosibirsk, Russia.

239. **V.A. Semikolenov, I.I. Il'ina, I.L. Simakova,**
Effect of Heterogeneous and Homogeneous Pathways on Selectivity of Pinane-2-ol to Linalool Isomerization,
10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, "SHHC-10", 2-6 July, Lyon, France. Abstracts, p. 148.
240. **N.V. Semikolenova, E.P. Talsi, D.E. Babushkin, A.P. Sobolev, V.A. Zakharov,**
Homogeneous and Supported Catalysts Based on 2,6-Bis(imine)Pyridyl Complexes of Fe and Co. Study on the Intermediates and Ethylene Polymerization,
10th International Symposium on Relation Between Homogeneous and Heterogeneous Catalysis, "SHHC-10", June, Lyon, France.
241. **V.E. Sharomov, A.V. Gubar, A.G. Okunev, Yu.I. Aristov, V.N. Parmon,**
Kinetics and Mechanism of Carbon Dioxide Sorption from Wet Gases by Composite Sorbents "K₂CO₃ in Porous Matrices",
XIX All-Russian School-Symposium of Young Scientists on Chemical Kinetics, 12-16 February, Klyaz'ma, Russia. Abstracts, p. 61.
242. **A.B. Shigarov, A.V. Kulikov, N.A. Kuzin, V.A. Kirillov,**
Modelling of Critical Phenomena for the Liquid/Vapor-Gas Exothermic Reaction on a Single Catalyst Pellet,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 142-145.
243. **V.V. Shinkarev, M.Yu. Lebedev,**
Peculiarities of Sulfur Deposition on the Filamentous Carbon upon H₂S Oxidation in the Excess of Oxygen,
III Scientific Technical Conference "Novel Chemical Technologies: Production and Application", August, Penza, Russia.
244. **N.B. Shitova, D.A. Shlyapin, E.A. Lobyntsev, P.V. Snytnikov,**
Cluster Pt₁₅ – Precursor of the Catalysts for Carbon Oxide Oxidation in the Presence of Hydrogen,
III All-Russian Conference on Clusters Chemistry "Polynuclear Systems and CO₂ Activation", 20-25 August, Kazan-Cheboksary, Russia. Abstracts, p. 48.
245. **D.A. Shlyapin,**
Effect of Preparation Conditions of Ru-Me/Sibunit Catalysts on their Activity in the Ammonia Synthesis,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, p. 198.
246. **D.A. Shlyapin, N.M. Dobrynkin, N.B. Shitova,**
Effect of the Nature and Method of Deposition of Alkali Component on the Activity of Ru-Me/Sibunit Catalysts in Low-Temperature Ammonia Synthesis,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptug, 13-15 June, Omsk, Russia. Abstracts.
247. **V.P. Shmachkova, N.S. Kotsarenko, M.A. Fedotov,**
An Effect of Composition of Phosphate-Alumina Complexes in the Solution on the Phase Composition of Solid Aluminium Phosphates,
III All-Russian Conference on Clusters Chemistry "Polynuclear Systems and CO₂ Activation", 20-25 August, Kazan-Cheboksary, Russia. Abstracts, p. 82.
248. **(A.S. Shmelev), I.A. Zolotarskii, S.I. Reshetnikov,**
Computational Systems for Chemical Technological Schemes Calculation,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.

249. **V.I. Simagina, I.V. Stoyanova, V.A. Yakovlev, V.A. Likholobov,**
Synthesis and Characterization of Supported Bimetallic Catalysts for Hydrodechlorination of Polychlorinated Compounds,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, p. 318.
250. **V.I. Simagina, I.V. Stoyanova, V.A. Yakovlev,**
Synthesis and Characterization of Supported Bimetallic Catalysts for Hydrodechlorination of Polychlorinated Compounds,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 8-P-49.
251. **A.A. Slepterev, E.N. Kudrya,**
Design of Modified Oxide and Palladium Catalysts for Mine Methane Combustion,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptug, 13-15 June, Omsk, Russia. Abstracts, p. 185.
252. **A.A. Slepterev, E.N. Kudrya, P.G. Tsyrlunikov,**
Design of Modified Oxide and Palladium Catalysts for Mine Methane Combustion,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, p. 194.
253. **P.V. Snytnikov, D.A. Shlyapin, E.A. Lobyntsev,**
Pt/C, Ru/C, Pd/C – Novel Catalysts for CO Oxidation in the Presence of Hydrogen,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, pp. 85-86.
254. **V.N. Snytnikov, Vlad.N. Snytnikov, V.O. Stoyanovsky,**
Methane Conversion with Vibrational-Excited Carbon Dioxide,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 4-P-11.
255. **G.P. Snytnikova, V.G. Stepanov, K.G. Ione,**
Production of Alkybenzenes over Zeolite Catalysts,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts, p. 71.
256. **O.A. Soboleva, L.V. Barysheva,**
Preparation and Investigation of Model Catalyst for Isobutane Dehydrogenation,
XXXIX International Science Student Conference, "Students and Scientific and Technological Advance. "Chemistry", 9-13 April, Novosibirsk, Russia. Abstracts, pp. 82-83.
257. **V.A. Sobyenin, V.D. Belyaev, V.V. Galvita, A.K. Demin, (P.E. Tsiakaras),**
Performance of a SOFC Fed by Ethanol Reforming Products,
International Conference on Solid State Ionics, 8-13 July, Cairns, Australia. Extended Abstracts, p. 150.
258. **V.A. Sobyenin, V.V. Galvita, V.D. Belyaev, G.L. Semin,**
Hydrogen Production by Steam Reforming of Ethanol or Dimethyl Ether,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 10-P-36.
259. **A.N. Startsev, G.I. Aleshina, D.G. Aksenov,**
A Temperature-Programmed Technique in Studying Sulfide Catalysts: Comparison of "Reduction" and "Desorption" Modes,
2nd International Symposium "Molecular Aspects of Catalysis by Sulfides", 14-18 May, Porquerolles, France. Abstracts, pp. 33-34.

260. **A.N. Startsev, I.I. Zakharov, V.N. Parmon,**
An Unexpected Phenomenon in Heterogeneous Catalysis: Oxidative Addition of Hydrogen to the Sulfide Catalysts,
10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, "SHHC-10", 2-6 July, Lyon, France.
261. **A.N. Startsev, I.I. Zakharov, V.N. Parmon,**
An Unexpected Phenomenon in Heterogeneous Catalysis: Oxidative Addition of Hydrogen to the Sulfide Catalysts,
2nd International Symposium "Molecular Aspects of Catalysis by Sulfides", 14-18 May, Porquerolles, France. Abstracts, pp. 15-16.
262. **(E.F. Stefoglo, V.I. Drobyshevich), V.A. Semikolenov, (I.V. Kuchin, O.P. Zhukova),**
Elevation of Performance of Gas-Liquid Reactors on Solid Catalyst,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 122-125.
263. **A.G. Stepanov,**
The New Routes for Hydrocarbon Conversion on Solid Acid Catalysts as Studied by Solid-State NMR,
International Catalysis Workshop for Young Scientists-2001 "New Perspectives on Catalysis for Sustainable Chemical Technologies", "ICWYS-2001", 23-27 September, Beijing, China. Abstracts, pp. 19-20.
264. **A.G. Stepanov, M.M. Alkaev, A.A. Shubin,**
Probing the Mobility of iso-Butyl Alcohol Inside Zeolite H-ZSM-5 by Deuterium Solid State NMR,
13th International Zeolite Conference, 8-13 July, Montpellier, France. Recent Research Reports, 13-RR-05.
265. **A.G. Stepanov, M.V. Luzgin, (H. Ernst, D. Freude),**
Conversion of n-Butene-1-¹³C on Zeolite H-Ferrite. *In situ* ¹³C MAS NMR Study,
13th International Zeolite Conference, 8-13 July, Montpellier, France. Recent Research Reports, 12-RR-02.
266. **A.G. Stepanov, A.A. Shubin, M.M. Alkaev, M.V. Luzgin, (H. Jobic, C.R.A. Catlow),**
Deuterium NMR Study of Alkanes Dynamics Inside Zeolite ZSM-5,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 147.
267. **V.G. Stepanov, K.G. Ione,**
"Zeoforming" Process for the Production of High-Octane Gasolines over Zeolite Catalyst,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts, p. 222.
268. **V.G. Stepanov, K.G. Ione,**
"Zeoforming" – Technology for Upgrading of Straight-Run Gasolines Fractions and Gas Condensates to High Octane Motor Fuels,
Conference "Low Tonnage Oil and Gas Processing in Republic Sakha (Yakutia)", 26-27 July, Yakutsk, Russia. Abstracts, pp. 153-160.
269. **V.G. Stepanov, S.V. Kapterev, L.P. Poslovina, Yu.V. Malozemov, K.G. Ione,**
Hexene-1 Oligomerization over Zeolite Catalysts,
Russian Conference "Actual Problems of Petrochemistry", 17-22 April, Moscow, Russia. Abstracts, p. 223.
270. **V.G. Stepanov, G.P. Snytnikova, K.G. Ione,**
A New Effective Process for Motor Gasoline Production over Zeolite Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 13-O-07.

271. **A.P. Suknev, (S.G. Masters), V.B. Goncharov, B.S. Bal'zhinimaev, (R. Fehrmann), A.V. Toktarev, L.G. Simonova, (V.V. Barelko),**
SCR by NH₃ over Impregnated Fiber-Glass Catalysts,
17th Meeting of the North American Catalysis Society "Horizons of Catalysis", 3-8 June, Toronto, Ontario, Canada.
272. **O.V. Sumenkova, A.D. Simonov, N.A. Yazykov,**
Catalytic Incineration of Municipal Sewage Sludge,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 222-225.
273. **E.P. Talsi, K.P. Brylyakov, A.P. Sobolev,**
EPR and NMR Spectroscopic Studies of the Reactive Intermediates of Homogeneous Catalytic Oxidation,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 151.
274. **V.V. Terskikh, I.L. Moudrakovskii, (C.I. Ratcliffe, J.A. Ripmeester, C.J. Reinhold, P.A. Anderson, P.P. Edwards),**
NMR and ESR of Alkali Metals Confined in Porous Matrices,
NATO ARW "Magnetic Resonance in Colloid and Interface Science", 26-30 June, St. Petersburg, Russia. Abstracts, p. 64.
275. **S.F. Tikhov, V.A. Sadykov, I.I. Bobrova, Yu.V. Potapova, V.B. Fenelonov, S.V. Tsybulya, S.N. Pavlova, A.S. Ivanova, V.Yu. Kruglyakov, N.N. Bobrov,**
Composite Steam Reforming Catalysts Prepared from Al₂O₃/Al Matrix-Precursor,
6th Natural Gas Conversion Symposium, 17-22 June, Girdwood Alaska, USA. Abstracts, p. 6.
276. **M.N. Timofeeva, M.M. Matrosova, G.M. Maksimov, T.V. Reshetenko, L.B. Avdeeva, E.A. Paukshtis, A.L. Chuvilin, V.A. Likholobov,**
Investigation of Adsorptive and Catalytic Properties of Heteropoly Acids with Various Compositions and Structures,
NATO ASI Polyoxometalate Molecular Science, 25 August-5 September, Tenerife, Spain. Abstracts.
277. **M.N. Timofeeva, M.M. Matrosova, G.M. Maksimov, T.V. Reshetenko, L.B. Avdeeva, E.A. Paukshtis, A.L. Chuvilin, V.A. Likholobov,**
Investigation of Adsorptive and Catalytic Properties of Heteropoly Acids with Various Compositions and Structures,
10th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, "SHHC-10", 2-6 July, Lyon, France. Abstracts, p. 160.
278. **M.N. Timofeeva, M.M. Matrosova, G.M. Maksimov, T.V. Reshetenko, L.B. Avdeeva, E.A. Paukshtis, A.L. Chuvilin, V.A. Likholobov,**
Investigation of Adsorptive and Catalytic Properties of Heteropoly Acids with Various Compositions and Structures,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-P-12.
279. **M.N. Timofeeva, Z.P. Pai, A.G. Tolstikov, P.V. Berdnikova, N.V. Selivanova, K.P. Brylyakov,**
Investigation of Biphasic Oxidation of Cyclic Olefins Catalyzed by Polyoxometalates with Hydrogen Peroxide,
NATO ASI Polyoxometalate Molecular Science, 25 August-5 September, Tenerife, Spain. Abstracts.
280. **A.V. Timoshok, O.Yu. Ovsyannikova, A.M. Volodin, (A. Lund),**
NO Molecules and Nitroxyl Mono- and Biradicals as Spin Probes for the Study of Oxide Catalysts,
NATO ARW "Magnetic Resonance in Colloid and Interface Sciences", 26-30 June, St. Petersburg, Russia. Abstracts, p. 154.

281. **A.V. Toktarev, S.V. Dudarev,**
The Fitting Equation for Zeolite Crystallization with Seeds,
13th International Zeolite Conference, 8-13 July Montpellier, France. Abstracts, 7 pp.
282. **M.M. Tokarev, (I.V. Koptuyug), N.M. Ostrovskii, N.A. Chumakova, L.Y. Ilyina, N.V. Vernikovskaya, N.N. Bukhavtsova, Yu.I. Aristov,**
Composite Sorbents “CaCl₂ in a Porous Matrix” for Gas Drying: Fixed Bed Experiments, NMR-Imaging, Modelling,
5th Italian Conference on Chemical Process Engineering, 20-23 May, Florence, Italy. Abstracts, pp. 191-196.
283. **N.N. Trukhan, V.N. Romannikov, (J. Mrowiec-Bialon, A.B. Jarzebski), O.A. Kholdeeva,**
New Applications of Mesoporous Ti-Containing Silicate Materials in Selective Oxidation. Structure-Selectivity/Activity Relationships,
4th World Congress on Oxidation Catalysis, “4WCOC”, 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.1, pp. 243-246.
284. **N.N. Trukhan, V.N. Romannikov, (J. Mrowiec-Bialoń, A.B. Jarzębski), O.A. Kholdeeva,**
Oxidation of 2,3,6-Trimethylphenol with H₂O₂ over Mesoporous Ti-Containing Silicate Materials,
5th European Congress on Catalysis, “EUROPACAT-V”, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 8-P-08.
285. **(B.J. Trznadel, A.M. Puziy, B. Charnas, O.I. Poddubnaya), M.S. Mel’gunov, (R. Leboda),**
On Surface Heterogeneity of Carbon-Silica Adsorbents Determined on the Basis of the Complex Adsorption Investigations,
4th International Symposium on Surface Heterogeneity Effects, August, Krakov, Poland. Abstracts, p. 51.
286. **(M.V. Tsodikov, Ye.A. Trusova, O.V. Bukhtenko, G.G. Hernandez), V.V. Kriventsov, V.V. Kalinkin, (M.C. Hidalgo, J.A. Navio),**
[Co,Cu]-TiO₂ Catalysts, Obtaining by Alkoxo-Method Tested in the Three-Way Conversion of CO, NO and C₃H₆,
5th European Congress on Catalysis, “EUROPACAT-V”, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 8-P-52.
287. **(M.V. Tsodikov, O.V. Bukhtenko, T.N. Zhdanova, I.A. Litvinova, L.E. Kitaev, L.N. Vasilieva), V.V. Kriventsov,**
Structure and Acid-Basic Properties of the Surface of Titanium Oxides Modified by P(3+; 5+); Cu(1+; 2+) and SO₄,
Russian Conference “Actual Problems of Petrochemistry”, 17-22 April, Moscow, Russia. Abstracts, p. 194.
288. **(M.V. Tsodikov, V.Ya. Kugel, F.Ya. Slivinskii), D.I. Kochubey, V.V. Kriventsov, (A.E. Gekhman, I.I. Moiseev),**
CO₂ Conversion Catalyzed by Hydrogen Accumulating System TiFe_{0.95}Zr_{0.03}Mo_{0.02},
III All-Russian Conference on Clusters Chemistry “Polynuclear Systems and CO₂ Activation”, 20-25 August, Kazan-Cheboksary, Russia. Abstracts, p. 45.
289. **L.T. Tsykoza, S.A. Yashnik, R.A. Shkrabina, Z.R. Ismagilov, E.V. Pluzhnikova, V.V. Kuznetsov, V.A. Sazonov,**
Optimum Parameters of Synthesis of Cu-ZSM-5 Catalyst for Reduction of NO_x with Hydrocarbons,
3rd European Workshop on Environmental Catalysis “Environmental Catalysis. A Step Forward”, “ENVICAT’2001”, 2-5 May, Maiori, Italy. Abstracts, p. 173.
290. **P.G. Tsyrunnikov,**
The New Approach to the Selection and Preparation of Heterogeneous Catalysts,
5th European Congress on Catalysis, “EUROPACAT-V”, 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-P-64.

291. **Yu.E. Tuzova**,
Construction of Kinetic Model of Catalytic Reaction Based on Experimental Data,
XXXIX International Scientific Student Conference "Students and Scientific and Technological Advance. Physics", 9-13 April, Novosibirsk, Russia. Abstracts.
292. **I.V. Vasilieva, S.V. Myakin, F.V. Sycheva, O.A. Cheremisina, L.B. Svatovskaya**,
Improving of the Hardness of Cement Mastic by Electron-Beam Treating of Oxide Fillers,
3rd International Conference "Chemistry of Highly-Ordered Substances and Scientific Bases of Nanotechnology", 26-29 June, St.-Petersburg, Russia. Abstracts, pp. 176-177.
293. **I.V. Vasilieva, S.V. Myakin, A.V. Makarov, (M. Lutsche)**,
Electron-Beam Treating of Polyethyleneterephthalate Films,
3rd International Conference "Chemistry of Highly-Ordered Substances and Scientific Bases of Nanotechnology", 26-29 June, St.-Petersburg, Russia. Abstracts, pp. 178-179.
294. **O.V. Vassiltsova, V.N. Parmon**,
Photochemical Properties of CdS Nanocrystallites in the Process of Electron Phototransfer through the Lipid Vesicle Membranes,
International Conference on Semiconductor Photochemistry, "SP-1", 23-25 July, Glasgow, UK. Abstracts, No 62.
295. **O.V. Vassiltsova, V.N. Parmon**,
Photochemical Properties of CdS Nanocrystallites in the Process of Electron Phototransfer through the Lipid Vesicle Membranes,
10th International Conference on Untraditional Photoactive Systems, "UPS-01", 4-8 September, Le Diablerets, Switzerland. Abstracts, p. 76.
296. **A.A. Vedyagin**,
Catalytic Dehydrogenation of Methanol over Copper-Containing Catalysts,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, p.17.
297. **A.A. Vedyagin**,
The Effect of the Reduction Temperature of Copper Containing Systems on their Catalytic Properties,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, 1-P-01.
298. **A.A. Vedyagin, S.V. Ignashin**,
Thermodynamic Peculiarities of Methanol Dehydrogenation,
13th All-Russian Symposium "Modern Chemical Physics", 25 September-6 October, Tuapse, Russia. Abstracts, p. 83.
299. **A.A. Vedyagin, N.O. Struikhina**,
Methanol Dehydrogenation over Copper Catalysts, Prepared from Various Precursors,
Scientific Youth Conference "Young Scientists on the Eve of the Third Millennium" Devoted to the 70th Anniversary of the Birthday of Prof. V.A. Koptug, 13-15 June, Omsk, Russia. Abstracts, p. 163.
300. **N.V. Vernikovskaya, (V.I. Drobyshevich, L.V. Yausheva), S.A. Pokrovskaya, N.A. Chumakova**,
Software "REACTOR" in Education Course of Chemical Engineering in Catalysis,
15th International Conference on Chemical Reactors, "CHEMREACTOR-15", 5-8 June, Helsinki, Finland. Abstracts, pp. 313-315.
301. **G.G. Volkova, L.M. Plyasova, A.N. Salanov, G.N. Kustova, T.M. Yurieva, V.A. Likholobov**,
Heterogeneous Catalysts for Halide-Free Carbonylation of Dimethyl Ether,
5th European Congress on Catalysis, "EUROPACAT-V", 2-7 September, University of Limerick, Limerick, Ireland. Abstracts, 1-P-30.

302. **A.M. Volodin**,
Spin Design of Metal Complexes in Zeolite Matrices,
11th International Conference “Magnetic Resonance in Chemistry and Biology”, 20-27 April,
Zvenigorod, Russia. Abstracts, pp. 146-147.
303. **A.M. Volodin**,
NO Molecule and Spin Design of Metal Complexes on the Surface of Oxide Catalysts,
13th All-Russian Symposium “Modern Chemical Physics”, 25 September-6 October, Tuapse, Russia.
Abstracts, p. 22.
304. **A.V. Vorontsov, D.V. Kozlov, E.N. Savinov, (L. Davydov, P.G. Smirniotis)**,
Study on TiO₂ Deactivation during Diethyl Sulfide (DES) Gas Phase Photooxidation,
6th International Conference on TiO₂ Photocatalytic Purification and Treatment of Water and Air,
25-29 June. Abstracts, pp. 52-54.
305. **I.S. Yakovleva, L.A. Isupova, (I.I. Gainutdinov, Yu.T. Pavlyukhin), V.A. Sadykov**,
Resonance Messbauer Spectroscopy to Study Coordination Surrounding and Valence State of Iron
Cations in Threefold Oxides with Perovskite Structure La_{1-x}Ca_xFeO₃,
*Scientific Youth Conference “Young Scientists on the Eve of the Third Millennium” Devoted to the 70th
Anniversary of the Birthday of Prof. V.A. Koptug*, 13-15 June, Omsk, Russia. Abstracts, pp. 195-196.
306. **S.A. Yashnik, L.T. Tsykoza, Z.R. Ismagilov, V.V. Kuznetsov, V.A. Ushakov**,
Manganese Containing Catalysts Supported on Highly Porous foam Materials for Automotive
Exhaust Purification,
*3rd European Workshop on Environmental Catalysis “Environmental Catalysis. A Step Forward”,
“ENVICAT’2001”*, 2-5 May, Maiori, Italy. Abstracts, p. 255.
307. **A. Yermakova**,
Rate of Catalytic Transformations and Macrokinetic Models of Catalytic Reactions,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk,
Russia.
308. **M.M. Yulikov, O.N. Martyanov, R.N. Lee, V.F. Yudanov**,
Size Phenomena in FMR Spectra of Nanoparticles,
International Conference of Magnetic Resonance in Colloid and Interface Science,
26-30 June, St. Petersburg, Russia. Abstracts, pp. 165-166.
309. **T.M. Yurieva, T.P. Minyukova, I.Sh. Itenberg, A.A. Khassin, I.I. Bobrova, G.N. Kustova,
I.A. Zolotarskii, V.N. Parmon**,
Ni-Containing Clays Catalysts for Methane Steam Reforming,
AIChE Spring National Meeting, Natural Gas Utilization Topical Conference, 22-26 April, Houston,
Texas. Proceedings, pp. 17-29.
310. **M.M. Yulikov, (K.A. Tarasov, V.P. Isupov), O.N. Martyanov, V.F. Yudanov**,
Superparamagnetic Resonance of Nanosized Metal Particles,
International Conference of Magnetic Resonance in Colloid and Interface Science,
26-30 June, St. Petersburg, Russia. Abstracts, pp. 167-168.
311. **A.N. Zagoruiko**,
Fundamental Basis for Design of Catalytic Reactors. Heat(Mass) Transfer in Catalytic Reactors,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk,
Russia.
312. **V.S. Zakharenko, A.N. Moseichuk**,
Photoinduced Processes on Gas Solid Interface,
International Conference on Semiconductor Photochemistry, “SP-1”, 23-25 July, Glasgow, UK.
Abstracts, p. 45.

313. **V.S. Zakharenko, A.N. Moseichuk, V.N. Parmon,**
Photoinduced Chemical Processes on Solid Tropospheric Aerosols,
8th Conference “Siberian Aerosols”, 27-30 November, Tomsk, Russia. Abstracts, p. 35.
314. **A.V. Zakharov, V.G. Stepanov, L.S. Filippova, K.G. Ione,**
Comparative Analysis of Technicoeconomic Figures of “Zeoforming” Process for the Production of High-Octane Gasolines at Small Refineries,
Russian Conference “Actual Problems of Petrochemistry”, 17-22 April, Moscow, Russia. Abstracts, p. 228.
315. **V.P. Zakharov, I.A. Zolotarskii, V.A. Kuz'min,**
Numerical Research of Mass Transfer on the Honeycomb Channel Walls,
15th International Conference on Chemical Reactors, “CHEMREACTOR-15”, 5-8 June, Helsinki, Finland. Abstracts, pp. 138-141.
316. **V.P. Zakharov, I.A. Zolotarskii, V.A. Kuz'min,**
Computational Study of Gas Flow through “Gauze Pad – Honeycomb” Catalytic System,
15th International Conference on Chemical Reactors, “CHEMREACTOR-15”, 5-8 June, Helsinki, Finland. Abstracts, pp. 272-273.
317. **V.A. Zakharov, I.I. Zakharov, E.P. Talsi, D.E. Babushkin, N.V. Semikolenova, V.N. Panchenko,**
Structure of MAO and Mechanism of Ion Pairs Formation for Catalyst Cp_2ZrMe_2/MAO ,
International Symposium on Future Technology for Polyolefin and Olefin Polymerization Catalysts, March, Tokyo, Japan.
318. **S.G. Zavarukhin, G.G. Kuvshinov,**
Modeling of Production of Filamentous Carbon from Methane on the IKU-59-1 Catalyst in Various-Type Isothermal Reactors,
15th International Conference on Chemical Reactors, “CHEMREACTOR-15”, 5-8 June, Helsinki, Finland. Abstracts, pp. 185-188.
319. **S.G. Zavarukhin, G.G. Kuvshinov,**
Modeling of Production of Filamentous Carbon from Methane on the IKU-59-1 Catalyst in Various-Type Isothermal Reactors,
III Scientific Technical Conference “Novel Chemical Technologies: Production and Application, August, Penza, Russia.
320. **S.G. Zavarukhin, (A.I. Yavorskii, A.V. Trachuk),**
Centrifugally-Bubbling Device,
III Scientific Technical Conference “Novel Chemical Technologies: Production and Application, August, Penza, Russia.
321. **G.A. Zenkovets, G.N. Kryukova, (Z. Sobalik), S.V. Tsybulya, V.N. Parmon,**
Catalytic Properties of Novel Nanostructured Vanadia-Based Catalysts in the Selective Catalytic Reaction of NO by NH_3 ,
4th World Congress on Oxidation Catalysis, “4WCOC”, 16-21 September, Berlin/Potsdam, Germany. Extended Abstracts, v.2, pp. 225-226.
322. **(Yu.N. Zhukov), A.S. Noskov, E.S. Borisova, L.Yu. Zudilina,**
Mathematical Modeling and Industrial Implementation of Unsteady State Method for Gas Purification from Nitrogen Oxides,
15th International Conference on Chemical Reactors, “CHEMREACTOR-15”, 5-8 June, Helsinki, Finland. Abstracts, pp. 316-317.
323. **I.A. Zolotarskii,**
Modern Trends in Development of Catalytic Technologies in Nitric Industry,
Extension Courses in the Field of Catalysts and Catalytic Processes, 24-29 September, Novosibirsk, Russia.
324. **I.A. Zolotarskii, V.A. Kuz'min, A.V. Muzykantov, E.L. Smirnov,**
Investigation of Radial Heat Transfer in Beds Packed by Regular and Shaped Particles,
15th International Conference on Chemical Reactors, “CHEMREACTOR-15”, 5-8 June, Helsinki, Finland. Abstracts, pp. 118-121.

AUTHOR'S INDEX

- Aksenov D. G.**, 163, 174, 187
Al't L. Ya., 96, 157
Aleshina G. I., 187
Alikina G. M., 94, 102, 103, 147, 149, 155, 156, 173, 184
Amosov Yu. I., 13
Andreev D. V., 120, 151
Andrievskaya I. P., 125, 147, 172
Andrushkevich T. V., 10, 43, 124, 141, 163, 183
Anikeev V. I., 9, 59, 134, 135, 141, 160, 163
Anisimov M. P., 68, 70, 132, 133, 141, 164
Anisimova L. M., 133, 141, 164
Anufrienko V. F., 92, 97, 98, 113, 148, 149, 161, 175, 184, 185
Aristov Yu. I., 9, 43, 56, 121, 122, 141, 144, 154, 156, 158, 164, 176, 180, 186, 190
Avdeev V. I., 77, 141
Avdeeva L. B., 109, 155, 183, 189
Ayupov A. B., 164, 168
Babushkin D. E., 41, 128, 158, 164, 186, 193
Badaev V. K., 129, 147
Baklanova O. N., 155
Bal'zhinimaev B. S., 13, 30, 92, 94, 95, 99, 123, 134, 141, 142, 150, 155, 157, 164, 165, 166, 169, 178, 189
Barysheva L. V., 165, 187
Batygina M. V., 165, 167, 168
Bavykin D. V., 165
Beck I. E., 123, 149, 176
Beloshapkin S. A., 102, 103, 149, 155, 156, 174, 184, 185
Belyaev V. D., 136, 145, 169, 170, 187
Belyaeva N. P., 134, 142
Belyi A. S., 16, 71, 72, 165
Berdnikova P. V., 189
Berezina A. S., 132, 141, 164
Bibin V. N., 185
Bobrin A. S., 13, 165
Bobrov N. N., 13, 38, 63, 93, 110, 142, 159, 165, 189
Bobrova I. I., 93, 110, 159, 165, 182, 184, 189, 192;
Bobrova L. N., 185
Bogdanov S. V., 180
Boldyreva N. N., 184
Boldyreva N. N., 94, 147, 173
Bondareva V. M., 43, 87, 124, 141, 151, 163, 179
Borbat V. F., 142; 166, 167
Borisova E. S., 165, 193
Boronin A. I., 107, 118, 135, 150, 153, 156, 166, 176
Bredikhin M. N., 182
Brylyakov K. P., 86, 142, 166, 185, 189
Bubnov A. V., 142, 166, 167, 180
Budneva A. A., 112, 116, 148, 151
Bukatov G. D., 127, 128, 142, 152, 166
Bukhavtsova N. M., 43, 141, 190
Bukhtiyarov V. I., 7, 41, 86, 95, 97, 111, 112, 142, 148, 157, 158, 166, 168, 175
Bulgakov N. N., 174, 184
Bulushev D. A., 118, 143
Bulusheva L. G., 166, 180
Bunina R. V., 102, 103, 149, 155, 156, 173, 182, 184, 185
Burgina E. B., 102, 104, 143, 154, 156, 174, 184, 185
Butenko Yu. V., 89, 108, 147, 150, 153, 166, 167, 177, 180, 183
Buyanov R. A., 10, 20, 60, 89, 95, 107, 109, 111, 143, 152, 161, 167, 178, 179
Byrdina N. A., 129, 147
Chermashentseva G. K., 113, 148
Chernov V. A., 81, 82, 83, 143, 144, 147, 158
Chernyavsky V. S., 117, 154, 181
Cherstyuk O. V., 167, 185
Chesalov Y. A., 183
Chesnokov V. V., 89, 96, 107, 109, 110, 142, 143, 145, 152, 155, 161, 167, 179
Cholach A. R., 90, 144, 167
Chumakova N. A., 14, 43, 125, 135, 141, 144, 160, 167, 174, 179, 190, 191
Chuvilin A. L., 89, 108, 109, 110, 119, 145, 147, 150, 153, 155, 156, 166, 167, 170, 177, 183, 185, 189
Danilova L. G., 127, 151, 153, 156, 178, 180; M. M., 137
Danilyuk A. F., 9, 163, 164
Davydova L. P., 85, 155, 184
Delii I. V., 166
Demanov Yu. K., 136, 151
Demeshkina M. P., 112, 113, 148, 161

- Demin A. K.**, 26, 29, 167, 187
- Derevyankin A. Yu.**, 91, 105, 106, 144, 145, 149, 155, 159, 184
- Detusheva L. G.**, 115, 144, 150
- Dobrynkin N. M.**, 165, 167, 168, 186
- Doronin V. P.**, 16, 38, 43, 72, 93, 103, 144, 149, 168, 184
- Dovlitova L. S.**, 85, 112, 115, 144, 155, 161, 168
- Drozdov V. A.**, 17, 93, 125, 144, 155, 160, 168
- Dubkov K. A.**, 100, 144, 153, 160, 181
- Dudarev S. V.**, 168, 190
- Duplyakin V. K.**, 16, 93, 144, 150, 155, 165, 178
- Echevskaya L. G.**, 126, 144, 152
- Echevsky G. V.**, 14, 38, 65, 164, 165, 167, 168, 175
- Elokhin V. I.**, 77, 143, 151, 169, 170, 178
- Ermakov D. Yu.**, 110, 145, 169
- Ermakova M. A.**, 110, 145, 169
- Ermolaev V. K.**, 117, 125, 145, 146, 160
- Fedorova N. K.**, 130, 152
- Fedotov M. A.**, 86, 87, 115, 117, 142, 144, 151, 165, 169, 170, 175, 186
- Fenelonov V. B.**, 8, 28, 38, 52, 90, 91, 93, 96, 102, 103, 105, 106, 107, 141, 144, 145, 149, 152, 155, 159, 169, 174, 184, 189
- Fialko E. F.**, 88, 146
- Filimonova S. V.**, 87, 145
- Filippova L. S.**, 193
- Fominsky S. A.**, 86, 142
- Frolova Yu. V.**, 102, 156, 182, 184, 185
- Galvita V. V.**, 136, 145, 170, 187
- Gavrilov V. Yu.**, 92, 161
- Gerasev A. P.**, 134, 145, 170
- Gladky A. Yu.**, 117, 146
- Glushenkov A. M.**, 177
- Gogin L. L.**, 185
- Goidin V. V.**, 170, 178, 179
- Golovanova O. A.**, 142, 166
- Golovin A. V.**, 159
- Goncharov V. B.**, 88, 99, 127, 146, 153, 155, 174, 189
- Gordeeva L. G.**, 164
- Gorodetskii V. V.**, 8, 26, 54, 77, 110, 146, 151, 169, 170, 178
- Gubar A. V.**, 180, 186
- Gudkov M. V.**, 134, 160
- Gulyaeva T. I.**, 93, 144, 150, 168
- Ignashin S. V.**, 191
- Il'ina I. I.**, 43, 108, 118, 122, 146, 156, 186
- Ilyin A. N.**, 183
- Ilyina L. Yu.**, 88, 141, 144, 149, 164, 176, 190
- Ione K. G.**, 33, 101, 146, 171, 178, 185, 187, 188, 193
- Ismagilov I. Z.**, 171, 172;
- Ismagilov Z. R.**, 10, 27, 30, 31, 34, 38, 41, 98, 99, 109, 124, 125, 131, 136, 146, 147, 153, 155, 160, 163, 167, 170, 171, 172, 173, 174, 176, 181, 182, 183, 190, 192
- Isupova L. A.**, 94, 147, 167, 173, 192
- Itenberg I. Sh.**, 113, 148, 175, 192
- Ivanchev S. S.**, 18, 129, 130, 131, 147, 152, 154, 173, 182
- Ivancheva N. I.**, 129, 147
- Ivanov A. A.**, 134, 142;
- Ivanov E. A.**, 173;
- Ivanov V. P.**, 93, 94, 147, 159, 167, 174, 184, 185
- Ivanova A. S.**, 10, 93, 101, 102, 103, 149, 155, 156, 159, 184, 189; A.S., 147
- Kachesova P. A.**, 142, 166
- Kaichev V. V.**, 86, 89, 95, 97, 112, 142, 148, 157, 158, 166, 175
- Kalinkin A. V.**, 77, 99, 110, 124, 125, 144, 146, 148, 149, 190
- Kanazhevskii V. V.**, 104, 148, 174
- Kapterev S. V.**, 188
- Karpyshev N. N.**, 86, 115, 142, 159
- Kashkin V. N.**, 174, 180
- Kazachkin D. V.**, 174
- Kerzhentsev M. A.**, 10, 31, 131, 160, 163, 167, 171, 172, 181, 182
- Khabibulin D. F.**, 87, 171, 174
- Khaikin S. Ya.**, 129, 130, 131, 147, 152, 154, 182
- Khairulin S. R.**, 124, 125, 146, 147, 170, 172, 173, 174
- Khairulina L. N.**, 121, 151, 179
- Khanaev V. M.**, 165
- Kharitonov A. S.**, 117, 154, 181
- Khasin A. V.**, 11, 183
- Khassin A. A.**, 11, 62, 112, 113, 148, 175, 192
- Khlebnikova T. V.**, 115, 159

- Kholdeeva O. A.**, 9, 57, 98, 106, 114, 117, 148, 155, 159, 175, 190
- Khomov V. V.**, 176
- Kikhtyanin O. V.**, 168
- Kildyashev S. P.**, 168
- Kireeva T. V.**, 17
- Kirillov V. A.**, 14, 29, 34, 41, 67, 134, 136, 137, 148, 150, 151, 157, 175, 178, 181, 186
- Kirillova N. V.**, 175, 177
- Klimov O. V.**, 168
- Klubin V. V.**, 129, 154
- Kochubey D. I.**, 7, 27, 38, 83, 84, 85, 92, 102, 104, 107, 143, 145, 148, 149, 150, 154, 155, 156, 157, 159, 163, 168, 174, 175, 184, 185, 190
- Kodenev E. G.**, 91, 105, 149, 168, 175
- Kolmogorov K. V.**, 17, 43
- Kolomiichuk V. N.**, 102, 155, 156, 184
- Komova O. V.**, 175, 176
- Korotkikh V. N.**, 13, 43, 180
- Koshcheev S. V.**, 107, 118, 153, 156, 166
- Kotsarenko N. S.**, 88, 104, 148, 151, 154, 174, 178, 185, 186
- Kovalenko G. A.**, 9, 59, 107, 149, 176;
- Kovalenko O. N.**, 124, 125, 148, 149
- Kovaleva L. A.**, 117, 148, 175
- Kovalyov E. V.**, 169
- Kozlov D. V.**, 192
- Kreichman G. S.**, 129, 154
- Krieger T. A.**, 85, 112, 113, 148, 155, 156, 161, 180, 183
- Kriventsov V. V.**, 83, 84, 85, 92, 102, 104, 143, 144, 148, 150, 154, 156, 159, 175, 184, 185, 190
- Krivoruchko O. P.**, 10, 108, 150, 176
- Kruglyakov V. Yu.**, 13, 93, 159, 189
- Kryukova G. N.**, 92, 93, 94, 147, 161, 173, 176, 193
- Kudrya E. N.**, 167, 187
- Kulikov A. V.**, 42, 136, 137, 148, 150, 151, 178, 186
- Kundo N. N.**, 9, 56, 124, 125, 148, 149, 152
- Kustova G. N.**, 112, 113, 148, 161, 175, 191, 192
- Kuvshinov D. G.**, 107, 149, 177, 178;
- Kuvshinov G. G.**, 14, 67, 110, 145, 169, 177, 178, 193
- Kuz'min V. A.**, 185, 193, 194
- Kuzin N. A.**, 136, 137, 148, 150, 151, 157, 175, 178, 186
- Kuzmin A. O.**, 118, 145, 177, 179; V. A., 182, 184, 185
- Kuznetsov V. L.**, 12, 25, 89, 108, 147, 150, 153, 166, 167, 177, 180, 183;
- Kuznetsov V. V.**, 99, 109, 146, 153, 183, 190, 192
- Kuznetsova E. V.**, 107, 149, 177;
- Kuznetsova L. I.**, 115, 144, 150, 170, 175, 176, 177, 182;
- Kuznetsova N. I.**, 115, 150, 170, 175, 177;
- Kuznetsova T. G.**, 102, 103, 149, 155, 156, 174, 184, 185
- Kvon R. I.**, 110, 148
- Lakhmostov V. S.**, 174
- Lapina O. B.**, 8, 26, 56, 87, 94, 95, 106, 151, 155, 157, 162, 171, 174, 177
- Larina T. V.**, 98, 113, 148
- Latkin E. I.**, 77, 151, 169, 178
- Lavrenov A. V.**, 136, 151, 178
- Lavrov G. A.**, 137, 157
- Lebedev M. Yu.**, 169, 178, 186
- Likholobov V. A.**, 12, 16, 20, 38, 41, 109, 114, 115, 116, 117, 144, 150, 151, 155, 159, 160, 161, 165, 170, 175, 177, 178, 183, 187, 189, 191
- Litvak G. S.**, 102, 156, 183, 184
- Lobyntsev E. A.**, 178, 186, 187
- Lopatkin S. V.**, 178
- Luk'yanov B. N.**, 137, 151, 178
- Luzgin M. V.**, 88, 99, 146, 151, 178, 188
- Lysova A. A.**, 177, 179
- Madyarov A. I.**, 174, 179
- Makarov A. V.**, 191
- Makarshin L. L.**, 120, 151
- Maksimov G. M.**, 84, 85, 116, 117, 148, 151, 159, 175, 179, 189
- Maksimovskaya R. I.**, 102, 104, 116, 117, 143, 148, 151, 154, 156, 159, 175, 179, 184
- Malakhov V. V.**, 7, 41, 85, 112, 115, 144, 152, 155, 161, 163, 168
- Malakhova I. V.**, 125, 160
- Malozemov Yu. V.**, 188
- Maltsev A. V.**, 180
- Mamatyuk V. I.**, 115, 159
- Martyanov O. N.**, 192
- Marunyak M. D.**, 165

- Mashkina A. V.**, 10, 59, 121, 151, 152, 179
- Matrosova M. M.**, 116, 117, 159, 189
- Matsko M. A.**, 126, 127, 151, 152
- Matveev A. V.**, 110, 149, 179;
- Matveev K. I.**, 12, 63, 122, 152, 153
- Matvienko L. G.**, 86, 118, 145, 158, 177
- Mel'gunov M. S.**, 90, 96, 107, 145, 152, 174, 190
- Mesh A. M.**, 130, 131, 147, 152
- Mikenas T. B.**, 87, 126, 127, 144, 151, 152
- Mikhailova I. A.**, 134, 157, 175
- Minyukova T. P.**, 112, 161, 192
- Mishakov I. V.**, 44, 96, 109, 145, 152, 155, 179
- Mogilnykh Yu. I.**, 107, 149
- Moiseeva M. E.**, 130, 147
- Mokrinskii V. V.**, 180
- Molchanov V. V.**, 95, 143, 152, 170, 175, 178, 179, 180
- Molina I. Yu.**, 85, 113, 148, 155
- Moroz B. L.**, 114;
- Moroz E. M.**, 41, 102, 122, 155, 156, 174, 180, 184, 185
- Moseichuk A. N.**, 180, 192, 193
- Moudrakovskii I. L.**, 189
- Murzakhmetov K. T.**, 118, 156
- Muzykantov A. V.**, 194
- Myakin S. V.**, 191
- Mysov V. M.**, 101, 146, 171
- Nikitenko S. G.**, 85, 90, 160, 163
- Nizovskii A. I.**, 17, 142, 166, 180
- Noskov A. S.**, 14, 29, 41, 66, 124, 125, 141, 153, 154, 160, 165, 167, 168, 174, 180, 193
- Nosov A. V.**, 87, 105, 145, 149
- Novgorodov B. N.**, 102, 104, 148, 155, 174, 184, 185
- Novopashina V. M.**, 125, 149
- Odegova G. V.**, 175
- Odyakov V. F.**, 122, 152, 153
- Ogorodnikova O. L.**, 183
- Okunев A. G.**, 43, 122, 156, 180, 186
- Oleinik L. V.**, 147
- Oruzheynikov A. I.**, 17, 180
- Ostrovskii N. M.**, 16, 43, 123, 124, 136, 141, 151, 153, 180, 183, 190
- Ovsyannikova I. A.**, 152, 173, 189
- Pai Z. P.**, 15, 181, 185, 189
- Pakhomov N. A.**, 38, 109, 111, 123, 143, 152, 153, 181
- Panchenko V. N.**, 127, 128, 153, 158, 161, 193
- Pankrat'ev Yu. D.**, 122, 154
- Panov G. I.**, 10, 41, 100, 117, 144, 154, 181
- Parmon V. N.**, 5, 9, 20, 27, 28, 29, 30, 34, 42, 43, 86, 88, 101, 110, 112, 113, 117, 118, 120, 121, 137, 138, 141, 142, 145, 146, 148, 149, 151, 153, 154, 157, 158, 164, 165, 167, 168, 171, 172, 175, 176, 177, 179, 180, 181, 182, 183, 184, 186, 188, 191, 192, 193
- Pashis A. V.**, 110, 148
- Paukshtis E. A.**, 13, 64, 87, 94, 95, 100, 102, 103, 104, 106, 112, 116, 117, 127, 144, 148, 149, 151, 153, 154, 155, 156, 157, 159, 164, 168, 174, 175, 178, 181, 184, 185, 189
- Pavlova S. N.**, 84, 93, 102, 104, 143, 150, 154, 156, 159, 182, 184, 185, 189
- Pavlyuchenko V. N.**, 18, 129, 147, 154, 182
- Pazhetnov E. M.**, 166
- Pershin A. N.**, 185
- Pestunova O. P.**, 172, 182, 183
- Pinaeva L. G.**, 99, 155
- Piryutko L. V.**, 117, 154, 181
- Plakhutin B. N.**, 41, 154
- Plaksin G. V.**, 16, 110, 154, 155
- Pluzhnikova E. V.**, 190
- Plyasova L. M.**, 85, 112, 113, 148, 155, 161, 183, 184, 191
- Podyacheva O. Yu.**, 136, 146, 183
- Pokrovskaya S. A.**, 174, 180, 191
- Polygalov Yu. I.**, 132, 141, 164
- Popova G. Ya.**, 43, 124, 141, 163, 183
- Poslovina L. P.**, 188
- Potapova Yu. V.**, 93, 155, 159, 185, 189
- Primachenko O. N.**, 129, 154, 182
- Prosvirin I. P.**, 166, 168
- Pushkarev V. V.**, 136, 146
- Reshetenko T. V.**, 109, 155, 183, 189
- Reshetnikov S. I.**, 14, 38, 118, 134, 142, 143, 173, 183, 186
- Resnyanskii E. D.**, 169

Rogov V. A., 7, 172, 173, 175, 176, 183, 184
Romanenko A. I., 108, 150, 153, 177, 183
Romannikov V. N., 105, 106, 144, 145, 149, 155, 158, 159, 175, 190
Rudina N. A., 107, 149, 153, 176
Rusina E. S., 173

Sadovskaya E. M., 99, 155
Sadykov V. A., 10, 26, 28, 38, 60, 84, 91, 93, 94, 102, 103, 104, 143, 145, 147, 149, 150, 154, 155, 156, 159, 167, 173, 174, 176, 182, 183, 184, 185, 189, 192
Sakaeva N. S., 166
Sakhaltueva L. G., 121, 151
Sal'nikov G. E., 115, 159;
Sal'nikov V. S., 125, 160, 178
Salanov A. N., 7, 52, 93, 97, 118, 119, 125, 141, 156, 159, 160, 173, 180, 182, 185, 191
Saputina N. F., 182, 185
Savelieva G. G., 96, 157, 167
Savinov E. N., 9, 30, 120, 160, 165, 177, 183, 185, 192
Savinova E. R., 118, 119, 145, 156, 163, 167, 177, 179, 185
Sazonov V. A., 98, 99, 146, 147, 171, 172, 190
Sazonova N. N., 174, 175, 184, 185
Selivanova N. V., 185, 189
Semikolenov V. A., 12, 38, 41, 108, 118, 122, 136, 145, 146, 156, 185, 186, 188
Semikolenova N. V., 126, 128, 144, 158, 166, 186, 193
Semin G. L., 136, 145, 170, 187
Serushkin M. I., 129, 147
Shaimordanov I. N., 132, 133, 141, 164
Sharonov V. E., 122, 156, 180, 186
Sherstyuk O. V., 119, 156
Shigarov A. B., 136, 137, 150, 151, 157, 178, 186
Shikina N. V., 98, 99, 125, 146, 147, 172, 173, 183
Shinkarev V. V., 178, 186
Shishkin G. V., 123, 149, 176
Shitova N. B., 96, 157, 168, 186
Shkrabina R. A., 98, 99, 124, 125, 146, 147, 172, 173, 190
Shlyapin D. A., 168, 186, 187
Shmachkova V. P., 88, 104, 148, 151, 154, 174, 178, 186
Shmakov A. N., 89, 97, 105, 106, 108, 141, 144, 145, 149, 150, 155, 158, 159
Shubin A. A., 76, 86, 87, 151, 156, 157, 158, 160, 174, 188
Sidelnikov V. N., 91, 162
Simagina V. I., 111, 157, 187
Simakov A. V., 11, 174, 175, 176, 184, 185
Simakova I. L., 108, 118, 122, 146, 156, 186
Simonov A. D., 14, 67, 137, 138, 141, 157, 181, 189;
Simonov P. A., 119, 156, 167, 185
Simonova L. G., 94, 95, 157, 164, 189
Slavinskaya E. M., 180
Slepterev A. A., 187
Smirnov E. L., 194;
Smirnov M. Yu., 96, 157
Smolikov M. D., 167
Snegurenko O. I., 182, 185
Snytnikov V. N., 9, 58, 158, 182, 186, 187; VI. N., 187
Snytnikova G. P., 187, 188
Sobolev A. P., 87, 126, 134, 144, 151, 186, 189
Soboleva O. A., 187
Sobyenin V. A., 10, 26, 29, 41, 136, 145, 167, 170, 182, 183, 187
Sorochinskaya O. V., 129, 154, 182
Sorokin A. M., 89, 158
Sorokina T. P., 43, 93, 144, 168, 184
Starokon E. V., 181
Startsev A. N., 12, 30, 163, 173, 174, 187, 188
Stasko S. N., 175
Stepanov A. G., 8, 53, 88, 151, 178, 188, 193;
Stepanov V. G., 101, 146, 171, 178, 187, 188
Stoyanov E. S., 115, 158, 183
Stoyanova I. V., 111, 157, 187
Stoyanovsky V. O., 182, 187
Struikhina N. O., 191
Suknev A. P., 99, 127, 153, 155, 189
Sumenkova O. V., 189
Svatovskaya L. B., 191
Sycheva F. V., 191

Talsi E. P., 7, 41, 52, 86, 128, 142, 158, 166, 186, 189, 193;
Talsi V. P., 17
Tanashev Yu. Yu., 121, 158
Tapilin V. M., 75, 90, 144, 158, 167
Teleshev A. T., 92, 159

- Terskikh V. V.**, 94, 95, 157, 189
- Tikhov S. F.**, 93, 155, 159, 189
- Timofeeva M. N.**, 116, 117, 151, 159, 185, 189
- Timoshok A. V.**, 189
- Titkov A. I.**, 185
- Tkachev A. V.**, 98, 155, 170
- Tokarev M. M.**, 43, 122, 141, 144, 154, 164, 176, 190
- Toktarev A. V.**, 95, 157, 164, 168, 185, 189, 190
- Tolstikov A. G.**, 15, 67, 86, 115, 142, 159, 189
- Tolstikova O. V.**, 115, 159
- Trenikhin M. V.**, 142, 166, 180
- Trukhan N. N.**, 44, 106, 159, 174, 175, 185, 190
- Tsybulya S. V.**, 7, 92, 93, 94, 102, 104, 147, 154, 156, 159, 161, 173, 176, 184, 189, 193
- Tsykoza L. T.**, 98, 99, 146, 147, 172, 190, 192
- Tsyrulnikov P. G.**, 16, 72, 125, 160, 168, 178, 187, 190
- Tulmankov V. P.**, 18
- Tuzova Yu. E.**, 191
- Tyshchishchin E. A.**, 122, 156
- Ushakov V. A.**, 124, 125, 146, 147, 172, 173, 175, 176, 183, 192
- Usoltseva A. N.**, 108, 150, 177
- Vanina M. P.**, 114, 148
- Varnek V. A.**, 166
- Vasenin N. T.**, 184
- Vasilieva I. V.**, 191
- Vassiltsova O. V.**, 191
- Vedenikin P. M.**, 182, 185
- Vedyagin A. A.**, 44, 191
- Vedyakin P. I.**, 137, 157
- Veniaminov S. A.**, 184, 185
- Vernikovskaya N. V.**, 43, 141, 144, 190, 191
- Vichkanov A. N.**, 142, 166
- Vlasov A. A.**, 91, 115, 144, 152, 162
- Volkova G. G.**, 11, 61, 191
- Volodin A. M.**, 96, 100, 104, 145, 154, 155, 160, 181, 189, 192
- Vorontsov A. V.**, 120, 160, 192
- Vostrikov Z. Yu.**, 182, 184, 185
- Yakovlev A. L.**, 156;
- Yakovlev V. A.**, 187
- Yakovleva I. S.**, 94, 147, 173, 192; V. N., 121, 151, 152
- Yakushko V. T.**, 93, 118, 156, 159
- Yashnik S. A.**, 98, 99, 124, 125, 146, 147, 172, 173, 183, 190, 192
- Yazykov N. A.**, 137, 138, 141, 157, 189
- Yermakova A.**, 38, 41, 134, 135, 141, 160, 163, 192
- Yudanov I. V.**, 146, 155;
- Yudanov V. F.**, 7, 192
- Yudina E. S.**, 134, 142
- Yulikov M. M.**, 192
- Yurchenko E. M.**, 158
- Yurieva T. M.**, 11, 29, 61, 62, 85, 112, 113, 136, 145, 148, 155, 161, 175, 191, 192
- Zabolotnaya G. V.**, 84, 102, 104, 143, 150, 154, 156, 184
- Zagoruiko A. N.**, 14, 38, 65, 166, 169, 192
- Zaikovskii V. I.**, 89, 91, 94, 95, 96, 102, 103, 104, 108, 112, 113, 148, 149, 150, 154, 155, 156, 157, 159, 161, 164, 168, 174, 184, 185
- Zakharenko V. S.**, 120, 154, 180, 182, 192, 193
- Zakharov A. V.**, 193;
- Zakharov I. I.**, 75, 127, 153, 161, 183, 188, 193;
- Zakharov V. A.**, 12, 41, 63, 75, 87, 126, 127, 128, 142, 144, 151, 152, 153, 158, 161, 166, 186, 193;
- Zakharov V. P.**, 193
- Zavarukhin S. G.**, 193
- Zenkovets G. A.**, 92, 161, 176, 193
- Zhdanov V. P.**, 77, 78, 79, 80, 91, 111, 135, 144, 161, 162
- Zhidomirov G. M.**, 7, 20, 21, 25, 28, 41, 51, 75, 76, 77, 141, 142, 156, 157, 160
- Zhizhina E. G.**, 122, 152
- Zhukov Y. N.**, 166
- Zolotarskii I. A.**, 13, 14, 38, 60, 174, 180, 182, 184, 185, 186, 192, 193, 194
- Zudilina L. Yu.**, 193
- Zudin V. N.**, 128, 158
- Zuev M. G.**, 171, 172, 180

C O N T E N T

BORESKOV INSTITUTE OF CATALYSIS OF THE SIBERIAN BRANCH OF THE RUSSIAN ACADEMY OF SCIENCES	5
STRUCTURE OF THE INSTITUTE.....	6
SCHOOLS OF THE BORESKOV INSTITUTE OF CATALYSIS	19
R&D ACTIVITY OF THE INSTITUTE.....	21
INSTRUMENT FACILITIES.....	22
INTERNATIONAL COOPERATION	23
CONFERENCE AND EXHIBITION ACTIVITIES.....	31
BORESKOV INSTITUTE OF CATALYSIS AS AN EDUCATIONAL CENTER	39
SCIENTIFIC SOCIAL LIFE	41
IMPORTANT RESULTS OF THE R&D BY THE BORESKOV INSTITUTE OF CATALYSIS FINISHED IN 2001	49
RESEARCH ACTIVITY	73
Quantum-Chemical Studies	75
Monte-Carlo Simulation to Study Physico-Chemical Processes	77
Development and Application of Physicochemical Methods for Catalysts Investigation.....	81
Nature, Mechanism and Physicochemical Essence of the Low-Waste, Environmentally Friendly Methods of Catalyst Preparation	92
Catalysis on Zeolites	98
Studies on Zirconia-Based Materials	101
Studies on Mesoporous Mesophase Materials	105
Carbon and Carbon Containing Materials.	107
Studies on Metal Catalysts.....	110
Copper-Containing Oxide Catalysts	112
Catalysis by Metal Complexes.....	114
Heteropolycompounds in Catalysis	116
Studies on Selective Catalytic Oxidation.....	117
Studies on Electrocatalytic Processes	118

Photocatalytic and Related Processes	120
Catalysis for Synthesis Sulfur-Organic Compounds.....	121
Heat Accumulation Processes	121
Biology Related Catalysis and Biotechnology.....	122
Catalyst Deactivation	123
Catalysts for Detoxication	124
Catalytic Combustion.....	125
Polymerization Processes	126
Aerosol Nucleation Processes	132
Mathematical Simulation of Processes and Reactors. Chemical Engineering.....	134
SCIENTIFIC PUBLICATIONS	139
Journal Publications and Monographs	141
Abstracts, Proceedings	163
AUTHOR'S INDEX	194
CONTENT	200

Annual Review
of Activities in Fundamental Areas

2001

Responsible Editor Acad. V. Parmon
Editor E. Mikhailenko
Technical Editor N. Poteryaeva
Translation into English E. Nikiforova

Edited and printed at Boreskov Institute of Catalysis

Подписано в печать 14.06.2002
Печ. л. 25,5

Формат 60x84/8
Заказ № 100

Гарнитура Таймс
Тираж 300

Отпечатано на полиграфическом участке издательского отдела Института катализа СО РАН

630090, Новосибирск, пр-т Академика Лаврентьева, 5