BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

ANNUAL REVIEW 2003

ANNUAL REVIEW
of Activities in Fundamental Areas
2002

BORESKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

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Dear Colleagues,

Let me present the ninth issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covering the year 2002.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and NIS, but also in many western and oriental countries. Since the sixties of the 20th century it remains the largest chemical research institution in the Asian part of Russia and has many deep and stable traditions in providing basic and applied research in nearly all fields of catalysis. The interests of BIC spread from the sophisticated areas of purely academic research to the real applied problems, including development of commercial catalysts and catalytic technologies.

The current features of BIC result from dramatic changes in Russia during the last decade and its entering the market economy. In spite of general economic instability in the country for the last decade, 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 2002 was very important for the life of BIC in many aspects. First of all, the Institute has condoned to sustain successfully in the extremely high financial instability of Russia in the middle 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 2002, 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. The major priority of the Institute in the year 2002 was participation in the very rigid competition to win the largest R&D grant of the nowadays Russia in the field of new catalysts and catalytic technology in oil refining. Since the spring of 2003, this project becomes the leading for the Institute's R&D activity for the next three years.

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 director of the Boreskov Institute of Catalysis is simultaneously the general director of the UIC. In 2002, the United Institute of Catalysis included 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 Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences (BIC) still remains the largest specialized institute working in the field of catalysis not only at the territory of Asian part of Russia, but in the world too. It is the only institution in the country fully specialized on the problems of catalysis and encompasses all its aspects from fundamental and theoretical to industrial mastering of new catalysts.

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

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

In 1984 Professor Zamaraev became the Director of the Institute of Catalysis, and since that time he was the real leader of all research and development activity of this huge (up to 1000 people in staff) Institute. K.I. Zamaraev, the former President of the International Union of Pure and Applied Chemistry, Foreign Fellow of the Indian National Science Academy and of the Korean Academy of Science and Technology, holder of the Silver Medal of the Royal Chemical Society of Great Britain as a centenary lecture, has passed away in the prime of his brilliant scientific career on 26 June 1996.

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

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

STRUCTURE OF THE INSTITUTE

The Institute of Catalysis with its Omsk and St. Petersburg Divisions currently has 1000 employees including researchers and their co-workers, of these 2 Members of the RAS, 4 Corresponding Members of the RAS, about 60 Professors, more than 200 have a Ph.D. degree, about 40 Ph.D. students, personnel of Service, Managing, Engineering and Pilot Departments to support and promote R&D activities. The Institute presents the unique society of qualified specialists in broad spectra of catalysts problems, able to solve any questions related to phenomena of catalysis, from theoretical problems like quantum-chemical calculations up to designing of industrial catalysts and processes.

The structure of the Institute incorporates 7 Scientific-Research Departments, Department of Applied Catalysis, Center for Catalyst Characterization and Testing, and Information Center. The structure of the Institute includes also scientific-supportive units, manufacturing facilities, administration and services.

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

The main directions of its activity are:

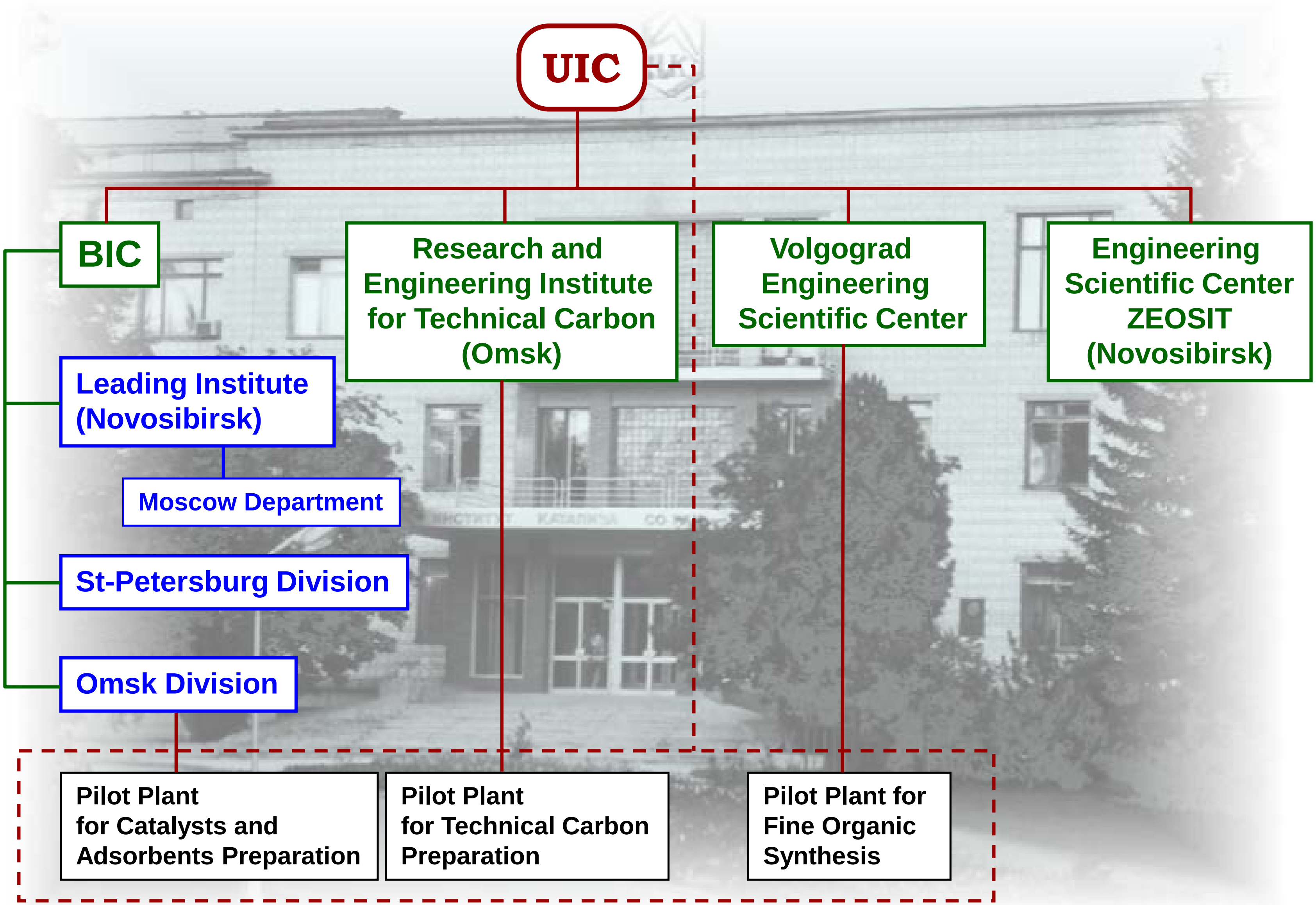
- Complex investigation and characterization of the catalysts by a set of modern physicochemical methods.
- Joint scientific projects with foreign firms and organizations on studying certain catalytic processes and catalysts for the purpose of their improvement.
- Development of modern standard experimental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

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

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

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

United Institute of Catalysis (UIC)



UIC

BIC

Leading Institute (Novosibirsk)

Moscow Department

St-Petersburg Division

Omsk Division

Research and Engineering Institute for Technical Carbon (Omsk)

Volgograd Engineering Scientific Center

Engineering Scientific Center ZEOSIT (Novosibirsk)

Pilot Plant for Catalysts and Adsorbents Preparation

Pilot Plant for Technical Carbon Preparation

Pilot Plant for Fine Organic Synthesis

STRUCTURE OF THE INSTITUTE

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

DIRECTOR

Directorate

Scientific Council

Research Departments

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
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 6 groups Head: Prof. V.A. Sobyanin

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
7 laboratories and 2 groups 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
Head: I.A. Zolotarskii

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. Eugenii 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 Technologies
Head: Prof. Vladimir I. Anikeev

DEPARTMENT OF HETEROGENEOUS CATALYSIS

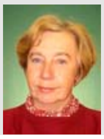
HEAD OF THE DEPARTMENT PROF. VLADIMIR A. SOBYANIN

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

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

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. Bair 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. Eugenii A. Paukshtis

Group of Catalysts Preparation
Head: Vasilii 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. ALEXANDER S. NOSKOV

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

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

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. Alexander 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

Group of Catalytic Technologies for Carbon Materials Synthesis,
Head: Dr. Dmitrii G. Kuvshinov

DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS

ACTING HEAD OF THE DEPARTMENT PROF. ZINAIDA 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 (VICE DIRECTOR)
PROF. VALERII K. DUPLYAKIN

SCIENTIFIC-RESEARCH SUBDIVISIONS

Laboratory of Catalytic Synthesis
Head: Prof. Vladimir A. Likholobov

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

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

Laboratory of Catalysis by Supported Metals
Head: Prof. Aleksander S. Belyi

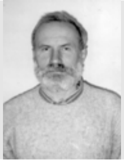
Laboratory of Kinetics and Modeling of Petrochemical Processes
Head: Prof. Nikolai M. Ostrovskii

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

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 rote of oxidation reactions;

- The influence of cation nearest environment on catalytic properties;

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

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

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

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

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

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

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

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

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

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

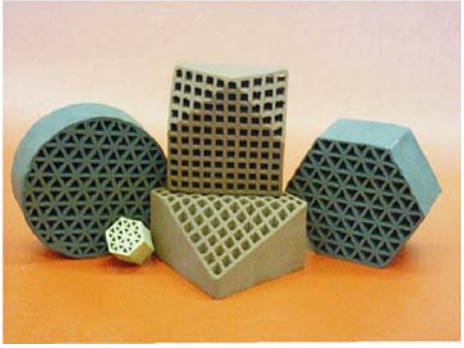
- Design of highly efficient catalysts of new generation for the production of key chemicals and oil processing
- Design of catalytic compositions and technologies for innovative application areas
- Development of innovative catalysts and catalytic technologies manufacturing complex chemicals and polymers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

Some R&D Priorities of BIC

- Catalysts for the processes of oil refineries
- Catalysts and catalytic technologies of the basic processes structurizing the chemical industry
- Catalysts and catalytic technologies for sulfur removal from the natural gas
- Catalysts and catalytic technologies for production of the main types of drugs and vitamins

- Catalysts and catalytic technologies for production of fertilizers and chemicals for protection of agricultural crops
- Catalysts and processes of polymerization
- Catalysts and catalytic technologies for environmental protection
- Composite materials with regulated properties for various application
- Catalysts and processes for renewable energetics as well as utilization and conversion of renewable raw materials and coal.

New industrial catalysts by BIC

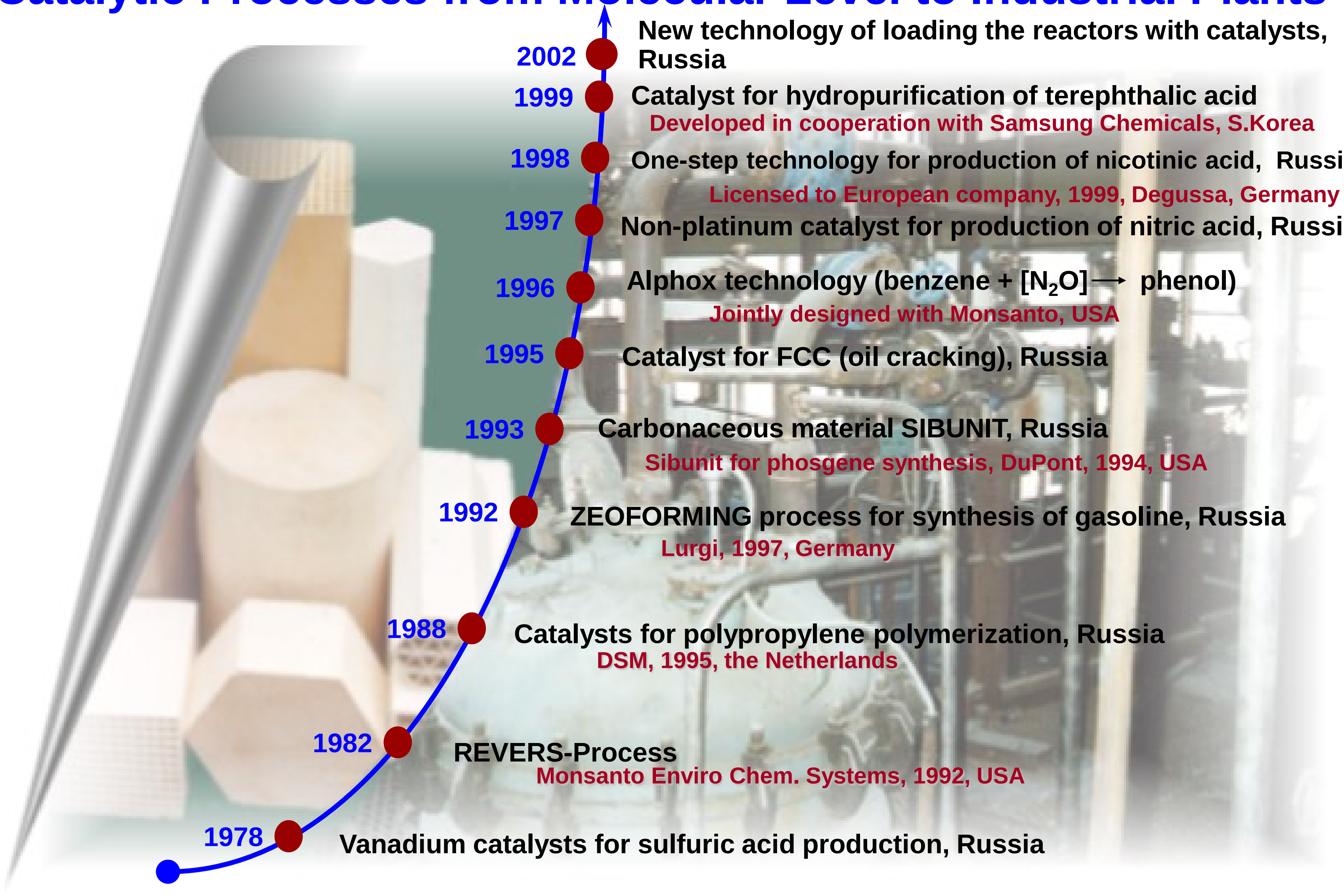


- Catalysts for inorganic synthesis
- Catalysts for organic and fine synthesis
- Catalysts for olefin polymerization
- Catalysts for oil processing
- High silica zeolites
- Catalysts for treatment of gaseous and liquid wastes of industries, energetics, transport, etc.
- Catalysts for treatment of technological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

New catalyst supports by BIC

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

Catalytic Processes from Molecular Level to Industrial Plants



2002 New technology of loading the reactors with catalysts, Russia

1999 Catalyst for hydropurification of terephthalic acid
Developed in cooperation with Samsung Chemicals, S.Korea

1998 One-step technology for production of nicotinic acid, Russia
Licensed to European company, 1999, Degussa, Germany

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

1996 Alphox technology (benzene + [N_2O] → phenol)
Jointly designed with Monsanto, USA

1995 Catalyst for FCC (oil cracking), Russia

1993 Carbonaceous material SIBUNIT, Russia
Sibunit for phosgene synthesis, DuPont, 1994, USA

1992 ZEOFORMING process for synthesis of gasoline, Russia
Lurgi, 1997, Germany

1988 Catalysts for polypropylene polymerization, Russia
DSM, 1995, the Netherlands

1982 REVERS-Process
Monsanto Enviro Chem. Systems, 1992, USA

1978 Vanadium catalysts for sulfuric acid production, Russia

1958

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

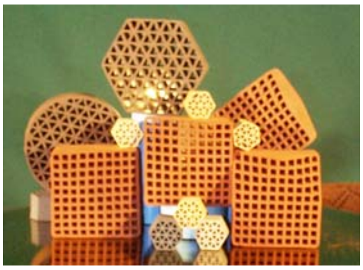
1990 - Russia

FORMALDEHYDE PRODUCTION FROM METHANOL OVER OXIDE CATALYST

1972 - Russia
1982 - Czech Republic, Bulgaria

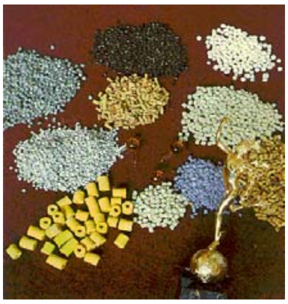
DEHYDROGENATION CATALYSTS FOR ELASTOMERS PRODUCTION

1974 - Russia



TECHNOLOGY OF ALUMINA PRODUCTION: NITRATE-AMMONIA TECHNOLOGY, THERMAL DECOMPOSITION WITH THE USE OF CHG, 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 H_2SO_4. Capacity up to 100 000 m^3/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

CATALYIC 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

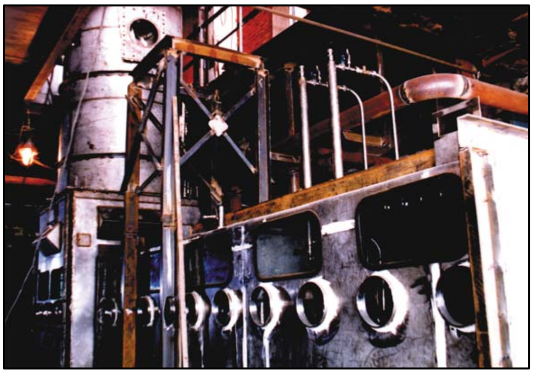
1992- Russia

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

INSTRUMENT FACILITIES

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

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

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

Analytical (composition of catalysts and catalytic reaction products)

Bulk composition

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

Phase analysis

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

Morphology

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

Surface

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

Molecular composition of individual compounds and their mixtures

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

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

Porosimetry
Calorimetry

Kinetic

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

Spectral methods

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

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. During the year 2002 108 scientists took part in measures abroad.

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.

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

Belgium	2	Hungary	2	Singapore	2
China	2	India	1	South Korea	1
Czech Republic	4	Israel	1	Spain	2
Egypt	2	Italy	4	Sweden	2
Finland	2	Japan	5	Switzerland	9
France	10	Netherlands	15	Turkey	2
Germany	14	Norway	2	USA	16
Greece	3	Poland	4	Yugoslavia	1
Hong Kong	1	Romania	1		

Visits of foreign specialists to the Boreskov Institute of Catalysis

Chile	2	Japan	10	Romania	1
Denmark	1	Netherlands	8	South Arabian Republic	1
France	7	Norway	2	South Korea	2
Germany	12	Poland	1	Taiwan	2
Greece	2	Portugal	1	UK	4
				USA	21

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-CNR**, Messina – **BIC**, Novosibirsk, "*Catalysis for Solving the Energy Problem*".

FRANCE

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

- Institute de Recherches sur la Catalyse, Villeurbanne on the BIC-IRC Twinning Programme:

1. *Membranes in Catalysis*
2. *Mechanistic Study of Catalytic Reactions by Transient Techniques. Experiment and Modeling*
3. *Dynamics of Adsorbed Species in Zeolites*
4. *Depollution of Organic Contaminants.*

- Université Pierre et Marie Curie, Paris on the project *"NMR Investigations of Supported Vanadium Catalysts"*.

INDIA

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

- **Central Salt&Marine Chemicals Research Institute**, Bhavnagar on the project *"Olefin Hydroformylation"*.
- **National Chemical Laboratory**, Pune on the project *"Design of Bifunctional Supported Non-Iron Catalysts for Low-Temperature Ammonia Synthesis"*.

POLAND

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

YUGOSLAVIA

The cooperation with the **University of Belgrade** was continued in the frame of the agreement between Serbian Academy of Sciences and Arts and Russian Academy of Sciences.

COOPERATION WITH FOREIGN ORGANIZATIONS IN THE FRAMEWORK OF BILATERAL AGREEMENTS

SPAIN

The cooperation with research institutions of Spain is:

“Development and Applications of New Theoretical Approach to Investigation of the Electronic Structure and Spectra of Fullerene-Like Systems", **Institute of Computational Chemistry**, Girona.

“Nanoparticles on the Base of Mixed Oxides of the Transition Metals. Catalytic and Photocatalytic Activity in the Ecological Processes, Oxides for Microelectronics”, **Sevilla Institute of Material Sciences**, Sevilla.

“Fundamental and Technical Aspects on In-situ Spectroscopy of Oxide Catalysts”, **Institute of Catalysis and Petrochemistry**, Madrid.

GERMANY

Cooperation in the frame of RAS-DFG agreement with the **Fritz-Haber-Institut der MPG**, Berlin and **Munich Technical University**, Munich.

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”*.

COOPERATION IN THE FRAME OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

I. Novel Nanocomposites of Nanocarbons: Synthesis, Characterization, Application

Project Coordinator:

Prof. Yu. Svirko, University of Joensuu, Finland

Participants:

Dr. J-M. Bonard, Ecole Polytechnique Federale de Lausanne, Switzerland
Dr. V. Kuznetsov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. N. Yudanov, Institute of Inorganic Chemistry, Novosibirsk, Russia
Dr. T. Kononenko, General Physics Institute, NSC, Moscow, Russia
Dr. A. Obraztsov, Moscow Lomonosov State University, Moscow, Russia
Dr. G. Mikheev, Institute of Applied Mechanics, Izhevsk, Russia.

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

Project Coordinator:

Prof. J. Ross, University of Limerick, 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 V_2O_5-TiO_2 System

Project Coordinator:

Prof. K. Jug, University of Hannover, 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. P. Tsiakaras, University of Thessaly, Greece

Participants:

Prof. V. Sobyanin, 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, Bremen, Germany
Prof. R. Imbihl, University of Hannover, 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. Keiski, University of Oulu, Linnanmaa, Oulu, Finland
Prof. J. Santamaria, University of Zaragoza, Zaragoza, Spain
Prof. P. Menon, University of Gent, Gent, Belgium.

VII. Development and Study of New Catalytic Systems Based upon Microdomain Textured Perovskites for Efficient Lean DeNOx Process, CO Removal and C_2H_6 Conversion

Project Coordinator:

Prof. R. Schloegl, Fritz-Haber-Institut der MPG, 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. The Nature of Sulfated Zirconia Strong Acidity

Project Coordinator:

Prof. J. Vedrine, 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.

IX. 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.

X. Advanced Highly Ordered Thermostable Nanoscale Silicates, Their Derivatives and Composite Materials

Project Coordinator:

Dr. A. Gedeon, Université Pierre et Marie Curie, Paris, France

Participants:

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

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

Project Coordinator:

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

Participants:

Dr. V. Zyryanov, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia
Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. L. Ivashkevich, Research Institute for Physical and Chemical Problems, Byelarus State University, Minsk, Byelarus
Prof. J. Criado, Sevilla Institute of Material Sciences, Sevilla, Spain.

GRANTS PROVIDED BY INTAS-RFBR

I. 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.

II. 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, Berlin, Germany

Participants:

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

III. 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. A. Payatakes, Institute of Chemical Engineering and High Temperature Chemical Processes, Rion-Achaia, Greece

Participants:

Prof. M. Ormerod, Keele University, Staffordshire, United Kingdom
Dr. A. Demin, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia
Prof. Ch. Comninellis, Swiss Federal Institute of Technology, Lausanne, Switzerland
Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Kozhukharof, University of Chemical Technology and Metallurgy, Sofia, Bulgaria
Dr. N. Zakarina, 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. J.-M. Cormier, University of Orleans, France
Dr. B. Potapkin, Russian Research Centre "Kurchatov Institute", Moscow, Russia
Prof. V. Kirillov, 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. 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, Pedagogical University of Czestochowa, Czestochowa, Poland
Prof. K. Warmuzinski, Institute of Chemical Engineering of the PAS, 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. K. Luyben, Delft University of Technology, The Netherlands

Participants:
Prof. J. Garcia Fierro, Institute of Catalysis and Petrochemistry, Madrid, Spain
Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. Yu. Plyuto, Institute of Surface Chemistry National Academy of Sciences of Ukraine, Kiev, Ukraine.

NATO PROGRAMME: SCIENCE FOR PEACE

I. Catalytic and Electrochemical Processes for SO_2 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.
Project Co-Directors:
Prof. R. Fehrmann, Technical University of Denmark, Denmark
Dr. V. Parvulescu, University of Bucharest, Bucharest, Romania
Dr. J. Winnick, Georgia Tech, Atlanta, USA
Mr. Yu. Zhukov, Byisk Oleum Plant, Byisk, Russia.

II. Development of Shape Steam Reforming Catalysts

NATO Country Project Director:
Prof. J.A. Mouljin, Delft Technological University, Delft, The Netherlands

Partner Country Project Director:
Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia

Project Co-Director:
Mr. S. Perezhogin, Ulba Metallurgical Plant, Ust-Kamenogorsk, Kazakhstan.

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

Project Co-Director:
Prof. R. Tsekov, University of Sofia, Sofia, Bulgaria.

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. Caldararu, Institute of Physical Chemistry "I.G. Murgulescu", Bucharest, Romania

Project Co-Directors:

Dr. G. Pop, Zecasin S.A., Bucharest, Romania
Prof. A. Startsev, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. J. Cejka, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
Ing. K. Svoboda, Chemopetrol, Litwinov, Czech Republic
Dr. M. Derewinski, Institute of Catalysis and Surface Chemistry, Krakow, Poland
Prof. A. Khan, University of Lund, Lund, Sweden.

CRDF

I. Infrared Studies of Nature of Solvated Proton

Project Coordinators:

Prof. E. Stoyanov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. Ch. Reed, University of California, Riverside, USA.

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

Project Coordinators:
Dr. O. Kholdeeva, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. C. Hill, Emory University, USA

III. Catalysis by *in-situ* Generated Oxidants

Project Coordinators:
Prof. V. Bukhtiyarov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. W. Goodman, Texas A&M University, USA.

IV. Nanocrystalline Oxides as Novel Catalytic Materials and Destructive Sorbents for Hazardous Compounds: Relationship Between Synthesis, Structure and Reactivity

Project Coordinators:
Prof. A. Volodin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. K. Klabunde, Kansas State University, USA.

INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)

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

Project Manager:

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

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

Project Manager:

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

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

Project Manager:

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

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

Project Manager:

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

CONFERENCE AND EXHIBITION ACTIVITIES

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

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 2002, the most important BIC's achievements in the area of applied catalysis were presented at the exhibitions:

- ***Second Moscow International Salon of Innovations and Investments***, February 6-9, Moscow, Russia. **Golden Medal** for "Organization of Production of Catalyst IC-8-21 for Propylene Polymerization"
- Exhibition of Developments of SB RAS ***"New Technologies and Materials in Industry"***, February 4-8, Izhevsk, Udmurtia Republic, Russia
- Exhibition ***"New Innovation Technologies in Petrochemistry, Tribotechnologies and Polymers"***, February 6-13, Kair, Egypt
- ***"High Technologies" – "HI-TECH-2002"***, April 22-26, Moscow, Russia
- Exhibition-Congress ***"Oil and Gas – 2002"***, May 15-17, Tomsk, Russia
- Exhibition-Seminar Dated to the Exit Session of Scientific Council on ***Regional Scientific-Technical Program "Sibir"***, May 28-30, Tyumen, Russia
- Exhibition Dated to the Joint Session of SB RAS and SB RAMC ***"Novel Technologies in Medicine"***, June 18-19, Novosibirsk, Russia
- International Industrial Exhibition ***"Science of Siberia-2002"***, October 29 – November 11, Novosibirsk, Russia. **Minor Golden Medal** for "Development of Technology on Production of Ecologically Safe Silicagel IC-01-2"
- ***Complex Exhibition Devoted to 300 Jubilee of St. Petersburg,*** November 11-14, London, UK
- Exhibition-Seminar of Developments of SB RAS, November 11-15, Khanty-Mansiisk, Russia
- Exhibition-Seminar ***"Energosberezhenie-2002"***, November 13-15, Tomsk, Russia. **Diploma** for "Catalytic Gas Heater "TERMOCAT-2M".

Solution of many specific problems requires joint efforts in order to promote its fastest accomplishing. 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. One of the directions of the scientific-organizational work carried out in the Institute is aimed on conducting conferences and seminars with the participation not only of Russian scientists and scientists from NIS, but foreign participants as well.

Russian–Dutch Workshop "Catalysis for Sustainable Development"

June 22-26, Novosibirsk, Russia

The Workshop was organized by Boreskov Institute of Catalysis, Schuit Institute of Catalysis (NIOK) and Scientific Council on Catalysis of the Russian Academy of Sciences. The Workshop title exactly depicts the global problem of the modern science. The scientists from all leading universities of The Netherlands, six Russian Universities, eleven Russian scientific centers as Moscow, St. Petersburg, Krasnoyarsk, Novosibirsk, Perm', Ekaterinburg, Samara, Tomsk, Omsk, Kazan, Irkutsk, Kirovo-Chepetsk, and a number of representatives from industrial companies of both countries took an active part in the work of the seminar. The goal of bilateral seminars, used as a traditional cooperation between academic institutions, is the discussion of joint research activities progress and development of new promising projects.

The cooperation between Russian and Dutch researchers in the field of catalysis was always a priority and it has received a fresh impetus in recent years. Every year NWO and RFBR announce competitions for joint Russian-Dutch projects in different fields. The year 2002 they have announced a competition in catalysis, which inspired the performance of the first joint seminar on catalysis.

The Workshop program has covered numerous problems that are solved by present-day catalysis. The scientific program included 8 plenary lectures, 25 oral presentations and 46 posters. The scope of the Workshop included:

- Fundamentals of catalysis: surface science and theory
- Homogeneous catalysis
- Catalysis for renewable energy production
- Environmental catalysis
- Kinetics and reactor modeling.

The participants and audience of the seminar have noted a high level of the Plenary Session.

R.A. van Santen (Eindhoven University of Technology, The Netherlands) - *"Molecular Modeling"*. The Density Functional Theory is successfully used to describe the experimental data on the reaction of selective toluene alkylation, which confirmed that the reaction is sterically controlled. On this basis, the reaction mechanism is suggested.

V.B. Kazansky (Zelinsky Institute of Organic Chemistry, Moscow, Russia) – *"Localization of Bivalent Transition Metal Ions in High Silica Zeolites Probed by Low Temperature Adsorption of Molecular Hydrogen"*. The lecture is devoted to a study of adsorption sites on the zeolites modified with bivalent metal cations as zinc. It was established that several adsorption sites appear in the samples with a low Si/Al ratio. When this ratio is high in the sample, only one adsorption site is observed. This observation is very important from an industrial standpoint, especially for oil refining. The work was performed in collaboration with the group of Prof. R.A. van Santen (Eindhoven University of Technology, The Netherlands).

V.N. Parmon (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Catalytic Methods of Energy Production from Renewable Sources and Materials"*. The lecture is devoted to novel catalytic technologies providing generation of heat and production of high-quality liquid fuels from renewable carbon-containing feedstock (primarily biomass) via utilization of nuclear and non-traditional energy sources as well as middle and low-potential waste. The emphasis has been placed on the most elaborated catalytic technologies as environmentally safe combustion of biomass in the fluidized catalyst bed, catalytic conversion of nuclear and solar energy and recuperation of low-potential heat using new composite materials as selective water sorbents.

H. Van Bekkum, A.C. Besemer* (Delft Universityof Technology, Julianalaan, The Netherlands; *SCA Hygiene Products, Zeist, The Netherlands) - *"Selective Oxidation of Carbohydrates with Focus on TEMPO Catalysis"*. The lecturer has stated that converting carbohydrates into carboxylates or polycarboxylates is an obvious way of upgrading renewables. The focus of the lecture is on the amazingly selective TEMPO-catalyzed primary alcohol oxidation of low and high molecular mass carbohydrate systems. Further trends are to apply cheap TEMPO derivatives and to develop immobilized TEMPO systems, and a major challenge is to find a salt-free method.

G.M. Zhidomirov, A.A. Shubin, V.B. Kazansky*, V.N. Solkan*, R.A. van Santen**, A.L. Yakovlev**, L.A.M.M. Barbosa** (Boreskov Institute of Catalysis, Novosibirsk, Russia; *Zelinsky Institute of Organic Chemistry, Moscow, Russia; **Eindhoven University of

Technology, Eindhoven, The Netherlands) - *"Structural Stability and Catalytic Reactivity of Zinc Ion Species in Zeolites"*. The quantum chemical methods are used to describe the atomic state of zeolite supported systems (MF1 type).

J.A. Moulijn, A. Stankewicz, F. Kapteijn (Delft University of Technology, The Netherlands) - *"The Potential of Structured Reactors in Process Intensification"*. Structured catalytic reactors have a large potential in Process Intensification. It is a breakthrough in chemical engineering. The lecture consisted of a general introduction in Process Intensification and a more specialized treatment of the most common type of structured reactors, the monolithic reactor. Multiphase systems were highlighted. The potential in fine chemistry was discussed explicitly. The new monoliths, designed in cooperation with the laboratory of Prof. Z.R. Ismagilov (Boreskov Institute of Catalysis, Novosibirsk, Russia), demonstrated increase in the efficiency of a number of important processes such as DeNOx, catalytic partial oxidation, etc.

Z.R. Ismagilov, O.Yu. Podyacheva, L.T. Tsykoza, V.N. Kruchinin, S.A. Yashnik, V.V. Kuznetsov, T.V. Reshetenko, H.J. Veringa* (Boreskov Institute of Catalysis, Novosibirsk, Russia; *ECN, The Netherlands) - *"Development of Advanced Catalysts for Environmental Protection"*. The paper reviews the main results obtained under three joint Russian-Dutch Projects supported by NWO and RFBR and considers the design of catalytic heat-exchanging reactors for highly effective combustion of fuels, and new efficient catalytic systems for selective reduction of nitrogen oxides by hydrocarbons as well as new ways for catalytic production of fuels from renewable sources.

C.J. Weststrate, A. Gluhoi, R.J.H. Grisel, **B.E. Nieuwenhuys** (Leiden Institute of Chemistry, The Netherlands) – *"Oxidation Reactions over Multicomponent Catalysts Consisting of Gold and a Transition/Rare Earth Metal Oxide"*. This fundamental study focuses on the problems of environment protection, such as cleaning of automotive exhaust, oxidation of carbon monoxide in the presence of hydrogen in order to clean hydrogen produced from hydrocarbon fuels for further using in fuel cells. The effect of the gold particle size and the effect of the presence of MO_x on the activity and the selectivity were discussed. On the basis of the results the authors proposed a formulation for a novel catalyst for the selective oxidation of CO. In addition, a mechanism was proposed for the relevant processes.

It should be noted that most of results presented in the plenary lectures were jointly performed by Russian and Dutch researchers and supported by the NWO and RFBR grants.

Oral contributions were presented by both well-known and young scientists.

The seminar programme perfectly combined the lectures devoted to fundamental investigations and applied R&D. The Poster Session reflected the main idea of the Seminar – performance of fundamental investigations and their purposeful implementation in industry. The posters devoted to the development of new catalytic systems and promising technologies have attracted considerable interest of the participants.

The special INTAS Session has been held as a part of the scientific program of the seminar.

The joint meeting of the Novosibirsk Branch of Mendeleev's Society and the Royal Chemical Society of The Netherlands (Prof. Rutger A. Van Santen is the chairman) was organized in the Workshop framework. The members of Society were greeted by a vice-president of the Society, a Corresponding Member of RAS, N.Z. Lyakhov (Director of the Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk). The chairman of the Novosibirsk branch of the Society, Academician V.N. Parmon presented very interesting information on the work of the regional branch. He has pointed to the positive changes in the development of Russian science that provide a revival of the Russian Chemical Society. Professor R.A. van Santen made a report on the work of the Royal Chemical Society of The Netherlands.

During the seminar, there was a meeting of Prof. N.S. Dikanskii (Rector/Head of the Novosibirsk University), Academician V.N. Parmon (Director of the Institute of Catalysis) and Prof. R. Van Santen (Head/Rector of the Eindhoven University). They have discussed new ideas for cooperation between the Universities, which would provide efficient training of students and post-graduates.

At the final sitting, it was decided to continue performance of bilateral meetings in order to discuss the obtained experimental results, estimate the state of the art and determine further research activities.

VI Russian Conference “Mechanisms of Catalytic Reactions”, “MCR-VI”

October 1-5, Moscow, Russia

The VI Conference “Mechanisms of Catalytic Reactions” was organized by**:**

- Ministry of Industry, Science and Technologies of the Russian Federation, Moscow
- Boreskov Institute of Catalysis, Novosibirsk
- Lomonosov Moscow State University, Moscow
- Scientific Council on Catalysis of the Russian Academy of Sciences
- Russian Foundation for Basic Research, Moscow
- International Association for the Promotion of Cooperation with Scientists from the New Independent States of the former Soviet Union (INTAS)
- Shimadzu Europe GmbH, Germany.

The financial support was given by: JSC “Uraltechnogenmet" (Kirovograd, Russia), SASOL Germany GmbH, UOP LLC, Bayer AG, Engelhard, ICI, Dow Chemical Company, Haldor Topsoe A/S.

The Conference was held at the Moscow Lomonosov State University. The five-day MCR-VI Conference program consisted of 11 plenary and 14 keynote invited lectures, 105 oral presentations and 160 posters of 250 participants from the NIS (Armenia, Byelarus, Kazakhstan, Russia, Ukraine) and also 35 participants from western countries (Austria, Finland, France, Germany, Hungary, Israel, Italy, Japan, Norway, Poland, UK, USA).

The plenary lectures were given by:

A.T. Bell (University of California, Berkeley, USA) – *“Applications of Density Functional Theory for the Identification of Reaction Pathways of Catalyzed Processes”*. The paper presents several illustrations to show how DFT can be used to identify critical features of the processes involved in N_2O transformation, and a newly developed method for identifying transition states and reaction pathways.

A.E. Gekhman (Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia) – *"Catalysis of Oxidation with Hydroperoxides: Molecular Pathways"*. The paper discusses the nature of intermediates upon oxidation with hydroperoxides.

B.N. Kuznetsov (Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia) – *"Modern Views on Mechanism of Catalyst Action in Conversions of Plant Polymers"*. The lecture presents the current state in the field of catalytic mechanisms of the processes of transformation of plant polymers. Latest ideas on the mechanism of catalytic depolymerization of plant carbohydrides and lignin of plant biomass, carbonization of plant polymers into carbon materials, etc. are discussed.

G.I. Panov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"New Oxidation Reactions in Organic Synthesis"*. The review of the gas-phase reactions involving N_2O as selective oxygen donor in organic synthesis was accompanied by demonstration of possible application of nitrous oxide in the liquid-phase oxidation, which open a new way for synthesis of various oxygenated organic products.

V.A. Sadykov, V.V. Lunin*, J.R.H. Ross** (Boreskov Institute of Catalysis, Novosibirsk, Russia; *Moscow Lomonosov State University, Moscow, Russia; **University of Limerick, Limerick, Ireland) – *"Mechanism of Nitrogen Oxides Selective Reduction by Hydrocarbons in the Excess of Oxygen: Intermediates, Their Reactivity and Routes of Transformation"*. This is a survey of systematic studies of the former process to demonstrate that strongly bonded surface nitrates are the key intermediates; their transformation resulting from interaction with hydrocarbons and oxygen is the limiting reaction stage.

O.N. Temkin, L.G. Bruk (Moscow Lomonosov State Academy of Fine Chemical Technology, Moscow, Russia) – *"Palladium(II,I,0) Complexes in Catalytic Oxidative Carbonylation Reactions"*. The role of Pd complexes in the oxidative carbonylation of alcohols and alkynes and mechanistic features of unusual oscillating oxidative carbonylation is discussed.

Yu.B. Monakov (Institute of Organic Chemistry, Ufa, Russia) – *"Organic Compound of Nontransition Metal and Ion-Coordinated Dienes Polymerization"*. The data presented allow to consider that the organic compound of nontransition metal play an important role both in active centers formation and functioning, and some times it plays the determinative role as transition metal compound (catalyst), that testifies to active center structure, containing both metals (transition and nontransition) in its composition.

A.Ya. Rozovskii (Topchiev Institute of Petrochemical Synthesis, Moscow, Russia) – *"Mechanism and Kinetics of C_1-Molecules Transformations over Cu-Based Catalysts"*. The author used his own and literature data to suggest a consistent scheme for the reactions of one-carbon molecules over copper-containing catalysts, among which were synthesis of methanol, Fischer-Tropsh synthesis, synthesis of dimethyl ether, methyl formate, steam reaction. The overall scheme of natural gas processing into motor fuels was discussed in conclusion.

H. Schulz (University of Karlsruhe, Karlsruhe, Germany) – *"The Mechanism of Fischer-Tropsch Synthesis"*. The mechanism of FT-synthesis is discussed in details on the basis of recently gained data.

The keynote sectional and oral presentations were scheduled in the following parallel sessions:

- ☐ *Reductive-Oxidative Heterogeneous Catalysis*
- ☐ *Acid-Base Heterogeneous and Homogeneous Catalysis*
- ☐ *Methods of Investigation of the Mechanisms of Catalytic Reactions.*

Session *"Catalytic Reactions in Membrane Reactors"* was organized to commemorate the 80th anniversary of the late Professor Vladimir Gryaznov. The Plenary Lecture "Scientific Activity of Academician V.M. Gryaznov" was given by **Prof. V. Yagodovskii** (Russian University of People's Friendship, Moscow, Russia).

It should be noted that a number of lectures were, in essence, the summary of long-term systematic studies in certain fields.

Organization of three Sessions appeared very effective for scientific discussions. This allowed indeed many speakers, among which were young scientists, to present oral communications. Many of these communications were of the same interest as those by venerable scientists. 24 INTAS projects were presented at all parallel Sessions of the Conference as oral and poster presentations.

Traditionally, much attention was paid at the Conference to application of physical (mainly spectral) methods for investigation of catalytic systems. It should be emphasized that this Session was of great interest to the Conference participants, the Conference hall often was overcrowded.

During the Conference, detailed discussions have been carried out aimed at elaboration of further plans of collaboration in various fields.

Presentation of a new Journal "Catalysis in Industry" was included in the Conference program.

The Conference was concluded with presentations of the Boreskov Institute of Catalysis (Academician V.N. Parmon) and the Moscow Lomonosov State University (Academician V.V. Lunin).

The Conference participants have approved the first iteration of the Statute of Russian Scientists.

International School-Conference on Catalysis "Catalyst Design"

December 2-6, Novosibirsk, Russia

The Conference was organized by the Boreskov Institute of Catalysis, Council of Young Scientists of the Boreskov Institute of Catalysis, Novosibirsk State University, Scientific Council on Catalysis RAS for young scientists (up to 35 years old).

The program included:

- Lectures of the leading scientists
- Oral and poster presentations of young scientists
- Practical seminars.

170 participants from 8 countries (United Kingdom, France, Germany, Austria, Poland, Ukraine, Kazakhstan, Russia) took part in the Conference.

The scope of the Conference covered the following topics:

- Mechanisms of heterogeneous catalysis, biocatalysis, electrocatalysis, and fine organic synthesis in catalysis
- Catalyst preparation
- Methods of catalyst investigations
- Catalysis for environmental protection
- Kinetics and modeling of catalytic reactions and reactors
- Legal assistance and estimation of intellectual property objects
- Ways of technology transfer
- Information retrieval of scientific and commercial data bases.

16 lectures of the leading scientists on the fundamental and applied catalysis as well as innovation activity and intellectual property protection were presented:

V.A. Semikolenov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Catalysis in Fine Organic Synthesis"*

N.A. Pakhomov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"The Supported Bimetallic Catalysts of Hydrocarbon Conversion: The Models of Active Component, Approaches to Purposeful Synthesis"*

A.N. Startsev (Boreskov Institute of Catalysis, Novosibirsk, Russia) - *"The Sulfide HDS Catalysts: From the Active Component Structure to Its Molecular Design"*

S. Knobl, G.A. Zenkovets*, G.N. Kryukova*, T.V. Larina*, V.F. Anufrienko*, **D. Niemeyer,** R. Schlögl (Fritz-Haber-Institut der MPG, Berlin, Germany; *Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Methods for Preparation and Characterisation of Heterogeneous Catalysts"*

V.L. Kuznetsov, Yu.V. Butenko (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Synthesis and Investigation of Carbon Nanostructures"*

E.A. Quadrelli, J.M. Basset, M. Chabanas, C. Copèret, J. Thivolle-Cazat, A. Lesage,* L. Emsley* (Laboratoire de Chimie Organométallique de Surface, Villeurbanne, France; *Laboratoire de Stéréochimie et des Interactions Moléculaires Lyon, France) – *"Surface Organometallic Ta(V) Carbenic Species: Mechanism of Grafting Reaction"*

Z.R. Ismagilov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Advanced Catalysts and Catalytic Processes for Environmental Protection"*

Yu.I. Aristov (Boreskov Institute of Catalysis, Novosibirsk, Russia) - *"Composites «An Inorganic Salt Confined to a Porous Host Matrix»: State of the Art"*

V.A. Sobyanin (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Electrocatalysis. Fuel Cells"*

E.M. Moroz (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"X-Ray Methods in Catalyst Investigations"*

D.I. Kochubey (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"EXAFS-Spectroscopy and Investigation of Nanomaterials"*

A. Yermakova (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Modeling of the Kinetics of Catalytic Reactions"*

N.A. Chumakova (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Some Mathematical Aspects of Dynamics of Catalytic Reactions Modeling"*

S.N. Zagrebelnyi (Novosibirsk State University, Novosibirsk, Russia) - *"Enzymes and Design of Biocatalysts"*

M.B. Demidov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Legal Assistance and Estimation of Intellectual Property Objects"*

V.A. Remnyov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Ways of Technology Transfer"*.

3 Practical seminars on physical chemistry and chemical kinetics, excursions to the laboratories of the Institute, Round Table on the activities of the Councils of Young Scientists, social program were organized for the participants.

As a whole the School-Conference demonstrated high activity of young scientists, their ability to be worthy representatives of Science.

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 beginning of the 2002 the "ZeoSit" Scientific and Engineering Center celebrates two remarkable professional events, in a way, anniversaries:

- Ten years since the first installation for production of high octane gasoline from condensed gas - "**Zeoforming**" process - has been started-up at Nizhnevartovsk GPP;
- 5 years of successful operation of the industrial plant “ZEOFORMING-40” on high-octane gasoline "Eurosuper-95" and liquefied gas production on "Zeoforming" technology on "Glimar" Rifinery, Poland.

✯

According to the SB RAS Presidium resolution **Dr. Dmitrii E. Babushkin** and **Dr. Ilya V. Yudanov** are among the winners of the Competition of Youth Projects devoted to the 100th Anniversary of Academician M.A. Lavrentiev.

✯

The Academician A. Balandin prize (after the name of the founder of scientific school in the field of catalysis, author of the multiplet theory of catalysis) has been presented to **Prof. Tamara V. Andrushkevich, Dr. Valentina M. Bondareva** and **Dr. Galina Ya. Popova** for the series of works *"Heterogeneous Catalytic Oxidation of the Basic Organic Compounds into Carboxylic Acids: Mechanism, Kinetics, Design of Catalysts"*. The prize is awarded once per three years for the best works in the field of catalysis.

The presented series of work is the development of efficient methods of catalytic heterophase synthesis of carbonic acids – acrylic, formic and nicotinic acids from acrolein, formaldehyde and 3-methylpyridine, correspondingly. These acids are the valuable chemical products, widely used in production of polymers, chemical fibers, fragrant.

✯

The Project by **Dr. Mikhail V. Luzgin** *“In situ Monitoring of Scrambling of Selective* ^{13}C *and* $^{1}H(^{2}H)$ *Labels in Hydrocarbon Transformation over Solid Acid Catalysts: Kinetics and Mechanism of Reaction”* became the winner of the Competition of the Projects of Young Scientists of Novosibirsk Scientific Center devoted to the 45th anniversary of SB RAS.

✯

According to the SB RAS Presidium resolution the Prizes in the Name of Prominent Scientists (Prize in the name of G.K. Boreskov) was awarded to **Dr. Alexander A. Khassin** for the work “Studying of the Nature of Interaction of Active Component with Undercoat in Co- and Ni-Containing Catalysts Based on Si- and/or Al-Containing Layered Structures”.

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Dr. Dmitrii E. Babushkin and **Dr. Oleg N. Martyanov** were awarded by the State Scientific Scholarship according to the SB RAS Presidium decree.

*

Winners of the Grants within the framework of the Program *“Outstanding Scientists, Young Professors and Doctors of Sciences”* are **Valerii I. Bukhtiyarov** (as Professor) and **Anatolii P. Sobolev** (as Doctor).

*

April, 20 marks 95th anniversary from the birthday of Academician Georgii K. Boreskov, founder and the first Director of the Institute of Catalysis. The grand meeting of the Scientific Council of the Institute included the opening address by Academician Valentin N. Parmon, who reminded about the main facts of the G.K. Boreskov biography and told about his role in the creation of the basis for sustainable development of the Institute, four scientific lectures by G.K. Boreskov followers and presentation of the English version of the book “Heterogeneous Catalysis”, issued in Russian in 1988.

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The Joint Scientific Council on Chemical Sciences of the SB RAS, as well as all the joint scientific councils of the Siberian Branch, plays a role of the specialized branch of the Russian Academy of Sciences, but with the less authorized state. The chemists of the Siberian Branch were sheltered by the Institute of Catalysis, and all the sessions according to the prevalent tradition are held in its conference hall. Unfortunately, they succeed in gathering for clear reasons not more often than two times a year, and if either the General Meeting of the Branch is simultaneously held or everybody has a weighty argument to justify considerable traveling and living expenses. Anyway, many people come, and the scientific secretaries of the institutes of other scientific centers always find time and opportunities to spend a workweek in Novosibirsk.

*

During the XXXIX Annual BIC's Competition of the Research Works the 1 Prize has got the work by **E.V. Starokon, K.A. Dubkov, V.I. Avdeev, S.F. Ruzankin, V.A. Utkin, V.A. Rogov, G.M. Zhidomirov, G.I. Panov** *“Liquid Phases Oxidation of Alkenes with Nitrous Oxide”*.

* * *

In 2001 the Science and Engineering Journal **"Catalysis in Industry"** was founded. The Chief Editor of the Journal is Academician V.N. Parmon. **"Catalysis in Industry"** unites the knowledge and experience of researchers, engineers, producers and consumers of catalysts. The Scope of the Journal:

- Total Problems of Catalysis
- Catalysis in Chemical and Petrochemical Industry
- Catalysis in Oil-Refining Industry
- Engineering Problems. Service and Production
- Production of Catalysts
- Catalysis and Environment Control
- Domestic catalysts. Producers
- In the World of Catalysis
- Information
- Chronicle

* * *

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

The Foundation is supported by IUPAC and some Russian sponsors.

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

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

Major part of Foundation means is spent on Zamaraev post-graduate scholarships, prizes and grants. Foundation plans to support the international cooperation of scientific youth in the field of chemical catalysis and chemical physics, i.e., their participation in international scientific conferences and seminars.

November, 2-7 Zamaraev ICSF jointly with State Committee on Preservation of the Environment held the VII International Student's Ecological Conference *"Ecology of Russia and Contiguous Territories. Ecological Catalysis"* at the Novosibirsk State University within the

Federal Programm "Integration". In the frame of the Conference Zamaraev Foundation held the All-Russian Competition "Student Scholarship –2002". **A. Sametova** (NSU, Novosibirsk), who prepared her degree work at the Institute of Catalysis, has got the Scholarship. The post-graduate scholarships have got **Pavel V. Snytnikov, Anna A. Lysova, Andrey V. Matveev, Vasilii E. Sharonov.**

✯

10 Ph.D. students and scientific employees of the Institute form the personnel of the **Council of Scientific Youth.** The main principle of the Council is submission of the interests of the youth in the Institute. It includes organization of competition of the youth projects, support of the young lecturers of higher educational establishments – employees of the Institute, organization of training for qualifying examinations for the Ph.D. degree, improvement of living conditions of the young scientists, and other directions of activity connected with the improving of a position of the young employees in the Institute.

✯

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

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

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

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

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

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

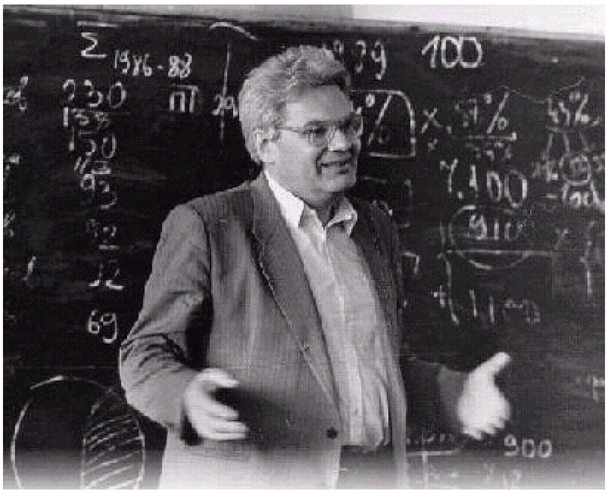
Of particular interest among the exhibit is the personal book collection of Georgii Konstantinovich including more than 1000 scientific volumes and 15 sets of Russian and foreign scientific journals. There are especially memorable copies with dedicatory inscriptions by the authors and the rarities published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

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

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

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

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



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

Kirill demonstrated his brilliant potentialities in sciences as early as his school years. He finished school as the Golden Medal winner; the medal is also stored in the Museum. He continued his education in the Mendeleev Institute of Chemical Technology in Moscow, but after the third year moved to the Moscow Physical and Technological Institute (MPhTI) in order to get a strong background in chemical physics. In the Museum, there are laboratory registries of post-graduate student Kirill Zamaraev and EPR spectra recorded by him during his post-graduate years.

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

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

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

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

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

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

IMPORTANT RESULTS
OF THE R&D ACTIVITY
OF THE BORESKOV INSTITUTE
OF CATALYSIS FINISHED IN 2002

Laboratory of Adsorption
Head: Prof. Valerii F. Yudanov

- The granular materials containing ferromagnetic nanoparticles have a quantity of unique properties due to relatively weak interparticle interactions. The interparticle coupling leads, for example, to giant magneto resistance, formation of different structures with ordered microcrystals magnetic moments, appearance of new phase transitions etc. In the field of chemical application such materials are presented as a wide range of catalysts. However till now there were no direct method to investigate the magnetic interparticle interactions.

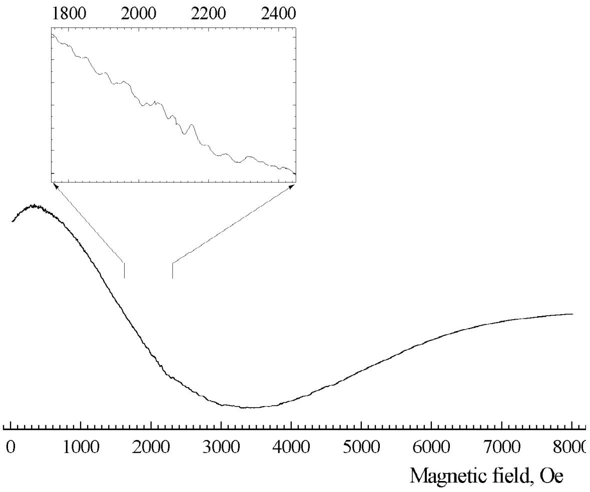


Fig. 1. Spectrum of ferromagnetic resonance of nickel powder in a paraffin matrix. According to electron microscopy, particles with sizes from 0.2 to 10 μm are present. Nickel content is ~5 wt %.

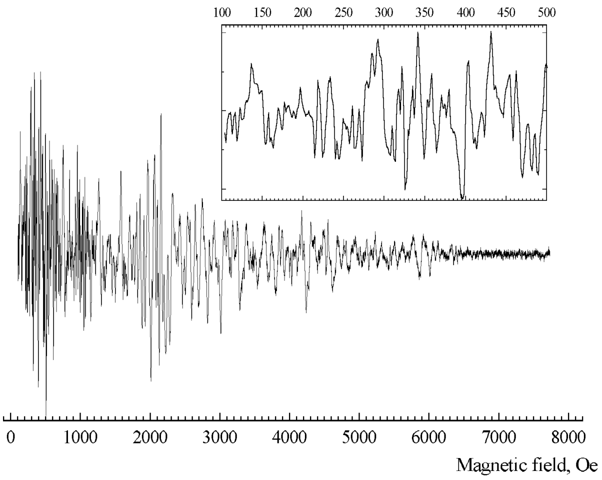


Fig. 2. Fine structure of the spectrum of ferromagnetic resonance of nickel powder prepared using ultrasonic dispersion in a molten paraffin matrix. Nickel content in the sample is ~1 wt %.

Such a possibilities are created owing to revealing in BIC the new type of Ferromagnetic Resonance Spectra of nanoparticles in structural inhomogeneous magnetics – Fine Structure of FMR spectra (FMR FS) (O.N. Martyanov, R.N. Li, V.F. Yudanov, JETP Letters, Vol. 75, No. 12, 2002, pp. 638–641). The spectra observed consist of the multitude of lines which are registered against the broad basic component (Fig. 1, 2). It was experimentally shown that the FMR spectra substructure appearance is connected with magnetisation processes, which take place in granular ferromagnets.

It was experimentally and theoretically shown that the physical origin of the narrow lines observed might be jumplike changes in the resonance conditions caused by a sharp change of the local magnetic field for each microcrystal. Such a situation could be realized due to jump of magnetization of the neighbor nanoparticles with external magnetic field increase (Fig. 3(a)).

The jumplike changes of magnetization of the nanoparticles are the result of interparticle interactions. Just the interparticle interactions in granular magnets provide, contrary to classical case of axial ferromagnetic crystal, multiple jumplike magnetic reversal in positive external magnetic field (Fig. 3(b)).

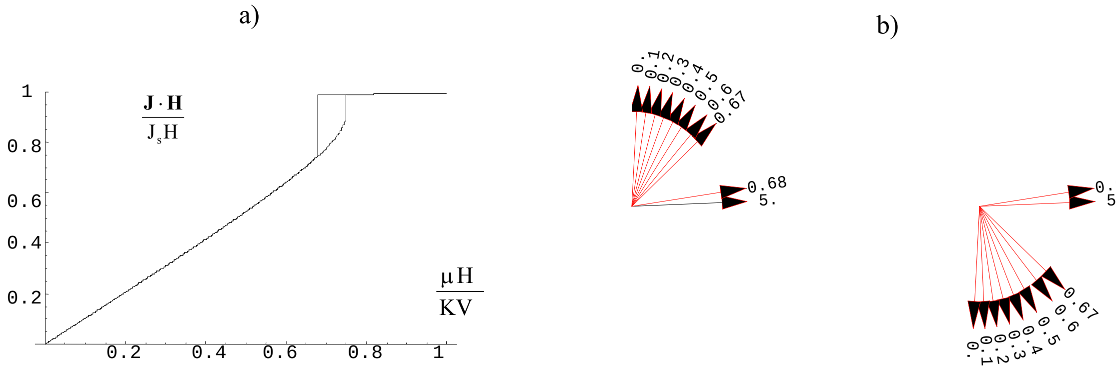


Fig. 3. (a) Variation of the projection of the total magnetic moment of a system of two particles onto the direction of the magnetic field as a function of an external magnetic field. The particles possess magnetic anisotropy and are related by a dipole–dipole interaction. The Hamiltonian of the system and its parameters are:

$$E = E_K + E_{dd} + E_H = -\frac{KV}{\mu^2}\left[(\mu_1 n_1)^2 + (\mu_2 n_2)^2\right] + \frac{d^2\mu_1\mu_2 - 3(d\mu_1)(d\mu_2)}{d^5} - H(\mu_1 + \mu_2),$$

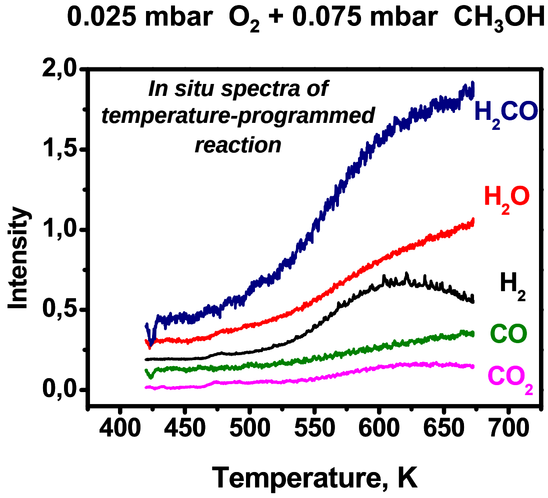
where K is the effective anisotropy constant, V is the volume of an isolated particle, $\mu_{1,2}$ are the vectors of the magnetic moments of the particles ($\mu=|\mu_1|=|\mu_2|$), $\mathbf{n}_{1,2}$ are the directions of the easy axes of the particles, and $\mathbf{d}$ is the vector characterizing their mutual arrangement.
(b) – rotation of the vectors of magnetization of the particles on changing the magnetic field from $H = 5KV/\mu$ to zero. At $H = 0.678KV/\mu$, the irreversible rotation of the magnetization vectors related to the disappearance of the "collinear" minimum occurs.

The phenomenon revealed essentially expands the potential of FMR in investigation of granular magnets and gives opportunity for the direct investigation of the magnetic interparticle interactions in nanomagnets. The analysis of FMR FS allows getting unique information about structure of heterogeneous catalysts, magnetic storage medium and geological species.

Surface Science Laboratory

Head: Prof. Valerii I. Bukhtiyarov

- A specialized VG ESCALAB "High Pressure" photoelectron spectrometer was modernized with the purpose to study heterogeneous catalytic reactions at pressures up to 0.5 mbar. Further modification of a VG ESCALAB "High Pressure" photoelectron spectrometer allowed increasing of the gas phase pressure over the surface of a heterogeneous catalyst up to 0.5 mbar during *in-situ* experiments. The modernized spectroscopic complex makes it possible to measure simultaneously both photoelectron spectra and mass-spectrometer signals, as well as control of the sample temperature in the course of the catalytic reaction. As consequence, both chemical compositions of the adsorbed layers on the catalyst surface and the gas phase can be analyzed together. Methanol oxidation to formaldehyde over Cu was found to proceed by several pathways including: 1) complete oxidation to CO_2 and H_2O, 2) selective oxidation to formaldehyde and H_2O, as well as two dehydrogenation reactions resulting in 3) formaldehyde and H_2, and 4) CO and H_2. Simultaneous measurement of O1s photoelectron spectra in the reaction mixture flow composed of methanol and O_2 over the catalyst showed a presence of two atomic oxygen species. One of them is oxygen adsorbed at the copper surface and another one is a novel state described as sub-oxide oxygen. The correlation between the intensity of XPS signal of sub-oxide oxygen and formaldehyde yield was additionally confirmed by steady state experiments. Results obtained show the availability of approach used for study the catalytic reactions mechanisms.



$2CH_3OH + O_2 \rightarrow 2H_2CO + 2H_2O$
(Selective oxidation)

$CH_3OH + 3/2O_2 \rightarrow CO_2 + 2H_2O$
(Consumption)

$CH_3OH \rightarrow H_2CO+H_2$
(Dehydrogenation)

$CH_3OH \rightarrow CO+2H_2$
(Dehydrogenation)

Laboratory of Investigations of Mechanisms of Catalytic Reactions

Head: Prof. Eugenii P. Talsi

➢ 1. In a study of the reaction system $MAO/(C_2H_5)_2ZrMe_2$, the size of the ion pair $[(C_5H_5)_2Zr(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$ was determined by pulsed field-gradient NMR of its cationic moiety. A mean effective hydrodynamic radius of 12.2-12.5 Å, determined from diffusion rates in benzene solution at different zirconocene and MAO concentrations indicates that the ion pair remains associated even at the lowest concentrations studied. The equilibrium constant for the reaction $[(C_6H_5)_2ZrMe^+...Me\text{-}MAO^-] + ½\ Al_2Me_6 \Leftrightarrow [(C_6H_5)_2Zr(\mu\text{-}Me)_2Al\ Me_2]^+[Me\text{-}MAO]^-$ changes at different Al/Zr ratios, this indicates that MAO contains various species that produce $[Me\text{-}MAO]^-$ anions with different Lewis basicities. The volume of the $Me\text{-}MAO^-$ anion suggests that it contains 150-200 Al atoms.

2. Spectroscopic monitoring of the cationic intermediates formed upon activation of metallocenes with methylaluminoxane (MAO) is crucial for the elucidation of the mechanisms of olefin polymerization. Recent NMR studies have provided important information on the structures of `cation-like` intermediates formed upon activation of Cp_2ZrMe_2 with MAO in toluene. It was shown, that the cationic complexes $[Cp_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ $Me\text{-}MAO^-$ **(III)** and $Cp_2ZrMe^+ \leftarrow Me^-\text{-}Al \equiv MAO$ (**IV**) were the major species at high Al/Zr ratios (200-4000). The complexes **III** and **IV** were proposed to be the precursors of the active centers for polymerization. In order to extend such studies to more complex and practically attractive

zirconocene catalysts, we report on the ^1H NMR characterization of 'cation-like' intermediates $[L_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ Me-MAO$^-$ (**III**), where L_2 are various cyclopentadienyl (Cp), indenyl (Ind) and fluorenyl (Flu) ligands. The following catalysts were studied: $(Cp\text{-}R)_2ZrCl_2$ (R= Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, Me_5, *n*Bu, *t*Bu), rac-ethanediyl$(Ind)_2ZrCl_2$, rac-$Me_2Si(Ind)_2ZrCl_2$, rac-$Me_2Si(1\text{-}Ind\text{-}2\text{-}Me)_2ZrCl_2$, rac-ethanediyl$(1\text{-}Ind\text{-}4,5,6,7\text{-}H_4)_2ZrCl_2$, $(Ind\text{-}2\text{-}Me)_2ZrCl_2$, $Me_2C(Cp)(Flu)ZrCl_2$, $Me_2C(Cp\text{-}3\text{-}Me)(Flu)ZrCl_2$, $Me_2Si(Flu)_2ZrCl_2$. For most of catalysts studied, broad resonances of **IV** were not detected at all or were observed only at low Al/Zr ratios, whereas only the 'cation like' complex $[L_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ Me-MAO$^-$ (**III**) was observed in the reaction solution at highest Al/Zr ratios. Despite the nonuniformity of their Me-MAO$^-$ counterions, the cationic parts of complexes **III** can be characterized by ^1H NMR spectroscopy equally well as for related complexes in reaction systems based on $[CPh_3][B(C_6F_5)_4]$.

3. Catalytic systems based on complexes of chromium with chiral Schiff bases are extensively studied as catalysts of asymmetric epoxidation of olefins and asymmetric Diels-Alder reactions. For the elucidation of the reaction mechanism, it is important to monitor *in situ* the structure of a catalyst. We have assigned for the first time the resonances in EPR and NMR spectra of the following three complexes Cr^{III}(salen)Cl, where salen=(S,S)-(+)-N,N'-bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanediamine; salen=N,N'-bis(salicylidene)-1,2-ethylenediamine; salen=racemic N,N'-bis(3,4,5,6-tetra-deuterosalicylidene)-1,2-cyclohexanediamine. These data allow monitor solution structure of enantioselective chromium catalysts.

Group of Scanning Spectroscopy
Head: Dr. Alexey N. Salanov

- Mechanism of oxygen interaction with Pd(110) monocrystal and regularities of CO oxidation in a wide range of reagents pressure (10^{-6}-10 Pa) and temperature (300-1200 K) has been studied. The role of chain reconstructive adsorptive and oxide structures in reaction of CO oxidation has been ascertained.

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

- The studies on the formation of silicate, alumino- and titanosilicate mesoporous mesophase materials of MCM-41 and SBA-15 type in the presence of SAS has been continued. Based on the aluminosilicate mesophase SBA-15 the composite mesostructured materials have been obtained, in which the main part of mesophase mesopores is filled with carbon from gas phase.

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

- *In situ* solid state ^{13}C NMR spectroscopy was applied to study the **reaction of *n*-but-1-ene on the prospective isomerization catalyst - zeolite ferrierite (H-FER)**. It has been established, that the conversion of but-1-ene over H-FER at 300-823 K included the following successive steps of the olefin conversion (depending upon the temperature): a double-bond-shift reaction, scrambling of the selective ^{13}C label in the formed *n*-but-2-ene, oligomerization (dimerization), conjunct polymerization, formation of condensed aromatics, and formation of the simple aromatics. Arguments in favor of either bimolecular or pseudo-monomolecular mechanisms are provided, excluding at the same time the monomolecular isomerization of n- to isobutene on a fresh sample. The arguments are based on selective label redistribution in the n-but-2-enes, the impossibility of the existence of isobutene inside the pores of the zeolite under static conditions and the observation of n-but-2-enes oligomerization (dimerization). Conjunct polymerization leads to the formation of alkyl-substituted cyclopentenyl cations (CPCs), which can serve as an intermediate for pseudomonomolecular isomerization. Carbonaceous deposits (polycyclic aromatics), which deactivate the catalyst in the isomerization reaction, are formed from the CPCs. Polycyclic aromatics are transformed into simple aromatics with methane and ethane evolution at 823 K.

In the study of the **dynamics of iso-butane inside the pores of the zeolite ZSM-5** by ^{2}H NMR it has been established that perdeuterated *iso*-butane-d_{10}, when it is adsorbed on zeolite ZSM-5, has been shown to exhibit a superposition of two ^{2}H NMR Pake-powder patterns with quadrupole constants C_Q=2.35 kHz and asymmetry parameter η=0.17 for the CD_3 groups and C_Q=23.0 kHz and η=0.20 for the CD groups at 153-373 K. The narrowed Pake-powder patterns have been interpreted in terms of the motional behavior of *iso*-butane molecule located at channel intersection site of the zeolite framework. Dynamic behaviour of *iso*-butane is complex and includes both fast intramolecular rotations and large amplitude librations of the molecule as a whole. For example, the motion of the CD group may be effectively described as consisting of the combination of the precession of the CD group around some axis Z which makes up the angle $\alpha \approx 50^{o}$ with the direction of C-D bond and fast hops of the axis Z itself between two equally populated orientations by the angle $\theta = 39^{o}$ (or 86^{o}). Simultaneously, fast rotation of the methyl groups around CD_3-CD axis occurs. The activation energies and rotational correlation times at 373 K have been estimated to be 13,5 kJ/mol and 41 ps for the methyl groups, and 17.7 kJ/mol and 1200 ps for the methene group, respectively.

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

- 1. The semi-empirical Method of Interacting Bonds (MIB) was used in the present work to clarify the mechanism of the title process. Various single crystal planes of Pt, Rh, Ir, Fe, and Re were examined with respect to the properties of the adsorbed NH_n species (n = 0; 1; 2; 3) by the semi-empirical MIB. The pronounced correlation between the experimental oscillatory behavior of a given single crystal surface and the respective calculated data is established. Those surfaces, where the combination reaction of the NH species can readily proceed theoretically, are active in the oscillatory behavior experimentally, and vice versa.

More than 20 novel satellites have been developed in DAPS spectra obtained after adsorption of various molecules on the Pt(100) single crystal surface. All of these satellites are of the same origin: they are called forth by the conjugate electron excitation, which includes the transition of the substrate core electron to the vacant state above the Fermi level accompanied by the excitation of the valence electron of adsorbed species to vacuum level, or excitation of the surface and bulk substrate plasmons.

2. Influence of adsorbed O_2 molecules on morphology of Pd-nanoparticles as well as Pd(110) plane was studied experimentally and by the theoretical Method of Interacting Bonds. The simulation has shown that the most energy favorable states for palladium are the multiple bonded states of atomic O_{ads} in the structures Pd_3-O_{ads} and Pd_4-O_{ads}. It has been shown that adsorption of atomic oxygen induces the morphology changes of Pd-nanocrystals and Pd(110) plane. In accordance with simulations the most stable cluster configuration for the 13-atomic cluster is the regular icosahedron. But adsorption of 9 oxygen atoms in the Pd_3-O_{ads} and Pd_4-O_{ads} states is accompanied by the structure transition and by transformation of the icosahedron into the cuboctahedron. That is of special interest in oxidative catalysis because of the morphological stability of nanoclusters in oxygen presence.

We have studied the adsorption of NO, O_2 and CO on Pd(110) surface by TDS method. The CO adsorption proceeds without dissociation. During nitric oxide adsorption single desorption peaks N_2, N_2O and O_2 were observed as a result of NO decomposition. The addition of oxygen was found to inhibit the process of NO dissociation. By analysis of TPR spectra of desorbing N_2 and CO_2 for different NO_{ads} + CO_{ads} coverages over Pd(110) and Pt(100) surfaces, we suggest an autocatalytic reaction in an “explosive” way. The unreconstructed Pt(100)-1×1 surface shows a high activity in the NO_{ads}+CO_{ads} reaction accompanied by N_2 and CO_2 peaks evolution (350 K). The reconstructed Pt(100)-hex surface appears to be less active under the same conditions (395 K). The Pd(110) surface shows a low activity (485 K). It may be that the 1×1 ⇔ hex phase transition is related with the “surface explosion” on (NO_{ads}+CO_{ads})/Pt(100). Since no structural phase transition was observed on the Pd(110) surface, the low activity of palladium is considered to reflect the different bonding energy of oxygen and nitrogen adatoms for Pt and Pd surfaces.

Detailed studies of the hysteresis phenomena and oscillatory reaction of CO oxidation on Pd(110) have been carried out with the molecular beam techniques. The modelling of self-oscillations and surface autowaves has been studied by the Monte-Carlo technique. It has been established that the surface phase transition $(1\times1) \rightarrow (1\times2)$, modeled as the adsorbed CO diffusion anisotropy, leads to the appearance of the reaction fronts elliptically stretched along the metal atom rows.

The results for $H_2 + O_{ads}$ reaction over Pd (110) single crystal surface has been studied. The contribution of spillover effect ($H_{ads}/Pd \rightarrow O_{2ads}/Ti^{3+}/TiO_2$) to the overall rate of H_2 oxidation has been studied as well. A series of activity sets: $Ti^{3+}/TiO_2 \ll Pd \sim Pd/Ti^{3+}/TiO_2$ have been determined.

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

- Based on the values of chemical shielding and quadrupolar tensors parameters obtained by SATRAS (SAtellite TRAnsition Spectroscopy) method for the highly crystalline individual compounds with well-known structures the new correlation between NMR parameters and local structure of vanadium sites was obtained.

At present seven types of vanadium sites could be recognized:

Tetrahedral vanadium sites of Q^0, Q^1 and Q^2 types could be revealed using correlation between the type (η_σ - chemical shielding asymmetry parameter) and value ($\Delta\sigma$ —CSA) of chemical shielding anisotropy (Fig. 1):

(i) Vanadium in regular tetrahedral oxygen environment (Q^0 type) has almost spherically symmetric chemical shielding tensor with small value of anisotropy ($\Delta\sigma<100$ ppm); quadrupolar constant C_Q varies from 1 to 6 MHz; chemical shielding asymmetry parameter varies from 0 up to 1.

(ii) Vanadium in slightly distorted tetrahedral sites with the adjacent tetrahedra sharing one common oxygen atom (Q^1 type) has an asymmetric chemical shielding tensor, but with larger value of anisotropy ($100<\Delta\sigma<200$ ppm); quadrupolar constant varies from 2.5 to 10 MHz; chemical shielding asymmetry parameter changes from 0.1 to 0.9.

(iii) Vanadium in strongly distorted tetrahedral sites with adjacent tetrahedra sharing two common oxygen atoms (Q^2 type) has an asymmetric chemical shielding tensor with large value of anisotropy ($200<\Delta\sigma<500$ ppm); quadrupolar constant varies from 2 to 7 MHz; chemical shielding asymmetry parameters changes from 0.6 to 0.8.

Whereas it is clear that vanadium sites in different *pyramid* couldn't be determined from Fig. 1. These sites could be recognized using the correlation between *effective* $\sigma_\perp$ estimated as ($\sigma_\perp \sim 1/2(\sigma_1 + \sigma_2)$, σ_i —components of CS-tensor) and quadrupolar coupling constant (C_Q) for the case of a large value of CSA (200 ppm$<\Delta\sigma$) and $\eta_\sigma<0.6$ (Fig. 2):

(iv) Vanadium in tetragonal pyramid of 4=2 type has an axially symmetric chemical shielding tensor with large value of anisotropy ($200<\Delta\sigma<500$ ppm); quadrupolar constant varies from 4 to 8 MHz; chemical shielding asymmetry parameters changes from 0 to 0.6, $\sigma_\perp \sim 200$–400 ppm .

(v) Vanadium in tetragonal pyramid of 4=1 type has an axially symmetric chemical shielding tensor with a large value of anisotropy ($400<\Delta\sigma<550$ ppm); quadrupolar constant varies from 1 to 3 MHz; chemical shielding asymmetry parameters changes from 0 to 0.2, $\sigma_\perp \sim 20$ -400 ppm.

(vi) Vanadium in trigonal pyramid of 3=1 type has an axially symmetric chemical shielding tensor with large value of anisotropy ($200<\Delta\sigma<500$ ppm); quadrupolar constant varies from 1 to 4 MHz; chemical shielding asymmetry parameters changes from 0 to 0.6, $\sigma_\perp \sim 400$–600 ppm.

(vii) Vanadium in V_2O_5 like species (distorted octahedral or trigonal bipyramidal of 3 =2 type) has an axially symmetric chemical shielding tensor with large value of anisotropy (500 ppm$<\Delta\sigma$); quadrupolar constant varies from 0 to 3 MHz; chemical shielding asymmetry parameters changes from 0 to 0.1, $\sigma_\perp \sim 200$–350 ppm.

Thus based on the correlations presented in Figs. 1 and 2 seven different types of vanadia sites could be determined in vanadia systems (Fig. 3).

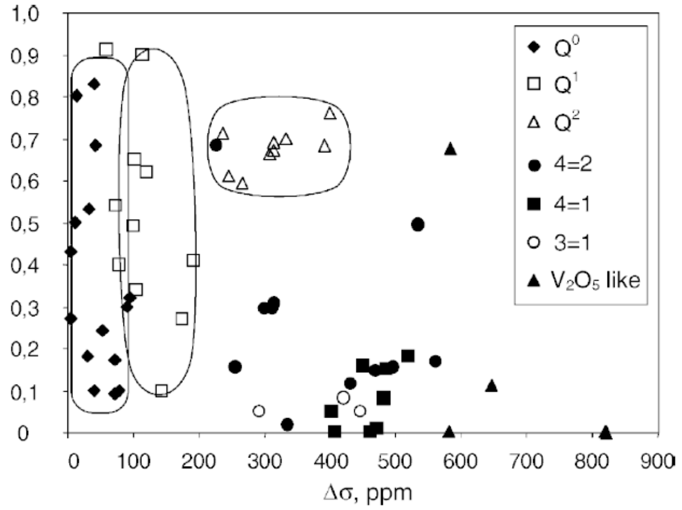


Fig. 1. Correlation between ^{51}V asymmetry (η_σ) and anisotropy parameters ($\Delta\sigma$) of chemical shielding tensor obtained for various vanadia compounds.

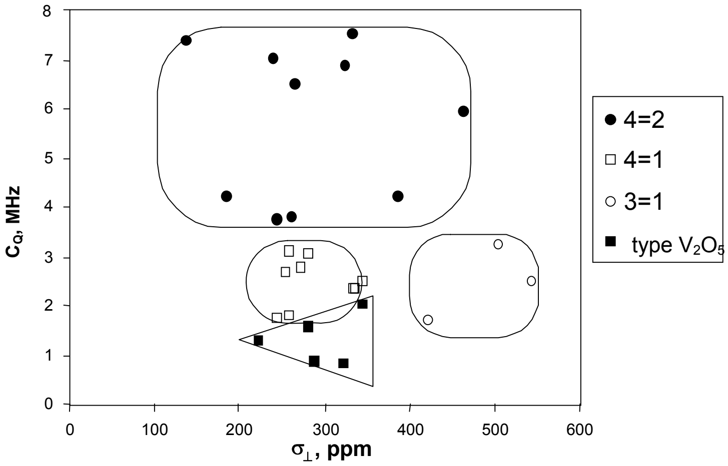


Fig. 2. Correlation between ^{51}V NMR chemical shielding tensor component ($\sigma_\perp$) and quadrupolar coupling constant (C_Q) for vanadium polyhedra with V=O bond having (200 ppm $<\Delta\sigma$ and η_σ <0 6).

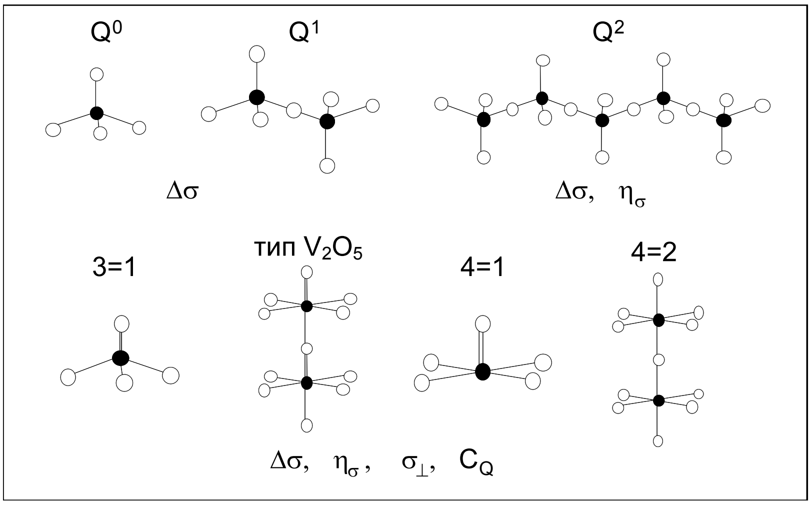


Fig. 3. The structures of vanadium sites, which could be determined from ^{51}V NMR parameters.

Laboratory of Energy Transforming Materials

Head: Dr. Yurii I. Aristov

1. A family of new working materials, so called Selective Water Sorbents (SWSs), is presented for sorption air conditioning. These materials are composites "hygroscopic salt inside porous matrix with open pores" and possess intermediate behaviour between solid adsorbents, salt hydrates and liquid absorbents, so that their water sorption properties can be controllably modified by varying a) porous structure of the host matrix, b) chemical nature of the impregnated salt and c) the amount of the salt inside the pores. For these materials the water sorption equilibrium and specific heat have been measured in a wide temperature and uptake range. This study shows that composites based on $CaCl_2$ and LiBr as impregnated salts and different micro- and mesoporous silica gels as host matrices are able to absorb up to 0.75 g H_2O per 1 g of the dry sorbent. After presentation of sorption equilibrium curves, the thermodynamic performance for their utilisation in heat pump and refrigeration systems is calculated. The results show that these new materials can operate with cycles whose maximum temperature is about 95°C (for cooling) and 140°C (for heating) that are lower than those for other pairs known so far. The values of COP are considerably higher than those reported for silica gel/water system at the same temperature of the heat source.

2. Water sorption equilibrium for SWS-1L ($CaCl_2$ in mesoporous silica) was measured at elevated temperature of 150 to 260°C and corresponding vapour pressure P_{H_2O} of 1.1 to 9.2 bar. A comparison of these data with those obtained at lower T (30–150°C) and P_{H_2O} (8–130 mbar) is made. All experimental data appear to lie on the same temperature independent curve "the water sorption *vs.* the relative vapour pressure", that indicates the universal mechanism of water sorption over the whole T-P range.

3. Thermal conductivity of the composite sorbents $CaCl_2/SiO_2$ and $LiBr/SiO_2$, was measured by the "hot wire method" under various conditions of vapour pressure P_{H_2O}, temperature T and water uptake w. The measurement ranges were chosen according to the operating

conditions of a typical sorption cooling cycle (10 mbar<P_{H_2O}<70 mbar, 40°C<T<130°C). The obtained results show that the sorbent thermal conductivity λ (T, P_{H_2O}, w) increases considerably with the uptake raise, while its dependence on pressure and temperature is, in the studied range, almost negligible. Finally, the influence of the thermal conductivity on the specific power of the sorption chiller is discussed.

4. The kinetics of water vapor sorption on two host materials; namely mesoporous silicagel and alumina, was studied in comparison with the two composites SWS-1L and SWS-1A formed by impregnating these two host matrices with $CaCl_2$. Moreover, the kinetics of water vapor sorption on microporous silicagel has been also investigated. The measurements have been carried out on 3 g samples of loose pellets on an isothermal wall under three different operating conditions of sorption heat pumps. The results obtained evidence a remarkable increase in the differential water loading of both SWS-sorbents over their host materials. However, and due to the increased diffusion resistance to water sorption resulting from the salt impregnation, the kinetics of water sorption into the host matrices is faster than that into the two SWS-composites. Moreover, SWS-1L is found to be faster than SWS-1A in sorbing water vapor. The differential water loading on microporous silica is about twice that on mesoporous silica and alumina, but the sorption kinetics are a little bit slower.

5. The sorbents of "potassium carbonate impregnated in porous matrix" type have been studied. The use of several complementary characterisation techniques such as XRA, IRS, TG, differentiating dissolution, low temperature nitrogen adsorption etc. revealed the texture of composites and the mechanism of CO_2 sorption. The crystallization water has been found to promote CO_2 sorption by impregnated potassium carbonate. Disperse potassium carbonate was shown to react with γ-alumina matrix forming the inactive potassium alumocarbonate phase, that results in the decrease of sorbent dynamic capacity. The alumocarbonate phase is unstable under air and degrades to potassium bicarbonate. The dynamic capacity of the sorbent after 10 cycles is 35 g CO_2/kg of sorbent at 20-80°C.

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

- 1. Method for catalytic afterburning of waste gases of the processes of sulfur production and processing was improved to allow the ignition temperature to be 200–300°C reduced.

2. H_2S oxidation by oxygen over vanadium catalysts was studied at the temperature higher and below the sulfur dew-point; the mechanism of the catalysts action was suggested.

3. The reaction of liquid-phase oxidation of hydrogen sulfide by oxygen in the presence of 2, 9, 16, 23- cobalt tetrasulfonate phthalocyanine (CoTSPh) and in the presence of NaCN was studied. In the presence of cyanide ions, catalytic activity of CoTSPh decreased sharply and, in addition, kinetics of liquid-phase oxidation of hydrogen sulfide was disturbed: The reaction was

of first order with respect to the catalyst (CoTSPh) in the absence of CN^- but not in the presence of these ions. The selectivity of CoTSPh for elemental sulfur decreases considerably in the presence of CN^- ions. Conditions of bonding cyanide ions were determined in order to provide the effective reaction.

4. A new reaction of catalytic dehydrogenation of propane by sulfur was thoroughly studied with reactant concentrations, reaction parameters and catalyst types varied over wide ranges.

5. The catalysts providing considerable variations in the burning rate and in dependence of the rate on pressure were developed for solid fuel compositions.

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

➢ The first titanium hydroperoxo complex $[Bu_4N]_4[PTi(OOH)W_{11}O_{39}]$ (**1**) has been isolated and comprehensively characterized. A compilation of UV-vis, IR, resonance Raman, ^{31}P and ^{183}W NMR, X-ray, cyclic voltammetry, and potentiometric titration data supports a monomeric Keggin type structure of **1** bearing one hydroperoxo ligand in an η^2-coordination mode. Contrary to all known titanium peroxo complexes, **1** is able to oxidize organic compounds under stoichiometric conditions. It has been demonstrated that **1** can be successfully used as a model compound for studying oxidation mechanisms of heterogeneous titanium-silicate catalysts. A detailed mechanistic study of the practically important oxidation of 2,3,6-trimethylphenol (TMP) to 2,3,5-trimethyl-*p*-benzoquinone (TMBQ) has been carried out using **1**. By contrast to the well-known titanium peroxo complex $[Bu_4N]_5[PTi(O_2)W_{11}O_{39}]$ (**2**), **1** readily reacts with TMP to give TMBQ and/or 2,2',3,3',5,5'-hexamethyl-4,4'-biphenol (BP). The product distribution depends on the TMP/**1** ratio and provides evidence in favor of a homolytic oxidation mechanism that implicates the formation of phenoxyl radicals. The rate law and lack of a k_{ArOH}/k_{ArOD} kinetic isotope effect for the stoichiometric TMP oxidation with **1** allow for the formation of an active η^1-intermediate, containing both the hydroperoxo moiety and the substrate, within which inner-sphere electron transfer occurs.

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

✱ 1. A laser-controlled subsonic flow reactor was designed for the process of methane dimerization.

The numerical model of a laser-controlled gas dynamic reactor was developed in cooperation with the Institute of Theoretical and Applied Mechanics SB RAS. The regimes were calculated and the factors affecting the reactor efficiency were analyzed. The gas dynamic catalytic reactor is a kind of channel; the reaction gas mixture with inclusions of catalytically active solids is passed through it. The energy needed for the endothermic reaction of pyrolysis is supplied a CO_2 laser radiation through a capillary face. The calculation model of the laser-heated catalytic gas dynamic reactor is based on the two-phase two-temperature model with three-channel energy exchange (thermoconductivity, radiation, chemical channel). The reaction pathway is considered which includes initiation of pyrolysis on the solid surface and evolution of the reaction chain in gas phase.

The limiting channel – formation of the first methyl radical – proceeds on the solid surface. Chain evolution and 'death' of radicals proceed in the bulk in accordance to the general gas-phase kinetics. Hydrogen radicals associate on the solid surface. The solid phase acquires energy by absorbing laser radiation and looses it via formation of radicals, via heat conductivity and via radiation that irreversibly escapes the system. The gas phase adopts energy from the laser radiation, radical recombination, and from the solid phase through its heat conductivity. The solid and gas phases are thermalized, each at its distinct temperature.

Scale analysis and computer simulations showed for the regimes achieved in a reactor at fixed parameters such as weight consumption, composition of the heterogeneous mixture and starting temperature that the results of conversion are strongly dependent on relationship of constant λ (characteristic of heat transfer between gas and solid) and K (catalyst activity).

2. Experimental studies were focused on catalytic activity of nanoparticles constituted by elements in proportion to their natural occurrence. Self-organization of gravitally unstable media with catalytic reactions was theoretically studied in terms of numerical modeling of the space chemical reactor of a protoplanetary disk. Regimes with instabilities of the disk matter were studied by varying the parameters over wide ranges. It was discovered that:

1. Freshly prepared nanoparticles constituted by elements in proportion to their natural occurrence can reveal a high catalytic activity.
2. Catalytic synthesis of organic compounds in a gravitally unstable circumstellar disk can stimulate formation of planets.

Group of Biocatalysis
Head: Galina A. Kovalenko

❋ Systematic studies of adsorptive immobilization of enzymes *glucoamylase* and *invertase* on macrostructured carbon-containing ceramic supports were aimed at development of highly stable heterogeneous biocatalysts for continuous processes of production of glucose syrups and starch treacles and of invert sugar from sucrose. The surface carbon layer with a loose filamentous structure formed by catalytic carbon (CFC) was shown to possess the optimal morphology for effective adsorption and stabilization of the enzymes under study, whereas the immobilized enzymes were relatively low stable on smooth graphite-like carbon. Kinetic regularities of starch hydrolysis and sugar inversion were studied. Michaelis-Menten constants were estimated for yeast invertase in the soluble and immobilized states. Kinetics of conversion of starch dextrins and sucrose were studied in variously designed flow bioreactors using the prepared differently shaped biocatalysts (granules, foam ceramics, honeycomb monoliths).

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

- The mechanism of dehydration of 2-propanol and the reverse reaction of propylene hydration in supercritical water (SCW) was proposed as corresponding to the mechanism of acid catalysis in solutions that led to conclude about the nature of influence of SCW density on the reaction rate. The rates of both direct and reverse reactions were shown to be in direct proportion to concentrations of the reactants and H_3O^+ ions playing the role of homogeneous catalysts. The true constant of the reaction rate was established not to depend on the SCW density.

EVM algorithm used for parametric identification of kinetic models was examined and improved.

Mathematical processing of experimental data and studies of kinetic regularities of interaction of methanol and hydrogen sulfide over heterogeneous catalyst ICT-31-1 was carried out.

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

- For the first time nanodispersed (~1.5 nm) Co^{2+} hydroxide, containing Co^{2+} cations in unusual terahedral oxygen coordination was synthesized. The tetrahedral Co^{2+} coordination was shown to be the result of size effect for $Co(OH)_2$ with the particles of various dispersion. The results obtained open principally new ways for synthesis of unique nanodispersed cobalt containing catalysts and high-tech materials for other fields of application.

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

- The influence of modifying additives nature and content on the activity and selectivity of supported catalysts in reaction of ethylmercaptane condensation into diethylsulfide has been revealed.

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

- **Vanadium-containing catalysts** are most selective and active among the binary and multicomponent oxide systems for oxidative dehydrogenation of ethane at the range of moderate temperatures (300–500°C).

The influence of the local structure of vanadium sits on ethane transformation was studied using model catalysts V_2O_5/Me_xO_y supported on oxides of various nature (TiO_2, Al_2O_3, Nb_2O_5, MgO, Sb_2O_5, TiO_2-ZrO_2 и TiO_2-SiO_2). Concentration of V_2O_5 was not higher than 70% in the monolayer coverage.

Ethylene was selectively formed over all the catalysts. The selectivity to the reaction products varied only slightly at 250–350°C but the further temperature elevation resulted in a more or less abrupt decrease in the selectivity to ethylene and, correspondingly, in an increase in the selectivity to carbon oxides. An only exception was the sample supported on alumina: A considerable increase in the selectivity to ethylene (from 30 to 72%) was observed with temperature elevation from 250 to 350°C.

With the supports used, the activity decreased in the series: TiO_2 > Nb_2O_5 > TiO_2-SiO_2 > TiO_2-ZrO_2 > MgO > Al_2O_3 > Sb_2O_5, while the initial selectivity to ethylene decreased in almost reverse series: Al_2O_3 > Sb_2O_5 > MgO > TiO_2-ZrO_2 ≈ TiO_2-SiO_2 > Nb_2O_5 > TiO_2.

^{51}V NMR spectra of the samples under study were complex, these were superposition of two or more lines different in shape and parameters of chemical shift tensor and quadrupole constants.

In most samples, vanadium cations were in predominantly oxygen tetrahedral environment. Vanadium cations in the octahedral environment strongly bonded to the support were only characteristic of the catalyst supported on TiO_2. The tetrahedral vanadium complexes differed in the degree of distortion and strength of bonding to the support.

The comparative catalytic and spectroscopic data revealed that octahedrally coordinated vanadium cations were most active to complete transformation of both ethane and ethylene but least selective to ethylene. The tetrahedrally coordinated vanadium cations were far less active but more selective. The most selective but least active among the catalysts under study were VO_x/Al_2O_3 and VO_x/Sb_2O_5, in which some part of vanadium complexes were bonded to the support as strongly as to form chemical compounds.

Kinetics of oxidative ammonolysis of acrylic acid nitrile (AAN) was studied over promoted bismuth-molybdenum (K-1) and iron-antimony (K-2) catalysts used for commercial production of AAN by oxidative ammonolysis of propylene.

Initially, both catalysts were almost equally active and selective in oxidative ammonolysis of propylene but the yields of AAN were different (73–75% over K-1 and 76–78% over K-2) due to specific consecutive transformations of AAN over these catalysts.

In the presence of oxygen and ammonia AAN is transformed into carbon oxides, prussic acid and nitrogen:

$$C_3H_3N + O_2 + NH_3 \rightarrow CO + CO_2 + HCN + N_2 + H_2O$$

Carbon oxides are mainly produced over K-1, carbon oxides and prussic acid over K-2.

Two pathways of formation of prussic acid, oxidative destruction and amination of AAN, were observed over K-2.

Kinetic equations for rates of formation of the reaction products over K-1 and K-2 are given in the Table:

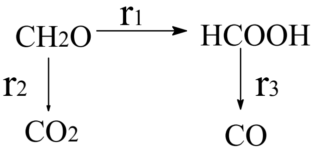
Catalyst	Kinetic equations
K-1	$R_{CO_x} = \frac{K_1C_1C_2}{1+K_2C_2+K_3C_3}$ $R_{HCN} = K_4C_1$
K-2	$R_{CO_x} = \frac{K_1C_1C_2}{K_2C_1+K_3C_2+K_4C_1C_2+K_5C_2C_3+K_6C_1C_2C_3}$ $R_{HCN} = \frac{K_7C_1C_2(0.5+K_8C_3)}{K_2C_1+K_3C_2+K_4C_1C_2+K_5C_2C_3+K_6C_1C_2C_3}$

*C_1, C_2, C_3 - concentrations of AAN, oxygen and ammonia, respectively.

The obtained kinetic dependencies elucidate why the antimony-based catalysts provide higher yields of AAN and prussic acid than molybdenum catalysts in industrial processes of oxidative ammonolysis of propylene. The former are less active to AAN transformation, and the latter are more active to formation of HCN. The data obtained demonstrate that prussic acid is preferably formed from acrylonitrile generated during oxidative ammonolysis of propylene while conversion of propylene into HCN is a less contributing pathway.

Kinetics of oxidation of formaldehyde into formic acid over V-Ti oxide catalyst was studied at 105, 120 and 140°C using the fraction 3×5 mm. The studies were focused on the influence of formaldehyde, oxygen and water at the stationary concentration ranges 0.5–5.0%, 0 –17.0% and 0–20 vol %, respectively.

Series-parallel pathway of formaldehyde transformations was established including formation of CO_2 and formic acid from formaldehyde by the parallel pathway and consecutive decomposition of formic acid into carbon monoxide and water. Kinetic equations that describe satisfactorily the experimental data are given in the Table:

Reaction pathway	Kinetic equations
 	$r_1 = \frac{K_1C_\phi\left(1+K_2C_{H_2O}\right)}{1+K_3C_\phi/C_{O_2}+K_4C_{H_2O}}$ $r_2 = \frac{K_5C_\phi}{1+K_6C_\phi/C_{O_2}+K_7C_{H_2O}}$ $r_3 = \frac{K_8C_{MK}}{1+K_9C_{MK}/C_{O_2}+K_{10}C_{H_2O}}$

where r_i are rates of formation of products; K_i constants; C_f, C_{fa}, C_{O2}, C_{H2O} - concentrations of formaldehyde, formic acid, oxygen and water, respectively.

Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov

➢ 1. Metal-carbon catalysts prepared by decomposition of hydrocarbons over iron group metals according to the carbide cycle mechanism were shown to allow highly efficient purification of n-butenes from butadiene and acetylene hydrocarbons. Ni-Cu-catalysts were chosen as the composition providing the selectivity as high as 96-98% for hydrogenation.

Metastable hexagonally structured carbide Ni_3C_{1-x} was formed as an intermediate in the course of hydrocarbon decomposition over Ni species. Due to its structure, the carbide microphase was decomposed to produce hexagonal nickel particles. As a result, two zones were generated in the nickel particle involved in the process of hydrocarbon decomposition and growth of a graphite filament. These are a zone with the initial cubic structure and another with the hexagonal structure.

2. Catalytic oxidation of solid organic compounds of plant origin possessing an extremely low solubility and reactivity was demonstrated to be possible under conditions of mechanochemical activation and high pressure with ursolic acid as an example.

3. The reasons for emergence of the *sphere of catalysis* – the space above a surface active site with a high concentration of radicals responsible for the radical chain process (RCP) of hydrocarbon pyrolysis – were analyzed in terms of thermodynamics and kinetics. The radical distribution through the sphere and technological sphere radius (that determines design of RCP catalysts and requirements for technological arrangement of the pyrolysis process) were calculated.

4. It was shown for the reaction of selective hydrogenation of acetylene into ethylene over Pd/C catalysts that palladium may occur in one of four states: dispersed Pd, Pd^+, Pd^{2+} and Pd intercalated between the graphite layers depending on the concentration of supported palladium (0.1 to 10 mol %) and crystallographic structure of graphite. Catalytic and other properties of palladium in these states are essentially different.

5. Two methods were developed for utilization of wastes from hydrocarbon chloride derivatives: (1) Decomposition into carbon and HCl by the carbide cycle mechanism and (2) Hydrodechlorination to produce HCl and a chlorine-free hydrocarbon mixture. The proposed methods were checked using a pilot installation.

6. New type graphite composites of loose feather-like morphology were synthesized by decomposition of mixtures of hydrocarbon chloride derivatives. A large surface area (up to 400 m^2/g), high adsorbability for hydrogen (up to 3 wt %) and porosity are characteristic of the composites. Individual feathers in the structures are arranged along the common axis at the angle of 60° with respect to one another; they are built-up by graphite flakes chaotically arranged therein.

Laboratory of Oxidative Catalysis over Zeolites

Head: Prof. Gennadii I. Panov

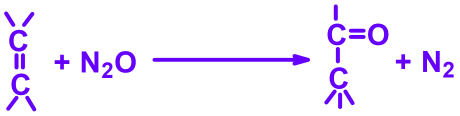
Laboratory of Quantum Chemistry

Head: Prof. Georgii M. Zhidomirov

- Carbonyl compounds (ketones and aldehydes) are classified among the most important organic chemicals. They are mostly synthesized using complex and low-effective technologies. One-step synthesis of carbonyl compounds via non-catalytic liquid-phase oxidation of alkenes with nitrous oxide (N_2O) is innovative method discovered recently at BIC. Experimental and quantum chemical studies have revealed that the oxidation mechanism is based on a remarkable ability of N_2O to interact directly with the double bond C=C and to donate the oxygen atom to the unsaturated carbon of the alkene at almost 100% selectivity.

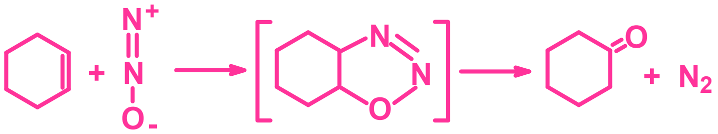
Using quantum chemical calculations full energetic description of the reaction pathway is given for the oxidation of cyclohexene to cyclohexanone, as an example. The data obtained are in good agreement with experimental results.

The new method was shown applicable for carbonylation of various types of alkenes (aliphatic, cyclic, heterocyclic and the derivatives) to produce intermediates for organic synthesis, polymers, pharmaceutics, perfumery, etc.



T = 200-250°C
S ≈ 95-99%

Mechanism

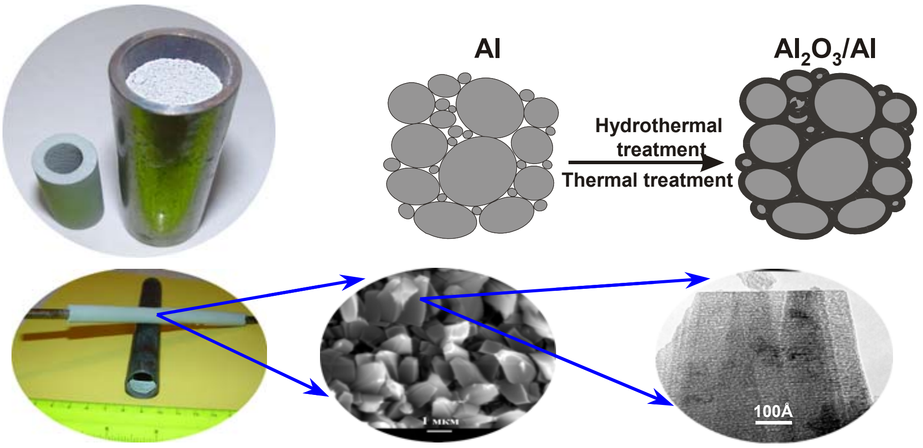


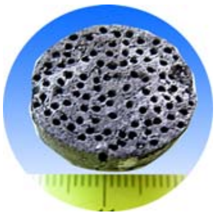
Laboratory of Catalysts for Deep Oxidation

Head: Prof. Vladislav A. Sadykov

- Synthesis of Al_2O_3/Al, $MeO_x/Al_2O_3/Al$, $Me^1/Me^2O_x/Al_2O_3/Al$ composites is based on the partial oxidation of aluminum in a confined space. The solid-phase volume increase results in the formation of a strong composite with macroporous structure. After calcination in air, this composite transforms into a strong cermet, in which aluminium particles are randomly distributed in an oxide matrix with microporous structure. Variety of method includes: 1) capsulation of low soluble powdered active component (AC) into the Al_2O_3/Al matrix; 2) introduction of soluble AC from liquid phase upon the impregnation of granulated composites; 3) modification in hydrothermal conditions on the stage of Al oxidation, 4) Al oxidation with water jointly with rigid constructive elements (tubes, sticks, gauzes) or 5) with burning at high temperature materials.

Basic stages of formation of cermets were studied: formation of powdered charge, hydrothermal oxidation, calcination in air. Structural, textural and mechanical properties of various type cermets were comprehensively studied. The deduced dependencies of specific pore volume and mechanical strength of the composites on parameters of charge and solid-phase aluminium oxidation can also be applied for a wide variety of processes of gas-solid interaction in closed volume. A number of catalysts were synthesized and characterized including systems with cobalt-based active components (for complete oxidation of CO and butane), perovskite- and intermetallide-based systems (for processing of methane), systems based on intermetallide hydrides (for Fischer-Tropsch process). Demonstration samples were prepared including the ones with cermet supported on the inner and/or outer side of tubes, as well as honeycomb structures, tubes and permeable porous materials.





Fields of application:

- **Catalytic and adsorptive processes with intensive heat transfer**
- **Gases and liquids filtration**
- **Compact catalytic devices with low hydraulic resistance and high mechanical strength**

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

The work deals with EPR and ESDR studies of electron states of copper depending on the method used for preparation of Cu-ZSM-5 (ion exchange, wet impregnation, deposition), basic conditions of synthesis (pH of copper solution, copper precursor, temperature etc.) and copper loading.

For calcined Cu-ZSM-5 samples treated in vacuum at 400°C, axial EPR spectra of O^- ion radicals with $g_{\perp}=2.05$ and $g_{\parallel}=2.02$, which are presumably assigned to linear $–O^-–Cu^+–O^-–Cu^+–O^-$ chains in zeolite channels, are observed against the background of EPR signal of isolated octahedral Cu^{2+} ions with different extents of tetragonal distortion.

The studies of the copper electron states in Cu-ZSM-5 have allowed a copper state with absorption bands at the unexpected region of 18000 to 23000 cm^{-1} to be discovered for the first time in the samples treated in vacuum at 150–400°C (Fig.). Along with this state, isolated Cu^{2+} ions (a.b. 12500–14000 cm^{-1}) and clustered copper oxide species (CTB 27000–32000 cm^{-1}) are observed. The discovered absorption bands (18000–23000 cm^{-1}) relate to the ligand-metal CTB in $–O^{2–}–Cu^{2+}–O^{2–}–Cu^{2+}–O^{2–}$–like chains in the zeolite channels. Probably, the chain structures are easy to reduce (they are even capable of self-reduction) and may play an important role, along with $Cu^{2+}\cdots Cu^{1+}$ sites (a.b. 15000–17000 cm^{-1}), in selective reduction of nitrogen oxides.

ADF quantum chemical calculations argue for the probable occurrence of charge transfer bands at 18000–23000 cm^{-1} for copper with coordination number equal to 2, such as linear $Cu^{2+}–O^{2-}–Cu^{2+}–O^{2-}–$ chains, and, in principle, for the possibility for intrachain reduction $Cu^{2+}O^{2-} \rightarrow Cu^{+}O^{-}$.

Formation of the chains is caused by copper hydrolysis during synthesis of Cu-ZSM-5 followed by stabilization of polynuclear $[Cu^{2+}O^{2-}]$ species in the zeolite channels. The ratio of copper states in Cu-ZSM-catalysts depends both on the preparation procedure and conditions (pH, concentration of copper salt solute, temperature) and on conditions of the thermal post-treatment in vacuum (temperature and time).

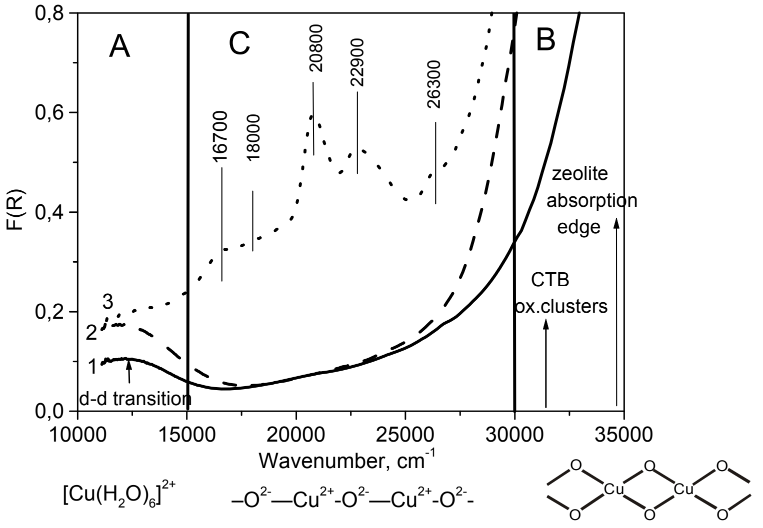


Fig. ESDR spectra of Cu-ZSM-5 sample, (1) – initial and treated in vacuum at 25°C (2) and 150°C (3)

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

- ***Fischer-Tropsch Synthesis:***

1. The new type of the catalyst bed for the Fischer-Tropsch synthesis was developed: **penetrable composite monoliths (PCM)** which are characterized by:

a high concentration of a catalytically active compound (0.9-1.1 g/cm^3);
a high heat-conductivity (above 3 W/(m s));
a high mechanical strength;
a penetrability, which is reasonable for Fischer-Tropsch synthesis (10^{-14} - $5 \cdot 10^{-13}$ m^2);
a well developed transport pore structure with the mean radius of ca. 2-5 μm and the concentration of ca 1 - $3 \cdot 10^9$ m^{-2}.

2. The effectiveness factor of the PCM catalyst usage in the three-phase operation mode is enough (60-70 %) to provide the high productivity of the PCM volume (2-3 times higher, than for the conventional slurry bed reactor). No catalyst is located in the closed pores.

3. Despite the PCM pore structure favors the intense mass-transfer and the mass-transfer restrictions are rather mild, the process performance is sensitive to the mean size of transport pores and to the dispersion of their size distribution. Therefore, studies on the way of the preparation of PCM samples with more homogeneous pore size distribution are necessary.

4. The effectiveness of the PCM technology has been demonstrated at 2.1 MPa and the sample size of ca. 3 cm^3. Due to a highly intense mass-transfer and high density of the active component loading, it can steadily provide the process STY of ca. 200 mg/(cm^3 hr) at 483 K. At that, the selectivity of the process on the base of PCM is maintained at the highest level ($\alpha = 0.84$; olefins content in the C_3-C_4 fraction above 55 %).

- ***Strong Metal Support Interaction in Co-Al Systems:***

The studies of the Co-Al catalyst derived from hydrotalcites were continued using the DRS UV-VIS spectroscopy and magnetic susceptibility. It was shown that:

1. DRS spectra and magnetic susceptibility data of the Co-Al hydrotalcite – oxide system can be considered in a reasonable and non-contradictory manner. The process of the calcination in the inert gas medium is accompanied by the decrease of the Weiss constant from +8 K to -90 K, indicating the destruction of the layered hydroxycarbonate structure and the formation of the mixed Co-Al oxide. The low value of the effective magnetic moment, μ_{Co}, and the structure of UV-VIS spectra evidence that the oxidation of Co^{2+} species to the low-spin Co^{3+} state occurs during the calcination of the samples in the inert gas medium. The obtained data are consistent with the earlier data on the Co-Al co-precipitated catalysts evolution during their activation and allow us to make more accurate conclusions on the cationic composition of the calcined samples.

2. The magnetization isotherms of the reduced samples allow one to conclude that metallic cobalt particles are formed during the reduction of the sample at the temperature above 480°C and to estimate the reduction extent of the samples. The concentration of metallic cobalt depends on the temperature of reduction a lot. The estimated values agree well with our earlier estimations made on the XPS data basis.

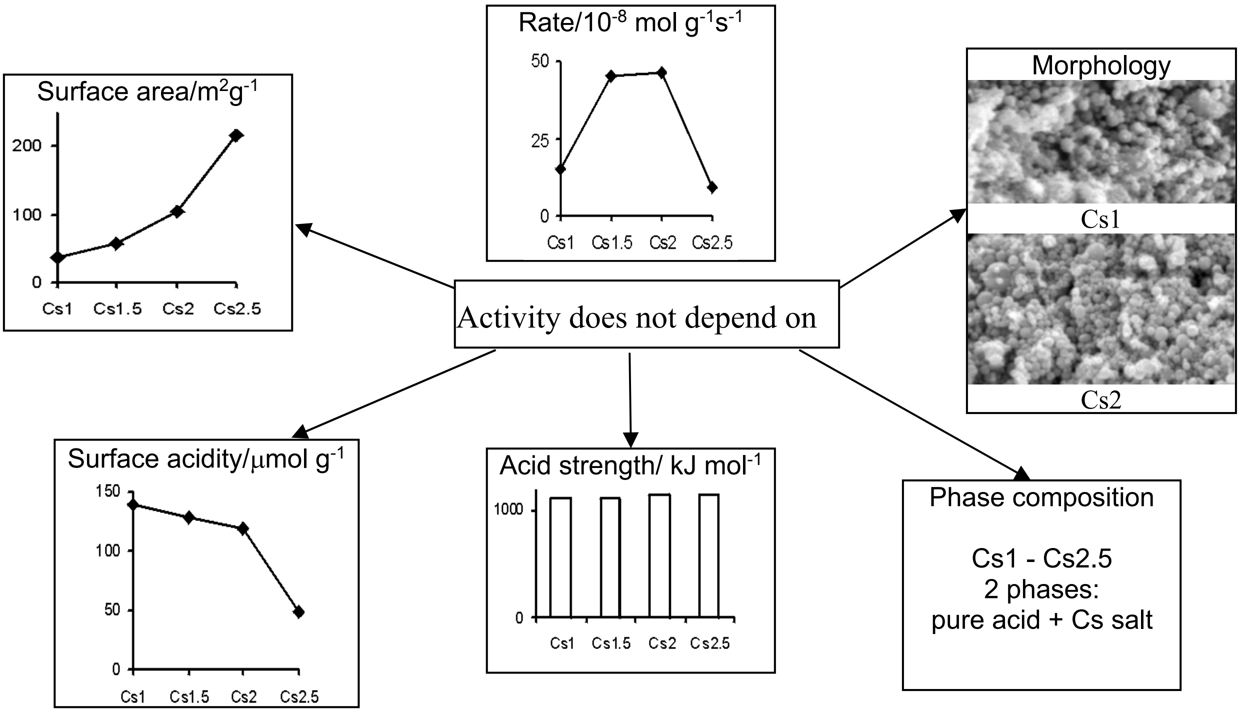
3. Paramagnetic and ferromagnetic contributions were distinguished for the sample reduced at 480°C (CA-LT). The spontaneous magnetization was found to increase monotonously with temperature in the range of 80-300 K. Besides, the saturation is achieved at a higher strength of the magnetic field in the low temperature experiments compared to those at room temperature. These anomalies are more expressed for sample CA-LT than for sample reduced at 620°C (CA-HT). This observation correlates with abnormal catalytic and physico-chemical properties of sample CA-LT reported earlier.

Group of Catalytic Synthesis of Oxygen-Containing Compounds

Head: Dr. Galina G. Volkova

- $Rh/Cs_xH_{3-x}PW_{12}O_{40}$ systems were comprehensively studied as catalysts for halide-free carbonylation of dimethyl ether to methyl acetate:

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



The best catalysts revealed activity one order of magnitude higher than rhodium salt of the same acid supported on silica – $Rh/H_3PW_{12}O_{40}/SiO_2$. What is the reason for such high activity of acidic cesium salts of 12-tungtophosphoric acids, especially Cs1.5 and Cs2? The XRD, ^{31}P NMR, BET, SEM and FTIR spectroscopy of pyridine adsorption were used for providing answer on this question. It was shown that activity of Cs1.5-2 salts was not directly depending on phase composition, surface area, morphology and on their surface acidity. The high catalytic behavior of Cs salts of $H_3PW_{12}O_{40}$ requires further detailed investigations.

Group of Catalysts and Processes Based on Heteropoly Acids

Head: Prof. Klavdii I. Matveev

- The results of earlier studies were used to prepare scientific and applied data for assembling and operation of a pilot installation in order to elaborate the new MEK-technology for synthesis of methylethylketon based on oxidation of commercial n-butene fractions by air oxygen. MEK synthesis will be achieved by three stages:

1. Oxidation of n-butenes into MEK over a Pd+HPA catalyst (aqueous solution of Pd salt and Mo-V-P heteropoly acid);

2. Steam stilling of MEK from the reduced catalyst species;
3. Regeneration of the oxidized (Pd+HPA) catalyst species through oxidation of its reduced form by air oxygen.

A number of original methods were developed for analytic control of the catalyst composition and operation after preparation or during operation.

Project documentations for construction of the pilot installation and catalyst production plant for the new ecologically sounds MEK process were prepared under supervision of the Group.

Laboratory of Sulfide Catalysts

Head: Prof. Anatolii N. Startsev

- The Laboratory has developed a new method of preparation of the sulfide catalysts, which do contain and do not contain the strongly bonded (occluded) hydrogen. For the first time it was found that the alumina supported sulfide Co and Ni catalysts contain the occluded hydrogen. The reverse conditions were found to prepare the same sulfide catalyst sample with and without occluded hydrogen.

Group of Catalysts on Carbon Supports

Head: Prof. Vladimir A. Semikolenov

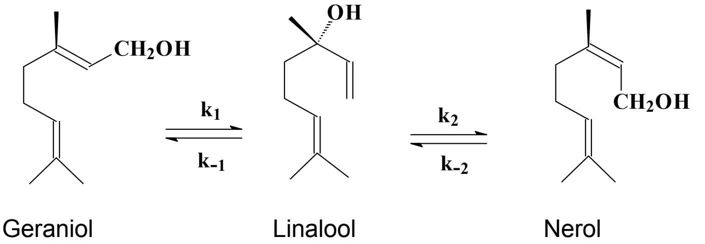
- ^{51}V NMR and UV spectroscopies were used for studying formation of catalytic system $[OV(OR)_3 + (Bu)_4N^+OH^- + ROH]$ from aqueous NH_4VO_3 solution. The factors were identified which caused formation of solid polyvanadates, reduction of V^{5+} and dehydration of ROH. The method was suggested for preparation of highly selective and thermostable catalytic system for isomerization of linalool.

Kinetic regularities of isomerization of linalool into geraniol and nerol were studied. The process was shown to proceed reversibly by the parallel pathway, the equilibrium constant (t-ROH $\rightleftharpoons$ n-ROH) and geraniol/nerol ratio being only slightly dependent on temperature. It was shown that the process temperature could be increased by 50–70°C and the contact time decreased from dozens of hours to 1–2 hours due to high thermal stability of catalytic system.

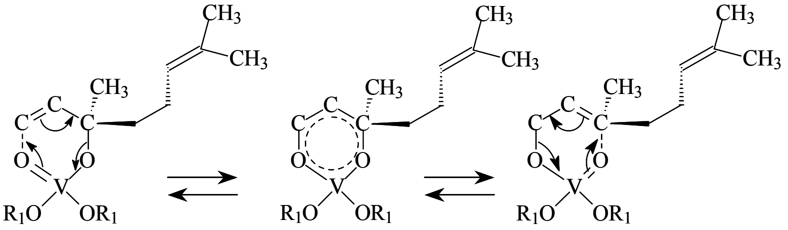
A combination of such techniques as ^{51}V NMR, highly effective gas-liquid chromatography and chromatomass spectrometry was used for studying the mechanism of allyl rearrangement over $OV(OR)_3$ complexes. Activation of ROH (ligand exchange linalool/geraniol/nerol) was shown to be very fast at the temperature as low as room temperature. Equilibrium constants of ligand exchange (t-ROH/n-ROH) were determined. The rate determining step of allyl rearrangement was found to be the redox process inside the coordination sphere of vanadium to produce cyclic six-membered intermediate.

The process of isomerization of linalool (including commercial linalool prepared by turpentine processing) was achieved in periodical and continuous modes using an enlarged laboratory installation. Pilot batches of geraniol + nerol mixtures of 99,6% purity corresponding to the perfumery quality were produced.

Process parameters:	New	Known
τ, h	1	30
Selectivity, %	92	90
T, °C	200	160

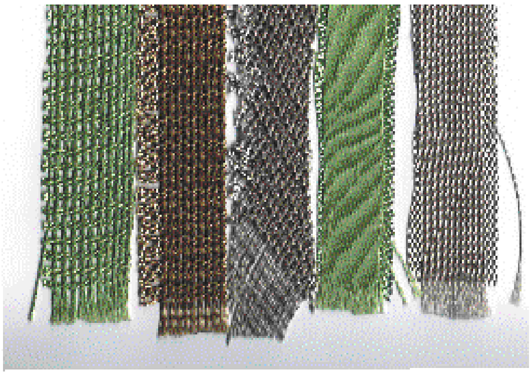


Catalytic system
$OV(OR)_3 + (Bu)_4N^+OH^-$



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

✱ Based on detailed studies of physico-chemical properties, as well as a structure of glass fiber materials the effective ways for introduction and stabilization of separate cations or clusters (mostly, Pt and Pd) into fiber bulk in depth of 100 Å were developed. Despite the extremely low noble metal content (~0,01% wt.) the catalysts revealed high performance in VOC oxidation, low temperature SO_2 oxidation, destruction of R-Cl's, selective hydrogenation of acetylene in $C_2H_2 + C_2H_4$ feedstock, $deNO_x$ with hydrocarbons, purification of diesel exhausts etc. Due to inaccessibility of active sites the glass fiber based catalysts were very stable against various poisons like S, P, H_2O, HCl etc. Moreover, the low pressure drop, uniform gas flow distribution, low internal diffusion limitations, as well as a flexibility to organize the structured beds of any shape and geometry makes these catalysts a very promising for industrial applications. The pilot testing under real waste gases demonstrate the high performance of glass fiber based catalysts in such reactions for environmental protection, as oxidative destruction of VOC from vent gases, SO_2 oxidation, purification of exhaust from diesel engine, as well as their high stability against poisons.

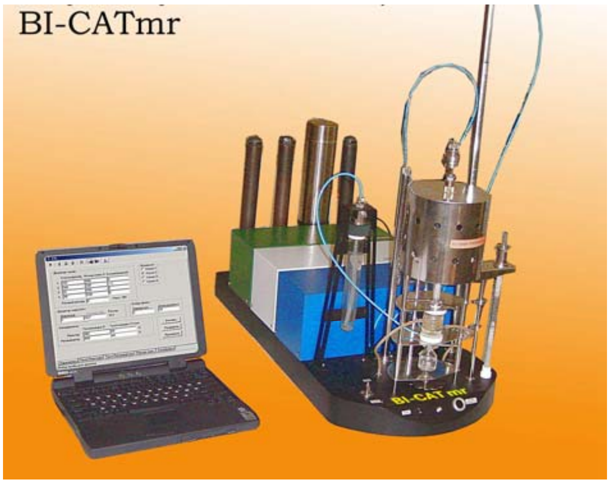


Laboratory of Catalyst Activity Testing

Head: Dr. Nikolai N. Bobrov

✱ A number of new models of versatile laboratory facilities are designed for physicochemical studies of various materials using static and dynamic methods:

- Flow circulation installation BI-CAT*rCH*$_4$ of fundamentally new type based on improved pulse digital gas batchers;
- Dynamic device BI-SORB*multy* (Sorbtometer-M) for determination of surface area of dispersed and porous materials based on one-point BET method and multipoint BET and STSA methods (in cooperation with the United Institute of Semiconductor Physics);
- BI-GAS*cleaner* systems for gas cleaning;
- Versatile catalytic flow installation BI-CAT*mr*;
- BI-SORB*poly* device for determination of volumes of absorbed gases;
- BI-GAS*flow* unit for preparation of gas mixture flows.



The designed physicochemical devices allow highly precise and productive characterization of catalytic properties of heterogeneous catalysts, as well as adsorptive properties of dispersed and porous materials, to be accomplished. Models of the new laboratory facilities meet all the up-to-date requirements but are several times less expensive than the currently used analogues. Some of them (pulse digital gas batchers, hydrostatic liquid batchers, flow circulation installations) are unique (no analogues worldwide) and covered by patents.

Laboratory of Zeolites and Acid Base Catalysis

Head: Prof. Eugenii A. Paukshtis

✱ Oxidative destruction of chlorobutane and dichloroethane over glass fiber catalysts are studied. Chlorobutane is shown to be completely oxidized in air into HCl, CO_2 and water at 500–550°C to produce no harmful chlorine and phosgene. Dichloroethane is oxidized into carbon dioxide, hydrogen chloride and water at the selectivity not lower than 96–97%, rest 3–4% are vinyl chloride. At 600°C dichloroethane is completely oxidized into carbon dioxide, hydrogen chloride and water.

Chlorination of n-octane by chlorine is studied using a set of various zeolites, glass fiber catalysts and oxides. Chlorine is shown to add preferably to the terminal carbon atoms at the temperature range between 50 and 250°C. Selectivity to 1-chlorooctane reaches 60% over zeolites and 70% over magnesia. Monochlorinaiton of octane reaches 95.5% over glass fiber catalysts, 4-chlorooctane being formed at a high selectivity.

Laboratory of Kinetics of Catalytic Processes

Head: Dr. Sergey I. Reshetnikov

❋ The laboratory-scale plant permitting *in-situ* product analysis has been constructed for rapid screening of the catalysts for chladone production.

Laboratory of Dynamics of Catalytic Processes

Head: Dr. Andrey N. Zagoruiko

❋ R&D work of the laboratory in the area of catalytic process and catalyst (ICT-27-40) for selective oxidation of H_2S into sulfur was successfully accomplished by creation of the first semi-industrial plant for cleanup of Claus process tail gases at Omsk Refinery (Omsk, Russia). Plant design capacity is equal to 10000 m^3 of tail gas per hour. Construction works and catalyst loading were completed. The startup of the plant is scheduled for the beginning of 2003.

Laboratory of Unsteady-State Catalytic Methods for Gas Purification

Head: Prof. Alexander S. Noskov

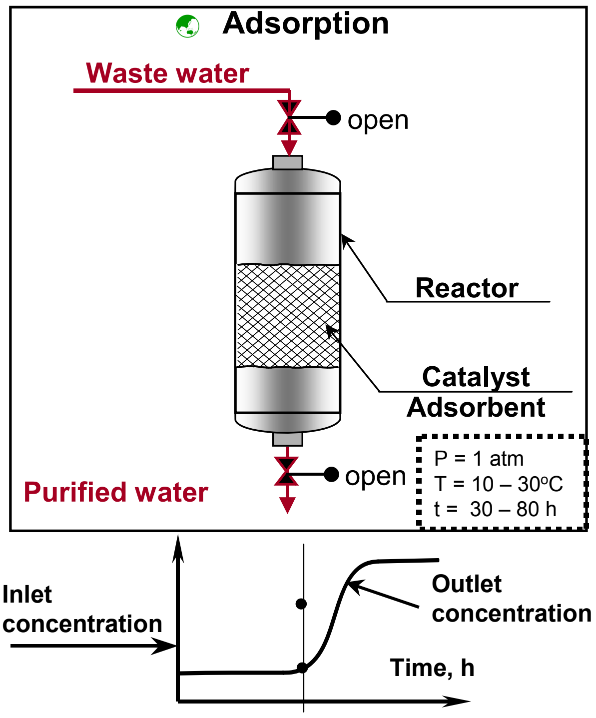
❋ 1. A mathematical model is developed and analyzed for the case of trapping of aerosol soot particles from diesel exhaust gases by fibrous materials. The model is based on non-stationary equations for concentrations of soot particles, O_2 and CO_2 in gas phase, soot concentration in solid phase, filter temperature, as well as the equation for pressure drop through the filter. A numerical algorithm based on the method of “straight lines” and the Rosenbrok method with automated step choice is realized for analysis of the model. Among the principal results is modeling of dynamic regimes of filling with soot and oxidative regeneration of the filter consisting of a catalyst supported on a fibrous material. It is shown by calculations that the efficiency of soot particle trapping is improved as the filter is filled with soot. The temperature regimes are determined which provide: a) preferable filling of the filter by soot; b) concurrent filling of the filter by soot, oxidation and filter autoregeneration. In the former case the filter filling by soot is accompanied by an increase in the pressure drop until the boundary value of 0.5 atm. In the latter case a minor increase in the pressure drop leads to some asymptotic level depending on the temperature of gases to be cleaned from soot. Basic parameters of soot catalytic filters are determined to provide higher than 80 – 85% efficiency. Technical data are prepared for designing of pilot filter models for bench testing (Co-workers: Group for Mathematical Methods for Catalytic and Adsorption Processes Modeling.

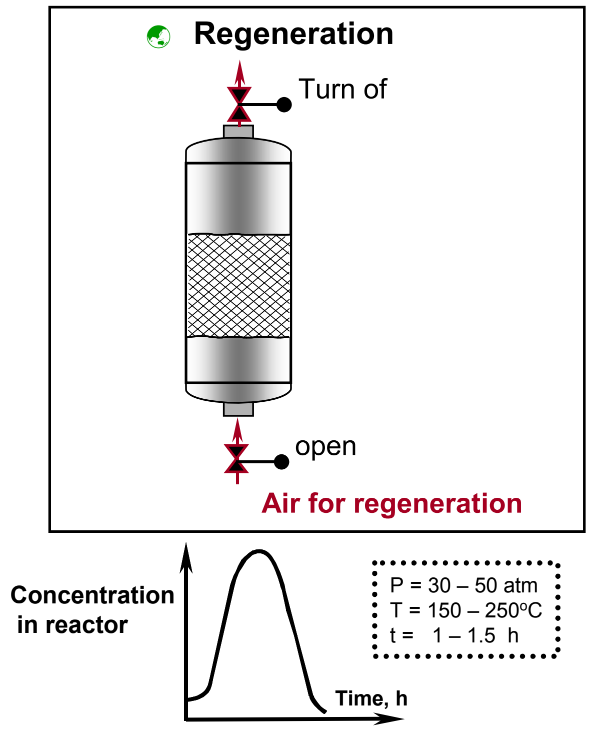
2. A liquid-phase catalytic adsorption method is developed for oxidative purification of technological solutions and industrial wastewater. The method allows aqueous solutions to be completely cleaned from toxic organic and inorganic compounds including various nitrogen compounds (ammonia, acetonitrile, aromatic compounds etc.), oxygen compounds (alcohols,

acids, esters of various composition), chloride and sulfur compounds (tetrachloromethane, dichloroethane, benzene chlorides, sulfides, thiols etc.).

The method is implemented by passing the aqueous solution to be cleaned through a granular bed of catalyst-adsorbent under standard conditions (20 °C, 1 atm) until contaminating impurities become detected in the outlet flow (typically, the adsorption stage takes 30 to 100 h). When so, the inlet temperature and pressure are increased by feeding air. The adsorbed impurities are rapidly oxidized into harmless compounds such as carbon dioxide, nitrogen, sulfates etc. (the catalytic stage takes 1 to 1.5 h) while the bed is recycled for the adsorption cleaning.

The method is tested on the pilot scale using wastewater from various industries and model mixtures of phenol and aniline. It is covered by Russian patent. The technology for utilization of industrial wastes is proposed on the bases of the said method, which also allows volatile exhausts from the existing wastewater treatment units to be prevented.





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

❋ Development project is accomplished to bring a demonstration semi-commercial 500 kWt heat generator based on catalytic combustion of solid fuel to the level of design objectives with respect to toxic wastes and capacity. Technical data for designing the prime model of serial commercial heat generators (500 kWt) for catalytic combustion of solid fuel are prepared and forwarded for implementation to the Novosibirsk Plant of Chemical Concentrates.

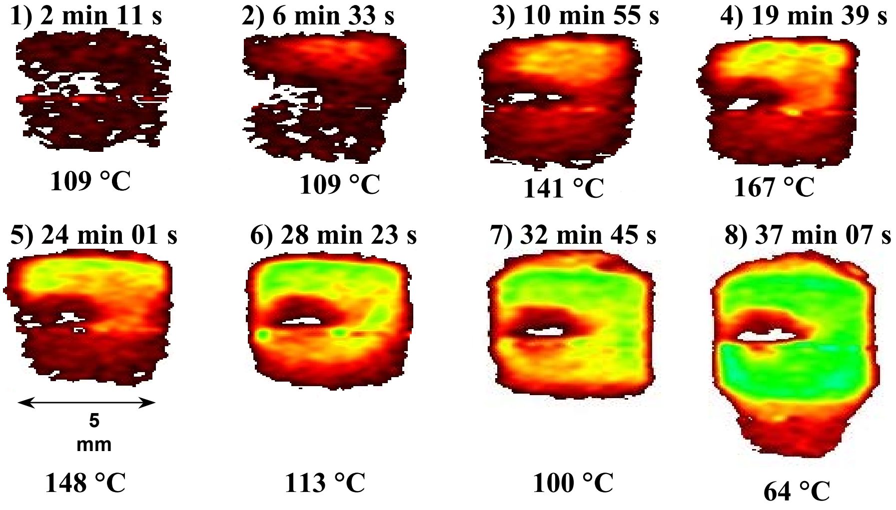
Laboratory of Multiphase Processes Modelling

Head: Prof. Valerii A. Kirillov

✱ The ^{1}H NMR imaging has been shown in the last years as a powerful nondestructive method for the *in situ* studies of material properties and various physical-chemical processes in porous media. Jointly with the International Tomography Center (Novosibirsk) ^{1}H NMR imaging has been applied to study the model reaction of heterogeneous catalytic α-methylstyrene hydrogenation at the pellet temperature 185 °C.

All ^{1}H NMR microimaging experiments were performed on a Bruker DRX spectrometer equipped with a vertical bore superconducting magnet and an imaging add-on device capable of providing pulsed magnetic field gradients of up to 100 G/cm.

Thus, the *in situ* NMR imaging demonstrates that impregnation of the porous catalyst with a liquid reagent under conditions of the simultaneous endothermic reagent evaporation and its exothermic hydrogenation can lead to the formation, inside the catalyst grain, of the two domains with the strongly differing liquid phase content: the upper part of the grain completely filled with the liquid phase and the lower part of the grain which is almost dry and filled with the gas-vapor phase where the vapor-phase hydrogenation occurs. The evaporation process occurs at the boundary between these two domains inside the grain. The location of the boundary depends on the liquid flow rate, thermal conductivity of the grain, and the ratio of the evaporation and hydrogenation rates. If the liquid supply to the grain is less than required for its full saturation, the impregnation of porous pellet is accompanied with the AMS evaporation and subsequent hydrogenation, that leads to the gradient of the grain temperature (up to 60^{0}C on the catalyst pellet 4-5 mm in size).



Thus, for the first time it has been demonstrated by the direct visualization of the spatial liquid distribution in the catalyst pellet upon AMS hydrogenation that the catalyst pellet filling with the liquid phase is strongly affected by the endothermic reaction accompanied by liquid-gas phase transition.

Group of Catalytic Technologies for Carbon Materials Synthesis

Head: Dr. Dmitrii G. Kuvshinov

- Dependence of scale effects on the composition and procedure of catalyst preparation during catalytic synthesis of nanofiber carbon materials was established.

It was demonstrated that world-level dispersed nickel catalysts for hydrogenation of benzene and food oils can be prepared based on the suggested method of heterophase sol-gel synthesis.

Department of Catalytic Processes of Fine Organic and Bioorganic Synthesis

Acting Head: Prof. Zinaida P. Pai

- Medication *Fluoxetin* (antidepressant) is synthesized in amount of 50 g from its molecular complexes with natural glycosides containing pentacyclic triterpene aglycones. The experimental batch of *Fluoxetin* is transmitted to the Pharmacological Laboratory (Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk) for testing for biological activity. The patent application is filed.

Omsk Division of the Boreskov Institute of Catalysis

Head: Prof. Vladimir A. Likholobov

- ***Development of catalysts of new generation and modernization of the reforming technology for production of high-octane gasolines including synthesis from unstable gas condensates***

The current state-of-the-art in the field of catalytic reforming of gasoline fractions and in the industry of reforming catalysts was assessed. The basic quality and operation parameters of the currently used and promising types of the catalysts were determined. The effect of promoting aluminium-platinum-rhenium catalysts with tin and zirconium was studied. The studies were focused on the influence of promoting procedures, nature of initial compounds, optimization of processes for preparation of two promising catalysts based on Pt-Re-Sn/Al_2O_3 (PR-53A) and Pt-Re-Zr/Al_2O_3 (PR-71) systems. The catalysts (produced as experimental batches) were tested for reforming of n-heptane and gasoline fractions 85–180°C and 105–175°C in comparison to Russian (PR-51) and exported commercial catalysts. The observed stability of new catalysts was not inferior to that of the analogues while the activity and selectivity were considerably (1.4 to

1.7 times) higher. Some ideas regarding the nature of modification of reforming active sites were suggested (Laboratory of Catalysis by Supported Metals, Prof. A.S. Belyi).

❋ ***Development of new technology for co-processing of C_3- C_4 hydrocarbons and gasoline fractions to produce motor fuels ("Biforming")***

Ryazan Oil Processing Plant affiliated by Tyumen Oil Co using the data of Omsk Department of the Boreskov Institute of Catalysis has accomplished the Project of reconstruction of the typical reforming installation for Biforming mode.

The pilot testing of the Biforming process as applied to the installation LG-35-11/300 at "LUKoil" Perm Oil Refining Plant has been carried out. It has been shown that replacement of catalyst R-56 (UOP, USA) by Russian PR-51 catalyst combined with the reconstruction of this installation for the Biforming mode demonstrated an increase of yield of high-octane component by 3-5% and decrease of benzene concentration from 2.5 to 0.7–1.0 vol. % (Laboratory of Catalysis by Supported Metals, Prof. A.S. Belyi).

❋ ***Development and improvement of technology for manufacturing of new reforming catalysts***

Technical and initial data for designing industrial facilities for manufacturing of up-to-date reforming catalysts were developed for implementation in a number of Russian companies. (Laboratory of Catalysis by Supported Metals, Prof. A.S. Belyi).

❋ ***Development of highly effective additives to cracking catalysts for improvement of octane number***

The composition of an additive to cracking catalysts developed for improvement of octane number allows extraction of butylenes (feedstock for alkylation processes) to be increased by 20%. The technology for the additive synthesis was adapted for real equipment of an industrial plant. The process will be implemented in 2003 (Laboratory of Zeolite-Containing Catalysts, Dr. V.P. Doronin).

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

❋ A detailed study of the parameters for SiO_2 preparation as a support for post-metallocene catalysts is performed and resulted in the selection of the optimum processing modes imparting silica with the ability to provide catalysts with the highest activity.

The optimum conditions are determined for the synthesis of SiO_2-supported catalysts based on bis(imino)pyridyl-iron chloride complexes affording ethylene polymerization activities in slurry and gas phase processes up to 35-40 tons PE/molcat.·MPa·hour. These catalysts are found to be active upon the additional introduction of a small amount of aluminum alkyls into the reaction medium.

Procedures for the synthesis of active supported catalysts based on nickel bromide diimine complexes are developed with the optimization of the process parameters. These catalysts provide ethylene polymerization activities up to 35-40 tons PE/molcat.·MPa·hour without any additional activation with aluminum alkyls.

The catalyst systems of this kind provide polyethylenes with various molecular weights and branching degree, the latter increasing with the polymerization temperature growth, i.e. at 30°C the number of CH_3-groups per 1000 C atoms is 11.6 whereas at 70°C this value is equal to 35.7. The branching degree is almost independent on ethylene pressure.

Samples of the developed supported catalysts are tested at the gas phase polymerization installation of the Share holding Company JSC Kazanorgsyntez using commercial raw materials. The obtained data are in agreement with R&D results.

RESEARCH ACTIVITY

Quantum-Chemical Studies

TWO FOLD COORDINATED SILICON ATOM: A HOLE TRAP IN SiO_2

V.A. Gritsenko*, A.V. Shaposhnikov*, G.M. Zhidomirov, M. Roger** (*Institute of Semiconductor Physics, Novosibirsk, Russia; **DRECAM, SPEC, Gif sur Yvette, France)

Solid State Commun., 121(6-7) (2002) pp. 301-304.

The capturing properties of a neutral diamagnetic two fold coordinated silicon atom with two paired electrons (silylene center =Si:) in SiO_2 are studied with *ab initio* density functional method. This defect was proved to be a hole trap in SiO_2. Hole capture results in creation of a paramagnetic two-fold coordinated silicon atom with unpaired electron =Si• (+). According to this prediction silylene centers can be with silicon-silicon bonds responsible for the positive charge accumulation in MOS devices at ionizing radiation

HOLE TRAPPING ON THE TWOFOLD-COORDINATED SILICON ATOM IN SiO_2

A.V. Shaposhnikov*, V.A. Gritsenko*, G.M. Zhidomirov, M. Roger** (*Institute of Semiconductor Physics, Novosibirsk, Russia; **DRECAM, SPEC, Gif sur Yvette, France)

Physics of the Solid State, 44(6) (2002) pp. 1028-1030.

The ability of a neutral diamagnetic twofold-coordinated silicon atom with two paired electrons (=Si: silylene center) in SiO_2 to capture charge carriers is investigated by the *ab initio* density-functional method. It is found that this defect is a hole trap in SiO_2. Hole trapping brings about the formation of paramagnetic twofold-coordinated silicon atoms with an unpaired electron =Si·. According to this prediction, the silylene center and the silicon–silicon bond can be responsible for the accumulation of the positive charge in metal–oxide–semiconductor structures under ionizing radiation.

CLUSTER MODELS OF THE VO_x/TiO_2 SUPPORTED CATALYST

E.P. Mikheeva, N.A. Kachurovskaya, G.M. Zhidomirov

Kinetics & Catalysis, 43(2) (2002) pp. 223-232.

Molecular structures of the active vanadium phase of the VO_x/TiO_2 supported catalyst are calculated in the framework of the cluster approximation of density functional theory (DFT). It is shown that vanadium can be stabilized on the anatase (001) surface both in the tetrahedral and octahedral coordination with the formation of monoxo- and dioxovanadyl structures. The energy of the dioxovanadyl structure binding to the support surface is 600–800 kJ/mol. The formation of dioxovanadyl structures from monoxovanadyl ones with the formation of water molecules is energetically favorable. The effect of support on the electronic state and acidic properties of the supported vanadium phase is discussed.

PERIODIC DFT STUDY OF ISOMORPHOUS INCORPORATION OF V ION INTO (100) AND (001) ANATASE SURFACE LAYER

N.A. Kachurovskaya, G.M. Zhidomirov, C. Minot* (*CNRS Université Pierre et Marie Curie, Paris, France)

Surface Review and Letters, 9(3-4) (2002) pp. 1425-1430.

Two models of V_2O_5 catalyst supported on TiO_2 are compared using DFT-GGA periodic calculations. In the first one, the energetically least favorable, a surface Ti atom of the TiO_2 anatase is substituted by a V atom, leading to a V^{+4} ion as active site. In the second model, the Ti atom is substituted by a VOH group; pentacoordinated V^{+5} ions are formed at the surface. This model leads to the most stable system with a gap between the occupied band mainly localized on the oxygen ions and the vacant band mainly localized on the metal ions. For the (100) face, it is concluded that the substitutions occur with the same energies at first neighbor or second neighbor metal positions. The adsorption energies are slightly larger for the (001) face that is more stable.

CLUSTER MOLECULAR MODELING OF STRONG INTERACTION FOR VO_x/TiO_2 SUPPORTED CATALYST

N.A. Kachurovskaya, E.P. Mikheeva, G.M. Zhidomirov

J. Molec. Catal. A: Chemical, 178(1-2) (2002) pp. 191-198.

Cluster molecular models of VO_x/TiO_2 catalytic system based on embedding process of V-ion in the anatase support were considered. Cluster structures of (001) anatase surface, containing one-and two-layer were constructed and isomorphous substitution of two Ti-ions on two V-ions were calculated. Comparison of the Bronsted acidic properties of V-OH group on the surface of V_2O_5 and supported VO_x/TiO_2 species showed that embedding procedure increases their acidic power and the influence of the second layer of the support is essentially important. Formation of ammonium ion under the adsorption of NH_3 on supported and unsupported vanadium oxide catalyst was considered and discussed.

CLUSTER MODELS OF Co^{2+} ION LOCALIZATION IN CATIONIC SITES OF ZSM-5 ZEOLITE

M.A. Kirillov, G.M. Zhidomirov

J. Struct. Chem., 43(2) (2002) pp. 246-249.

A DFT quantum chemical calculations have been performed for Co^{2+} localized in α-, β- and γ-cationic sites of zeolite ZSM-5. Local geometry of Co^{2+} ions in oxygen surrounding has been characterized. It has been revealed that energy of ion stabilization increases in the raw $\alpha\rightarrow\beta\rightarrow\gamma$.

DFT CLUSTER MODEL OF HYDROPEROXIDE ACTIVATION INTERMEDIATES IN Ti-CONTAINING POROUS SILICATES

M.A. Milov, G.M. Zhidomirov

React. Kinet. & Catal. Lett., 75(1) (2002) pp. 147-155.

Various intermediates of hydroperoxide activation on Ti-containing microporous and mesoporous silicates were studied using the DFT cluster model approach. Lowering the coordination number of Ti(IV) ions in the matrix was found to destabilize the peroxide form =Ti(OO) and to hinder the formation of singlet dioxygen.

THE NEST DEFECT AS A PLACE OF STABILIZATION OF TRANSITION ELEMENTS IONS IMPLANTED IN HIGH-SILICA ZEOLITES. CLUSTER CALCULATION OF Fe(II), Fe(III) ENTRAPPED IN ZEOLITE MATRIX

S.F. Ruzankin, I.V. Shveigert, G.M. Zhidomirov

J. Struct. Chem., 43(2) (2002) pp. 250-254.

Density functional theory is used for cluster calculation of the structure of nest defects in zeolites. The hydroxyl groups of defects forms the ordered structure, stabilized by H-bonds. The entrapping of Fe(II) and Fe(III) ions of chloride compounds by nest defects is discussed for two limiting cases of “rigid” and “labile” lattices, and the resulting structures are compared. The entrapped Fe(II) and Fe(III) ions are regarded as the precursors for centres of selective oxidation, formed upon N_2O decomposition and the difference in oxygen atom stabilization over these centres is estimated.

PROPERTIES OF THE ADSORBED OXYGEN FORMS ON A DEFECTIVE SURFACES Ag(111). THE THEORETICAL ANALYSIS BY DFT METHOD

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

J. Struct. Chem., 43(1) (2002) pp. 26-32.

A cluster model of an Ag12-3O (AS_V) adsorption center using layered Ag oxide as a prototype is proposed. The model includes a cation vacancy V on the Ag(111) surface and oxide type subsurface oxygen atoms Oox. Density functional theory (DFT) (B3LYP/LANL1MB approximation) is used to analyze the electronic structure of AS_V and oxygen adsorption on this center, AS_V+O→ AS-O. As shown by the calculations, the adsorbed O is associated with the subsurface O atoms Oss to form structures similar to metal ozonides - Ag-Oss-Oep-Oss-Ag-Oox-Ag, containing electrophilic oxygen Oep along with the oxide oxygen Oox. The optical spectra of the AS_V and AS-O centers were calculated by the CI method with single excitations (CIS). For AS_V, the most intense absorption bands were obtained in the region 500-700 nm. Oxygen association is accompanied by a sharp decrease in spectrum intensity in the range 600-700 nm and an increase in the intensity of the peak at 500 nm. Vibration frequencies and (IR) intensities were determined for the AS_V and AS-O centers. The AS_V center exhibits a characteristic spectrum in the region 350-500 cm^{-1}, which corresponds to the frequency spectrum of the surface oxide Ag_2O. For associated oxygen forms (AS-O center), the calculations predict additional peaks around 980, 640, and 230 cm^{-1}. These peaks are due to the vibrations of the Oss-Oep-Oss structural unit, stabilized at the cation vacancy.

A DFT QUANTUM-CHEMICAL STUDY OF ION PAIRS FORMATION FOR THE CATALYST Cp_2ZrMe_2/MAO

I.I. Zakharov, **V.A. Zakharov**

Macromol. Theory Simul., 11(3) (2002) pp. 352-358.

A process of ion-pair formation in the system Cp_2ZrMe_2/MAO has been studied by means of DFT quantum-chemical calculations for MAOs with different structures and reactive sites. An interaction of Cp_2ZrMe_2 with a MAO of the composition $(AlMeO)_6$ results in the formation of a stable molecular complex $Al_5Me_6O_5Al(Me)O\text{-}Zr(Me)Cp_2$ with an equilibrium distance *r*(Zr-O) of 2.15 Å. The interaction of Cp_2ZrMe_2 with "true" MAO of the composition $(Al_8Me_{12}O_6)$ proceeds with a tri-coordinated aluminum atom in the active site $(OAlMe_2)$ and yields the strongly polarized molecular complex or the μ-Me-bridged contact ion pair (**d**) $[Cp_2(Me)Zr(\mu Me)Al{\equiv}MAO]$ with the distances *r*(Zr-μMe) = 2.38 Å and *r*(Al-μMe) = 2.28 Å. The following interaction of the μ-Me contact ion pair (**d**) with $AlMe_3$ results in a formation of the trimethylaluminum (TMA)-separated ion pair (**e**) $[Cp_2Zr(\mu Me)_2AlMe_2]^+\text{-}[MeMAO]^-$ with *r*[Zr-(MeMAO)] equal to 4.58 Å. The calculated composition and structure of ion pairs (**d**) and (**e**) are consistent with the ^{13}C NMR data for the species detected in the Cp_2ZrMe_2/MAO system. An interaction of the TMA-separated ion pair (**e**) with ethylene results in the substitution of $AlMe_3$ by C_2H_4 in a cationic part of the ion pair (**e**), and the following ethylene insertion into the Zr-Me bond. This reaction leads to formation of ion pair (**f**) of the composition $[Cp_2ZrCH_2CH_2CH_3]^+\text{-}[Me\text{-}MAO]^-$ named as the propyl-separated ion pair. Ion pair (**f**) exhibits distance *r*[Zr-(MeMAO)] = 3.88 Å and strong C_γ-agostic interaction of the propyl group with the Zr atom. This propyl-separated ion pair (**f**) is supposed to be an active center for olefin polymerization.

ION PAIRS FORMATION FOR CATALYST Cp_2ZrMe_2/MAO. A DFT QUANTUM CHEMICAL STUDY

V.A. Zakharov, I.I. Zakharov

*"Future Technology for Polyolefin and
Olefin Polymerization Catalysis"*,
Eds. M. Terano, T. Shiono,
Technology and Education Publishers, Tokyo, 2002,
pp. 117-123.

Process of ion pairs formation in system Cp_2ZrMe_2/MAO has been studied by means of DFT quantum chemical calculations for different types of MAO with different reactive sites. Two possible structures have been calculated for "true" MAO with composition $(Al_8Me_{12}O_6)$: μ-Me bridged contact ion pair $[Cp_2(Me)Zr(\mu Me)][MAO]$ (I) and $AlMe_3$-separated ion pair $[Cp_2Zr(\mu Me)_2AlMe_2]\text{---}[MeMAO]$ (II). These structures are being in equilibrium; the structure (II) is considered as precursor of active sites.

AB INITIO CALCULATION OF THE STRUCTURE OF THE SURFACE COMPOUNDS OF OZONE AND OXYGEN ON Ni(110) BY DENSITY FUNCTIONAL THEORY

I.I. Zakharov, I.N. Shapovalova*,
O.I. Zakharova*, G.O. Tatarchenko*,
N.F. Tyupalo* (*Severodonetsk Technological Institute, Severodonetsk, Ukraine)

J. Struct. Chem., 42(6) (2001) pp. 1064-1070.

The method of density functional theory (exchange correlation functional Becke3LYP) was used to analyze dissociative and molecular type adsorption of O_3 on nickel. The energetic profile was calculated for the reaction of ozone destruction $(O_3)_{gas} \rightarrow (O_3)_{ads} \rightarrow (O_2)_{ads} + ½\, O_2 \uparrow$ on a surface cluster Ni_{10}. Unlike the oxygen species weakly bonded to transition metals, ozone was shown to form a strongly bonded surface compound on the nickel surface. An attemp was made to estimate the heat of oxygen adsorption on the "defect" surface of nickel quantitatively in terms of the model of surface cluster Ni_{13} with a vacancy. Positions of "surface" nickel atoms before and after interaction with the adsorbate were calculated. Relaxation of "surface" nickel atoms was shown to be of importance for the adsorption process. Possibility of stabilization of the ozone-like molecular oxygen species on the transition metal surface under conditions of high oxygen coverage was discussed.

BONDING IN THE OXO FERROUS IRON SPECIES: A COMPLETE ACTIVE-SPACE SELF-CONSISTENT-FIELD THEORY VERIFICATION OF THE MOLECULAR-OXYGEN-LIKE PATTERN

I.L. Zilberberg, R.W. Gora*, G.M. Zhidomirov,
J. Leszczynski** (*Wroclaw University of Technology, Wroclaw, Poland; **Computational Center for Molecular Structure and Interactions, Jackson State University, Jackson, USA)

J. Chem. Phys., 117(15) (2002)
pp. 7153-7161.

The bonding of atomic oxygen to ferrous iron was studied using the $Fe(OH)_2$ system as a model of the ferrous iron center. All lowest triple, quintet, and septet states of $OFe(OH)_2$ were studied at the complete active-space self-consistent-field theory level augmented by multireference second-order-perturbation theory. In addition the density functional theory with three-parameter exchange functional of Becke and correlation functional of Lee, Yang, and Parr has been applied to this system. The ground state has been found to have $^5A_1$ symmetry. The electron configuration responsible for this state is similar to that of molecular oxygen: there are the doubly occupied σ and π shells and singly occupied π^* orbitals. The only difference revealed in this study is the presence of nonbonding half-filled d_δ orbitals.

REDUCTION OF NITROAROMATIC COMPOUNDS ON THE SURFACE OF METALLIC IRON: QUANTUM CHEMICAL STUDY

**I.L. Zilberberg, A. Pelmenschikov*,
Ch.J. Mcgrath**, W.M. Davis**,
D. Leszczynska***, J. Leszczynski***
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Intern. J. Molec. Sci., 3 (2002) pp. 801-813.

The initial reduction steps of nitroaromatic compounds on the surface of metallic iron have been studied theoretically using nitrobenzene (NB) as a representative of nitroaromatic compounds. The quantum chemical cluster approximation within the semiempirical Neglect of Diatomic Differential Overlap for Metal Compounds method was applied to model the Fe(110) crystallographic surface, taken as a representative reactive surface for granular iron. This surface was modeled as a 39-atom two-layer metal cluster with rigid geometry. The associative and dissociative adsorption of nitrobenzene was considered. Based on our quantum chemical analysis, it is suggested that the direct electron donation from the metal surface into the π^* orbital of NB is a decisive factor responsible for subsequent transformation of the nitro group. Molecularly adsorbed NB interacts with metal iron exclusively through nitro moiety oxygen which occupy tri-coordinated positions on surface The charge transfer from metal to NB of approximately 2 atomic units destabilizes the nitro group. As a result, the first dissociation of the N-O bond goes through a relatively low activation barrier. The adsorbed nitrosobenzene is predicted to be a stable surface species, though still quite labile.

SYMMETRICAL CONDITIONS FOR THE STATE COUPLING COEFFICIENTS IN THE OPEN-SHELL SCF THEORY

B.N. Plakhutin

"*Reviews of Modern Quantum Chemistry*", Ed. K.D.Sen, World Scientific, 2002, v. I, pp. 16–42.

A general approach has been developed to define the state coupling coefficients, a_{mn} and b_{mn}, that are used in the open-shell SCF theory to specify an electronic state under consideration. The new method is intended for the high-symmetry nonlinear molecules having the degenerate open-shell configuration γ^{N} ($\gamma = e, t, g, h$; dim $\gamma = 2, 3, 4, 5$), and involves two main parts: (i) representation of a state energy and electron repulsion integrals in terms of the "integral invariants" $H^k(\gamma,\gamma)$ which are molecular analogues of the Slater integrals $F^k(l,l)$; and (ii) new symmetrical constraints on the γ^{N} state coupling coefficients. The new approach has been thoroughly tested for the icosahedral structures $C_{20}{}^{n-}$ (n = 0, 1, 2) having the configuration g^{N} (N = 2, 3, 4). For these systems non-empirical SCF calculations of both the Roothaan and 'non-Roothaan' g^{N} states have been performed. For independent verification, these systems have been also calculated by method FCI-RAS-γ^{N} ("Full CI in the Restricted Active Space γ^{N} ").

ELECTRONIC STRUCTURE CALCULATIONS OF Cu AND Pt CRYSTALS IN CONFINED BASIS OF FUNCTION SET

V.M. Tapilin

J. Struct. Chem., 42(2) (2002) pp. 214-219.

The energy positions and energy of Cu and Pt crystals formation are calculated in the standard basis of atomic functions and in confined basis of function set with polynomial tails. Comparison of the results of calculation reveals that the accuracy of calculation in confined basis of function set is comparable to those in the basis of standard functions at approximately twofold time shortening.

MECHANISM OF OLEFIN EPOXIDATION BY TRANSITION METAL PEROXO COMPOUNDS

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"Computational Modelling of Homogeneous Catalysis",
Eds. F. Maseras and A. Lledós,
Kluwer Academic Publishers, Dordrecht, 2002,
Chapter 12.

Density functional calculations on model systems show that olefin epoxidation by peroxo complexes of early transition metals (Mo, W, Re) in general proceeds by direct transfer via spiro-type transition structures, rather than via insertion. Oxygen transfer by hydroperoxo complexes is at least competitive, if not preferred for Mo, while it is clearly preferred for Ti. A simple MO analysis allows to rationalize many trends (e.g. effects of the metal center and of additional base ligands) found for the computational results.

CARBON MONOXIDE ADSORPTION ON PALLADIUM NANOPARTICLES: A RELATIVISTIC DENSITY FUNCTIONAL STUDY

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J. Chem. Phys., 117(21) (2002) pp. 9887-9896.

Large octahedral and cuboctahedral palladium clusters, ranging from Pd_{55} to Pd_{146}, have been investigated by means of all-electron relativistic density functional calculations. Adsorption of CO molecules on the (111) facets of these clusters was also studied. In particular, the paper is focused on the interaction of CO (a single molecule per facet) with threefold hollow sites to inspect the variation of the calculated adsorption parameters with cluster size. It is considered how observables calculated for that adsorption position on cluster facets relate to adsorption properties of the corresponding site at the single crystal surface Pd(111). It is demonstrated for the first time that, with three-dimensional cluster models proposed here, one can reach cluster size convergence even for such a sensitive observable as the adsorption energy on a metal surface. The authors also addressed size effects on interatomic distances and the cohesive energy of bare Pd nanoclusters whose structure was fully optimized under the imposed O_h symmetry constraint. These quantities were found to correlate linearly with the average coordination number and the inverse of the cluster radius, respectively, allowing a rather accurate extrapolation to the corresponding values of Pd bulk. Finally, it was considered the size convergence of adsorption properties of the *optimized* Pd clusters, as probed by CO adsorption. It was also outlined implications of using these symmetric clusters for investigating adsorption and reactions on oxide-supported nanoparticles of model Pd catalysts

DETERMINATION OF HYPERFINE TENSOR COMPONENTS FROM NUCLEAR FREQUENCIES AT CANONICAL ORIENTATIONS OF THE *g*-TENSOR

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J. Mag. Res., 155(1) (2002) pp. 100-105.

The analytical procedure for the determination of all components of the symmetric hyperfine tensor of the I=1/2 nucleus in the *g*-tensor coordinate system is described, assuming that nuclear frequencies corresponding to the principal directions of the *g*-tensor and exact values of the external magnetic field (or nuclear Zeeman frequencies) are experimentally available.

LATTICE DEFECTS AND OXYGEN ABSORPTION/MIGRATION IN CERIA/CERIA-ZIRCONIA SOLID SOLUTIONS: ANALYSIS BY SEMIEMPIRICAL INTERACTING BONDS METHOD

N.N. Bulgakov, V.A. Sadykov, V.V. Lunin*, E. Kemnitz** (*Lomonosov Moscow State University, Moscow, Russia; **Humboldt-Universität, Berlin, Germany)

React. Kinet. & Catal. Lett., 76(1) (2002)
pp. 103-110.

Semiempirical Interacting Bonds Method was used to calculate the enthalpies of oxygen removal from the bulk of ceria and ceria-zirconia solid solutions. The energy of the bulk reduction was obtained to agree reasonably with the experimental data when the complex defect comprised of the oxygen vacancy and interstitial oxygen atom surrounded by six cations was suggested to emerge due to an oxygen removal from the bulk. The zirconium cations dissolved in ceria affect the energies of the bulk reduction and bulk oxygen mobility due to a decrease in the local Me-O coordination number from 8 to 7.

SURFACE ENERGIES AND HEATS OF OXYGEN ADSORPTION IN CERIA/CERIA-ZIRCONIA SOLID SOLUTIONS: ANALYSIS BY SEMIEMPIRICAL INTERACTING BONDS METHOD

N.N. Bulgakov, V.A. Sadykov, V.V. Lunin*, E. Kemnitz** (*Lomonosov Moscow State University, Moscow, Russia; **Humboldt-Universität, Berlin, Germany)

React. Kinet. & Catal. Lett., 76(1) (2002) pp. 111-116.

Semiempirical Interacting Bonds Method (IBM) in the slab approximation with due regard to relaxation after the free surface formation was used to calculate the surface energies and enthalpies of oxygen adsorption on the surface of ceria-based solid solutions. The IBM-estimated surface energies agree well with the published values obtained using electrostatic models or the periodic *ab initio* Hartree-Fock code CRYSTAL. The most weakly bound forms of the surface oxygen appear to be located at the (111) face on the cerium cations which have complex defects of non-stoichiometry in the subsurface layer.

A Monte Carlo Simulation to Study Physico-Chemical Processes

A MONTE CARLO SIMULATION OF THE DEVELOPMENT OF SURFACE ROUGHNESS AND ITS EFFECT ON THE DISSOLUTION KINETICS OF SiO_2 AEROGELS

S.I. Prokopiev, A.G. Okunev, Yu.I. Aristov

Colloid J., 64(1) (2002) pp. 95-100.

The development of surface roughness during dissolution of spherical particles is studied by the Monte Carlo method. The simulation results are used to analyze the dissolution kinetics of silicon dioxide aerogels in an aqueous solution of alkali (NaOH). The suggested model is shown to be suitable for describing the experimental dissolution curves obtained for aerogels with a small diameter of primary particles (3.5 and 2.9 nm). For aerogels with larger particles, a good agreement with the experiment can be achieved under the additional assumption that only part ($p < 1$) of the particle surface is originally active in dissolution; the best agreement is reached at $p \approx 0.5$. In the kinetic regime of dissolution, the dissolution rate may be more than three times higher (owing to the formation of rough surfaces of primary particles with relatively large diameters, 40 atoms or more) than the rate calculated for the same parameters within the framework of the modified Delmon model, which does not make allowance for the development of roughness. Relatively small particles (with the diameter of less than 15 atoms) are dissolved before a significant roughness can be developed; therefore, the kinetic curves obtained for both models have virtually identical shapes in this case. The formation of roughness has an especially large effect on the dissolution of intermediate-size particles, whose dissolution time has the same order of magnitude as the time required for establishment of the steady-state roughness.

MONTE CARLO SIMULATIONS OF OSCILLATIONS, CHAOS AND PATTERN FORMATION IN HETEROGENEOUS CATALYTIC REACTIONS

V.P. Zhdanov

Surf. Sci. Rep., 45 (2002) pp. 231-326.

Experimental studies employing surface-science methods indicate that kinetic oscillations, chaos, and pattern formation in heterogeneous catalytic reactions often result from the interplay of rapid chemical reaction steps and relatively slow complementary processes such as oxide formation or adsorbate-induced surface restructuring. In general, the latter processes should be analyzed in terms of theory of phase transitions. Therefore, the conventional mean-field reaction-diffusion equations widely used to describe oscillations in homogeneous reactions are strictly speaking not applicable. Under such circumstances, application of the Monte Carlo method becomes almost inevitable. In this review the advantages and limitations of employing this technique are discussed and it has been shown what one can reach on this way. Attention is focused on Monte Carlo simulations of CO oxidation on (100) and (110) single-crystal Pt and polycrystal Pt, Pd and Ir surfaces and of NO reduction by CO and H_2 on Pt(100). CO oxidation on supported nm catalyst particles and NO reduction on composite catalysts also are discussed. The results presented show that with the nowadays computer facilities the MC technique has already became an effective tool for analyzing temporal oscillations and pattern formation on the nm scale in catalytic reactions occurring both on single crystals and supported particles.

BISTABILITY IN CATALYTIC REACTIONS ON THE nm SCALE

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

Surf. Sci., 496(3) (2002) pp. 251-263.

Monte Carlo simulations of the bistable kinetics of CO oxidation occurring on nm-sized catalyst particles are presented. The analysis is focused on the simplest case when reaction runs primarily on the (111) facets. Specifically, the catalyst particle is represented by a truncated triangular lattice. The lattice size, L, is varied from 100 down to 3. The model takes into account specifics of oxygen adsorption on the (111) face of fcc metals (in particular, oxygen adsorption on nearest-neighbour sites is prohibited). The results, obtained with qualitatively realistic ratio of the rates of elementary reaction steps, indicate that the hysteresis in the reaction kinetics is nearly independent of L for $L>10$. For small lattices with $L\sim5$, the hysteresis disappears. The implications of these findings for interpretation of experimental data are briefly discussed.

KINETIC OSCILLATIONS ON nm-SIZED CATALYST PARTICLES: OXIDE MODEL

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

Surf. Sci., 511(1-3) (2002) pp. 23-33.

Monte Carlo simulations of kinetic oscillations in the CO-O_2 reaction occurring on nm-sized supported catalyst particles are presented. The model used includes the conventional Langmuir-Hinshelwood mechanism of CO oxidation and oxide formation and removal. The analysis is focused on such aspects as CO supply via the support, role of this supply in synchronization of oscillations on adjacent catalyst particles, and cooperative effects in the oxide formation.

KINETIC OSCILLATIONS ON nm-SIZED CATALYST PARTICLES: SURFACE RESTRUCTURING

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

Surf. Sci., 513(1) (2002) L385-L390.

Monte Carlo simulations of kinetic oscillations in the CO-O_2 reaction occurring on a (100) facet of a nm-sized supported Pt particles are presented. The model includes the conventional Langmuir-Hinshelwood mechanism of CO oxidation and CO- and O-induced restructuring of the facet. The facet size is varied from 50x50 to 5x5. With decreasing size, oscillations become more irregular. More or less regular oscillations accompanied by formation of CO islands are found for the sizes down to 15x15. Practically, this means that for observation of such oscillations the particle diameter should be above ~4 nm. These findings are in agreement with available experimental data.

PATTERN FORMATION IN THE A+B_2 REACTION WITH ANISOTROPIC LATERAL ADSORBATE-ADSORBATE INTERACTIONS

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

Europhys. J. B, 27(4) (2002) pp. 541-547.

Monte Carlo simulations of the formation of (1x2) islands in the case of the $2A+B_2 \rightarrow 2AB$ reaction occurring via the Langmuir-Hinshelwood mechanism on a square lattice under steady-state conditions are presented. The model employed takes into account the effect of anisotropic lateral B-B interactions on the rates of B diffusion and elementary reaction events. The results obtained with qualitatively realistic ratio of the rate of elementary reaction steps indicate that the average island size depends on the details of diffusion and reaction dynamics in a similar way as in the earlier studied case of the simplest A+B reaction running via the Eley-Rideal mechanism.

CELLULAR OSCILLATOR WITH A SMALL NUMBER OF PARTICLES

V.P. Zhdanov

Europhys. J. B, 29(3) (2002) pp. 485-489.

Monte Carlo simulations of the formation of oscillatory spatio-temporal spark-like patterns in the model completely stochastic cellular Ca^{+2} oscillator show that in order to observe this phenomenon the minimum average number of Ca^{+2} ions in the cytosol may be as low as about 50.

CONFORMATIONAL DYNAMICS IN ENZYMATIC REACTIONS

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

Europhys. Lett., 57(2) (2002) pp. 295-301.

Lattice Monte Carlo simulations of the product-formation step in rapid enzymatic reaction occurring via the conventional Henri-Michaelis-Menten mechanism are presented. The reaction is considered to be limited by reconfiguration of the enzyme structure. The effect of the conformational dynamics on the apparent parameters characterizing the reaction kinetics is demonstrated to be hidden. In particular, the pre-exponential factor of the reaction rate constant is nearly equal to that for elementary moves of the protein chain forming the enzyme.

EXACT RESULTS FOR LONG-RANGE BRIDGE-MEDIATED ELECTRON TRANSFER

V.P. Zhdanov

Europhys. Lett., 59(5) (2002) pp. 681-686.

The rate constant of long-range electron transfer is proportional to $|V_{DA}|^2$, where V_{DA} is the electronic coupling between the donor and acceptor. Particles located between the donor and acceptor may increase the coupling by forming a bridge for electron tunneling. Analysing this effect, an accurate asymptotic expression for V_{DA} in the case when the interaction of an electron with the donor, acceptor and bridge is represented as a sum of the Dirac delta functions is derived. Comparing the exact results with those obtained by using the conventional approach based on combination of atomic orbitals, it has been shown that the latter approach may overestimate V_{DA} by several orders of magnitude.

SIMULATIONS OF GLYCOLYTIC OSCILLATIONS IN CELLS WITH COMPARTMENTS

V.P. Zhdanov

Intern. J. Bifurc. Chaos, 12(7) (2002) pp. 1643-1652.

Monte Carlo simulations of glycolytic oscillations inside the cell with a chemically inactive compartment are presented. 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 in the area between the external membrane and the compartment. The model parameters are chosen so that the typical size of oscillatory patters is comparable with the cell size. Although the compartment does not directly participate in the reaction, its presence is found to amplify irregular oscillations provided that the compartment size is appreciable and it is located in the center of the cell.

SIMULATION OF MAINTENANCE OF THE EPIDERMIS

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

Phys. Chem. Chem. Phys., 4(19) (2002) pp. 4609-4611.

A 3D lattice Monte Carlo model of self-renewal of the epidermis, including division of cells located in the innermost layer, death of cells in the upper layers, and cell diffusion between the layers is proposed. The results of simulations indicate that the dependence of the epidermis thickness, L, on the model parameters is extremely weak. For example, the two orders of magnitude increase in the cell life expectancy results in increase of L only by a factor of two.

COMMENT ON "MONTE CARLO SIMULATIONS FOR A LOTKA-TYPE MODEL WITH REACTANT DIFFUSION AND INTERACTIONS"

V.P. Zhdanov

Phys. Rev. E, 65(3) (2002) 033101 (3 pages).

Discussing the effect of adsorbate-adsorbate lateral interactions on the kinetics of heterogeneous catalytic reactions, G. Zvejnieks and V.N. Kuzovkov [*Phys. Rev. E*, 63 (2001) 051104] conclude that in the case of adsorbed particles the Metropolis Monte Carlo dynamics is meaningless and propose to use their own dynamics, which is equivalent to the Glauber dynamics. In this Comment, it is shown that these and some other conclusions and prescriptions by Zvejnieks and Kuzovkov are not in line with the general principles of simulations of rate processes in adsorbed overlayers.

nm-SIZED METAL PARTICLES ON A SEMICONDUCTOR SURFACE, SCHOTTKY MODEL, etc.

V.P. Zhdanov

Surf. Sci., 512(1-2) (2002) L331-L334.

In the case of metal particles fabricated on a semiconductor surface, the Fermi levels in the two materials must be coincident. This condition is fulfilled due to charge redistribution near the interface. The available estimates of the transferred charge are based on the models constructed in analogy with the Schottky model describing the interface between a bulk metal and semiconductor. Specifically, the charge supplied or accepted by donors is assumed to be balanced by the charge located on the metal-semiconductor interface. It is shown that such models are not directly applicable to supported nm-sized metal particles, because in order to have no electric field inside a particle the available charge should be distributed nearly uniformly over the whole particle surface. According to analysis, the transferred charge is appreciably smaller than that predicted earlier.

NEW STATISTICAL LATTICE MODEL OF A SUPPORTED NANOPARTICLE: INFLUENCE OF DISSOCIATIVE ADSORPTION ON THE EQUILIBRIUM SHAPE AND SURFACE MORPHOLOGY OF A PARTICLE

E.V. Kovalev, V.I. Elokhin, A.V. Myshlyavtsev, B.S. Bal'zhinimaev

Doklady Phys. Chem., 381(6) (2001) pp. 309-313.

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.

Development and Application of Physicochemical Methods for Catalysts Investigation

N-BUTENE CONVERSION ON H-FERRITE STUDIED BY ^{13}C MAS NMR

A.G. Stepanov, M.V. Luzgin, S.S. Arzumanov, H. Ernst*, D. Freude* (*Universität Leipzig, Leipzig, Germany)

J. Catal., 211(1) (2002) pp. 165-172.

^{13}C MAS NMR analysis of the hydrocarbon products formed from the selectively ^{13}C-labeled *n*-but-1-ene on zeolite ferrierite (H-FER) in a closed batch reactor revealed the following successive steps of the olefin conversion with temperature increase from 300 to 823 K: a double-bond-shift reaction, scrambling of the selective ^{13}C label in the formed *n*-but-2-ene, oligomerization (dimerization), conjunct polymerization, formation of condensed aromatics, and formation of the simple aromatics. Arguments in favor of either bimolecular or pseudo-monomolecular mechanisms are provided, excluding at the same time the monomolecular isomerization of *n*- to isobutene on a fresh sample. The arguments are based on selective label redistribution in the *n*-but-2-enes, the impossibility of the existence of isobutene inside the pores of the zeolite under static conditions and the observation of *n*-but-2-enes oligomerization (dimerization). Conjunct polymerization leads to the formation of alkyl-substituted cyclopentenyl cations (CPCs), which can serve as an intermediate for pseudo-monomolecular isomerization. Carbonaceous deposits (polycyclic aromatics), which deactivate the catalyst in the isomerization reaction, are formed from the CPCs. Polycyclic aromatics are transformed into simple aromatics with methane and ethane evolution at 823 K.

OLEFIN AS AN INTERMEDIATE IN *n*-BUTANE ISOMERIZATION ON SULFATED ZIRCONIA. AN *IN SITU* ^{13}C MAS NMR STUDY OF *n*-OCTENE-1 CONVERSION

A.G. Stepanov, M.V. Luzgin, V.N. Sidelnikov

Catal. Lett., 78(1) (2002) pp. 153-156.

By using *in situ* ^{13}C MAS NMR and *ex situ* GC-MS, the analysis of hydrocarbon products formed from n-octene-1 adsorbed on sulfated zirconia catalyst (SZ) has been performed. It is shown that a mixture of alkanes and stable alkyl substituted cyclopentenyl cations (CPC) is formed as the basic reaction products. Formation of both alkanes and CPC from n-octene-1, a precursor of C_8^+ cation, the key intermediate in n-butane isomerization via a "bimolecular pathway", implies that formation of the isomerized alkane occurs by a complex process of "conjunct polymerization", rather than isomerization itself. CPC deposited on the SZ surface can be in charge of the catalyst deactivation.

DYNAMICS OF ISOBUTANE INSIDE ZEOLITE ZSM-5. A STUDY WITH DEUTERIUM SOLID-STATE NMR

A.G. Stepanov, M.M. Alkaev, A.A. Shubin, M.V. Luzgin, T.O. Shegai, H. Jobic* (*Institut de Recherches sur la Catalyse, CNRS, Villeurbanne, France)

J. Phys. Chem. B, 106 (2002) pp. 10114-10120.

Perdeuterated *iso*-butane-d_{10}, when it is adsorbed on zeolite ZSM-5, has been shown to exhibit a superposition of two ^{2}H NMR Pake-powder patterns with quadrupole constants $C_Q = 2.35$ kHz and asymmetry parameter $\eta = 0.17$ for the CD_3 groups and $C_Q = 23.0$ kHz and $\eta = 0.20$ for the CD group at 153-373 K. The narrowed Pake-powder patterns have been interpreted in terms of the motional behavior of *iso*-butane molecule located at channel intersection site of the zeolite framework. Dynamic behavior of *iso*-butane is complex and includes probably both fast intramolecular rotations and large amplitude librations of the molecule as a whole. For example, the motion of the CD group may be effectively described as consisting of the combination of the precession of the CD group around some axis Z which makes up the angle $\alpha \approx 50^\circ$ with the direction of C-D bond and fast hops of the axis Z itself between two equally populated orientations by the angle $\Theta = 39^\circ$ (or 86°). Simultaneously, fast rotation of the methyl groups around CD_3–CD axis occurs. The activation energies and rotational correlation times at 373 K have been estimated to be 13.5 kJ/mol and 41 ps for the methyl groups, and 17.7 kJ/mol and 1200 ps for the methene group, respectively.

^{14}N, ^{17}O, ^{103}Rh NMR STUDIES OF Rh(III) STATE IN DILUTED NITRIC ACID SOLUTIONS

M.A. Fedotov

Russ. J. Coord. Chem., 28(8) (2002) pp. 573-580.

The state of rhodium(III) in nitric acid solutions diluted with 3M HNO_3 or water was studied by ^{14}N, ^{17}O, and ^{103}Rh NMR methods. The ^{103}Rh NMR chemical shifts significantly depend on the ionic background of the solution. Concentrated nitric acid solutions (c_{Rh} = 0.5–1 mol/l) diluted 100 to 200 times retain the polynuclear Rh(III) forms with double (μ-NO_3, μ-OH) bridges. The predominant form in the diluted solutions is a dimer.

NMR STUDY OF DECOMPOSITION OF MONOETHANOLAMINE UNDER CONDITIONS OF INDUSTRIAL GAS TREATMENT

V.P. Talzi, S.V. Ignashin

Russ. J. Appl. Chem., 75(1) (2002) pp. 80-85.

The main impurities in aqueous solution of monoethanolamine used in various stages of gas treatment at the Omsk Oil Refinery Joint-Stock Company were identified by ^{1}H and ^{13}C NMR spectroscopy. A mechanism of their formation was proposed. A probable dependence of service characteristics of the absorbent on its composition was considered.

STRUCTURE OF GLASSES IN THE Na_2SO_4-P_2O_5-H_2O SYSTEM

A.M. Nepomiluev*, R.N. Pletnev*, O.B. Lapina, S.G. Kozlova*, V.G. Bamburov* (*Institute of Solid-State Chemistry, Ekaterinburg, Russia)

Glass Physics & Chemistry, 28(1) (2002) pp. 1-4.

The structure of sulfate–phosphate glasses is investigated by high-resolution ^{31}P solid-state nuclear magnetic resonance with magic-angle sample spinning (^{31}P MAS NMR spectroscopy). The structure parameters that account for the number of different types of phosphorus–oxygen structural units involved in the glass network are determined, and the main structural units of the glasses under investigation are revealed. The role of H_2O and Na_2SO_4 as modifiers of the structural network of sulfate–phosphate glasses is clarified.

ACTIVATION OF DIMETHYL ZIRCONOCENE BY METHYLALUMINOXANE (MAO) – SIZE ESTIMATE FOR Me-MAO$^-$ ANIONS BY PULSED FIELD GRADIENT NMR

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J. Amer. Chem. Soc., 124 (2002) pp. 12869-12873.

In a study of the reaction system MAO/$(C_5H_5)_2ZrMe_2$, the size of the ion pair $[(C_5H_5)_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ [Me-MAO]$^-$ was determined by Pulsed Field-Gradient NMR of its cationic moiety. A mean effective hydrodynamic radius of 12.2-12.5 Å, determined from diffusion rates in benzene solution at different zirconocene and MAO concentrations indicates that the ion pair remains associated even at the lowest concentrations studied. At elevated concentrations, aggregation to ion quadruples or higher aggregates is indicated by an apparent size increase and by shifts of the C_5H_5 and Me ^{1}H NMR signals. The equilibrium constant for the reaction $[(C_5H_5)_2ZrMe^{+}\cdots Me\text{-}MAO^{-}] + ½\ Al_2Me_6 \equiv [(C_5H_5)_2Zr(\mu\text{-}Me)_2AlMe_2]^{+}\ [Me\text{-}MAO]^{-}$ changes at different Al/Zr ratios; this indicates that MAO contains various species which produce $Me\text{-}MAO^{-}$ anions with different Lewis basicities. The volume of the $Me\text{-}MAO^{-}$ anion suggests that it contains 150-200 Al atoms.

APPLICATION OF NMR MICROIMAGING IN CATALYSIS

I.V. Koptyug*, L.Yu. Ilyina, A.V. Matveev, V.N. Parmon, R.Z. Sagdeev* (*International Tomography Center, Novosibirsk, Russia)

Chem. Phys., 21(1) (2002) pp. 71-82.

NMR microimaging is applied to study dynamics of mass transport upon the preparation of supported catalysts, in the course of drying of porous materials, moisture adsorption by adsorbents impregnated with hygroscopic salts, and also for detection of spatial velocity maps of liquid phase distribution in the transport channels of monolithic catalysts. The discussion of obtained results in the context of possible application of this method for heterogeneous catalysis demonstrates the perspectivity of this method at comprehensive approach to the investigation of all aspects, influencing the efficiency of catalytic reactor action.

APPLICATION OF ^{1}H NMR MICROIMAGING TO THE *IN SITU* INVESTIGATION OF LIQUID EVAPORATION FROM THE OBJECT MODELLING POROUS SOLIDS

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(*International Tomography Center, Novosibirsk, Russia)

Doklady Chemistry, 376(6) (2001) pp. 777-781

In this study for the first time the experiments are carried out when the operating reactor is placed directly inside the NMR imaing probe. It gives opportunity to study heat regimes of catalyst grain operation and to characterize experimentally the liquid phase distribution inside the porous particle directly in the course of catalytic reaction. The application of NMR microimaging for investigation of chemical reaction inside the porous catalyst grain with the participation of gaseous and liquid reagent gives possibility to visualize the mechanism of liquid phase distribution within the porous grain in the conditions of chemical and phase transformations and to develop the physico-chemical model for analysis of critical phenomena on the porous catalyst grain.

NMR IMAGING OF THE DISTRIBUTION OF THE LIQUID PHASE IN A CATALYST PELLET DURING α-METHYLSTYRENE EVAPORATION ACCOMPANIED BY ITS VAPOR-PHASE HYDROGENATION

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(*International Tomography Center, Novosibirsk, Russia)

JACS, 124(33) (2002) pp. 9684-9685.

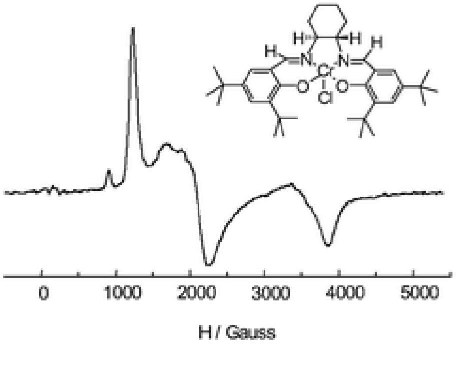
This communication reports the first application of NMR imaging to study the progress of a multiphase heterogeneous catalytic reaction *in situ*. Various stationary regimes of α-methylstyrene (AMS) hydrogenation on a single $Pt/\gamma\text{-}Al_2O_3$ catalyst pellet have been investigated. The two-dimensional maps of the liquid-phase distribution within the pellet have been obtained in the course of the catalytic reaction, with the pellet temperature rising up to 185°C. The large liquid-phase concentration gradients have been shown to exist under conditions of liquid AMS evaporation accompanied by its vapor-phase hydrogenation. It has been demonstrated that despite a substantial broadening of the NMR lines of liquids permeating porous solids the quantification of the relative amounts of AMS and the major reaction product cumene with spatial resolution across the pellet is feasible.

EPR AND ^{1}H NMR SPECTROSCOPIC STUDY OF THE Cr^{III}(SALEN)Cl CATALYSTS

K.P. Bryliakov, M.V. Lobanova, E.P. Talsi

J. Chem. Soc., *Dalton Trans.,* 11 (2002)
pp. 2263-2265.

An EPR and ^{1}H, ^{2}H NMR study of the Cr^{III}(salen)Cl type complexes was performed for the first time; the X-band EPR spectra of the *S*= 3/2 Cr^{III}(salen)Cl complexes were interpreted using analytical expressions to reveal the *g*-factors and fine structure parameters, and assignment of the ^{1}H and ^{2}H NMR resonances was made.



ROLE OF Mn (IV) SPECIES IN Mn(SALEN) CATALYZED ENANTIOSELECTIVE AEROBIC EPOXIDATIONS OF ALKENES: AN EPR STUDY

K.P. Bryliakov, O.A. Kholdeeva, M.P. Vanina, E.P. Talsi

J. Molec. Catal. A: *Chemical*, 178(1) (2002) pp. 47-53.

Using EPR spectroscopy, high valence Mn(salen) complexes were monitored in Mn^{III}(salen)/ isobutyraldehyde/O_2 and Mn^{III}(salen)/ pivalaldehyde/O_2 catalytic systems in the absence and in the presence of *N*-methylimidazole (*N*-Me-Imd), where Mn^{III}(salen) (**1**) is (S,S)-(+)-N,N'-bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanediamino-manganese(III) chloride. Interaction of **1** with aliphatic aldehydes in the presence of O_2 was found to give a mixture of oxo manganese(IV) species L_1(salen)Mn^{IV}=O (2) with various axial ligands L_1 (L_1=Cl^-, $RCOO^-$). They display EPR signals having close g values of c.a. 5.2 with resolved hyperfine structures from one manganese (A = 75 G, ^{55}Mn, I=5/2). In the presence of *N*-Me-Imd, new manganese(IV) complexes were detected. The first one was shown to be an antiferromagnetically coupled mixed-valence $[(salen)Mn^{IV}(\mu_2\text{-}O)_2Mn^{III}(salen)]^-$ dimer having 16-line EPR signal at g = 2. The second one is probably (salen)Mn^{IV}(OOCOR)*N*-Me-Imd acylperoxo complex (**2**) (g = 4.2 (R = $CH(CH_3)_2$), or g = 4.7 (R = $C(CH_3)_3$), unresolved manganese hyperfine structure). Possible roles of each complex in the enantioselective alkene epoxidations are discussed.

ELECTRONIC STATE OF VANADIUM IONS IN $Li_{1+x}V_3O_8$ ACCORDING TO EPR SPECTROSCOPY

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J. Solid State Chem., 163(2) (2002) pp. 421-426.

EPR spectroscopy is used to study the electronic state of vanadium ions in HT- and LT-$Li_{1+x}V_3O_8$. It is shown that in both cases the EPR spectra observed are attributed to vanadyl VO^{2+} ions (localized electron centers) with weak exchange interaction. The other type of registered electrons is characterized by larger mobility through a few V^{5+} ions, i.e., by a higher degree of delocalization (electron gas). Based on the analysis of the temperature dependence of the EPR line width, it is stated that the exchange interaction between localized electron centers proceeds through electron gas. It is found that HT-$Li_{1+x}V_3O_8$ differs from LT-$Li_{1+x}V_3O_8$ by the sloping form of its spectrum at g range connected with two types of VO^{2+} ions different in the direction of the crystal field axis corresponding to a short $V{=}O^{2+}$ bond.

ELECTRONIC STATE OF RHENIUM COMPLEXES WITH OCTAHEDRAL CHALCOCYANIDE CLUSTER ANIONS $[Re_6Q_8(CN)_6]^{3-}$ (Q = S, Se, Te). EPR AND MAGNETIC SUSCEPTIBILITY STUDIES

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Russ. J. Coord. Chem., 28(8) (2002) pp. 554-556.

Compounds $(Ph_4P)_3[Re_6S_8(CN)_6]$ (**I**), $(Ph_4P)_2(H)[Re_6Se_8(CN)_6]\bullet 4H_2O$ (**II**), and $(Bu_4N)_2(H)[Re_6Te_8(CN)_6]\bullet 2H_2O$ (**III**) were synthesized and studied using EPR spectroscopy and magnetic susceptibility methods. The $[Re_6Q_8(CN)_6]^{3-}$ cluster anions (Q = S, Se, Te) were found to be paramagnetic; at 300 K, μ_{eff} of complexes **I**, **II**, and **III** is equal to 2.01, 1.90, and 1.96 μ_B, respectively. Magnetic susceptibility χ measured in the 2–300 K range suggested insignificant exchange interaction between paramagnetic centers. The parameters of the EPR spectra of complexes **I** and **II** (g = 2.51 and 2.56; ΔH = 330 and 460 G, respectively) indicated that the unpaired electron is located near S or Se atoms.

PULSED EPR STUDY OF THE $(NO)_2$-Na^+ TRIPLET STATE ADSORPTION COMPLEX

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Chem. Phys. Lett., 349(5-6) (2001) pp. 511-516.

The $(NO)_2$-Na^+ triplet state complex stabilised in Na-A zeolites at low temperature was studied by pulsed EPR. The 3-pulse ESEEM spectra at 5 K were analysed by simulations in the time-domain, followed by Fourier transformation. The ESEEM was attributed to the interaction with Na^+. The hyperfine coupling **A**(^{23}Na)=(4.6, 4.6, 8.2) MHz and nuclear quadrupole **Q**(^{23}Na)=(0.3, 0.3, -0.6) MHz tensors are of comparable magnitude as in the NO-Na^+ complex determined earlier. The complexes are proposed to be either pairs of NO-Na^+ or ON-Na^+-NO.

THE SPECTROSCOPIC STUDY OF THE MODIFIED POLYTETRAFLUOROETHYLENE

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J. Struct. Chem., 43(1) (2002) pp. 64-68.

IR and ^{19}F NMR spectroscopy were used to study the effect of thermal gas dynamic destruction of polytetrafluoroethylene (PTFE) on its microscopic and permolecular structure and dynamic properties. It was shown that thermal gas dynamic dispergation results in the transformation of polytetrafluoroethylene macromolecules structures. The possible mechanism of PTFE depolimerization is generation of oligomers with terminal groups $—CF_3$ and $—CF=CF_2$.

IN SITU IR SPECTROSCOPIC STUDIES OF HCOOH DECOMPOSITION OVER V-Ti-O CATALYST

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T.V. Andrushkevich, E.S. Stoyanov

React. Kinet. & Catal. Lett., 76(1) (2002) pp. 123-129.

Decomposition of formic acid over V-Ti-O catalysts was studied by *in situ* IR spectroscopy. Four surface compounds, among which are H-bonded acid, one mono- and two bidentate formates (BF1 and BF2), were identified in the temperature range of 100-190°C. The activation energy and rate of the BF2 decomposition were found equal to those for the CO formation. This equality points to the involvement of BF2 in the HCOOH decomposition into carbon monoxide.

IR SPECTROSCOPIC CHARACTERIZATION OF NH_4-ANALCIME

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Yu.V. Seryotkin*, S.G. Shulgenko* (*Institute of Mineralogy and Petrography, Novosibirsk, Russia)

Physics & Chem. of Minerals, 29(9) (2002) pp. 617-623.

The IR spectrum of ammonium-exchanged natural analcime (basalt, Nidym River, Siberian platform) exhibits several features that suggest a lowered symmetry for the NH_4^+ ion and that this is influenced by hydrogen bonding within the framework. These features are: the pronounced splitting into three components and high-frequency shift of the ν_4-bending mode; appearance of the ν_1-stretching mode which is predicted to become IR-active when the ideal T_d symmetry of NH_4^+ ion is violated, and the low-frequency shift of the ν_1- and ν_3-stretching modes. The absence of absorption lines in the 1800-2400-cm^{-1} region indicates that hydrogen bonding between the framework and the NH^+_4 ion is very weak. The three-component splitting of the ν_4-bending mode indicates that the symmetry of NH^+_4 ion is lower than C_{3v}. This implies that at least two N-H bonds of the NH^+_4 ion are disturbed by hydrogen bonding. Computer analysis of the normal vibrations of the NH^+_4 molecule for different symmetry types (using harmonic approximation) indicates that the best fit to the observed ν_4 triplet frequencies for C_1 symmetry implies a deviation of the valent angle δH-N-H from ideal T_d symmetry of around ±2.5°. The factors governing the behaviour of the NH^+_4 ion in the analcime structure are discussed. The geometry of the nearest environment of the NH^+_4 ion in the analcime structure is analyzed with respect to the present IR data.

ACIDITY OF HETEROPOLY ACIDS WITH VARIOUS STRUCTURES AND COMPOSITIONS STUDIED BY IR SPECTROSCOPY OF THE PYRIDINIUM SALTS

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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 CF_3SO_3H and $HClO_4$. $H_3PW_{12}O_{40}$ was the strongest acid.

THE ROLE OF HYDROGEN BONDS IN THE PRESSURE-INDUCED STRUCTURAL DISTORTION OF 4-HYDROXYACETANILIDE CRYSTALS

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V.P. Baltakhinov (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia;
**Philipps University of Marburg, Marburg/Lahn, Germany)

Polish J. Chem., 76(9) (2002) pp. 1333-1346.

Results of X-ray diffraction and IR-specroscopy studies of the role of hydrogen bonds in the structural distortion of the monoclinic and the orthorhombic polymorphs of paracetamol induced by hydrostatic pressure (up to 4-5 GPa) are analyzed. Two groups of phenomena were studied: (i) the anisotropic structural distortion of the same polymorph, (ii) transitions between the polymorphs induced by pressure. The bulk compressibilities of the two polymorphs are practically equal. The anisotropy of pressure-induced structural distortion is qualitatively different. Lattice expansion in particular crystallographic directions was observed for the monoclinic polymorph. With increasing pressure the intermolecular NH...O and OH...O hydrogen bonds contracted and the intramolecular angles between the planes of the phenyl ring and the acetamide group decreased. Pressure-induced transitions between the polymorphs were poorly reproducible and limited by nucleation of the new polymorph.

SEPARATE MEASUREMENT OF THE ACTIVE COMPONENT AND SUPPORT TEMPERATURES FOR THE Ni/MgO CATALYST IN THE COURSE OF AN EXOTHERMAL REACTION BY *IN SITU* HIGH-TEMPERATURE X-RAY POWDER DIFFRACTION

L.M. Plyasova, T.A. Krieger, A.A. Khassin, V.N. Parmon

Doklady Phys. Chem., 382 (4-6) (2002) pp. 47-50.

A method was developed using *in situ* XRD for direct measurement of real temperature of nanoparticles of a supported active component (specifically, nickel metal) and a support (specifically, magnesia) under conditions of an exothermic reaction. Hydrogenation of CO was used as the exothermic reaction. The temperature dependence of the lattice constant of metal nickel at 200 to 350°C in a mixture of CO and hydrogen was shown to be far from linear with a maximum at about 300°C. It was concluded that the said behavior of the lattice constant resulted from overheating of the active species against the support temperature in the course of exothermic hydrogenation of CO. The maximal lattice constant of nickel metal at the range of 250 to 300°C was found to correspond to overheating ΔT (250±25°C) of nickel nanoparticles with respect to the support temperature.

SURFACE PROPERTIES OF ALUMINAS AS STUDIED BY THE ELECTRON-NUCLEAR DOUBLE RESONANCE METHOD

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Russ. J. Phys. Chem., 75(4) (2001) pp. 629-635.

XRD analysis, electron paramagnetic resonance (EPR), and electron–nuclear double resonance (ENDR) in conjunction with molecular anthraquinone probe, were used to study the properties of various aluminas. It was demonstrated that the use of the ENDR method for analyzing the hyperfine coupling of the unpaired electron with the aluminum and hydrogen nuclei of the paramagnetic species arising at the surface upon anthraquinone adsorption makes it possible to determine the structure of surface complexes even when EPR spectra are insufficiently resolved. It was established that various complexes are formed at the surface of the aluminas due to changes in the positions of acceptor surface sites participating in the reaction.

AN ION CYCLOTRON RESONANCE STUDY OF REACTIONS BETWEEN MOLYBDENUM OXIDE IONIC CLUSTERS AND AMMONIA

V.B. Goncharov, E.F. Fialko

Russ. J. Phys. Chem., 76(9) (2002) pp. 1454-1460.

Reactions between molybdenum oxygen-containing clusters $Mo_xO_y^+$ (x = 1-3, y = 1-9) and ammonia were studied by ion cyclotron resonance. The formation of several nitrogen-containing ions including the $Mo_3O_7N_2^+$ complex with molecular nitrogen was observed. The upper and lower limits of bond energies in the complexes were estimated (kcal/mol): Mo^+–NH (<92), MoO^+–NH (<117), MoO_2^+–NH (<71), $Mo_2O_5^+$–NH_3 (>56), $Mo_3O_8^+$–NH_3 (>58), $Mo_3O_8^+$-NH (>44), $Mo_3O_7(NH_3)^+$–NH_3 (>58), $Mo_3O_7^+$–2NH (>88), $Mo_3O_7^+$–N_2 (>112) in the Mo=N–N=Mo structure, and $Mo_3O_7^+$–N_2 (>56) in the Mo–N=N–Mo structure.

STRUCTURE AND REACTIVITY OF MOLYBDENUM OXIDE CLUSTER IONS IN GAS PHASE

V.B. Goncharov, E.F. Fialko

J. Struct. Chem., 43(5) *(*2002) pp. 838-843.

A combination of cyclotrone ion resonance technique and Knudsen effusion source was used for preparation of a set of ion clusters of molybdenum oxide $Mo_xO_y^+$ (x = 1 –5, y = 1 – 15). Dependencies of the concentrations of various molybdenum oxide ions on retention time, as well as reactions of the ions with carbon monoxide were studied. It was shown that the structure of $Mo_xO_y^+$ (x>3) ions comprises a cyclic fragment Mo_3O_9. Bond energies of oxygen involved in $Mo_xO_y^+$ ion clusters were estimated.

AN INFORMATION MEASURING SYSTEM FOR THERMODESORPTION STUDIES

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Instrum. & Experim. Techniques, 45(1) (2002) pp. 50-54.

An information measuring system for studying surface phenomena by the thermodesorption technique is described. The temperature of the sample under study is controlled in a wide dynamic range (from 70 to 1500 K) in steps of 0.06 K. The applicability of the proposed algorithm to the control of the sample temperature in the process of temperature-programmed desorption is demonstrated. A technique for determining the parameters of the control law is described.

ADSORPTION OF NITROGEN, OXYGEN, AND ARGON VAPORS ON SUPERMICROPOROUS OXIDES

V.Yu. Gavrilov

Kinetics & Catalysis, 43(4) (2002) pp. 580-584.

The adsorption of N_2, O_2, and Ar vapors on a number of supermicroporous tin dioxide and zirconia xerogels at 77.4 K was studied. The micropore volumes calculated with the use of sorbate densities at the corresponding temperature were found to be in satisfactory agreement for all of the sorbates. At the same time, the volumes of larger pores measured using nitrogen were greater than the values found with other sorbates. The previously found behavior of oxygen and nitrogen molecules in the geometrically restricted space of supermicropores was substantiated. In particular, this behavior manifests itself in a change in the adsorption properties of a unit surface area of supermicropores as compared with the surface of mesopores. However, the effects of this kind were not found for the argon–nitrogen sorbate pair.

CHEMICAL INHOMOGENEITY IN MATERIALS WITH f-ELEMENTS: OBSERVATION AND INTERPRETATION

I.G. Vasilyeva

J. Alloys & Compounds, 323-324 (2001) pp. 34-38.

Novel possibility to control local chemical inhomogeneities, acting on functional properties of materials, appeared due to the differential dissolution (DD) technique. A series of materials, such as thin films ZnS·EuS/Si and $YBa_2Cu_3O_x$/sapphire, crystals $TmBa_2Cu_3O_x \cdot CaO$, powders γ-$Ce_2S_3 \cdot Na_2S$ and $LaFeO_3 \cdot CaO$ have been analyzed and the DD patterns with different profiles of kinetic curves of elements dissolving and stoichiograms were collected. The origin of the local inhomogeneities was established by analysis of these profiles. The inhomogeneity manifested itself as separate phases, as spatial compositional nonuniformity of solid solutions, as the grain surface enriched by doping elements, as non-stoichiometry produced by undesired doping with the container or substrate elements. In all cases, the DD results were compared with those obtained by other assessment techniques.

ANALYSIS OF SURFACE LAYERS OF PARTICLES OF ATMOSPHERIC AEROSOLS OF EASTERN SIBERIA BY METHOD OF SECONDARY IONIC MASS-SPECTROMETRY

V.P. Ivanov, S.N. Trukhan, D.I. Kochubey, O.G. Netsvetaeva*, T.V. Khodzher* (*Limnological Institute, Irkutsk, Russia)

Chem. for Sustainable Devel., 10(4) (2002) pp. 593-600**.**

Element and phase composition of surface layers of particles of atmospheric aerosols (AA) (collected over Irkutsk, Listvyanka and Ulan-Ude regions) were analyzed by method of Secondary Ionic Mass-Spectrometry. It was established that erosion of alumosilicate soil is a source of atmospheric aerosols. The surface of AA is covered with adsorbed hydrocarbons, N-containing compounds and water and partly with organic particles 30 nm in size.

STUDY OF ATMOSPHERIC AEROSOLS BY X-RAY ABSORPTION SPECTROSCOPY USING SYNCHROTRON RADIATION

V.V. Kriventsov, A.N. Shmakov, V.P. Ivanov, S.N. Trukhan, D.I. Kochubey, O.G. Netsvetaeva*, T.V. Khodzher* (*Limnological Institute, Irkutsk, Russia)

Chem. for Sustainable Devel., 10(5) (2002) pp. 609-613.

Spectra of aerosols collected over the Lake Baikal region were studied using synchrotron radiation. It has been shown that phase composition of atmospheric aerosols and oxidation level of 3d-elements of these aerosols may be determined by methods of XANES and X-Ray absorption spectroscopy using synchrotron radiation.

PHYSICO-CHEMICAL STUDY ON THE STATE OF COBALT IN A PRECIPITATED COBALT-ALUMINUM OXIDE SYSTEM

A.A. Khassin, V.F. Anufrienko, V.V. Ikorskii, L.M. Plyasova, G.N. Kustova, T.V. Larina, I.Yu. Molina, V.N. Parmon

Phys. Chem. Chem. Phys., 17 (2002) pp. 4236-4243.

The evolution of Co–Al (1:1) hydroxycarbonate with a hydrotalcite-like structure during its consequent calcination in an inert gas flow and reduction in H_2 has been studied by means of X-ray diffraction, infrared spectroscopy, UV–VIS diffusive reflectance spectroscopy and magnetic susceptibility measurements. The oxidation of Co^{2+} species to Co^{3+} state during the calcination in the inert gas medium occurs simultaneously with the formation of a highly inverted anion-modified spinel-like structure. The samples reduced at 480°C and 620°C contain metallic cobalt particles. Ferromagnetic and paramagnetic contributions are distinguished and evaluated. The spontaneous magnetization of the sample reduced at 480°C increases monotonously with the temperature in the range of 78–300 K. The correlation of the results with earlier data on physico-chemical and catalytic properties has been discussed.

HIGH-TEMPERATURE XRD STUDIES OF THE PHASE TRANSFORMATIONS IN MnO_X-Al_2O_3 CATALYST FOR DEEP OXIDATION OF HYDROCARBONS

T.A. Krieger, S.V. Tsybulya, P.G. Tsyrulnikov

React. Kinet. & Catal. Lett., 75(1) (2002) pp. 141-146.

Dynamic transformations of MnO_x/Al_2O_3 catalysts for the high-temperature deep oxidation of hydrocarbons have been investigated by high-temperature *in situ* XRD. It is shown, that catalyst is a nanoheterogeneous system and that active manganese-alumina phase is a product of destruction of a $Mn_{3-x}Al_xO_4$ solid solution, which is in equilibrium at the synthesis temperature but metastable at lower temperatures.

STRUCTURE AND COMPOSITION OF THE ANIONIC CHLORIDE COMPLEXES OF COPPER(II) AS THE PRECURSORS OF CATALYSTS FOR C-Cl BOND METATHESIS

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Kinetics & Catalysis, 43(3) (2002) pp. 408-411.

The chloride complexes of copper(II) (catalysts or catalyst precursors for various reactions of halogenated hydrocarbons) were characterized using electron, EPR, and EXAFS spectroscopy. It was found that chlorocuprates occur as mononuclear ($[CuCl_4]^{2-}$), binuclear ($[Cu_2Cl_6]^{2-}$), and, probably, polynuclear species in chlorobenzene solutions. The Cu–Cl bond length in $[CuCl_4]^{2-}$ is 2.25 ±0.2 Å, which is close to the same values for crystalline tetrachlorocuprates. It was assumed that the chloride complexes of copper with counterions occur as globules in chlorobenzene.

STUDY OF THE SURFACE STRUCTURE OF NICKEL NANOPARTICLES CATALYZING FILAMENTARY CARBON GROWTH BY EXAFS: ADSORPTION OF PROBE MOLECULES

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Topics in Catalysis, 18(1) (2002) pp. 91-94.

This work is attempted to apply EXAFS technique using probe molecules for studying the surface of Ni catalysts for carbon production. It has been demonstrated that H_2Se is suitable for the probe molecule method. It was shown that (100) and (110) planes of the nanocrystals of nickel catalysts providing formation of filamentary carbon are mainly formed by one-layer height steps.

INVESTIGATION OF THE DISTORTION OF THE CRYSTAL LATTICE FOR HTSC MATERIAL OF $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.10}$ BY X-RAY DIFFRACTION, NEUTRON POWDER DIFFRACTION AND EXAFS-SPECTROSCOPY

S.G. Titova*, D.O. Shorikov*, I. Bryntse, V.F. Balakirev*, V.I. Voronin***, D.I. Kochubey, S.G. Nikitenko** (*Metallurgical Institute, Ekaterinburg, Russia; **University of Stockholm, Stockholm, Sweden; ***Institute of Metal Physics, Ekaterinburg, Russia)

Surface Investigation. X-Ray, Synchrotron and Neutron Techniques, 7 (2002) pp. 44-48.

Using high resolution X-Ray and Neutron Powder Diffraction it was shown for $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.10}$ compound, that at $T_o \sim T_c + 13$ K, T_c=127 K, copper and oxygen atoms belonging to "superconducting" CuO_2-planes, shift from their positions. This leads to a split of the CuO_2-layers. Below temperature T_o the decrease of the distortion is connected with development of superconducting fluctuations. EXAFS spectroscopy at temperatures 300, 140 and 110 K confirms appearance of such distortion in CuO_2-planes at T_o and their reduction below this point.

X-RAY DIFFRACTION AND EXAFS SPECTROSCOPY STUDY OF REACTIONS IN DIFFUSION-HARDENING ALLOYS ON THE BASE OF THE Cu-Ga SYSTEM

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Surface Investigation. X-Ray, Synchrotron and Neutron Techniques, 7 (2002) pp. 25-28.

Reaction of the formation of diffusion-hardening alloys on the base of the Cu-Ga system was studied by different structural methods with the application of synchrotron radiation from the VEPP-3 storage ring. It was shown, that complex of structural methods allows one to study this process in details.

APPLICATION OF MULTILAYER BIMIRROR MONOCHROMATOR FOR EXAFS SPECTROSCOPY OF FLUORIDE COMPOUNDS

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Surface Investigation: X-Ray, Synchrotron and Neutron Techniques, 1 (2002) pp. 63-66.

The possibility to use the W/Si multilayer mirrors as dispersion optical elements in order to obtain EXAFS spectra of light atoms in the soft X-ray range was studied. The EXAFS spectrum of cryolite (Na_3AlF_6) near fluorine K edge was measured and subsequent data processing was performed. The results obtained are in a good agreement to the well-known structural data of this compound. Thus, in spite of relatively low energy resolution the multilayer mirrors were shown to be used successfully in EXAFS spectroscopy of light elements starting with fluorine up to higher-Z elements.

SURFACE STRUCTURES IN THE SMSI STATE; Pd ON (1 × 2) RECONSTRUCTED $TiO_2(110)$

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J. Phys. Chem. B, 106(18) (2002) pp. 4688-4696.

Scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), and X-ray photoelectron spectroscopy (XPS) were used to investigate the thermal stability of Pd(111) islands and thin films on $TiO_2(110)$-(1×2). Two new nano-structures were observed to form on the surface of the Pd by annealing to 973 K. Atomic resolution STM images show a "pinwheel" super-structure. One domain has a $\begin{pmatrix}7 & 2\\ 5 & 7\end{pmatrix}$ unit cell with respect to the Pd(111) whereas the other domain has a $\begin{pmatrix}7 & 5\\ 2 & 7\end{pmatrix}$ unit cell. Coexisting with this phase is a structure consisting of zigzag rows that run along the close-packed directions of the Pd(111) islands. This has a rectangular unit cell incommensurate with both the substrate $TiO_2(110)$ and the Pd(111) islands. STM shows these two structures merge with no noticeable domain barriers or steps, suggesting a close relationship between the two. LEED shows several distinct, overlapping patterns that can be identified with the surface structures observed; TiO_2 (110)-(1 × 2), Pd(111)-(1 × 1), the hexagonal pinwheel structure, and the rectangular zigzag unit cell. XPS at normal and grazing emission show the encapsulating layer to be composed of TiO_x with Ti predominantly in $\sim 2^+$ or 3^+ oxidation states. The proposed models are structurally consistent with the LEED and STM data and have stoichiometries of TiO and $TiO_{1.4}$, chemically consistent with the XPS spectra. The STM images of the zigzag bear a strong similarity to structures seen for annealed Pt islands on $TiO_2(110)$-(1 × 1) and TiO_x supported on Pt(111), while the pinwheel structure is similar to annealed Cr on Pt(111).

THE STRUCTURE OF Si NANOCRYSTALS ON SiC

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J. Electron Micr., 50(4) (2001) pp. 311-319.

Si nanocrystals grown on cubic SiC have been characterized using high-resolution transmission electron microscopy. At lower temperatures nanocrystals grow in two different orientations, whereas at higher temperatures they grow in a single preferred orientation. The nanocrystals are shown to be unstrained; in some cases possibly due to the presence of a thin amorphous wetting layer.

DIRECT OBSERVATION OF DEFECT-MEDIATED CLUSTER NUCLEATION

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Nature Materials, 1(2) (2002) pp. 102-105.

Ion implantation is widely used to introduce electrically or optically active dopant atoms into semiconductor devices. At high concentrations, the dopants can cluster and ultimately form deactivating precipitates, but deliberate nanocrystal formation offers an approach to self-assembled device fabrication. However, there is very little understanding of the early stages of how these precipitates nucleate and grow, in no small part because it requires imaging an inhomogenous distribution of defects and dopant atoms buried inside the host material. The work demonstrates this, and addresses the long-standing question of whether the cluster nucleation is defect-mediated or spontaneous. Atomic-resolution illustrations are given for the chemically dissimilar cases of erbium and germanium implanted into silicon carbide. Whereas interstitial loops act as nucleation sites in both cases, the evolution of nanocrystals is strikingly different: Erbium is found to gather in lines, planes and finally three-dimensional precipitates, whereas germanium favours compact, three-dimensional structures.

HYDROXYAPATITES IN THE MAN BLOOD

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Surface Investigation. X-Ray, Synchrotron and Neutron Techniques, 7 (2002) pp. 72-76.

Two morphological types of hydroxyapatite (HAP) microcrystals in the solid residues of blood plasma and lymph were found by transition electron microscopy methods.

SYNTHETHIS AND CHARACTERIZATION OF THE Ti-DOPED NANOSTRUCTURAL V_2O_5

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Mater. Science & Engin. A., 343(1-2) (2002) pp. 8-12.

Using scanning and analytical transmission electron microscopies (TEM), the morphology and structure of nanostructurally assembled V_2O_5 doped with Ti has been studied. It was found that the bulk structure of the oxide particles crystallized in rod-like shape is of the V_2O_5 type whereas Ti atoms are located mainly on the thin surface layer of the rods. Such surface coating is nonuniform and contains up to 3 at.% of titanium. Modification of the oxide sample with titanium atoms seems to stabilize the V_2O_5 structure against electron beam irradiation.

THE STUDY OF $^1A_1 \Leftrightarrow ^5T_2$ SPIN TRANSITION IN $Fe_xNi_{1-x}(HTRZ)_3(NO_3)_2 \cdot H_2O$ (HTRZ = 1,2,4-TRIAZOLE)

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J. Struct. Chem., 43(4) (2002) pp. 649-656.

Solid phases of compositions $Fe_xNi_{1-x}(Htrz)_3(NO_3)_2 \times H_2O$ ($0.4 \le x \le 0.8$) and $Ni(Htrz)_3(NO_3)_2 \times H_2O$ are synthesized and characterized using magnetochemical and XRD techniques, electron and IR spectroscopies. The heterometal phases are characterized using the stoichiographic method of differentiating dissolution

(DD). Values for x are determined by two methods, *viz.* atomic adsorption and DD. Magnetochemical data show that the synthesized solid phases possess high-temperature spin transfer (ST) $^1A_1 \Leftrightarrow {}^5T_2$, which is preserved at $0,5 \le x \le 0,8$ but disappears at $x = 0.4$. ST is accompanied by thermochromism (color transfer rose ⇔ white for $0,6 \le x \le 1$ and rose ⇔ light lilac for $x = 0.5$). As x decreases, a decrease in the temperature of the direct (on heating, T_c) and reverse (on cooling, $T_c\downarrow$) transitions, a decrease of the hysteresis value (DT_c), as well as diffusion of ST are observed.

INFLUENCE OF CONSECUTIVE REDUCTION AND OXIDATION TREATMENT ON THE MAGNETIC PROPERTIES OF COPPER CHROMITE

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J. Struct. Chem., 43(2) (2002) pp. 274-278.

An influence of consecutive reduction and oxidation treatment of copper chromite on the magnetic properties has been studied by methods of magnetic susceptibility and low-temperature neutronography. The magnetic ordering with T_c=130 K has been shown to disappear upon copper chromite reduction in temperature region 453—643 K. The magnetic properties were not restored completely after reoxidation. Magnetic properties changes upon reduction and reoxidation agree with its structure changes.

NOISE-LIKE MAGNETIC RESONANCE FINE STRUCTURE FOR FERROMAGNETIC POWDERS: DIPOLE-DIPOLE INTERACTION EFFECTS

M.M. Yulikov, O.N. Martyanov, V.F. Yudanov

Appl. Magnetic Resonance, 23(1) (2002) pp. 105-112.

A noiselike fine structure of ferromagnetic resonance spectra in magnetic powders was investigated after ultrasonic treatment. Magnetic interactions between particles are proved to have an influence upon the fine structure formation. After decreasing dipole-dipole magnetic interactions in dilute suspension a special order appears in fine-structure spectra, which is generally the same for different systems.

FINE STRUCTURE OF FERROMAGNETIC-RESONANCE SPECTRA OF DISPERSE MAGNETS

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JETP Letters, 75(12) (2002) pp. 638-641.

The technique of ferromagnetic resonance (FMR) was used for the investigation of nickel powders dispersed in a diamagnetic solid matrix. The fine structure of FMR was studied, which was observed against a background of broad featureless FMR lines of conventional unoriented polycrystals. A model is suggested according to which the narrow lines observed appear in the FMR spectra because of jumplike changes in the resonance conditions caused by a sharp change in the magnetization of the sample due to a change in the external magnetic field. In contrast to the Barkhausen effect, the fine structure detected in the FMR spectra in this case is observed in stronger fields characteristic of the processes of magnetization rotation. It is shown that the physical origin of magnetization jumps in this case may be magnetic interparticle interactions as well as complex anisotropy of particles.

INFLUENCE OF OXYGEN NONSTOICHIOMETRY ON THE SPECTRAL PROPERTIES OF SOLID SOLUTIONS $LaNb_{2-2x}Ta_{2x}VO_{9-\delta}$ (x=0-0.4) AND $LaTa_{2-2x}Nb_{2x}VO_{9-\delta}$ (x=0-0.1)

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J. Solid State Chem., 167(1) (2002) pp. 73-79.

Phase equilibria in the $LaVO_4$-Nb_2O_5-Ta_2O_5 system were analyzed. New solid solutions $LaTa_{2-2x}Nb_{2x}VO_{9-\delta}$ (x=0-0.1) and $LaNb_{2-2x}Ta_{2x}VO_{9-\delta}$ (x=0-0.4) were detected in this system. The structures of the vanadate-niobate $LaNb_2VO_9$ and vanadate-tantalate $LaTa_2VO_9$ are not known. The structures of the vanadate-tantalate $LaTa_2VO_9$ and $LaTa_2VO_9$-based solid solutions are similar to the structure of $LaTa_7O_{19}$, which refers to the hexagonal crystal system. The influence of the oxygen nonstoichiometry $\delta(x)$ on crystallochemical characteristics and spectral properties of these solid solutions were examined by the X-ray phase analysis, IR and radio spectroscopic methods. A correlation between the nonstoichiometry $\delta(x)$ and the volume of a unit cell

$V(x)$ of solid solutions $LaTa_{2-2x}Nb_{2x}VO_{9-\delta}$ was found. The IR spectrum of $LaTa_2VO_{9-\delta}$ transformed in going from $\delta = 0$ to $\delta \neq 0$. Two types of VO_4 tetrahedra were formed in solid solutions $LaNb_{2-2x}Ta_{2x}VO_{9-\delta}$ depending on $\delta(x)$.

TEST OF AEROGEL COUNTERS FOR THE KEDR DETECTOR

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Nucl. Instrum. & Methods in Phys. Res. A, 478(1-2) (2002) pp. 353-356.

The project of Cherenkov counters based on Aerogel, wavelength SHIfter, and PHotomultipliers (ASHIPH) for the KEDR detector is described. The quality of particle identification with the ASHIPH counters has been measured for the first time. Tests have been carried out at the Dubna accelerator. For a momentum of 1.2GeV/c, the p/K separation is 4.5s. In comparison with direct light collection on PMTs, the ASHIPH method allows to diminish the number of PMTs essentially.

NUCLEATION RATE SURFACE TOPOLOGIES FOR BINARY SYSTEMS

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J. Phys. Chem. B, 105(47) (2001) pp. 11817-11822.

Recent experiments have found that two nucleation rate surfaces can be observed for two different critical embryo phases (solid and liquid) near the triple point of the condensing species. Direct experimental evidence was presented of the existence of two independent nucleation rate surfaces with one of them existed over metastable vapor-liquid-phase equilibrium lines. These results force more careful consideration of the role of metastable phase equilibria in the topology of nucleation rate surfaces. In the present study, the topology of the nucleation rate surface for a binary vapor in which partial solubility of the condensed components is considered. Schematic multiple surfaces over the phase diagram with a eutectic point, presenting two-channel nucleation, are constructed. Vapor-liquid nucleation in a carrier gas in most cases is a binary system with partial solubility of condensate. It is reasonable to propose that multiple nucleation rate surfaces are common phenomena for many systems. Sulfur hexafluoride-*n*-pentanol nucleation was experimentally studied using a flow diffusion chamber. The experimental results for *n*-pentanol-sulfur hexafluoride at total pressures of 0.10, 0.20, and 0.30 MPa are presented. All experimental conditions were recalculated to correspond to a nucleation temperature of 255.0 K. The observed convoluted lines of $\ln J$ plotted against $\ln S$ provide experimental evidence of the existence of multiple nucleation rate surfaces. It can be anticipated that a variety of multiple nucleation rate surfaces, such as presented here, will be detected soon. Obviously, the application of one-component nucleation theory for such systems with multiple nucleation rate surfaces will not be consistent with the data. Separation of the multiple nucleation surfaces reduces the problem to a simpler one-channel treatment of nucleation. It will then be possible to construct a consistent nucleation theory for a given series of compounds.

STOICHIOGRAPHIC METHODS IN THE ANALYSIS OF SUBSTANCES OF UNKNOWN COMPOSITION

V.V. Malakhov

J. Analyt. Chem., 57(10) (2002) pp. 869-874.

A hierarchic structure of concepts of the chemical composition of substances, including substances of unknown composition, was proposed on the basis of physicochemical criteria. The latest achievements in the theory and practice of standardless stoichiographic methods for determining the molecular composition of substances (differentiating dissolution and ion chromatography) were considered.

STOICHIOGRAPHY: NEW WAYS FOR DETERMINING CHEMICAL COMPOSITION AND REAL STRUCTURE OF MATERIALS

V.V. Malakhov

Eurasian ChemTech J., 3(3) (2001) pp. 141-155.

The principles of stoichiography and novel reference-free methods of molecular and phase analysis for complex unknown mixtures are considered. The stoichiography can be inferred from stoichiometry of mass transfer of unsteady homo- and heterophase processes and joins both operations:

separation of mixture by means of chromatography, electromigration, dissolution or others and determination of stoichiometry of a substance flow with time. The stoichiography allows a chemical compound to be determined by its primary property, namely, by stoichiometry of elemental composition. Stoichiograms provided a basis for such type of information. They are time variances of molar ratio for mass transfer rates of chemical elements from multielement substances. Invariancy to concentration and temperature of solvents, hydrodynamic regime is a fundamental property of the stoichiograms in the case of individual compounds. Therefore the stoichiograms are kept constant and are equal to formula stoichiometric coefficients of the individual compound. Theory and methodology of new stoichiographic methods, differential dissolution and ion-chromato-stoichiography are presented. New equipment, stoichiograph, and a new procedure of differential dissolution, stoichiographic titration, are discussed here in details. Applications of differential dissolution to analyze multielement and polyphase crystalline and amorphous samples are given.

STUDY OF PHASE COMPOSITION OF ATMOSPHERIC AEROSOLS BY STANDARD-FREE STOICHIOGRAPHIC METHOD OF DIFFERENTIAL DISSOLUTION

V.V. Malakhov, A.A. Vlasov, L.S. Dovlitova

Chem. for Sustainable Devel., 10(5) (2002)
pp. 643-650.

The standard-free stoichiographic method of differential dissolution (DD) was used for studying stoichiometric and quantitative composition of solid phases, including phases of variable composition, of multiphase multielement atmospheric aerosols. Contents of water-soluble phases of a number of metals (presumably, metal hydroxosulfates), of the individual phase of calcium (presumably, calcium carbonate), of the phase of calcium sulfate and two phases of aluminosilicates were determined in the aerosol sample coughed by a filter in one of the Novosibirsk regions. Contents of a number of impurity elements were determined in these phases formed by main elements constituting the aerosols (Si, S, Al, Fe, Mg, Ca, K, Na). In the phases formed by the main aerosol constituents, Mg and Ca, and Sr and Ba microelements, the qualitative ratios of all these elements was determined with the groups of earth metal (Mg, Ca, Sr and Ba) as an example. It was concluded that the possibility of acquiring intimate quantitative data on the phase composition of the aerosols is of vital importance for studying various aspects related both to the mechanisms of generation and evolution of atmospheric aerosols and to their influence on the environmental state.

ULTRAFAST GAS CHROMATOGRAPHY

V.N. Sidelnikov, Y.V. Patrushev, V.N. Parmon

"Principles and Method for Accelerated Catalyst Design and Testing",
NATO Science Series. Kluwer Academic Publishers.
Mathematics, Physics and Chemistry,
69 (2002) pp. 257-275.

The paper discussed the ways of accelerating the chromatographic analysis based on GC run parameters as a carrier gas linear velocity, an elevation of the temperature or establishing a high rate of temperature programming. Another approach to high speed GC is based on short columns with a small diameter application. The last way results in necessity to apply extremely small amount of substance for separation. This condition appreciably reduces application of narrow bore column in chromatography. But loading opportunities of a column for high speed separations could be expended via using, instead of a single capillary, a batch of capillaries operating as a single chromatographic column – multicapillary (MCC). Further the reasons for peak broadening over MCC are discussed. The efficiency of such columns depends on the dispersion of the capillary radius and on the way of liquid phase loading. This efficiency can be improved by using the loading methods designed in order to take into account correlation between the film thickness and capillary radius.

Nature, Mechanism and Physicochemical Essence of the Environmentally Friendly Methods of Catalyst Preparation

AN ANOMALOUS EFFECT OF SILICA ON THE REDUCTION OF NICKEL NANOPARTICLES

M.A. Ermakova, D.Yu. Ermakov, L.M. Plyasova, G.G. Kuvshinov

Russ. J. Phys. Chem., 76(4) (2002) pp. 665-668.

The reduction of nickel–silica systems synthesized by the heterophase sol–gel method was studied over the entire concentration range. It was found that, as the silica content of the system is increased from 0 to 34 wt %, the reduction temperature increases, whereas the average size of nickel crystallites decreases from 44 to 5–6 nm. However, a further increase in the silica content produced an unexpected result: the reduction temperature decreased, whereas the average size of nickel crystallites increased to 15 nm.

MORPHOLOGY AND TEXTURE OF SILICA PREPARED BY SOL-GEL SYNTHESIS ON THE SURFACE OF FIBROUS CARBON MATERIALS

M.A. Ermakova, D.Yu. Ermakov, G.G. Kuvshinov

Kinetics & Catalysis, 43(3) (2002) pp. 427-432.

Silica materials are synthesized by the sol–gel method including the deposition of tetraethoxysilane on various micro- and nanocarbon fibers. The use of nanofibrous carbon as a template makes it possible to prepare thermally stable mesoporous SiO_2 samples with unusually high surface areas (up to 1255 m^2/g) and high porosity (up to 5.6 cm^3/g). These silica materials and aerogels prepared by supercritical drying have comparable pore volumes. It is found by high-resolution electron microscopy that a thin-wall matrix permeated by channels is a prevailing structure of silica materials. When some catalytic fibrous carbons are used as templates, silica nanotubes can be prepared.

A SOL-GEL DERIVED CuO_x/Al_2O_3-ZrO_2 CATALYST FOR THE SELECTIVE REDUCTION OF NO BY PROPANE IN THE PRESENCE OF EXCESS OXYGEN

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Catal. Lett., 78(1-4) (2002) pp. 111-114.

Copper catalysts supported on alumina-doped zirconia were prepared by sol-gel processing followed by supercritical drying or aging in the mother solution at 100°C. After drying and calcination, the catalyst supports were impregnated with a copper(II) nitrate aqueous solution by the incipient wetness method to achieve a Cu loading of about 2%. The samples showed ~ 90% NO conversion at 350-400°C. The catalytic performance of these systems appears to be determined by the degree of clustering of copper cations as probed by FTIR spectroscopy of adsorbed CO.

MECHANOCHEMICAL SYNTHESIS AND CATALYTIC PROPERTIES OF THE CALCIUM FERRITE $Ca_2Fe_2O_5$

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Kinetics & Catalysis, 43(1) (2002) pp. 122-128.

The formation of the real structure of calcium ferrite prepared by the calcination of a mechanochemically activated hydroxide mixture at 600–1100°C was studied by X-ray diffraction analysis, electron microscopy, thermal analysis, Moessbauer spectroscopy, IR spectroscopy, small-angle X-ray scattering, and secondary-ion mass spectrometry. It was found that low-temperature calcium ferrite is an anion-modified oxide, in which the ordering of oxygen vacancies was incomplete. Regions with a disordered structure were detected on the surface of crystallites. As the calcination temperature was increased, the brownmillerite crystal structure was improved and the intercrystalline boundaries were formed and then annealed. At the surface, these processes were accompanied by a change in the predominant form of adsorbed NO from nitrosyl to dinitrosyl species. An increase in the specific catalytic activity of samples with calcination temperature can be associated with the perfection of the brownmillerite structure and with a change in the state of adsorption centers.

PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF $La_{1-x}Ca_xFeO_{3-0.5x}$ PEROVSKITES PREPARED USING MECHANOCHEMICAL ACTIVATION

L.A. Isupova, S.V. Tsybulya, G.N. Kryukova, G.M. Alikina, N.N. Boldyreva, A.A. Vlasov, O.I. Snegurenko, V.P. Ivanov, V.N. Kolomiichuk, V.A. Sadykov

Kinetics & Catalysis, 43(1) (2002) pp. 129-138.

The phase composition of $La_{1-x}Ca_xFeO_{3-0.5x}$ perovskites synthesized from preactivated oxides was studied by powder X-ray diffraction analysis and differential dissolution. The system does not form a continuous series of homogeneous solid solutions. No intermediate samples from this series are monophasic. It was found that the synthesis under nonequilibrium conditions (mechanical activation + calcination at 900°C for 4h) resulted in nonequilibrium microheterogeneous solid solutions with degrees of calcium substitution for lanthanum of no higher than 0.5. A longer calcination (for 16 h) or an increase in the calcination temperature of solutions up to 1100°C decreased the calcium content of the samples down to $x \sim 0.2$ because of the formation of a brownmillerite phase. The catalytic activity of the test samples in the oxidation of CO changed nonmonotonically with x, and it was maximum at $x = 0.5–0.6$, which correlates with the maximum density of interphase boundaries in these samples.

MECHANOCHEMICAL SYNTHESIS OF PEROVSKITE DEEP OXIDATION CATALYSTS $La_{1-x}Ca_xFeO_{3-0.5x}$

L.A. Isupova, I.S. Yakovleva, S.V. Tsybulya, G.N. Kryukova, N.N. Boldyreva, A.A. Vlasov, V.A. Rogov, V.A. Sadykov

Chem. for Sustainable Devel., 10(1-2) (2002) pp. 27-38.

XRD, SIMS, BET, MDPD, TPR, and HREM were used to study the effect of time of mechanical treatment (MT) of the mixture of simple La_2O_3, CaO and Fe_2O_3 oxides and the temperature of subsequent calcination on the phase composition, real structure and catalytic properties of substituted $La_{1-x}Ca_xFeO_{3-0.5x}$ ($0 \leq x \leq 1$) perovskites in CO catalytic oxidation. The phase composition and microstructure of MT samples differ significantly from those of ceramic samples: no Grenier phase $La_{0.33}Ca_{0.67}FeO_{2.67}$ and micro-heterogeneous solid composite $La_{0.5}Ca_{0.5}FeO_{2.75}$ were found in ceramic samples; independently of the time of treatment and Ca content, the MT samples are composed of the perovskite and brown millerite phases. The microstructure of MT samples ($T_{calc}<1100°C$) is distinguished by disordered stacking of microblocks of those phases. An increase in the calcination temperature and MT time does not lead to an increase of the amount of ternary oxides and calcium content in solid solution. The microstructure of samples obtained by ceramic synthesis is suggested to arise due to decomposition of the high-temperature (1100°C) homogeneous solid solution during its cooling. By contrast, MT does not result in formation of such solution due to short time of thermal annealing. Specific catalytic activity of samples in the reaction of CO catalytic oxidation was found to correlate with the density of extended defects (inter-phase and inter-grain boundaries) and the amount of reactive oxygen easily removed by H2-TPR at middle (350-400 °C) temperatures.

THE USE OF MECHANICAL ACTIVATION IN MANUFACTURING RECHARGEABLE LITHIUM ACCUMULATORS

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Chem. for Sustainable Devel., 10(1-2) (2002) pp. 81-88.

Mechanical activation (MA) in high-energy planetary activators is used to prepare disperse and disordered cathode ($LiMn_2O_4$, $LiCoO_2$ and $Li_{1+x}V_3O_8$) and anode ($Li_4Ti_5O_{12}$) materials, as well as solid oxide electrolytes ($La_{0.67-x}Li_{3x}TiO_3$) for rechargeable lithium accumulators. The effect of various factors including mechanical and structural properties of initial reagents, oxidation degree of transition metal ions, etc., on mechano-chemical synthesis is investigated. The features of the crystal and electronic structure of the synthesized compounds are studied using different methods in comparison with the materials obtained by the traditional ceramic method.

DISORDERING AND ELECTRONIC STATE OF COBALT IONS IN MECHANOCHEMICALLY SYNTHESIZED $LiCoO_2$

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J. Solid State Chem., 165(1) (2002) pp. 56-64.

Mechanical activation (MA) combined with heat treatment at moderate temperatures was used to prepare disordered and highly dispersed $LiCoO_2$ starting from the mixtures of various cobalt precursors (CoOOH, $Co(OH)_2$, and Co) and LiOH. X-ray powder diffraction and IR spectroscopy were used to investigate the phase composition and the crystal structure of as-prepared samples, while the electronic state of cobalt ions was characterized by diffuse reflectance electron spectroscopy. MA of the LiOH+CoOOH mixture led to the formation of LT-$LiCoO_2$ with a cubic spinel-related structure. Heat treatment at 600°C of the latter resulted in the formation of HT-$LiCoO_2$ with a hexagonal layered structure similar to ceramic $LiCoO_2$. However, as-prepared HT-$LiCoO_2$ is characterized by $Co^{3+}O_6$ octahedra less perfect than those of ceramic $LiCoO_2$. All MA-$LiCoO_2$ samples are exclusively described by localized *d* electrons.

MECHANOCHEMICAL SYNTHESIS OF TANTALATES OF RARE EARTH METALS

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Chem. for Sustainable Devel., 10(1-2) (2002) pp. 141-146.

The investigation of phase composition in Y_2O_3-Ta_2O_5 and La_2O_3-Ta_2O_5 systems is carried out at mechanical activation and subsequent heat treatment. In Y_2O_3-Ta_2O_5 system the interaction of components is observed during mechanical activation. Heating of mechanically activated intermixtures of oxides leads to the formation of orthotantalates of yttrium and lanthanum. Temperature and time of complete interaction of components is much less than in a traditional ceramic method. The new convenient method of synthesis of tantalates of rare-earth metals is developed.

APPLICATION OF MECHANOCHEMICAL CATALYSIS TO THE SYNTHESIS OF BORIC ACID ESTERS

V.V. Molchanov, V.V. Goidin, A.V. Golovin,
Yu.B. Zolotovskaya, S.V. Bogdanov, A.M. Volodin

Kinetics & Catalysis, 43(4) (2002) pp. 536-541.

The syntheses of triisopropyl borate and other boric acid esters under conditions of mechanochemical activation with the use of zeolite catalysts were found to be highly efficient. The proposed method exhibits the following advantages over known methods: short synthesis times, low energy consumption, higher yields of target products, and the absence of byproducts. The mechanism of the catalytic esterification of boric acid under conditions of mechanochemical activation is discussed.

MECHANO-CHEMICAL REACTIONS AT HIGH PRESSURE OF THE GAS PHASE

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Chem. for Sustainable Devel., 10(1-2) (2002) pp.133-140.

It is demonstrated with many examples that conducting mechano-chemical reactions at increased pressure of the gas medium allows one to synthesize new compounds, to conduct catalytic reactions in solid, to find new more efficient routes for reactions, both in inorganic and in fine organic synthesis. At hydrogen pressure of 2-10 MPa, the hydrides of magnesium and intermetallic compounds are synthesized, including previously unknown hydride of the magnesium-copper intermetallide. At increased oxygen pressure, lower oxides of manganese are transformed into active manganese dioxide, which is efficient oxidizer for the processes of fine organic synthesis. Catalytic reactions are conducted under the conditions of mechanical activation at increased pressure of hydrogen, oxygen, and ammonia. Solid-phase hydrogenation of a series of organic compounds allows one to selectively reduce functional groups and unsaturated bonds. Hydro-dechlorination of toxic chlorinated aromatic compounds has been performed, including complete destruction of 1,2,3,4-tetrachlorodibenzo-p-dioxin. At increased oxygen pressure, oxidative transformations of ursolic acid are performed. At increased ammonia pressure, the amide of ursolic acid is obtained. At increased temperature and increased hydrogen pressure, hydro-alumination of heptene-1 and dihydromyrcene is performed, leading to the formation of the corresponding aluminum derivatives R_3Al.

APPLICATION OF MECHANOCHEMISTRY IN HYDROMETALLATION REACTIONS

A.I. Lukashevich, V.V. Molchanov, V.V. Goidin, R.A. Buyanov, G.A. Tolstikov

Chem. for Sustainable Devel., 10(1-2) (2002) pp. 109-112.

The mechanochemical method of active aluminium preparation was developed. Also technique of preparation of aluminiumorganic derivatives from unsaturated hydrocarbons is fulfilled. Possibility of realization of hydroalumination under the conditions of mechanochemical activation in drums of planetary mills was demonstrated for the first time. Butyllithium via reaction of a butenes mixture with a lithium hydride in conditions of a mechanochemical activation was synthesized.

SOME OPPORTUNITIES OF APPLYING MECHANOCHEMICAL METHODS IN FINE ORGANIC SYNTHESIS

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Catalysis in Industry, 6 (2002) pp. 2-14.

Opportunities of applying mechanochemical activation (MCA) to carry out reactions of fine organic synthesis (FOS) are shown. The works gives the results of determining a range of practically important reactions of FOS, which can be carried out under the MCA conditions over a catalyst. Taking caryophyllen-a-oxide, benzamide, n-nitrodiphenyl, and hexachlorobenzene as examples, opportunities of catalytic solid-phase hydrogenation of unsaturated bonds and functional groups are shown. A high efficiency of mechanochemical catalysis is demonstrated for reducing destruction of chlorinated dioxine. A new high-performance method of producing triisopropyl borate being favorably characterized by short duration and low energy consumption is found. Taking ursolic acid and betulin as an example, an opportunity is shown to involve insoluble and not readily soluble phytogenous compounds in the oxidation reactions, expanding the basis for chemistry and technology of processing renewable plant raw materials and disclosing a way to synthesis of new biologically active systems. For the first time, the mechanochemical reactions were carried out under the conditions of high pressure and elevated temperature, taking hydroaluminizing of dihydromyrcen and heptene-1 as examples. Examples are given where MCA is used for preparation of reagents used in FOS. Application of mechanical activation permits to produce highly-dispersed metals of high reactivity, mechanical aluminum alloys for carrying out hydroaluminizing reactions, magnesium intermetallide hydrides as effective reducing agents, and active manganese dioxide for oxidizing reactions.

SYNTHESIS OF FRAMEWORK COMPLEX ZIRCONIUM PHOSPHATES VIA MECHANOCHEMICAL ACTIVATION OF MIXED SOLID SALTS

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Chem. for Sustainable Devel., 10(1-2) (2002) pp. 179-186.

Results of systematic studies of framework zirconium phosphates synthesis via mechanical activation (MA) of the mixture of solid salts followed by the hydrothermal treatment (HTT) in the presence of surfactants, drying and calcination in air are considered. Application of modern physical methods sensitive to the state of bulk and surface of nano-systems (XPD, SAXS, TEM, EXAFS, FTIRS, SIMS, UV-vis) allowed to elucidate genesis of those complex systems containing different stabilizing/modifying cations and anions. The local structure of zirconium phosphate nuclei formed in the course of MA and spatial distribution of guest cations within those nanoparticles strongly depend on the composition of starting solid reagents, which determines a mode of the acid-base interaction in the activated mixture. These properties determine in turn realization of different mechanisms of complex framework phosphates crystallization under HTT - either via oriented stacking of primary particles (occurs even in neutral or alkaline solutions) or by dissolution-precipitation route in acid solutions. Factors determining the structural type, thermal stability, surface composition and solubility of crystalline complex zirconium phosphates prepared via MA route were elucidated and analyzed as dependent upon the composition and genesis of those systems.

HONEYCOMB-SUPPORTED PEROVSKITE CATALYSTS FOR HIGH-TEMPERATURE PROCESS

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A.N. Salanov, N.N. Boldyreva, E.S. Rusina,
I.A. Ovsyannikova, V.V. Rogov, R.V. Bunina,
V.A. Sadykov

Catal. Today, 75(1-4) (2002) pp. 305-315.

Pechini route [US Patent No. 3,330,697 (1967)] was used for supporting perovskite-like systems on thin-wall corundum honeycomb support to prepare catalysts for high-temperature processes of methane combustion and selective oxidation into syngas. In this preparation, the surface of corundum monoliths walls was shown to be covered by strongly adhering porous perovskite layer formed by rounded crystals. At high temperatures when pore diffusion is expected to affect catalysts performance in fast reactions, this spatial distribution of the active component could be attractive. In the kinetically controlled region of methane oxidation, samples prepared via Pechini route possess activity comparable with that of samples made via support wet impregnation with mixed nitrate solutions, when an active component is uniformly distributed across the wall thickness. Corundum-supported lanthanum manganite and ferrite are the most active in the reaction of methane combustion, while its selective oxidation into syngas effectively proceeds on supported lanthanum cobaltite and nickelates. Corundum-supported perovskites are more thermally stable as compared with those on γ-alumina support.

EFFECT OF THE CONDITIONS OF THERMAL TREATMENT OF MOLYBDENUM-TITANIUM AND VANADIUM-MOLYBDENUM-TITANIUM OXIDE CATALYSTS ON PORE STRUCTURE FORMATION

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S.V. Tsybulya, V.N. Parmon

Kinetics & Catalysis, 43(4) (2002) pp. 573-579.

The effect of the conditions of thermal treatment on the texture formation in molybdenum–titanium oxide (Mo–Ti–O) and vanadium–molybdenum–titanium oxide (V–Mo–Ti–O) catalysts was studied. It was found that the presence of MoO_3 in the Mo–Ti–O catalyst resulted in the stabilization of the surface area of anatase and in the retention of the fine pore structure upon thermal treatment because of the insertion of highly dispersed molybdenum crystallites into the aggregates of anatase crystallites, preventing from their agglomeration over a wide range of temperatures. In the presence of MoO_3 and V_2O_5 in the catalyst, anatase particles underwent agglomeration as the temperature was increased. This resulted in a more drastic decrease in the specific surface area and an increase in the pore size, as compared with binary samples, because of the formation of a thermally labile vanadium–molybdenum compound at the surface of anatase.

EFFECT OF THERMAL ACTIVATION OF SUPPORTED CATALYSTS Pt/MeO_x, WHERE $MO_x = Al_2O_3$, CeO_2, La_2O_3, AND ZrO_2, FOR COMPLETE OXIDATION

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Kinetics & Catalysis, 43(3) (2002) pp. 379-384.

A sharp increase in the atomic catalytic activity (ACA) of supported platinum catalysts in the model reaction of *n*-pentane complete oxidation is found on going from the preliminary calcination temperature of 500-600°C to a temperature of 700°C. ACA increases by an order of magnitude for the $Pt/\nu\text{-}Al_2O_3$ system, ~3 times for Pt/ZrO_2, and ~1.5 times for Pt/CeO_2. The per-gram activities of all catalysts decrease because of a decrease in the dispersion of supported platinum with an increase in the temperature of preliminary calcination.

PHASE TRANSFORMATION IN THE THERMOACTIVATED MnO_x-Al_2O_3 CATALYTIC SYSTEM

P.G. Tsyrulnikov, S.V. Tsybulya, G.N. Kryukova, A.I. Boronin, S.V. Koshcheev, T.G. Starostina, A.V. Bubnov, E.N. Kudrya

J. Molec. Catal. A: Chemical, 179(1-2) (2002) pp. 213-220.

The phenomenon of the sharp increase of activity in reactions of deep oxidation found for the manganese oxide–alumina system calcined at 900–1000°C was named as thermoactivation effect. This effect was shown to be associated with phase transformations in this system. Peculiarities of phase transformations in the MnO_x/Al_2O_3 system after its calcination at 950°C for 1–10 h were studied with XRD, TEM, XPS methods; the catalysts activity in deep oxidation of *n*-pentane was measured in a flow-circuit setup. It was found that a set of phase transformations occurred in the system, starting from the formation of the metastable nonstoichiometric manganese–alumina cubic spinel (after 1–2 h calcination) and nonequilibrium solid solution of Mn^{3+} ions in the structure of γ-Al_2O_3 which decomposes producing high-temperature aluminas modified by manganese ions and particles of imperfect β-Mn_3O_4 phase doped with aluminium ions. Increase of the calcination time to 10 h and more results in the formation of biphasic system composed of α-Al_2O_3 and nanocrystalline β-Mn_3O_4 modified by Al^{3+} ions. These transformations are associated with the maximum activity showed by catalysts calcined for 5-6 h in the reaction of *n*-pentane combustion.

COPPER REINFORCED CATALYSTS ON A HEAT-EXCHANGE SURFACE FOR NITROBENZENE HYDROGENATION TO ANILINE

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Kinetics & Catalysis, 43(6) (2002) pp. 830-837.

The methods of X-ray diffraction, mercury porosimetry, and electron microscopy are used to study the texture and phase composition of nickel–aluminum supports obtained by the sintering of nickel and aluminum powders reinforced by a stainless steel grid and distributed over a heat-exchange surface, as well as copper catalysts for nitrobenzene hydrogenation to aniline supported on these materials. The catalysts prepared using this procedure are active in this reaction and make it possible to carry it out without substantial overheatings of the surface.

SYNTHESIS AND PROPERTIES OF HIGHLY POROUS $MeO_x/Al_2O_3/Al$ COMPOSITES (Me=Mg, Ca, La, Ti, Al)

S.F. Tikhov, Yu.V. Potapova , V.A. Sadykov, A.N. Salanov, S.V. Tsybulya, G.S. Litvak, L.F. Melgunova

React. Kinet. & Catal. Lett., 77(2) (2002) pp. 267-275.

The influence of various oxide additives, such as CaO, MgO, La_2O_3, TiO_2, and alumina on the reactivity of aluminium particles during their hydrothermal oxidation as well as on the thermal decomposition of hydroxides during the composite preparation has been studied. For some promoters, these additives were found to affect the crushing strength of composite granules and their microporous structure.

SULFIDE CATALYSTS SUPPORTED ON Al_2O_3. VI. SYNTHESIS OF CATALYSTS WITH THE USE OF BINUCLEAR MOLYBDENUM(V) COMPLEXES WITH SULFUR-CONTAINING LIGANDS

Yu.M. Serebrennikova, M.A. Fedotov, S.G. Nikitenko, D.I. Kochubey, A.N. Startsev

Kinetics & Catalysis, 43(4) (2002) pp. 585-591.

A new method was developed for the preparation of sulfide catalysts supported on aluminum oxide. The surface assembling of a direct precursor of the active component was used in this method. The method consists in the sequential immobilization of binuclear molybdenum complexes with S-containing ligands on the support surface followed by the immobilization of nickel (cobalt) compounds at the surface molybdenum complexes. The complexation and structure of the resulting complexes in solution and the structure of surface complexes were studied by ^{95}Mo and ^{17}O NMR, IR, and EXAFS spectroscopy. The surface assembling of a direct precursor of the active component of sulfide hydrodesulfurization catalysts was demonstrated using IR and EXAFS spectroscopy. The activity of the resulting catalysts in a model reaction of thiophene hydrogenolysis was comparable to the activity of sulfide catalysts of the metal complex origin and was much higher than the activity of commercial catalysts and catalysts prepared by impregnation.

SYNTHESIS OF Fe/C NANOCOMPOSITES UPON ARC-HEATED DECOMPOSITION OF IRON PENTACARBONYL

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Chem. for Sustainable Devel., 10(6) (2002) pp. 781-788.

Fibrous material consisting of filamentous crystals of iron carbide is synthesized.

FORMATION OF POROUS VERMICULITE STRUCTURE IN THE COURSE OF SWELLING

L.G. Gordeeva, E.M. Moroz, N.A. Rudina, Yu.I. Aristov

Russ. J. Appl. Chem., 75(3) (2002) pp. 357-361.

The effect of swelling conditions on the vermiculite pore structure was studied by X-ray diffraction analysis, mercury porosimetry, and scanning electron microscopy. The closed porosity of the samples was estimated. A possibility for purposeful modification of vermiculite pore structure by varying the swelling temperature and heating rate was evaluated.

THE STRUCTURE OF OXIDE Ga-Sb-Ni-P-W-O/SiO$_2$ CATALYST AND ITS CATALYTIC PROPERTIES IN PROPANE AMMOXIDATION

G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya, V.F. Anufrienko, T.V. Larina, E.B. Burgina

Kinetics & Catalysis, 43(3) (2002) pp. 384-390.

The structure of the multicomponent catalyst $Ga_1Ni_1P_2W_{0.5}Sb_6O_x/SiO_2$ and its catalytic properties in propane ammoxidation are studied. The catalyst is nanostructured and consists of noncoherently spliced blocks of a multiply promoted phase with a structure of gallium antimonate, which covers SiO_2 particles with a thin layer. In the multiply promoted compound with a structure of gallium antimonate, Ni^{2+} ions partially substitute for Ga^{3+} and W^{6+} ions partially substitute for Sb^{5+}. This leads to an increase in the crystalline lattice parameters a and c. Phosphate ions are stabilized in the region of block interfaces. The catalyst is characterized by high efficiency in propane ammoxidation.

PROMOTING EFFECT OF GOLD ON THE STRUCTURE AND ACTIVITY OF Co/KAOLIN CATALYST FOR THE 2,3-DIHYDROFURAN SYNTHESIS

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Catal. Commun., 3(8) (2002) pp. 341-347.

The promoting effect of gold and the influence of the thermal pretreatment of the cobalt/kaolin catalysts on the reducibility, catalytic activity and selectivity has been studied. The catalytic properties were tested in the cyclodehydration of 1,4-butanediol. The gold-promoted catalysts are more selective than their non-promoted analogues. The modification by gold leads to the formation of new cobalt species, being reducible at significantly lower temperatures in comparison to those of the non-promoted catalysts. This effect of gold results not only on the dispersion, but also on the structure of the metallic cobalt phases.

STRUCTURE OF A PLATINUM-ALUMINA CATALYST PREPARED FROM THE CARBONYL CLUSTER $H_2[Pt_3(CO)_6]_5$

D.I. Kochubey, N.B. Shitova, S.G. Nikitenko

Kinetics & Catalysis, 43(4) (2002) pp. 555-560.

The state of a platinum carbonyl cluster in an initial aqueous acetone solution and its transformations on the surface of aluminum oxide in the course of catalyst preparation were studied by EXAFS spectroscopy. It was found that water enters the polynuclear framework of the dissolved cluster (the Pt–O distance is 2.55 Å, where O is the oxygen atom of water). Structural changes in the supported cluster in the course of catalyst preparation exhibited a strong interaction of platinum with alumina (the Pt–O distance is 1.92–1.95 Å), beginning at the step of $H_2[Pt_3(CO)_6]_5$ adsorption. This interaction was retained upon the subsequent high-temperature treatments of the catalyst. The structures of samples prepared from platinum carbonyl and chloroplatinic acid were significantly different. In the former case, a surface prototype was formed from the initial cluster; in the latter case, the sample consisted of platinum metal clusters of a considerable size.

STRUCTURE OF MoS_2-BASED CATALYSTS FOR HYDRODESULFURIZATION PREPARED VIA EXFOLIATION

D.I. Kochubey, V.P. Babenko

React. Kinet. & Catal. Lett., 77(2) (2002) pp. 237-243.

The structure distortions of the bend type are shown to be a reason of the lower coordination numbers for the MoS_2 based catalysts for hydrodesulfurization.

STRUCTURAL ARRANGEMENT OF Fe-Sb-O CATALYSTS

G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya

Kinetics & Catalysis, 43(5) (2002) pp. 698-710.

In iron–antimony catalysts containing excess antimony oxide and consisting of a mixture of $FeSbO_4$ and α-Sb_2O_4 phases, the structure of iron antimonate changes compared to the catalyst with an equimolar composition, which is the pure $FeSbO_4$ phase. In the presence of excess antimony oxide in the near-surface layer of iron antimonate, extended defects with a structure of crystallographic shift are formed. These accumulate overstoichiometric antimony. Such a structural change is associated with changes in the acid–base properties and the surface oxygen binding strength.

ELECTRON-BEAM MODIFICATION OF THE SURFACE OF OXIDE MATERIALS (SiO_2 AND $BaTiO_3$)

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St. Petersburg, Russia)

Russ. J. Phys. Chem., 76(1) (2002) pp. 71-76.

Variations in the functional composition under the action of accelerated electrons was analyzed for the surface of oxide materials (A-175 Aerosil and barium titanate). The dependence of the content of Lewis and Broensted sites and their mutual conversion on the absorbed dose exhibit extremal behavior. The mechanisms of the variation of the functional composition of the surface were established to be related to the following rearrangements of the surface layer structure under the action of increasing absorbed dose. At doses below 100 kGy, the physically sorbed molecules of water dissociate into radicals and react with siloxane groups to form hydroxyls. At higher doses, a dehydration of the surface occurs. Electron-beam processing was demonstrated to be a promising method for controlled modification of the surface of oxides.

DISPERSING EFFECTS ON THE DONOR-ACCEPTOR PROPERTIES OF THE SURFACE OF FERROELECTRICS

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Russ. J. Phys. Chem., 76(9) (2002) pp. 1472-1476.

The distributions of donor–acceptor centers on the surface of dispersed barium titanate and a VS-1 ceramic material based on barium titanate and distribution changes after treatment with a dispersing agent and during dispersion were studied by adsorption of acid–base indicators. The obtained data can be used to rationally select the type of dispersing agents and determine the nature of interphase interactions during dispersion.

MODIFICATION OF MELAMINE-FORMALDEHYDE OLIGOMERS WITH ACRYLAMIDE

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Plolymer. Sci., ser. A, 44(12) (2002) pp. 1235-1239.

Reactions occurring in melamine–formaldehyde–acrylamide systems in weakly alkaline (pH 8) and weakly acidic (pH 6) media were studied. Possible mechanisms for the incorporation of acrylamide fragments into the melamine–formaldehyde oligomers were considered. It was shown that the addition of acrylamide units to melamine–formaldehyde oligomers proceeds via two stages: the formation of the methylol derivative of melamine and the interaction of acrylamide with methylol groups. This sequence of reactions can be realized only in acidic media.

COMPOUND LATEXES FOR ANTISTATIC COATINGS

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Russ. J. Appl. Chem., 75(10) (2002) pp. 1705-1708.

Compound latexes based on amine-containing styrene-acrylate copolymers and hollow particles of a polystyrene-based copolymer as a filler were studied. With this filler, it is possible to prepare antistatic pigmented coatings with increased surface hardness, decreased density, and surface resistivity ρ_s of the order of 10^8 Ω.

PREPARATION OF NANOCOMPOSITES BY ALKOXYSILANE HYDROLYSIS IN A POLYPROPYLENE MATRIX

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S.Ya. Khaikin, A. Hesse*, S.V. Myakin (*Borealis AG, Linz, Austria)

Polymer Sci., ser. A, 44(6) (2002) pp. 623-627.

Conditions for the formation of 20- to 100-nm silica or siloxane particles in PP by the hydrolysis of different alkylsilanes directly in a polymer matrix were determined. It was shown that the process could be performed both in a granulated PP and during its melt extrusion. Under certain processing conditions, the resulting nanocomposites were found to exhibit higher stiffness, impact strength, and transparency as compared to the initial PP. This improvement of the material properties is due to the structuring effect of nanoparticles formed by hydrolysis.

CATALYSTS AND THE PROGRESS OF POLYOLEFINE PRODUCTION PROCESSES

S.S. Ivanchev

Catalysis in Industry, 6 (2002) pp. 15-26.

The main stages of development and improvement of different generation of catalysts for olefine polymerization and concerned variants of technology and hardware implementation at the industrial production of polyolefines are analyzed taking possible regulation of assortment and possible application into account. Realization of polymerization (suspension, solution, gas-phase) process presents particular demands to the structure and properties of used polymerization catalysts and it is tied in with optimal variants of application of the polymers produced. The latest achievements in the field of development of new catalytic systems on the basis of metallocenes and postmetallocenes systems are briefly considered. The analysis made illustrates that the catalytic systems are a key for improvement of the structure and operational properties of polyolefines and realization of polymerization process.

THE ROLE OF SURFACTANTS IN THE FORMATION OF HIGHLY DISPERSED IRON-ZIRCONIUM OXIDE COMPOSITES WITH UNIFORM PORES

A.S. Ivanova, M.A. Fedotov, G.S. Litvak,
S.N. Trukhan, V.P. Ivanov

Kinetics & Catalysis, 43(1) (2002) pp. 139-145.

The effects of the nature and concentration of surfactants and the preparation conditions on the genesis of iron–zirconium composites with a $[Fe^{3+}]/[Zr^{4+}]$ ratio of 0.123 were studied. The effect of surfactants on the physicochemical properties of precipitates is determined by the conditions of synthesis. The amount of surfactants retained by the precipitate at pH ~ 3 is about an order of magnitude greater than at pH ~ 9. The thermolysis of samples synthesized at acidic pH is accompanied by the dehydration and dehydroxylation of iron–zirconium composites as well as by the decomposition and destruction of surfactants. In the latter processes, compounds or their fragments capable of reducing some phases are removed in a stepped-up manner. The specific surface area of oxide systems formed in this way is at most 100–150 m^2/g. In the pH range corresponding to the complete precipitation of the components, highly dispersed single-phase and uniformly porous composites are formed. The choice of a surfactant, its fraction, and preparation conditions enables the preparation of oxides with specific surface areas of 100–400 m^2/g. The average pore diameter of the samples ranges from 3.0 to 27.0 nm, and the total pore volume ranges from 0.20 to 0.38 cm^3/g.

NANOCRYSTALLINE MgO AS A DEHYDROHALOGENATION CATALYST

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V.V. Chesnokov, A.M. Volodin, V.I. Zaikovskii,
R.A. Buyanov, K.I. Klabunde* (*Kansas State University, Manhattan, USA)

J. Catal., 206(1) (2002) pp. 40-48.

Nanocrystalline MgO has been found to be an efficient dehydrohalogenation catalyst. Its reaction with different chlorobutane isomers or 1-bromobutane results in topochemical transformation of the MgO phase to $MgCl_2$ or $MgBr_2$ accompanied by a sharp decrease in the catalyst surface area and increase in its activity. The resulting magnesium chloride and magnesium bromide are very active catalysts for HCl and HBr elimination from halogenated hydrocarbons. The reaction mechanism changes from predominantly E2 elimination on MgO to mostly E1 elimination over $MgCl_2$ and $MgBr_2$, which act as Lewis acids. It was also found that

$MgBr_2$ could be completely converted back to MgO by calcination in oxygen at 500°C degrees while $MgCl_2$ oxidation did not occur under similar conditions.

ROLE OF ACID SITES IN FORMATION OF SUPPORTED METALLOCENE-BASED CATALYSTS FOR OLEFIN POLYMERIZATION

N.V. Semikolenova, V.N. Panchenko, I.G. Danilova, E.A. Paukshtis, L.G. Echevskaya, E.P. Talsi, V.A. Zakharov

Mendeleev Chemistry J., XLV(4) (2001) pp. 68-74.

The work summarizes data on generation of active component of supported metallocene catalysts and its reaction ability. The acid centers of methylalumoxane (MAO) and other cocatalysts, and their effect on the catalytic activity of metallocene systems have been studied.

The data obtained show that difference in the acid centers nature of the supports (MAO and $MgCl_2$) results in the formation of active centers of different types in supported catalysts SiO_2/MAO/zirconocene и $MgCl_2$/zirconocene. The results obtained may serve as a base for purposeful synthesis of highly active supported metallocene-based catalysts, prospective for production of polymers with predetermined properties.

Studies on Kinetics and Mechanism of Catalytic Reactions

KINETIC PECULIARITIES IN THE LOW-TEMPERATURE OXIDATION OF H_2S OVER VANADIUM CATALYSTS

P.N. Kalinkin, O.N. Kovalenko, O.B. Lapina, D.F. Khabibulin, N.N. Kundo

J. Molec. Catal. A: Chemical, 178(1-2) (2002) pp. 173-180.

H_2S oxidation by oxygen over V_2O_5/Al_2O_3, V_2O_5/TiO_2, V_2O_5/SiO_2, $V_2O_5/Al_2O_3/TiO_2$ catalysts was studied at the temperature below the sulfur dew-point. High activity and the oscillation nature of the oxidation process were demonstrated for the catalysts with low V_2O_5 contents (2–5 wt.%) supported on Al_2O_3, TiO_2 or a combination thereof. An increase in the V_2O_5 concentration up to 10–20 wt.% resulted in lowering of the catalytic activity and oscillation ability. The oscillations were not determined using V_2O_5/SiO_2 and pure V_2O_5 catalysts. Difference between pure V_2O_5, catalysts with high- and low-loaded V_2O_5 catalysts was accounted for by the structure of V^{5+} species formed in catalysts. The high activity of the catalysts with the low vanadium content supported on Al_2O_3, TiO_2 or combinations thereof was attributed to vanadium species bound directly to the surface.

REACTION KINETICS OF 2-PROPANOL DEHYDRATION IN SUPERCRITICAL WATER

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Kinetics & Catalysis, 43(2) (2002) pp. 189-194.

A study of the kinetics and mechanism of chemical reactions in supercritical fluids is considered. An experimental procedure was proposed for examining reversible chemical reactions in supercritical water. The reaction kinetics of 2-propanol dehydration in supercritical water was studied. It was found that the uncatalyzed reactions of olefin hydrogenation by hydrogen dissolved in supercritical water occur at high rates near the critical point of water. The experimental data on the dehydration of 2-propanol in supercritical water are adequately described by first-order reaction rate equations. The rate constants and activation energies of 2-propanol dehydration near the critical point of supercritical water were found.

KINETIC EVIDENCE FOR THE IDENTICAL NATURE OF ACTIVE CENTERS FOR PARTIAL AND DEEP OXIDATION OF ETHYLENE ON SILVER

A.V. Khasin

React. Kinet. & Catal. Lett., 76(2) (2002) pp. 327-334.

Kinetics of interaction of ethylene with pre-adsorbed oxygen on a silver film was studied at 473 K and different initial values of surface coverage with oxygen. Dependencies of the initial rates of partial and deep ethylene oxidation on the oxygen surface coverage manifest themselves as peaked curves with coinciding maxima. The results are considered as evidence that the processes of partial and deep ethylene oxidation on silver, when they occur at optimal conditions, proceed *via* identical active centers.

THEORETICAL CONCEPT OF NONBRANCHED RADICAL-CHAIN REACTIONS INVOLVING CATALYSTS

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Kinetics & Catalysis, 43(2) (2002)
pp. 170-174.

The foundations of the theoretical concept of nonbranched radical-chain reactions involving heterogeneous catalysts are considered for hydrocarbon pyrolysis. These include the phenomenological model and the concept of the "catalysis sphere." Surface active sites S participate in chain propagation along with hydrocarbon radicals from the gas phase. Surfaces show either inhibiting or neutral action depending on the $E_{S\text{-}R}$ bond energy. If the $E_{S\text{-}R}$ value is comparable with the energy of the breaking bond in the reacting molecule, the reaction accelerates due to the acceleration of either the heterogeneous or homogeneous component of the overall rate of the process. In the latter case, the catalyst ensures the generation of additional radicals for the gas phase, which result in the formation of a catalysis sphere. The catalysis sphere is defined, the radical distribution in it is presented, and its properties and role in radical-chain processes are discussed.

SIMULATIONS OF THE REACTION KINETICS ON nm SUPPORTED CATALYST PARTICLES

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Catalysis at Nanoparticle Surfaces,
Eds. A. Wieckowski et al., Marcel Dekker, 2002,
pp. 31-45.

The reaction kinetics on supported nm-sized catalyst particles may be quite different compared to those observed on macroscopic poly- or single-crystal surfaces, because the very function of the catalyst is often affected by decreasing the particle size, due to inherent factors connected with the properties of small particles alone, or as a result of new kinetic effects arising on the nm scale. These proven or suspected differences between supported catalysts and macroscopic surfaces have long been recognized to be a central part of the so-called "structure-gap" and "pressure-gap" problems in catalysis. To bridge these gaps and to form a conceptual basis for the understanding of reactions occurring on supported catalysts, in the present review the results of simulations scrutinizing qualitatively new effects in the reaction kinetics on the nm scale is summarized. The attention is paid to such factors as reactant supply via the support, interplay of the reaction kinetics on different facets, adsorbate-induced reshaping of catalyst particles, selectivity on the nm scale, and oscillatory and chaotic kinetics on nm catalyst particles. The kinetics of growth of nm particles is briefly discussed as well.

IMPACT OF SURFACE SCIENCE ON THE UNDERSTANDING OF KINETICS OF HETEROGENEOUS CATALYTIC REACTIONS

V.P. Zhdanov

Surf. Sci., 500(1-3) (2002) pp. 966-985.

The kinetics of chemical reactions in gas and liquid phases is usually described by employing the conventional mass-action law equations. The laws governing the kinetics of heterogeneous catalytic reactions are as a rule much more complex due to adsorbate-adsorbate lateral interactions, surface heterogeneity, spontaneous and adsorbate-induced changes in a surface, and/or limited mobility of reactants. The importance of these factors was recognized by the heterogeneous catalysis community far before the surface science era. Only with the development of surface science, however, has it become possible to study in detail the non-ideality of rate processes on solid surfaces. In the present paper, the main conceptual results currently available in this field are summarized and the impact of surface science on its development is illustrated. Specifically, it is outlined the approaches used to describe elementary reaction steps and the whole reaction kinetics near and far from equilibrium, including such topics as kinetic phase transitions, pattern formation, kinetic oscillations and chaos, and pressure- and structure-gap problems. All these phenomena and problems are demonstrated to provide promising opportunities for further experimental and theoretical studies.

KINETIC ASPECTS OF THE STRUCTURE-GAP PROBLEM IN HETEROGENEOUS CATALYSIS

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Catal. Lett., 81(3-4) (2002) pp. 141-145.

Analyzing one of the possible schemes of the NO-CO reaction occurring on nm-sized supported Rh or Pd particles, it has been shown that, due to the purely kinetic effects related to the interplay of the reaction kinetics on the (111) and (100) 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. The dependence of the turnover reaction rate on the fraction of adsorption sites belonging to the (100) facet is found to exhibit a broad maximum at f= 0.4.

NANOFACET-RESOLVED CO OXIDATION KINETICS ON ALUMINA-SUPPORTED Pd PARTICLES

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Chem. Phys. Lett., 354(5-6) (2002) pp. 403-408.

Employing a multi-molecular-beam approach, the angular distribution of CO_2 molecules formed during CO oxidation under steady-state conditions on well oriented and shaped nm-sized Pd crystallites grown on an ordered alumina film have been measured. The experiment is combined with kinetic Monte Carlo simulations based on a realistic structural model. The results obtained allows (i) to differentiate between local reaction rates on the particle nanofacets and (ii) to conclude that oxygen diffusion on and between the (111) facets is rapid compared to reaction.

1,2-BIS(ARYLIMINO)ACENAPHTHYL NICKEL BROMIDE COMPLEXES AS CATALYSTS OF ETHYLENE POLYMERIZATION

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Polymer Sci., Ser. A., 44(9) (2002) pp. 931-935.

The kinetics of ethylene polymerization initiated by four novel methylaluminoxane-activated diimine $NiBr_2$ complexes bearing bulky cyclic substituents at the *o*-position of an aryl group was studied. The activity of the synthesized complexes in polymerization was determined in the temperature range from 4 to 70°C and an ethylene pressure of 0.3 MPa. The structure and thermal characteristics of the as-prepared polyethylene samples were estimated by FTIR spectroscopy and DSC. It was shown that, as the temperature increases, the rate of the process passes through a maximum whose position depends on the structure of the complex and temperature. Polyethylene synthesized at 0.3 MPa is characterized by the presence of short-chain branching containing from 3.5 to 63 CH_3 groups/1000 C and, accordingly, a density varying from 940 to < 910 kg/m^3. The molecular mass of the tested polymers varies from $\sim 1\ 10^6$ to $\sim 1 \cdot 10^3$.

DEHYDROGENATION OF METHANOL OVER COPPER-CONTAINING CATALYSTS

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Appl. Catal. A: General, 237(1-2) (2002) pp. 171-180.

The catalytic properties in methanol dehydrogenation of copper metal formed as a result of reduction by hydrogen of copper-containing oxides with different structure: copper chromite (tetragonally distorted spinel), copper hydroxysilicate (Chrysocolla), and copper-zinc hydroxysilicate (Zincsilite) have been studied. This process proceeds via successive reactions:

(I) $2CH_3OH=CH_3OOCH+2H_2$ and
(II) $CH_3OOCH=2CO+2H_2$.

The methyl formate selectivity for the catalysts studied was close to 1.0 at low methanol conversion, $X \leq 0.1$, where the dehydrogenation process is represented by reaction (I), occurring far from its equilibrium. At $0.2 \leq X \leq 0.55$, the selectivity decreases with increasing conversion, and the ratio of the activities in successive reactions may serve as a comparative characteristic for the catalysts. At high conversions, when reaction (I) is close to its equilibrium, selectivity is independent of the properties of studied catalysts and depends on the methanol conversion.

Reaction (I) shows low sensitivity to the state of metal copper of reduced catalysts and, hence, low sensitivity to the composition and structure of oxides-precursors. The catalysts' activity in reaction (II) greatly depends on the state of metal copper in the catalysts. It was assumed that the catalyst activity in methyl formate conversion to CO and H_2 and, hence, the selectivity of methanol dehydrogenation with respect to methyl formate in the region of moderate methanol conversion depends on the strength of interaction between metal copper particles and catalyst oxide surface, which is determined by the composition and structure of oxide-precursor.

TEMPERATURE DEPENDENCY OF BENZENE HYDROGENATION ON THE SULFIDE CATALYSTS

M.V. Sidyakin, A.N. Cholodovitch, S.I. Reshetnikov, E.A. Ivanov, A.N. Startsev

React. Kinet. & Catal. Lett., 77(2) (2002) pp. 287-292.

Non-Arrhenius temperature dependence of benzene hydrogenation was found for sulfide alumina-supported (Ni,Mo) and (Ni,W) catalysts under unsteady-state reaction conditions. It was shown that the observed decrease in the catalyst activity at high temperature could not be explained by the increasing role of the reverse reaction. The activity decrease was supposed to result from the catalyst reduction with the reaction mixture.

PHYSICOCHEMICAL MOTIVE FORCES AND TRENDS IN THE NATURAL SELECTION AND EVOLUTION OF PREBIOTIC AUTOCATALYTIC SYSTEMS

V.N. Parmon

Russ. J. Phys. Chem., 76(1) (2002) pp. 126-133.

A complex kinetothermodynamic analysis was performed for systems containing a set of noninteracting molecules, i.e., autocatalysts that are products of chemical transformations of the common starting substrate (“food”). It was shown that a delay in food supply to a system, i.e., a decrease in the volume of the common food niche, may be responsible for the phenomenon of natural selection, which is a consecutive extinction of autocatalysts having the lowest steady-state chemical potential. The conclusion that natural selection for the systems under study is accounted for by the retardation of their metabolic and assimilative reactions in the course of transformations of the starting substrate was drawn irrespective of the degree of deviation of the autocatalytic system from thermodynamic equilibrium. Thus, the hypothesis based indirectly on the Prigogine theorem of minimum rate of entropy production (only for steady states near thermodynamic equilibrium) was confirmed: evolution of living systems in the course of natural selection results in a decrease in the rate of metabolic processes.

CATALYTIC AND PHYSICOCHEMICAL PROPERTIES OF OXIDATIVE CONDENSATION PRODUCTS IN THE OXIDATIVE DEHYDROGENATION OF PROPANE BY SULFUR DIOXIDE ON SiO_2

I.G. Danilova, E.A. Paukshtis, A.V. Kalinkin, A.L. Chuvilin, G.S. Litvak, A.A. Altynnikov, V.F. Anufrienko

Kinetics & Catalysis, 43(5) (2002) pp. 698-710.

The effect of the deposition of oxidative condensation products in the reaction of oxidative propane dehydrogenation in the presence of SO_2 on the catalytic, acid–base, and texture characteristics of silica was studied. It was found that the oxidative condensation products exhibited high catalytic activity in this reaction. The carbonization of silica from 0 to ~40 wt % was accompanied by an increase in the yield of propylene from 3.4 to 46 mol % (640°C; a $C_3H_8/SO_2/He + N_2$ mixture, 10:10:80 vol %). Further accumulation of condensation products resulted in a considerable decrease in the pore volume and radius; this imposed diffusion limitations on both propane conversion and selectivity to propane conversion products. The nature of active and deactivated condensation products was studied by DRIFT spectroscopy, diffuse-reflectance UV–VIS spectroscopy, EPR spectroscopy, XPS, thermal analysis, and electron microscopy.

NON-CATALYTIC LIQUID PHASE OXIDATION OF ALKENES WITH NITROUS OXIDE. I. OXIDATION OF CYCLOHEXENE TO CYCLOHEXANONE

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

React. Kinet. & Catal. Lett., 76(2) (2002) pp. 401-406.

A very efficient way of alkenes oxidation to carbonyl compounds is discovered. It is based on remarkable ability of nitrous oxide to interact directly with the double C=C bonds of liquid alkene and to transfer its oxygen, without catalyst aid, to unsaturated carbon atom with nearly 100% selectivity. This oxidation method can be applied to a wide range of organic compounds including aliphatic, cyclic, heterocyclic alkenes and their numerous derivatives.

NON-CATALYTIC LIQUID PHASE OXIDATION OF ALKENES WITH NITROUS OXIDE. II. OXIDATION OF CYCLOPENTENE TO CYCLOPENTANONE

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

React. Kinet. & Catal. Lett., 77(1) (2002)
pp. 197-205.

A very efficient way of cyclopentanone production *via* selective liquid phase oxidation of cyclopentene with nitrous oxide is reported. When contacting liquid cyclopentene at high temperature, nitrous oxide is able to interact directly with the C=C double bond of the hydrocarbon and transfer its oxygen to unsaturated carbon atom. The reaction occurs without catalyst with nearly 100% selectivity.

PROCEDURE FOR STUDYING THE STEADY-STATE KINETICS OF OXIDATION OF GASEOUS SUBSTRATES BY HYDROGEN PEROXIDE IN A LIQUID PHASE

A.O. Kuzmin, V.N. Parmon

Kinetics & Catalysis, 43(6) (2002)
pp. 774-777.

A procedure was developed for studying the steady-state kinetics of oxidation of various gaseous substrates by hydrogen peroxide under conditions of the continuous release of gaseous products. The steady state of a system was provided by continuously injecting hydrogen peroxide at low conversions of the oxidized substrate. The process was monitored by measuring substrate losses in a gas phase rather than the buildup of products. This allowed us to avoid difficulties associated with further oxidation of the products.

STATIONARY KINETICS OF LIGHT OLEFIN OXIDATION BY HYDROGEN PEROXIDE IN AQUEOUS ALKALI SOLUTIONS IN THE PRESENCE OF Fe(III) OXIDE

A.A. Lysova, A.O. Kuzmin, G.L. Elizarova, V.N. Parmon

Kinetics & Catalysis, 43(6) (2002)
pp. 778-784.

The steady-state kinetics of ethylene and propylene oxidation by hydrogen peroxide in the presence of Fe(III) oxide in aqueous solutions with the permanent adding of H_2O_2 to the reaction medium was studied. The use of an original method for the study of the steady-state reaction kinetics with gas chromatographic detection of substrate consumption from the gas phase made it possible to estimate the apparent rate constants of ethylene oxidation, the ratio of the rate constants of propylene and ethylene oxidation, the reaction orders with respect to the substrate and oxidant concentration, the dependence of the apparent rate constant of ethylene oxidation on the catalyst weight and on the pH of solution, and the apparent activation energy of the process under condition of substrate distribution between the gas and liquid phases. It was found that the kinetic isotope effect in ethylene oxidation is almost absent when completely deuterated ethylene is used.

Catalysis on Zeolites

HYDROISOMERIZATION OF *n*-HEXADECANE ON BIFUNCTIONAL CATALYSTS BASED ON ZEOLITES WITH DIFFERENT STRUCTURES

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Petroleum Chemistry, 42(3) (2002)
pp. 192-198.

The influence of the ratio between the hydrogenating–dehydrogenating and acidic functions of bifunctional catalysts prepared from crystalline aluminosilicates and silicaaluminophosphates of different structural types on the selectivity of *n*-hexadecane transformation in a hydrogen atmosphere was studied. The ratio of the hydroisomerization to hydrocracking products was shown to be determined by the ratio of the acidic to hydro–dehydrogenating activities of the catalyst and the structural characteristics of the initial zeolite or silicaaluminophosphate. The dependence of the amount of isoparaffins on the crystallographic size of channels of the base zeolite is nonmonotonic in character, with a maximum at 0.62–0.63 nm, which corresponds to the kinetic diameter of monomethylisoparaffins.

INFLUENCE OF HYDROGEN ON THE CONVERSION OF A MIXTURE OF C_6-C_8 HYDROCARBONS OVER IRON-CONTAINING ZEOLITE H-ZSM-5

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(*Novosibirsk State University, Novosibirsk, Russia)

Petroleum Chemistry, 42(3) (2002)
pp. 199-204.

The influence of the composition of the reaction medium on the conversion of a hydrocarbon mixture, which simulates feedstock for the zeoforming process in group composition; was studied with the purpose of obtaining high-octane gasolines and their components over a catalyst containing zeolite with isomorphously substitutable aluminum and iron atoms. Decationated zeolite ZSM-5, which was crystallized in the presence of iron compounds and whose framework contains isomorphously substituting iron atoms, is active in redox reactions and possesses a hydrogenating function. In the presence of hydrogen, the conversion of hydrocarbons on this zeolite follows the bifunctional mechanism. Hydrogenation reactions compete with hydrogen redistribution reactions in intermediate olefinic fragments, resulting in an increase in the yield of light paraffins C_1–C_4 and isoparaffins as products and a decrease in the formation of aromatic hydrocarbons.

DETECTION OF O^- RADICAL ANIONS IN Cu-ZSM-5 ZEOLITES AFTER HEAT TREATMENT

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Dokady Chemistry, 386(4-6) (2002) pp. 273-276.

The axial EPR spectra with $g_\perp = 2.05$ and $g_{||} = 2.02$ are detected for the samples of Cu-ZSM-5-zeolites obtained by ion-exchange from copper acetate and copper ammine after thermal treatment at 500°C. These spectra may be conditioned by line chains $O^- \cdots Cu^+ \cdots O^- \cdots Cu^+ \cdots O^- \cdots$ in zeolite channels. It is supposed that "internal" redox in the chains $\cdots O^- \cdots Cu^+ \cdots O^- \cdots Cu^+ \cdots O^- \cdots \leftrightarrow \cdots O^{2-} \cdots Cu^{2+} \cdots O^{2-} \cdots Cu^{2+} \cdots O^{2-} \cdots$ is conditioned by the effect of water molecules, shifting the balance to the right. Besides the EPR spectra of ion-radicals O^-, there are also observed EPR spectra of isolated Cu^{2+} ions with various extent of tetragonal distortion of octahedrons, stabilized on the external surface of zeolite between the crystallites.

EVOLUTION OF IRON STATES AND FORMATION OF α-SITES UPON ACTIVATION OF FeZSM-5 ZEOLITES

K.A. Dubkov, N.S. Ovanesyan*, A.A. Shteinman*, E.V. Starokon, G.I. Panov (*Zeolites Institute of Problems of Chemical Physics, Chernogolovka, Moscow Region, Russia)

J. Catal., 207(2) (2002) pp. 341-352.

Mössbauer spectroscopy *in situ* was used to study the effect of high-temperature activation on the evolution of iron introduced into a ZSM-5 zeolite matrix by various methods. The activation process (calcination in air, in vacuum, or in the presence of water vapor) was shown to cause an intensive reduction of iron, yielding two types of dinuclear Fe^{2+} complexes, which may comprise more than 60% of the total metal content. Reduced Fe^{2+} ions are stable in the presence of O_2 but are reversibly oxidized to Fe^{3+} by nitrous oxide, generating active α-oxygen species, which bring unique oxidation properties to the zeolite. After coordinative saturation by adsorbed water molecules, both iron complexes show identical Mössbauer spectra, which are close to the spectra of dinuclear iron sites in the MMO enzyme. A thorough quantitative comparison between the number of α-oxygen atoms and the number of Fe atoms involved in redox transition shows that α-sites are dinuclear complexes in which both Fe atoms are capable of α-oxygen generation.

NEW WAY FOR PREPARATION OF HYDROQUINONE AND CATECHOL USING NITROUS OXIDE AS OXIDANT

D.P. Ivanov, V.I. Sobolev, L.V. Pirutko, G.I. Panov

Adv. Synth. Catal., 344(9) (2002) pp. 986-995.

Synthesis of dihydroxybenzenes (DHB) via the gas-phase oxidation of phenol with nitrous oxide in the presence of benzene was studied. Addition of benzene to the feed mixture greatly improves the selectivity and catalytic stability of the Fe-containing ZSM-5 zeolite, what previously was considered to be a main obstacle to the development of a new process.

Reaction conditions strongly affect distribution of the DHB isomers: the ratio of hydroquinone to catechol may vary from 1.4 to 10, with the resorcinol fraction being nearly constant and comprising 3-5%. The 40 h experiments on the oxidation of a phenol-benzene mixture demonstrated high efficiency of the formed FeZSM-5 catalyst. At good stability, the catalyst provides 97% phenol selectivity referred to DHB and 85-90% N_2O selectivity referred to the sum of DHBs and phenol. New process for hydroquinone and catechol synthesis based on the neat oxidation of benzene with recycling the phenol as an intermediate product is suggested.

Studies on Zirconia-Based Materials

CATALYTIC PROPERTIES OF THE THERMAL DECOMPOSITION PRODUCTS OF $Zr(SO_4)_2•4H_2O$

N.S. Kotsarenko, V.P. Shmachkova

Kinetics & Catalysis, 43(2) (2002) pp. 280-283.

The catalytic activity of the thermal decomposition products of $Zr(SO_4)_2•4H_2O$ in the reactions of 1-butene isomerization to 2-butenes, isobutanol dehydration, and *n*-butane skeletal isomerization was studied. Their behaviors in typical acid reactions and in skeletal isomerization were found to be considerably different. In the first two reactions, which occur with the participation of proton sites, the activity of zirconium sulfates was an extremal function of hydrate calcination temperature. Zirconium sulfate calcined at 400-550°C was the most active catalyst. The reasons for such behavior are discussed. In the skeletal isomerization of *n*-butane, crystalline zirconium sulfate was practically inactive, and it became active only after degradation. The results suggest that the activation of *n*-butane molecules do not occur at proton sites.

EFFECT OF THE SULFATE SULFUR CONTENT AND THE PREPARATION PROCEDURE ON THE CATALYTIC PROPERTIES OF SULFATED ZIRCONIUM OXIDE

V.P. Shmachkova, N.S. Kotsarenko

Kinetics & Catalysis, 43(4) (2002) pp. 550-554.

The effects of the composition and the procedure of preparing sulfated zirconium oxides on their catalytic properties in the reactions of 1-butene isomerization to 2-butenes and isobutanol dehydration were studied. The activity was found to depend on the nature of parent zirconium oxide, the sulfate sulfur content, and the temperature of calcination. Catalysts prepared from a crystalline oxide exhibited the highest activity. Their activity depends on the sulfate sulfur content. The calcination of catalysts at temperatures higher than 400°C resulted in a detectable loss of sulfate. The activity of sulfated oxides prepared from an amorphous oxide was noticeably lower; it depended only slightly on the temperature of calcination and sulfate sulfur content. The catalytic behavior of the sulfated oxide in both of the reactions is indicative of the absence of superstrong proton sites. Based on the results, assumptions on the nature of formed surface compounds were made.

NEW APPROACH TO PREPARATION AND INVESTIGATION OF ACTIVE SITES IN SULFATED ZIRCONIA CATALYSTS FOR SKELETAL ISOMERIZATION OF ALKANES

N.A. Pakhomov, A.S. Ivanova, A.F. Bedilo*, E.M. Moroz, A.M. Volodin (*Kansas State University, Manhattan, USA)

Stud. Surf. Sci. & Catal., 143 (2002) pp. 353-360.

Catalysts active in the isomerization of n-butane have been synthesized by depositing sulfate ions on well-crystallized defective cubic structures based on ZrO_2. This technique for introduction of sulfates does not result in any significant changes in the bulk properties of zirconium dioxide matrix. Active sulfated catalysts were prepared on the basis of cubic solid solutions of ZrO_2 with calcium oxide and on the basis of cubic anion-doped ZrO_2. The dependence of the catalytic activity on the amount of calcium appeared to have a maximum corresponding to 10 mol. % Ca. Radical cations formed after adsorption of chlorobenzene on activated catalysts have been used as spin probes for detection of strong acceptor sites on the surface of the catalysts and estimation of their concentration. A good correlation has been observed between the presence of such sites on a catalyst surface and its activity in isomerization of n-butane.

CATION/ANION MODIFIED CERIA-ZIRCONIA SOLID SOLUTIONS PROMOTED BY Pt AS CATALYSTS OF METHANE OXIDATION INTO SYNGAS BY WATER IN REVERSIBLE REDOX CYCLES

V.A. Sadykov, T.G. Kuznetsova, S.A. Veniaminov, D.I. Kochubey, B.N. Novgorodov, E.B. Burgina, E.M. Moroz, E.A. Paukshtis, V.P. Ivanov, S.N. Trukhan, S.A. Beloshapkin, Yu.V. Potapova, V.V. Lunin*, E. Kemnitz, A. Aboukais***** (*Lomonosov Moscow State University, Moscow, Russia; **Institute for Chemistry, Humboldt-Universität Berlin, Germany; ***Universite du Littoral-Cote d"Opale Dunkerque, France)

React. Kinet. & Catal. Lett., 76(1) (2002) pp. 83-92.

Ca and/or F-modified fluorite-like Ce-Zr-mixed oxides have been prepared by Pechinis method. The bulk structure of samples was characterized by XRD, EXAFS and FTIRS of the lattice modes. The surface properties were studied by SIMS and FTIRS of adsorbed CO and surface hydroxyls. The specific reactivity of the surface oxygen, its amount, coefficients of bulk and near-surface diffusion, as dependent upon the sample composition and temperature, were estimated using sample reduction by CO in the pulse/flow mode. Insertion of fluorine into the lattice results in decreasing the degree of oxygen polyhedra distortion, thus decreasing the amount of reactive oxygen and diffusion coefficients. Calcium and Pt addition counteracts this effect. At 500^{o}C for Pt-supported Ce-Zr-O samples including those modified by Ca and F, the lattice oxygen is easily removed by methane generating CO and hydrogen with high selectivity. Reoxidation of reduced samples by water or carbon dioxide at the same temperature restores the oxygen capacity producing more hydrogen or carbon monoxide.

STRUCTURE OF ZIRCONIA NANOPARTICLES USED FOR PILLARING OF CLAY

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Mat. Res. Symp. Proc., 703 (2002)
pp. 529-534.

SAXS and EXAFS were applied to study genesis of polynuclear zirconium hydroxyspecies in pillaring solutions as dependent upon the zirconium concentration, addition of alkaline-earth chlorides and aging. After the montmorillonite clay pillaring, the structure of zirconium nanopillars was characterized by applying X-ray structural analysis, UV-Vis, FTIRS of adsorbed CO and nitrogen adsorption isotherms. Main pillaring species appear to be nanorods comprised of several Zr_4 tetramers. Basic structural features of the tetramers are preserved in zirconia nanoparticles fixed between alumosilicate layers in pillared clays. In calcined samples, those nanoparticles contain only bridging hydroxyls and/or oxygen anions responsible for bonding within pillars and between pillars and clay sheets.

Carbon and Carbon Containing Materials

MORPHOLOGY AND STRUCTURE OF CARBON RESULTING FORM DECOMPOSITION OF CHLOROHYDROCARBONS ON NICKEL AND COBALT CONTAINING CATALYSTS

I.V. Mishakov, V.V. Chesnokov, R.A. Buyanov, A.L. Chuvilin

React. Kinet. & Catal. Lett., 76(2) (2002)
pp. 361-367.

Morphology of carbons deposited from chlorohydrocarbons on $Ni(Co)/Al_2O_3$ has been investigated. It has been established that carbon filaments consist of imperfect graphite layers and possess high adsorption capacity towards hydrogen.

TRANSFORMATION OF DIAMOND NANOPARTICLES INTO CARBON ONIONS UNDER ELECTRON IRRADIATION

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Phys. Chem. Chem. Phys., 4(10) (2002)
pp. 1964-1967.

The irradiation-induced transformation of diamond nanoparticles (DNP) to spherical onions and onion-like carbon was studied *in situ* by high-resolution transmission electron microscopy (HRTEM) and electron energy loss spectroscopy (EELS). The process was observed in a transmission electron microscope operated at 200 kV without additional specimen heating. Estimated current density was in the range 20–40 A cm^{-2}. The onion-like particles formed from the diamonds were found to be quite stable to further electron irradiation. The changes in chemical bonding were also confirmed by EELS, revealing an increasing role of bonds with sp^2 hybridization in the irradiated material. The mechanism of structural transformation is discussed.

THE FORMATION OF CARBON-CONTAINING DEPOSITS IN THE OXIDATION OF C_2-C_4 ALCOHOLS AND ETHYLENE GLYCOL ON THE SURFACE OF SILVER CATALYSTS

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Russ. J. Phys. Chem., 76(8) (2002) pp. 1266-1270.

The morphology and formation of carbon deposition products on a massive silver catalyst in partial oxidation of monoatomic C_2–C_4 alcohols and ethylene glycol were studied gravimetrically and by scanning electron microscopy. The structure and reactivity of the alcohols were shown to be related to the structure of carbon-containing deposits formed in their oxidation.

THE ROLE PLAYED BY CARBON DEPOSITION PRODUCTS IN PARTIAL OXIDATION OF ETHYLENE GLYCOL TO GLYOXAL ON A COPPER CATALYST

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Russ. J. Phys. Chem., 76(8) (2002) pp. 1271-1274.

The scanning electron microscopy and thermographic and elemental analysis methods were used to show that two different types of carbon deposition products were formed on the surface of copper depending on the content of oxygen in the reaction mixture, namely, graphite-like films and oxycarbonaceous fibers. The interaction of ethylene glycol with the surface of copper catalysts treated in reaction media of various compositions was studied by the method of programmed-temperature reactions. The formation of graphite-like structures was observed on nonoxidized copper surface regions and resulted in blocking surface active centers. Carbon deposition products of the second type, carbonaceous fibers, were formed under the action of oxygen-containing reaction media. Growth of fibers was accompanied by the emergence of high-dispersity copper crystallites, which intensified the synthesis of glyoxal.

ONION-LIKE CARBON AND DIAMOND NANOPARTICLES FOR OPTICAL LIMITING

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S. Couris*, S. Korovin, P. Detkov**,**
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Chem. Phys. Lett., 357(5-6) (2002) pp. 336-340.

The present study reports on the experimental investigation of the nonlinear optical response of polydispersed and ultradispersed diamond powders and onion-like carbon structures in water suspension. It has been found that the onion-like carbon structures exhibit much stronger optical limiting action compared with the diamond powder suspensions. It is also shown that under our experimental conditions the nonlinear refraction of the onion-like structures was negligible.

DEFECT INDUCED LOWERING OF WORK FUNCTION IN GRAPHITE-LIKE MATERIALS

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Diamond & Related Materials, 11 (2002) pp. 813–818.

Different carbon materials have shown unusually high efficiency of electron field emission. The device application of the carbon cold cathodes requires a fundamental understanding of the emission mechanism. The emission properties of carbon thin films grown by chemical vapor deposition are described. The structure, phase composition and electronic properties peculiar to the film material were investigated. New model of electron emission sites and mechanism of field electron emission are proposed. In accordance with the proposed model the electron emission in carbon materials occurs from sp^3-like defects in a sp^2 network of graphite-like material. The corresponding mechanism of field emission consists of electrons escaping into vacuum by tunneling from the Fermi level of the graphite material through the atomically thin sp^3-like layer and the energy barrier on its surface.

THERMODYNAMIC ANALYSIS OF NUCLEATION OF CARBON DEPOSITS ON METAL PARTICLES AND ITS IMPLICATIONS FOR THE GROWTH OF CARBON NANOTUBES

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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, it was concluded 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 was proposed that the nucleus have 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.

METHANE PYROLYSIS OVER CARBON CATALYSTS

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Eurasian ChemTech J., 3(2) (2001) pp. 67-72.

Methane pyrolysis at the temperature range of 550-1000°C in gas flow reactor with fixed bed of mixed catalysts based on carbon materials of various structure (fullerene cocoons, fullerene black, vacuum black, cathode deposit, onion-like carbon, glassy carbon, carbon fibers, mineral shungite and graphite) has been studied. Methane pyrolysis products, including stoichiometric amount of hydrogen are C_3-C_4 alkanes, C_2-C_4 alkenes, aromatics and pyrolytic carbon. Methane pyrolysis is carried out both on a catalytic surface and in a volume and contribution of the surface is determined by pyrolysis temperature. Materials with curved carbon surface show an activity in methane dehydrogenation at lower temperatures, than materials with planar basic structure elements. Materials with a small specific surface area favor methane aromatization at 950–1000°C with formation of mainly benzene, toluene and naphthalene. The primary activation of C–H bond in methane at temperatures of lower than 850°C, as well as the multiple dehydrogenation conversions resulting in the formation of pyrolytic carbon and its precursors (aromatics), are, probably, heterogeneous reactions.

FORMATION OF CARBON FILAMENTS FROM 1,3-BUTADIENE ON Fe/Al_2O_3 CATALYSTS

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

Kinetics & Catalysis, 43(5) (2002) pp. 677-683.

The formation of carbon filaments with different crystallographic and morphological characteristics in the course of 1,3-butadiene decomposition on Fe/Al_2O_3 catalysts at low (500-600°C) and high (700-800°C) temperatures was considered in terms of a carbide cycle mechanism. The conditions of formation and decomposition of an iron carbide phase in the course of formation of graphite nanotubes in the low-temperature region were studied.

IRON CONTAINING CATALYSTS OF METHANE DECOMPOSITION: ACCUMULATION OF FILAMENTOUS CARBON

L.B. Avdeeva, T.V. Reshetenko, Z.R. Ismagilov, V.A. Likholobov

Appl. Catal. A: General, 228(1-2) (2002) pp. 53-63.

Iron-containing catalysts were tested in methane decomposition reaction at moderate temperature and pressure 1 bar in order to evaluate their catalytic properties and produce catalytic filamentous carbon (CFC). Catalyst preparation method and composition of the catalysts were found to influence their properties. The best performance was found with coprecipitated Fe-Co-Al_2O_3 catalysts, where carbon capacity has achieved 52.4 g/g_{cat}. TEM investigations have shown that carbon nanotubes were formed.

GAS-PHASE SYNTHESIS OF NITROGEN-CONTAINING CARBON NANOTUBES AND THEIR ELECTRONIC PROPERTIES

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Physics of the Solid State, 44(4) (2002) pp. 652-655.

Nitrogen-containing carbon nanotubes are synthesized using a gas-phase reaction. The synthesis of nitrogen-doped carbon nanotubes from 100 to 500 Å in diameter is accomplished through pyrolysis of acetonitrile (CH_3CN) at a temperature of 800°C. Cobalt and nickel metallic particles formed upon thermal decomposition of a mixture of maleate salts are used as catalysts. The materials synthesized are investigated by scanning and transmission electron microscopy. Analysis of the X-ray photoelectron spectra demonstrates that the content of nitrogen atoms in three nonequivalent charge states is approximately equal to 3%. A comparison of the X-ray fluorescence spectrum of the carbon nanotubes synthesized through electric-arc evaporation of graphite and the X-ray fluorescence spectrum of the nitrogen-containing carbon nanotubes prepared by catalytic decomposition of acetonitrile indicates that, in the latter case, the spectrum contains a certain contribution from the sp^3 states of carbon atoms. The temperature dependencies of the electrical conductivity for different types of multi-walled carbon nanotubes are compared. The difference observed in the temperature dependencies of the electrical conductivity is associated with the presence of additional scattering centers in nitrogen-containing carbon nanotubes.

CARBON-SUPPORTED PALLADIUM-RUTHENIUM CATALYST FOR HYDROPURIFICATION OF TEREPHTHALIC ACID

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Appl. Catal. A: General, 225(1-2) (2002) pp. 131-139.

The ruthenium-incorporated catalyst, (0.3%Pd-0.2%Ru)/CCM (carbon carbonaceous composite material) catalyst, has been studied as a candidate to replace an existing 0.5%Pd/C catalyst for hydropurification of crude terephthalic acid; it gives an excellent performance and is a promising catalyst. It has been confirmed that the (0.3%Pd-0.2%Ru)/CCM catalyst has higher stability in actual commercial condition and aging in lab condition compared with a commercial catalyst. The increased stability may be explained as the effect of ruthenium to prevent the sintering of supported metal particle. The (0.3%Pd-0.2%Ru)/CCM catalyst shows equal or less amount of side reaction of benzene ring hydrogenation. The dust from carbon support can also be decreased from the (0.3%Pd-0.2%Ru)/CCM catalyst due to the increased strength of the CCM. The (0.3%Pd-0.2%Ru)/CCM catalyst may be very competitive to the existing catalyst due to the inexpensive ruthenium and expected long life of the catalyst.

INFLUENCE OF RUTHENIUM ADDITION ON SINTERING OF CARBON-SUPPORTED PALLADIUM

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Appl. Catal. A: General, 227(1-2) (2002) pp. 117-123.

Carbon-supported palladium catalysts are widely used in hydrogenation reactions. Palladium particles are observed to sinter in the course of the reaction, particularly at high temperatures, that results in the catalyst deactivation. A prospective way for stabilization of palladium particles on the active carbon surface is introduction of another metal, for example ruthenium, therein.

The present work was aimed at studying the influence of the Ru addition on the phase composition, dispersion and sintering resistance of metal particles of catalysts for hydropurification of terephthalic acid (TPA).

THE TEMPERATURE DEPENDENCE OF THE ELECTRICAL RESISTIVITY AND THE NEGATIVE MAGNETORESISTANCE OF CARBON NANOPARTICLES

A.I. Romanenko*, O.B. Anikeeva*, A.V. Okotrub*, L.G. Bulusheva*, V.L. Kuznetsov, Yu.V. Butenko, A.L. Chuvilin, C. Dong, Y. Ni**** (*Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institute of Physics, Chinese Academy of Sciences, Beijing, China)

Physics of Solid State, 44(3) (2002) pp. 487-489.

Temperature dependencies of the electrical resistivity of samples of carbon nanoparticles obtained from nanodiamonds by annealing at 1800, 1900, and 2140 K were studied. The magnetoresistance of these samples was measured at 4.5 K. Data on the positive magnetoresistance obtained in fields above 3 T were used to estimate the mean free path l of carriers at liquid-helium temperature, $l \sim 12$ Å for a sample annealed at 1800 K, $l \sim 80$ Å for a sample annealed at 1900 K, and $l \sim 18$ Å for the case of annealing at 2140 K. The samples annealed at 1800 and 2140 K exhibit a negative magnetoresistance in fields below 2 T. The carrier concentrations n in the samples annealed at 1800 and 2140 K were estimated as $n \sim 8 \cdot 10^{21}$ and $3 \cdot 10^{21}$ cm^{-3}, respectively.

PHYSICOCHEMICAL ASPECTS OF PREPARATION OF CARBON SUPPORTED NOBLE METAL CATALYSTS

P.A. Simonov, V.A. Likholobov

Catalysis at Nanoparticle Surfaces,
Eds. A. Wieckowski, E.R. Savinova, C.G. Vayenas, 2002, Marcel Dekker, Inc., New York, pp. 379-407.

A literature survey. Publications which deal with studying an interaction of noble metals nanoparticles with the surface of porous quasi-graphitic carbon materials are considered. A critical analysis of mechanisms of the formation of carbon-supported metal catalysts is also done.

METHOD OF UTILIZATION OF CHLOROHYDROCARBONS ON NICKEL AND COBALT-BEARING CATALYSTS

I.V. Mishakov, R.A. Buyanov, V.V. Chesnokov

Catalysis in Industry, 4 (2002) pp. 33-39.

Methods of utilization of chlorohydrocarbons on Ni/Al_2O_3, $Ni\text{-}Pd/Al_2O_3$, and Co/Al_2O_3 catalysts according to the mechanism of carbide cycle for the purpose of producing carbon composite materials and by hydrodechlorination with production of proper hydrocarbons have been considered. Stability of metals to deactivation under the effect of HCl is shown to decrease in the series of Ni>Co>Fe. The morphology of carbon, which is formed on Ni/Al_2O_3 catalyst during decomposition of 1,2-dichlorethane, has been studied. The pilot tests on decomposition of 1,2-dichlorethane in two modes on enlarged plant with rotating reactor were carried out.

SILICON CARBONITRIDE FILMS AS A PROMISING MATERIAL SYNTHESIZED FROM NEW SOURCES

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Chem. for Sustainable Devel., 9(7) (2001) pp. 23-27.

Silicon carbonitride films were synthesized by means of the chemical vapour deposition (CVD) process in the scheme with remote plasma. Initial compounds were the silyl derivatives of 1,1-dimethyl hydrazine: dimethyl(2,2-dimethylhydrazino)-silane and dimethyl-bis-(2,2-dimethylhydrazino)silane. The molecules of the monomers contain the bonds Si-N, Si-C and C-N, which are necessary for the formation of silicon carbonitride.

Studies on Metal Catalysts

THE Pt-CONTAINING CATALYSTS ON FIBER GLASS WOVEN SUPPORTS: FEATURES AND PROSPECTS OF THEIR APPLICATION

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Catalysis in Industry, 5 (2002) PP. 33-39.

Physico-chemical and structural properties of Pt supported on leached fiber glass materials have been studied. According to TEM and XPS data, there are two types for Pt appearance depending on the synthesis method: on the surface and in the bulk of glass fiber. By testing of the catalysts in the reactions of deep oxidation of n-butane, SO_2 oxidation to SO_3 and selective catalytic reduction of NO by propane in the presence of O_2 excess it was shown that the localization of Pt in the fiber's bulk results in enhanced catalytic activity and catalyst stability at high temperatures in the presence of SO_2 and H_2O. These characteristics along with other exploitation advantages such as high tensile strength, low hydraulic resistance, improved mass and heat transfer determine the prospects of industrial application of the Pt-containing catalysts on fiber glass woven supports. In particular, there is a real possibility to substitute the laborious in exploitation granular catalyst beds for the structured pile made up by the elementary catalytic layers.

CATALYSTS BASED ON FIBERGLASS SUPPORT: IV. PLATINUM CATALYSTS BASED ON FIBERGLASS SUPPORT IN OXIDATION OF HYDROCARBONS (PROPANE AND *n*-BUTANE) AND SULFUR DIOXIDE

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Kinetics & Catalysis, 43(1) (2002) pp. 61-66.

Platinum catalysts (0.003–0.52% Pt) based on leached sodium silicate and boron silicate fiberglass supports are studied in the complete oxidation of hydrocarbons (*n*-butane and propane) and high-temperature SO_2 oxidation. It was shown that platinum localized in the bulk of the glass matrix show a higher activity and thermal stability than metal particles supported on the outer surface of fiberglass. The experimental results for hydrocarbon oxidation on platinum-containing fiberglass gauzes at short contact times are discussed.

CATALYSTS BASED ON FIBERGLASS SUPPORTS. V. ABSORPTION AND CATALYTIC PROPERTIES OF PALLADIUM CATALYSTS BASED ON A LEACHED SILICA-FIBERGLASS SUPPORT IN THE SELECTIVE HYDROGENATION OF AN ETHYLENE-ACETYLENE MIXTURE

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Kinetics & Catalysis, 43(4) (2002) pp. 542-549.

The absorption and catalytic properties of palladium catalysts (0.01% Pd) based on leached soda–silica fiberglass supports were studied in the selective hydrogenation of acetylene as the constituent of an ethylene–acetylene mixture. It was found that fiberglass catalysts exhibited much higher selectivity than traditional supported Pd catalysts. It was suggested that the high selectivity in the reaction of acetylene hydrogenation resulted from the selective absorption (diffusion) of acetylene in the bulk of fiberglass, where Pd microparticles are localized.

CO OXIDATION OVER A Pt-Rh SYSTEM. I. REACTION ON INDIVIDUAL METALS

A.V. Kalinkin, A.V. Pashis, V.I. Bukhtiyarov

React. Kinet. & Catal. Lett., 77(2) (2002) pp. 255-261.

The reaction of CO oxidation over thin films of rhodium and platinum prepared by vacuum evaporation of the metals on an inert support has been investigated at low pressures ($P < 2\times10^{-5}$ mbar). Rhodium has been found to be more active than platinum in this reaction. The reasons of the higher activity of Rh are discussed.

ETHANOL DECOMPOSITION OVER Pd-BASED CATALYST IN THE PRESENCE OF STEAM

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React. Kinet. & Catal. Lett., 76(2) (2002) pp. 343-351.

Catalytic decomposition of ethanol in the presence of steam over Pd supported on a porous carbonaceous material was studied. XPS and TEM were used for the catalyst characterization. Experiments were performed under atmospheric pressure, temperature of 320-360°C and H_2O/C_2H_5OH molar ratio 8.1. It was found that the catalyst exhibited a high activity and long-term stability for the ethanol decomposition into a gas mixture containing carbon oxides, methane and hydrogen.

Pd-Au/SIBUNIT CARBON CATALYSTS: CHARACTERIZATION AND CATALYTIC ACTIVITY IN HYDRODECHLORINATION OF DICHLORODIFLUOROMETHANE (CFC-12)

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J. Catal., 209(2) (2002) pp. 528-538.

A series of Sibunit carbon-supported palladium–gold catalysts prepared by different methods (wet and incipient wetness impregnation and direct redox reaction) were characterized by various techniques and investigated in the reaction of dichlorodifluoromethane with dihydrogen. The direct redox method resulted in a higher degree of Pd–Au alloying than the impregnation procedures. A temperature-programmed hydride decomposition (TPHD) study appears to be a very promising technique for characterization of Pd–Au bimetal. A clear correlation between TPHD spectra and X-ray diffraction data for Pd–Au catalysts allows proposal of the former technique for diagnosing the quality of Pd–Au alloying. The selectivity toward difluoromethane (desired reaction product) was increased upon introducing gold to palladium; however, this enhancement depended very much on the degree of Pd–Au alloying. For the catalysts prepared by the direct redox reaction method the selectivity for difluoromethane increased from <70 (for Pd) to nearly 90% for bimetallic samples at the highest temperature of screening, 180°C. Such a high selectivity enhancement was not observed for Pd–Au/C catalysts prepared by impregnation methods, which showed a lesser degree of Pd–Au alloying. During the reaction of dichlorodifluoromethane hydrodechlorination substantial amounts of carbon dissolve in the bulk of the palladium (or Pd-rich alloy) phase. Independent studies with a model Pd/SiO_2 catalyst showed that this carbon originates from the CFC molecule, not from the carbon support. It is interesting that a massive carbiding of palladium takes place at a very early stage of the reaction, when also the most important changes in catalytic behavior occur. Thus, it may be speculated that the surface state of the working catalyst must be correlated with the extent of the bulk carbiding. An easy removal of carbon from palladium by hydrogen at the reaction temperature confirms our earlier idea that methane formation from dichlorodifluoromethane may occur via hydrogenation of C_1 surface species.

INFLUENCE OF MODIFYING ADDITIVES ON ELECTRONIC STATE OF SUPPORTED GOLD

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J. Molec. Struct., 642 (1-3) (2002) pp. 129-136.

Using the methods of IR spectroscopy of adsorbed CO, electron spectroscopy of diffuse reflectance, XRD, XPS, EXAFS and electron microscopy the influence of modifying additions of Ce, Zr, La and Cs oxides on the surface electronic states of supported gold have been studied. The additions of Ce and Zr oxides stabilize the ionic states of supported gold and increase the effective charge of the ions. In contrast, La and Cs oxides lower the effective charge of gold cation and favor their fast reduction.

EFFECT OF THE STRUCTURE OF CARBON NANOFIBERS ON THE STATE OF AN ACTIVE COMPONENT AND ON THE CATALYTIC PROPERTIES OF Pd/C CATALYSTS IN THE SELECTIVE HYDROGENATION OF 1,3-BUTADIENE

V.V. Chesnokov, I.P. Prosvirin, N.A. Zaitseva, V.I. Zaikovskii, V.V. Molchanov

Kinetics & Catalysis, 43(6) (2002) pp. 838-847.

The state of highly dispersed palladium particles supported on filamentous carbon was studied using high-resolution electron microscopy, XPS, and X-ray diffraction analysis. Three types of filamentous carbon were used, in which the basal planes of graphite were arranged along, across, and at an angle to the nanofiber axis. The amount of supported palladium was 0.25–5.8 wt %. The structure of the carbon support was found to affect the properties of the active component. Highly dispersed palladium particles exhibited the strongest interaction with a carbon surface formed by the butt ends of graphite (002) layers. This interaction resulted in electron transfer from the metal to the support and in the stabilization of palladium in the most dispersed state. A change in the properties of palladium particles caused a change in the catalytic properties of Pd/C catalysts in the reaction of selective 1,3-butadiene hydrogenation to butenes. The strong interaction of Pd^{2+} with the butt ends of graphite resulted in the stabilization of palladium in an ionic state. An increase in the fraction of Pd^{2+} in the catalysts was responsible for a decrease in both the overall activity and selectivity of Pd/C catalysts in the reaction of 1,3-butadiene hydrogenation to butenes.

KINETICS OF THE HYDROGENATION OF α-PINENE TO *cis*- AND *trans*-PINANES ON Pd/C

I.I. Il'ina, I.L. Simakova, V.A. Semikolenov

Kinetics & Catalysis, 43(5) (2002) pp. 645-651.

The liquid-phase hydrogenation of α-pinene on a Pd/C catalyst at 0-100°C and hydrogen pressures of

1–11 atm was studied. It was found that the order of reaction with respect to pinene increased with hydrogen pressure and did not depend on temperature, whereas the selectivity of *cis*-pinane formation decreased with temperature and increased with hydrogen pressure. A mechanism was proposed for the hydrogenation of α-pinene. According to this mechanism, the selectivity of *cis*-pinane formation depends on the following two factors: (a) a temperature-dependent equilibrium between adsorbed α-pinene species, which are *cis*- and *trans*-pinane precursors, and (b) competition between the hydrogenation and β-H-elimination of surface σ-pinanyl complexes. The ratio between the rates of these reactions depends on the concentration of surface hydride species, and this concentration depends on the pressure of hydrogen.

KINETICS OF THE HYDROGENATION OF PINANE HYDROPEROXIDE TO PINANOL ON Pd/C

I.I. Il'ina, I.L. Simakova, V.A. Semikolenov

Kinetics & Catalysis, 43(5) (2002) pp. 652-656.

The liquid-phase hydrogenation of pinane hydroperoxide (PHP) to pinanol on a Pd/C catalyst at 20–80°C and hydrogen pressures of 1–11 atm was studied. It was found that the rate of hydrogenation decreased with PHP concentration. The rate of PHP hydrogenation dramatically increased as the pressure of hydrogen was increased in a range of 2.5–3 atm. A mechanism was proposed for the hydrogenation of PHP. According to this mechanism, the step of hydrogen activation (homolytic or heterolytic addition) depends on the redox properties of the catalyst surface (the ratio between adsorbed PHP species and H_2). It was found that pinanol can be prepared with high selectivity by the hydrogenation of PHP on a Pd/C catalyst under mild conditions.

KINETICS OF CATALYST POISONING DURING CAPILLARY CONDENSATION OF REACTANTS

N.M. Bukhavtsova, N.M. Ostrovskii

Kinetics & Catalysis, 43(1) (2002) pp. 73-80.

The influence of the capillary condensation of reactants on the poisoning of Pt/SiO_2 catalysts by thiophene is studied experimentally for *p*-xylene hydrogenation at T = 60 and 80°C. The poisoning kinetics is independent of a catalyst and its rate decreases with a decrease in temperature. Poisoning during capillary condensation is 1.5–6 times slower than that in the gas phase, depending on the fraction of surface platinum in the pores filled with a liquid. The poisoning of the catalyst active sites in the pores filled with a liquid requires less sulfur at the same deactivation degree. The number of sulfur atoms per one platinum atom necessary for the complete poisoning of platinum in the gas phase is higher than that in the case of capillary condensation by a factor of 1.4–1.5.

Catalysis for Synthesis of Sulfur-Organic Compounds

CATALYTIC SYNTHESIS OF SOME SULFUR-CONTAINING HETEROCYCLIC COMPOUNDS

A.V. Mashkina

Chem. of Heterocyclic Comp., 38(5) (2002)) pp. 503-523.

Researches on the synthesis of sulfur-containing heterocyclic compounds at the Boreskov Institute of Catalysis are reviewed. They include the synthesis of thiolane by the recyclization of THF in hydrogen sulfide; the synthesis thiacycloalkanes by the hydrogenation of thiophenes; the synthesis of 4-methylthiazole by the reaction of SO_2 with methylisopropylideneamine; the synthesis of thiophenes by the heterocyclization of aliphatic compounds of sulfur and dehydrogenation of thiacycloalkanes; the synthesis of thiolane 1,1-dioxide by the hydrogenation of 2- and 3-thiolene 1,1-dioxides and 3-alkoxythiolane 1,1-dioxides; the synthesis of sulfoxides by the oxidation of thiacycloalkanes with atmospheric oxygen.

GAS-PHASE THIOPHENE HYDROGENATION TO TETRAHYDROTHIOPHENE OVER SULFIDE CATALYSTS

A.V. Mashkina, L.G. Sakhaltueva

Kinetics & Catalysis, 43(1) (2002) pp. 107-114.

Thiophene hydrogenation to tetrahydrothiophene over supported transition metal sulfides is studied. Comparison of the atomic catalytic activity at T = 240°C and P = 2 MPa showed that aluminosilicate-supported PdS is one to two orders of magnitude more active than Rh, Ru, Mo, W, Re, Co, and Ni sulfides on various supports. These metal sulfides are arranged in the following series according to the rate of tetrahydrothiophene formation: Pd >> Mo > Rh ≥ Ru> Re > W > Co > Ni. The reaction over sulfide catalysts is assumed to occur through thiophene activation on proton centers and coordinatively unsaturated cations of metal sulfides and additionally on the proton centers of support in the case of palladium catalysts.

KINETIC STUDY OF CATALYTIC HYDROGENATION OF THIOPHENE ON A PALLADIUM SULFIDE CATALYST

A. Yermakova, A.V. Mashkina, L.G. Sakhaltueva

Kinetics & Catalysis, 43(4) (2002) pp. 528-535.

The kinetics of thiophene hydrogenation on a palladium sulfide catalyst is studied at high hydrogen pressures. The reaction mainly occurs via the consecutive scheme: the reaction of thiophene with hydrogen results in the formation of tetrahydrothiophene, which partially decomposes under the action of hydrogen to yield butane and hydrogen sulfide. A kinetic model describing the reaction rates and the selectivity to tetrahydrothiophene at 0.2–3.0 MPa and 493–533 K is proposed. The rate constants and activation energies are determined. The effect of temperature and pressure on the maximal yield of tetrahydrothiophene is examined.

THE INFLUENCE OF A SUPPORT ON THE ACTIVITY AND SELECTIVITY OF SULFIDE CATALYSTS FOR THIOPHENE HYDROGENATION TO TETRAHYDROTHIOPHENE

A.V. Mashkina, L.G. Sakhaltueva

Petroleum Chemistry, 42(5) (2002) pp. 335-340.

Thiophene hydrogenation to tetrahydrothiophene (THT) in the gaseous phase at an elevated temperature and a high hydrogen pressure in the presence of transition metal sulfides supported on carbon, aluminum oxide, silica gel, and aluminosilicate was examined. High selectivity for THT formation was exhibited by tungsten, molybdenum, and ruthenium sulfides supported on different carriers, as well as by aluminosilicate- or silica gel-supported palladium sulfide. The THT selectivity in the presence of supported palladium and cobalt sulfides increases with increasing Brönsted acidity of the catalyst surface. The lowest rate of THT formation was observed on nickel sulfide, regardless of the support nature, and the highest one was achieved on palladium sulfide supported on different carriers; an especially high activity was displayed by palladium sulfide on aluminosilicate. The catalyst activity is enhanced with increasing dispersion of metal sulfides in the support and upon their partial reduction with hydrogen.

SELECTIVE HYDROGENATION OF DIETHYL DISULFIDE TO ETHANETHIOL IN THE PRESENCE OF SULFIDE CATALYSTS

A.V. Mashkina, L.N. Khairulina

Kinetics & Catalysis, 43(2) (2002) pp. 261-267.

The gas-phase reaction of diethyl disulfide hydrogenation at atmospheric pressure in the presence of supported transition metal sulfides was studied. The reaction of diethyl disulfide with hydrogen at T = 200°C resulted in ethanethiol, and the selectivity to ethanethiol was no lower than 94%. The selectivity decreased at a higher temperature because of diethyl disulfide decomposition to ethylene and hydrogen sulfide. The reaction of diethyl disulfide in the presence of hydrogen occurred at a higher rate and selectivity than that in an atmosphere of helium. The activity of metal sulfides supported on aluminum oxide was higher than on the other studied supports — aluminosilicate, silica gel, and a carbon support. Metal sulfides supported on Al_2O_3 were arranged in the following order according to their activity: $Rh > Ru > Mo \geq Pd > Ni > W$. Bimetallic catalysts were less active than monometallic catalysts. The activity of catalysts increased with the sulfide sulfur content; the partial reduction of metal sulfides also increased the catalytic activity.

CATALYTIC REACTIONS OF *n*-PROPANOL AND *n*-BUTANOL WITH HYDROGEN SULFIDE

A.V. Mashkina, L.N. Khairulina

Kinetics & Catalysis, 43(5) (2002) pp. 684-690.

The transformations of *n*-propanol and *n*-butanol in an H_2S atmosphere at T = 300-350°C and P = 0.1 MPa in the presence of acid–base catalysts were studied. Only alcohol dehydration with the release of alkenes occurred at a high rate on catalysts with strong proton sites (tungstosilicic and tungstophosphoric acids on SiO_2 or a decationized high-silica zeolite), whereas alcohol thiolation with the formation of alkanethiols also occurred on catalysts with Lewis acid sites (Al_2O_3; NaX; MgO; Cr/SiO_2; and Al_2O_3 modified with W, K, Na, K_2WO_4, or Na_2WO_4). The rate of reaction decreased with decreasing strength of Lewis acid sites and with increasing strength of basic sites; however, the selectivity of thiol formation increased. Alumina modified with alkaline additives was the most selective catalyst. In the presence of this catalyst, an alcohol selectively reacted with H_2S to form an alkanethiol, and the alkanethiol underwent partial decomposition with the release of an alkene and H_2S at a long contact time.

CATALYTIC PROCESSES OF SYNTHESIS OF ORGANIC SULFUR COMPOUNDS

A.V. Mashkina

Catalysis in Industry, 3 (2002) pp. 4-11.

The results of the studies made in Boreskov Institute of Catalysis in the field of catalytic synthesis of some organic sulfur compounds are generalized. Alkylmercaptans are synthesized as a result of the reaction of regular structure alcohols with hydrogen sulfide and the decomposition of dialkylsulfides. When hydrogenating di- and polysulfides by molecular hydrogen, alkyl and arylmercaptans have been obtained. Synthesis of dimethylsulfide was performed on the basis of methanol and hydrogen sulfide and that of dialkylsulfides with R = C_1 - C_4 was performed using lower alkylmercaptans contained in gases. Thiolane was produced by recycling tetrahydrofuran in the hydrogen sulfide medium, and thiolanes were produced by hydrogenating thiophenes. The process of synthesis 4-methyltiazol is based on interaction of sulfur dioxide with methyl isopropylidenimine. Oxidizing processes of dimethylsulfide into dimethyl sulfoxide by oxygen of the air and hydrogenating processes of sulfolene-3 into sulfolane were developed. Effective catalysts were developed for the whole of the cited processes, and optimal conditions of their realization.

Catalysis by Metal Complexes and Heteropolycompounds

STUDY OF THE ETHYLENE POLYMERIZATION OVER HOMOGENEOUS AND SUPPORTED CATALYSTS BASED ON 2,6-BIS(IMINO)PYRIDYL COMPLEXES OF Fe(II) AND Co(II)

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J. Molec. Catal. A: Chemical, 182-183(1-2) (2002) pp. 283-294.

The kinetic data on ethylene polymerization over homogeneous catalysts based on 2,6-bis[1-(2,6-dimethylphenylimino)ethyl]-pyridineiron(II) and cobalt(II) chlorides ($LMCl_2$, M = Fe, Co) with different aluminium-organic activators (MAO, $AlMe_3$, $Al(i\text{-}Bu)_3$) are reported. $LFeCl_2$ is very effective with $AlMe_3$ and $Al(i\text{-}Bu)_3$ as activator and $LCoCl_2$ is highly active in the presence of $AlMe_3$. For MAO as activator, the activity depends on the content of free $AlMe_3$ in MAO. Maximal activity has been found for MAO completely purified from free $AlMe_3$. According to ^1H and ^2H NMR study, formation of the similar neutral intermediates of the type $[LFe(II)Me(\mu\text{-}Me)_2AlMe_2]$ have been detected for $LFeCl_2/AlMe_3$ and $LFeCl_2/MAO$ catalysts. In the system $LCoCl_2/MAO$, the complex of the type $LCo(II)Me(X)\cdot MAO$ (X = Me or Cl) with terminal Co–Me group is detected. Interaction of $LCoCl_2$ with $AlMe_3$ results in the formation of diamagnetic Co(I) species.

Highly active supported catalysts $SiO_2/LFeCl_2+AlR_3$ and $SiO_2/MAO/LFeCl_2$ have been prepared. In contrast to homogeneous systems, the supported catalysts are stable at elevated temperatures of polymerization (70°C) and produce high molecular mass polyethylene with improved morphology.

METHYL-VERSUS-CHLORIDE EXCHANGE AS A MEASURE OF ELECTRON DENSITY AT THE METAL CENTER OF RING-SUBSTITUTED ZIRCONOCENE COMPLEXES

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Organometallics, 21(5) (2002) pp. 920–923.

Methyl-versus-cloride exchange equilibria between different zirconocene complexes provide a sensitive measure of relative electron densities at the Zr centers of these complexes. As expected, methyl and trimethyl silyl substituents increase the electron density at the Zr center of a bis(cyclopentadienyl) Zr(IV) complex; the same holds for a dimethyl silyl bridge. In bis(indenyl) complexes, on the other hand, electron density at the metal center is reduced and substituent and bridge effects are different from those observed in bis(cyclopentadienyl) Zr(IV) complexes.

HIGHER TERPENES IN THE SYNTHESIS OF CHIRAL P- AND N-CONTAINING LIGANDS FOR METALLOCOMPLEX CATALYSTS OF ASYMMETRIC REACTIONS

A.G. Tolstikov, O.V. Tolstikova,
T.B. Khlebnikova, N.N. Karpyshev

Chemistry and Computational Simulations. Butlerov Communications, 7 (2002) pp. 1-7.

Starting from the optically pure phytogenous terpenoids: (α)-santonin, dehydroabietic and levopimaric acids the synthesis of chiral phosphorous- and nitrogen-containing ligands for metallocomplex catalysts of asymmetric transformations has been performed. The original procedure for synthesis of chiral bisphosphines and bisphosphinites with a decahydrophenanthrene fragment has been developed. This compounds have been used as ligands to synthesize cationic Rh(I)-complexes – catalysts for enantioselective hydrogenation of unsaturated substrates. The amines, isocyanates and isothiocyanates prepared from dehydroabietic acid have been taken as precursors for the chiral Schiff bases, ureas and thioureas containing an octadecahydrophenanthrene fragment. The obtained optically active nitrogen-containing compounds have served as ligands for a synthesis of cationic and neutral *in situ* Rh(I) and Ru(II) complexes tested in enantioselective hydrogen-transfer reduction of acetophenone with 2-propanol. Purposeful transformations of (α)-methyldesmotropsantonin – methylated product of dienone-phenolic rearrangement of natural sesquiterpene (-)-(α)-santonin – have been studied. As the result the chiral salicylaldimines used as chiral ligands for V(V) *in situ* peroxooxocomplexes have been prepared.

HETEROGENEOUS CATALYSTS FOR HALIDE-FREE CARBONYLATION OF DIMETHYL ETHER

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G.N. Kustova, T.M. Yurieva, V.A. Likholobov

Catal. Lett., 80(3) (2002) pp. 175-179.

Acidic cesium salts of 12-tungstophosphoric acid promoted with rhodium, Rh/$Cs_xH_{3-x}PW_{12}O_{40}$ ($1.5 \le x \le 2$ and Rh≥0.1%), were shown to be novel and effective catalysts for halide-free carbonylation of dimethyl ether (DME) to methyl acetate. The catalysts were characterized by chemical analysis, nitrogen adsorption, XRD, SEM, TGA-DTA and IR spectroscopy. Their behavior may be explained by assuming that (1) activation of the C—O bond in the DME molecule and formation of a metal-alkyl bond occurs in the presence of the strong acid sites and (2) these strong acid sites act in conjunction with Rh carbonyl complexes, which are responsible for CO insertion and acetate formation.

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

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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 $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{q-}$ ($n_{av} = 3$), 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 $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{q-}$ ($n_{av} \approx 10$) + $[(VO)_3(PW_9O_{34})_2]^{9-}$ 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.

FORMS OF Rh(III) IN NITRIC ACID SOLUTIONS

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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 Rh(-OH)(-ONO_2)Rh; terminal positions of the central atoms are occupied by water molecules. It was found that the isotopic equilibrium $^{14}NO^{3-}$/$^{15}NO^{3-}$ of the bridging ligand sets in at an abnormally high rate, at which the isotopic exchange $H_2{}^{17}O/H_2{}^{16}O$ 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.

ADSORPTION OF $H_3PW_{12}O_{40}$ BY POROUS CARBON MATERIALS

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T.V. Reshetenko, L.B. Avdeeva, E.A. Paukshtis,
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Russ. Chem. Bull., 2 (2002) pp. 243-248.

Adsorption of $H_3PW_{12}O_{40}$ from water and organic oxygen-containing solvents (AcOH, Me_2CO, MeOH) by carbon mesoporous materials, *viz.*, Sibunit and catalytic filamentous carbons (CFC), was studied. The amount of irreversibly sorbed heteropolyacid is 50-100 mg g^{-1} of support and decreases in the series of solvents: $H_2O > Me_2CO > AcOH > MeOH$. The adsorption capacity of CFC depends on the specific surface, total pore volume, and microstructure of the CFC fiber.

CATALYTIC SYSTEMS BASED ON PLATINUM AND HETEROPOLY COMPOUNDS FOR OXIDATION OF HYDROCARBONS WITH A DIOXYGEN-DIHYDROGEN GASEOUS MIXTURE

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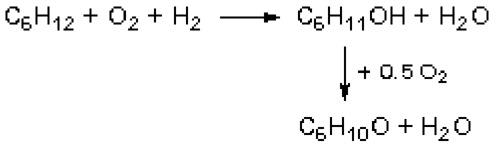
V.A. Likholobov

Russ. Chem. Bull., 6 (2002) pp. 975-981.

The oxidation of cyclohexane, saturated and aromatic hydrocarbons with an O_2-H_2 gaseous mixture was applied to study the catalytic properties of bicomponent systems based on platinum and heteropoly compounds (HPC). The consumption of gases and the yield of the products depend on the surface area, accessibility of the platinum species to the reactant, and composition of the HPC. The solid Pt samples suspended in an HPC solution, the Pt(5%)-PMo_{12}/Al_2O_3 bicomponent supported system, and the solid bicomponent sample prepared from the $[Pt(NH_3)_4][H_2PMo_{12}O_{40}]_2$ $7H_2O$ complex salt were used as catalysts. Among the catalysts with the same molar compositions of the active components, the bicomponent materials are much more active in the oxidation than a combination of the Pt catalyst with an HPC solution. The bulk catalyst is a crystalline solid substance with the HPC structure with incorporated Pt species. Molybdenum is predominantly oxidized, and platinum is present in both the reduced and ionic states. The oxidation of saturated hydrocarbons affords alcohols and ketones. The yield of the positional isomers of the oxygenated products increases in the series primary << secondary< tertiary C-atoms. Benzene and toluene are converted into the corresponding phenols in equal yields. The scheme proposed for oxidation assumes the participation of the active hydroxyl radical.



Photocatalytic and Related Processes

ROUTES OF PHOTOCATALYTIC DESTRUCTION OF CHEMICAL WARFARE AGENT SIMULANTS

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New J. Chemistry, 26 (2002) pp. 732-744.

Selected imitants of chemical warfare agents such as dimethyl methylphosphonate (DMMP), diethyl phosphoramidate (DEPA), pinacolyl methylphosphonate (PMP), butylaminoethanethiol (BAET) were subjected to photocatalytic and sonophotocatalytic treatment in aqueous suspensions of TiO_2. Complete conversion of the same mass of imitants to inorganic products was obtained within 600 min for DMMP, DEPA, PMP, but required a longer time for BAET. Sonolysis accelerated photodegradation of DMMP. No degradation was observed without ultraviolet illumination. Final products of degradation were PO_4^{3-}, CO_2 for DMMP and PMP, PO_4^{3-}, NO_3^-(25%), NH_4^+(75%), CO_2 for DEPA, and SO_4^{2-}, NH_4^+, CO_2 for BAET. The number of main detected intermediate products increases in the order DMMP (7), DEPA (9), PMP (21), and exceeds 34 for BAET. Degradation of DMMP mainly proceeds through consecutive oxidation of methoxy groups and then the methyl group. Dimethyl hydroxymethylphosphonate and dimethylphosphate testify to the parallel oxidation of the methyl group. Destruction of DEPA mainly starts with cleavage of the P–NH_2 bond to form diethyl phosphate, which transforms further into ethyl phosphate. Oxidation of α and β carbons of ethoxy groups to form ethylphosphonoamidate, hydroxyethyl ethylphosphonoamidate and other products also contributes to the destruction. Photocatalytic degradation of PMP mainly starts with oxidation of the pinacolyl fragment, methylphosphonic acid and acetone being the major products. Oxidation of BAET begins with dark dimerization to disulfide, which undergoes oxidation of sulfur forming sulfinic and sulfonic acids as well as oxidation of carbons to form butanal, aminobutane, etc., and cyclic products such as 2-propylthiazole. A scheme of degradation was proposed for DMMP and DEPA, and starting routes for PMP and BAET. Quantum efficiencies of complete mineralization calculated as reaction rate to photon flux ratio approximate 10^{-3} %.

CHEMICAL PROCESSES PHOTOINDUCED ON SOLID TROPOSPHERIC AEROSOLS

V.S. Zakharenko, A.N. Moseichuk, V.N. Parmon

Atmospheric and Oceanic Optics, 15(5-6) (2002) pp. 448-452.

Experimental results obtained indicate that organofluorine and organochlorine compounds containing hydrogen atoms experience destructive photosorption on MgO aged for a long time in air under conditions close to the tropospheric ones. The photosorption rate is higher for halogen-containing hydrocarbons (HCH) including fluorine while being several times lower for chlorine-containing hydrocarbons. The amount of photosorbed HCH at room temperature and at the pressure of 1 Pa can exceed 15% of MgO surface that confirms the hypothesis of a substantial contribution of the photoprocesses on the MgO surface to removal of these HCH from the troposphere. The absence of photosorption activity with respect to HCH on γ-Al_2O_3 (S_{sp} = 150 m^2/g) and SiO_2 (S_{sp} = 500 m^2/g) is connected with the difference in crystallinity of the studied oxide powders.

DESTRUCTIVE PHOTOSORPTION OF HALOGEN CONTAINING HYDROCARBONS BY ATMOSPHERIC SOLID AEROSOLS IN CONDITIONS CLOSE TO THE TROPOSPHERIC ONES

V.S. Zakharenko, V.N. Parmon

Chem. for Sustainable Devel., 10(5) (2002) pp. 585-592.

Experimental results on studying the interaction of halogen containing hydrocarbons with Mg-, Al-, Si-oxides of laboratory and commercial preparation in darkness and under solar tropospheric radiation are presented. These oxides correspond by their chemical composition to main components of solid atmospheric aerosols. The obtained experimental results evidence that P-, Cl-organic compounds containing hydrogen atoms, are destructively photosorbed on MgO, exposed to the air for a long time, with formation of magnesium halogenide. The rate of photosorption is higher for halogen containing hydrocarbons (HCH) containing fluorine, and is several times less for chlorine-containing hydrocarbons. The quantity of photosorbed HCH at room temperature and pressure 1Pa may exceed 15% of MgO surface manolayer. Interaction of MgO with HCH leads to their removal from atmosphere in conditions close to tropospheric ones up to partial pressure less than 10^{-6} Pa. The results obtained evidence the essential contribution of photo processes on the MgO surface in removal of HCH from tropospheric gase phase.

SPACE CHEMICAL REACTOR OF PROTOPLANETARY DISK

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Advances in Space Research, 30(6) (2002) pp. 1461-1467.

It was found that the protostar accretion disk is the place of organic compounds synthesis from simple molecules. The mass of the matter moving around the synthesis zone is comparable to the solar mass. The formed amount of organic substance may be limited by the instability of collective dynamics of solids in the disk.

Studies on Electrocatalytic Processes

STRUCTURE AND DYNAMICS OF THE INTERFACE BETWEEN A Ag SINGLE CRYSTAL ELECTRODE AND AN AQUEOUS ELECTROLYTE

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Faraday Discuss., 121 (2002) pp. 181-198.

The aim of this work is to elucidate the initial steps of the electrochemical oxidation of Ag(111) in alkaline electrolytes. Electrochemical as well as *ex situ* (XPS) and *in situ* (SHG) spectroscopic techniques are used to reconstruct the Ag(111)/electrolyte interface as a complex dynamic entity. Moving in the direction from negative to positive potentials it is first observed specific adsorption of hydroxide ions, which starts at *ca.*–1.1 V *vs.* Ag/Ag_2O in 0.1 M NaOH. SHG data prove that hydroxide retains its negative charge. At –0.3 V oxidation of the surface sets in with the formation of negatively charged adsorbed oxygen species and Ag^+ ions, which give rise to peaks at 528.2±0.2 eV and at 367.7 eV in the O 1s and the Ag $3d_{5/2}$ XP spectra, respectively. Around –0.1 V the adlayer is transformed into an ordered surface oxide phase, which grows *via* a nucleation and growth mechanism. Above the reversible Ag/Ag_2O potential the 2D Ag(I) oxide transforms into a 3D Ag(I) oxide. The electrochemical oxidation is compared with the previously studied gas-phase process, demonstrating both remarkable similarities as well as some differences.

THE STRUCTURE ANALYSIS OF THE ACTIVE CENTERS OF Ru-CONTAINING ELECTROCATALYSTS FOR THE OXYGEN REDUCTION. AN *IN SITU* EXAFS STUDY

N. Alonso-Vante*, I.V. Malakhov, S.G. Nikitenko, E.R. Savinova, D.I. Kochubey (*Laboratory of Electrocatalysis, Université de Poitiers, Poitiers, France)

Electrochim Acta, 47 (22-23) (2002) pp. 3807-3814.

A family of novel catalysts for oxygen electroreduction is presented, based on nanostructured Ru_xX_y chalcogenide compounds (X=S, Se, Te). EXAFS data suggest that the catalysts have a core of ruthenium atoms, which has triangular coordination and a direct metal-metal bond. Depending on the chalcogen, the Ru-cluster consists of two or three metal layers of different size and mutual co-ordination with chalcogen atoms coordinated to the periphery of the cluster. Variation of the chalcogen type affects the size of the Ru-cluster and the strength of its interaction with the chalcogen. This influences the interaction of Ru-clusters with oxygen and thus their activity in the reduction of molecular oxygen.

IN SITU EXAFS STUDY TO PROBE ACTIVE CENTERS OF Ru-CHALCOGENIDE ELECTROCATALYSTS DURING OXYGEN REDUCTION REACTION

I.V. Malakhov, S.G. Nikitenko, E.R. Savinova, D.I. Kochubey, N. Alonso-Vante* (*Laboratory of Electrocatalysis, Université de Poitiers, Poitiers, France)

J. Phys. Chem. B., 106(7) (2002) pp. 1670-1674.

Novel cluster Ru chalcogenide materials $Mo_xRu_ySe_z$ and Ru_xTe_y were studied *in situ* using EXAFS in the transmission mode during the oxygen reduction reaction. Reversible changes in the structure of the active center were revealed for the electrochemical reaction as a function of the applied electrode potential. The shift of the potential in the anodic direction from 0.08 to 0.78 V versus *rhe* (reference hydrogen electrode) in the presence of oxygen resulted in an increase of the Ru-O and simultaneous decrease of the Ru-Ru coordination numbers in the first coordination shell of Ru. Along with the variation of the coordination numbers, reversible changes of the coordination distances were observed: a decrease of the Ru-O and an increase of the Ru-Ru distance with the positive polarization. These changes witness the distortion of the catalytic center upon oxygen adsorption. A tentative mechanism of oxygen activation on Ru_xX_y cluster materials is proposed on the basis of the *in situ* EXAFS data.

PERFORMANCE OF A SOFC FED BY ETHANOL REFORMING PRODUCTS

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Solid State Ionics, 152-153 (2002) pp. 551-554.

Performance of a Pt based anode solid oxide fuel cell (SOFC) fed with a gas mixture containing H_2, CO and

CH_4 (molar ratio 1:1:1) produced by external ethanol decomposition was studied. Experiments were performed at atmospheric pressure in the temperature range 660–800 °C and anode potential vs. air −0.78 to −0.23 V. It was shown that at low temperature (660 °C), the outlet gas contained the products of complete oxidation of the gas mixture, while high temperature (800 °C) facilitated synthesis gas production.

Biology Related Catalysts and Biotechnology

MACROSTRUCTURED CARBONIZED CERAMICS AS ADSORBENTS FOR IMMOBILIZATION OF GLUCOAMYLASE

G.A. Kovalenko, O.V. Komova, A.V. Simakov, V.V. Khomov, **N.A. Rudina**

J. Molec. Catal. A: Chemical, 182-183(1-2) (2002) pp. 73-80.

Macrostructured carbonized ceramics have been synthesized and studied for the immobilization of glucoamylase. Carbon layer of different morphology, in particular of filamentous one, has been obtained on the surface of honeycomb monoliths and foam ceramic supports. The effects of morphology of surface carbon on adsorption and biocatalytic properties of immobilized glucoamylase, namely, on the stability and the activity of biocatalyst in continuous starch hydrolysis, have been investigated.

CARBON-CONTAINING MACROSTRUCTURED CERAMIC SUPPORTS FOR ADSORPTIVE IMMOBILIZATION OF ENZYMES AND BACTERIA. I. ADSORPTION OF GLUCOAMILASE

G.A. Kovalenko, O.V. Komova, A.V. Simakov, N.A. Rudina, V.V. Khomov

Biotechnology, 3 (2002) pp. 55-66.

A comparative investigation on the adsorptive immobilization of *glucoamylase* on carbonised ceramic monoliths with honeycomb structure has been carried out. Glucoamylase adsorption has been found to depend strongly on *morphology* of surface carbon layer. The catalytic synthesis of *filamentous carbon* on the ceramic monoliths surface has led to obtaining the efficient adsorbents with the highest adsorptive capacity ensuring tight attachment of the enzyme that is important for the development of heterogeneous biocatalyst for starch hydrolysis.

CARBON-CONTAINING MACROSTRUCTURED CERAMIC SUPPORTS FOR ADSORPTIVE IMMOBILIZATION OF ENZYMES AND BACTERIA.
II. BIOCATALYTIC PROPERTIES OF ADSORBED GLUCOAMILASE

G.A. Kovalenko, O.V. Komova, A.V. Simakov, L.V. Perminova, V.V. Khomov, O.Yu. Borovtsova, N.A. Rudina

Biotechnology, 5 (2002) pp. 81-93.

Systematic studies on the development of highly stable heterogeneous biocatalyst for the process of continuous starch hydrolysis based on the immobilized glucoamylase have been carried out. Carbonized ceramics with surface layer of filamentous carbon appeared to be optimal adsorbents and supports for immobilization of glucoamilase. The stability of glucoamilase on such adsorbents is an order higher then in solution. The immobilized glucoamilase maintains its high biological activity during 1-1,5 years keeping at room temperature. The studies of fermentative activity of obtained heterogeneous biocatalysts in flow reactors have shown that diffusion is a limiting step of the starch hydrolysis. Different ways to decrease the diffusion restrictions have been suggested, including purposeful synthesis of supports with complicated geometrical structure containing large transport pores.

CHEMICAL RIBONUCLEASES.
IV. AN ANALYSIS OF THE DOMAIN STRUCTURE OF CHEMICAL RIBONUCLEASES BASED ON 1,4-DIAZABICYCLO[2.2.2]OCTANE

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Russ. J. Bioorg. Chem., 28(4) (2002) pp. 331-341.

Artificial ribonucleases of the **ABLkCm** series were synthesized. They consist of a lipophilic alkyl radical (Et, *n*-$C_{14}H_{29}$, or *n*-$C_{15}H_{31}$) **A**, an “RNA-binding domain" **B** (bisquaternary salt of 1,4-diazabicyclo[2.2.2]octane), a "catalytic domain" **Cm** [histamine (**C1**) or histidine (**C3**) residue], and a "linker" **Lk** that joins the "domains" **B** and **Cm** [here, k is the number of methylene units (one or three) in the linker]. The effect of the "domain structure" on the catalytic properties of the chemical ribonucleases was analyzed using seven compounds of this series (**ABL1C1**, **ABL3C1**, **ABL3C3**, **AC1**, **AB**, **BL2**, and **BL3C3**). The catalytic activity of the compounds was assessed in the reaction of hydrolysis of the *in vitro* transcripts of human $tRNA^{Lys}$ and yeast $tRNA^{Asp}$ under physiological conditions. It was shown that only chemical ribonucleases that involve all the fragments of the **ABLkCm** construct can hydrolyze the substrate tRNA at a high rate (90% of tRNA is hydrolyzed for 10 h at 37°C). The activity of the compounds is largely determined by the presence of a long lipophilic radical linked to 1,4-diazabicyclo[2.2.2]octane and a long linker, which joins the RNA-hydrolyzing and RNA-binding domains. The results indicate an important role of hydrophobic interactions in the acceleration of the RNA hydrolysis reaction.

DESIGN AND SYNTHESIS OF ARTIFICIAL RIBONUCLEASES BASED ON 1,4-DIAZABICYCLO[2.2.2]OCTANE AND IMIDAZOLE

D.A. Konevetz*, I.E. Beck, G.V. Shishkin*, V.V. Vlassov*, V.N. Silnikov (*Novosibirsk Institute of Bioorganic Chemistry, Novosibirsk, Russia)

Russ. Chem. Bull., 51(7) (2002) pp. 1100-1111.

The review surveys the results of our studies devoted to the design of highly efficient catalysts of hydrolysis of the phosphodiester bonds in RNA. These catalysts contain the imidazole residue in the catalytic domain, one or several bis-quaternized rings of 1,4-diazabicyclo[2.2.2]octane as a polycationic RNA-binding domain, and a lipophilic radical. A versatile approach to artificial ribonucleases of this type was proposed, which allows one to vary not only the number of positive charges in the RNA-binding domain, the structure of the catalytic site, and their mutual arrangement but also the domain structure of the molecule as a whole. Analysis of the catalytic properties of the synthesized constructs makes it possible to optimize the domain structure and the geometry of the molecule ensuring its maximum ribonuclease activity.

EFFECT OF HETEROGENEOUS AND HOMOGENEOUS PATHWAYS ON SELECTIVITY OF PINANE-2-OL TO LINALOOL ISOMERIZATION

V.A. Semikolenov, I.I. Il'ina, I.L. Simakova

J. Molec. Catal. A: Chemical, 182-183(1-2) (2002) pp. 383-393.

The regularities of pinane-2-ol isomerization over block catalyst under reagent pressure of 2–45 Torr and within a temperature range of 450–620°C were studied. A scheme of key product - linalool, as well as side products - hydrocarbons and 5-membered cyclic alcohols formation was suggested. Light hydrocarbons C_1–C_6 are formed by gas phase free radical pathway of pinane-2-ol destruction, hydrocarbons C_{10} by linalool dehydration over catalyst surface acid centers, 5-membered cyclic alcohols by linalool intermolecular cyclization.

The reaction rate constants of *cis*/*trans*-pinane-2-ol conversion to linalool and its following cyclization to 5-membered alcohols were evaluated. The linalool formation mechanism including the intermolecular interaction of OH group proton resulting in pinane ring opening was suggested.

A NEW ENVIRONMENTALLY FRIENDLY METHOD FOR THE PRODUCTION OF 2,3,5-TRIMETHYL-*P*-BENZOQUINONE

O.A. Kholdeeva, N.N. Trukhan, M.P. Vanina, V.N. Romannikov, V.N. Parmon, J. Mrowiec-Białoń*, A.B. Jarzębski* (*Institute of Chemical Engineering, Gliwice, Poland)

Catal. Today, 75(1-4) (2002) pp. 203-209.

A new environmentally friendly method for the production of 2,3,5-trimethyl-1,4-benzoquinone (TMBQ, Vitamin E precursor) based on the oxidation of 2,3,6-trimethylphenol (TMP) with aqueous H_2O_2 over various Ti-containing mesoporous silicate materials is reported. Both well-organized mesoporous mesophase materials (Ti-MMM), having hexagonal arrangement of uniform mesopores, and amorphous TiO_2-SiO_2 mixed oxides (aerogels and xerogels) produced TMBQ with good to high yield. All the materials studied have been proved to operate as truly heterogeneous catalysts. No titanium leaching occurred from the solid matrixes during the oxidation process. Titanium dispersion and its accessibility were found to be crucial factors determining the catalytic properties. For samples with similar titanium loading, both the catalytic activity and TMBQ yield appeared to fall in the order TiO_2-SiO_2 aerogel > Ti-MMM >

TiO_2-SiO_2 xerogel and correlate with average mesopore diameter and mesopore volume. The best results (96-98% selectivity to TMBQ at 99-100% TMP conversion) were obtained with TiO_2-SiO_2 aerogels, containing 1.7-6.5 wt.% Ti.

SYNCHRONIZATION OF METABOLIC OSCILLATIONS: TWO CELLS AND ENSEMBLES OF ADSORBED CELLS

V.P. Zhdanov, B. Kasemo

J. Biol. Phys., 27 (2001) pp. 295-311.

Synchronization of metabolic oscillations was treated in two cells and in ensembles of cells adsorbed at the liquid-solid interface. (i) Synchronization of oscillations in two cells is assumed to occur via perturbation of the metabolite concentration near one cell due to the metabolite diffusion flux from another cell. This direct channel of synchronization may be important if the distance between two cells is comparable with the cell diameter. The corresponding coupling coefficient is found to be proportional to the metabolite diffusion coefficient and inversely proportional to the cell radius and the distance between the cells. (ii) In the case of ensembles of adsorbed cells, synchronization of oscillations is considered to be indirect, i.e., to occur via the metabolite concentration formed outside the cells near the interface due to metabolite diffusion from the cells. A general integral equation relating the metabolite concentration near the interface with concentrations inside the cells has been derived.

Heat Accumulating Materials

A FAMILY OF NEW WORKING MATERIALS FOR SOLID SORPTION AIR CONDITIONING SYSTEMS

Yu.I. Aristov, G. Restuccia*, G. Cacciola*, V.N. Parmon (*Institute of Accumulation and Transformation of Energy, Messina, Italy)

Appl. Therm. Engin., 22(2) (2002) pp. 191-204.

In this communication a family of new working materials, so called Selective Water Sorbents (SWSs), is presented for sorption air conditioning. These materials are composites “hygroscopic salt inside porous matrix with open pores” and possess intermediate behaviour between solid adsorbents, salt hydrates and liquid absorbents, so that their water sorption properties can be controllably modified by varying a) porous structure of the host matrix, b) chemical nature of the impregnated salt and c) the amount of the salt inside the pores. For these materials the water sorption equilibrium and specific heat have been measured in a wide temperature and uptake range. This study shows that composites based on $CaCl_2$ and LiBr as impregnated salts and different micro- and mesoporous silica gels as host matrices are able to absorb up to 0.75 g H_2O per 1 g of the dry sorbent. After presentation of sorption equilibrium curves, the thermodynamic performance for their utilisation in heat pump and refrigeration systems, is calculated. The results show that these new materials can operate with cycles whose maximum temperature is about 95 °C (for cooling) and 140 °C (for heating) that are lower than those for other pairs known so far. The values of COP are considerably higher than those reported for silica gel/water system at the same temperature of the heat source.

SELECTIVE WATER SORBENTS FOR MULTIPLE APPLICATIONS. 12. WATER SORPTION EQUILIBRIUM AT ELEVATED TEMPERATURES

M.M. Tokarev, A. Freni*, G. Restuccia*, Yu.I. Aristov (*Institute of Accumulation and Transformation of Energy, Messina, Italy)

React. Kinet. & Catal. Lett., 76(2) (2002) pp. 295-301.

In this communication the experimental data are presented on water sorption equilibrium for SWS-1L ($CaCl_2$ in mesoporous silica) measured at elevated temperature of 150° to 260°C and corresponding vapour pressure P_{H_2O} of 1.1 to 9.2 bar. A comparison of these data with those obtained at lower T (30°–150°C) and P_{H_2O} (8–130 mbar) is made. All experimental data appear to lie on the same temperature independent curve “the water sorption *vs.* the relative vapour pressure”, that indicates the universal mechanism of water sorption over the whole T-P range.

NEW COMPOSITE SORBENT “$CaCl_2$ IN MESOPORES OF MCM-41” FOR SORPTION COOLING/HEATING

M.M. Tokarev, L.G. Gordeeva, V.N. Romannikov, I.S. Glaznev, Yu.I. Aristov

Intern. J. Thermal Science, 41(5) (2002) pp. 470-474.

New working material "$CaCl_2$ confined to mesoporous host matrix MCM-41" is synthesised and studied keeping in mind its application for sorption cooling/heating. For this *mesoporous* system water sorption isobars, isosters and isotherms are obtained at temperature 293-423 K and vapour partial pressure 8.7 – 50.3 mbar. The water sorption is found to be a combination of liquid absorption and heterogeneous adsorption. The results obtained evidence considerable change of the salt properties due to its confinement to the MCM-41 nanopores. Brief comparison of this sorbent with a pure silica gel for cooling/heating application is done.

THERMAL CONDUCTIVITY OF SELECTIVE WATER SORBENTS UNDER THE WORKING CONDITIONS OF A SORPTION CHILLER

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G. Restuccia*, Yu.I. Aristov (*Institute of Accumulation and Transformation of Energy, Messina, Italy)

Appl. Therm. Engin., 22(14) (2002)
pp. 1631-1642.

This paper presents the experimental data on the thermal conductivity of the composite sorbents $CaCl_2/SiO_2$ and $LiBr/SiO_2$, measured by the "hot wire method" under various conditions of vapour pressure P_{H2O}, temperature T and water uptake w. The measurement ranges were chosen according to the operating conditions of a typical sorption cooling cycle (10 mbar < P_{H2O} < 70 mbar, 40°C <T< 130°C). The obtained results show that the sorbent thermal conductivity λ (T, P_{H2O}, w) increases considerably with the uptake raise, while its dependence on pressure and temperature is, in the studied range, almost negligible. Finally, the influence of the thermal conductivity on the specific power of the sorption chiller is discussed.

WATER SORPTION ON "LiBr IN POROUS CARBONS"

L.G. Gordeeva, A. Freni*, G. Restuccia*,
Yu.I. Aristov (*Institute of Accumulation and Transformation of Energy, Messina, Italy)

Fuel Processing Technology, 79(3) *(*2002)
pp. 225-231.

Water sorption equilibrium of LiBr confined to pores of a mesoporous synthetic carbon Sibunit and a macroporous expanded graphite (samples SWS-2C and SWS-2EG, respectively) was studied. Isobars of water sorption on these composites are measured at vapor pressure 6-81 mbar and temperature 30-135°C. The type of sorption equilibrium for the two composites appears to be quite different. The isobars for SWS-2EG have a plateau corresponding to 1 molecule of H_2O adsorbed by 1 molecule of LiBr, that indicates the formation of crystalline hydrate $LiBr{\cdot}H_2O$ inside pores with a monovariant type of equilibrium. At lower temperature the equilibrium becomes divariant that is typical for LiBr–water solutions. On the contrary, the water sorption equilibrium for SWS-2C is divariant over the whole temperature and pressure range that means no crystalline hydrates are formed inside Sibunit pores. This distinction possibly results from differences in a pore structure of the host carbons. The composite sorption capacity can reach 0.6–1.1 g H_2O per 1 g of the dry sorbent at relative humidity 70%. The advanced sorption capacity makes the sorbents promising for gas drying, thermal storage of energy and other applications.

Catalysts for Detoxication Processes

STUDY OF THE REACTION OF HIGH-TEMPERATURE H_2S DECOMPOSITION ON METAL OXIDES (γ-Al_2O_3, α-Fe_2O_3, V_2O_5)

T.V. Reshetenko, S.R. Khairulin, Z.R. Ismagilov,
V.V. Kuznetsov

Intern. J. Hydrogen Energy, 27(4) (2002)
pp. 387-394.

Experimental study of the reaction of heterogeneous decomposition of the hydrogen sulfide on bulk oxides γ-Al_2O_3, α-Fe_2O_3 and V_2O_5 in the interval of temperatures 500-900ºC has been performed. Reaction orders by H_2S for γ-Al_2O_3 and V_2O_5 are 2.0, and for α-Fe_2O_3 - 2.6; effective activation energies are respectively 72, 94 and 103 kJ/mole. Using the ESDR and XRD methods, it is shown that in the course of hydrogen sulfide decomposition reaction, the reduction of transition metal oxide catalysts (α-Fe_2O_3 и V_2O_5) and also the formation of sulfides under the influence of reaction media proceed. Interaction of hydrogen sulfide with aluminum oxide at low temperatures leads to formation of adsorbed species of H_2S as fragments HS^- and S^{2-}, which upon heating at 100-700ºC transfer into different species of sulfur: c-S_8, c-S_{12}, S_4. In separate experiments it was demonstrated that the higher the temperature of H_2S interaction with Al_2O_3, the larger number of adsorbed sulfur species are observed in the spectra. Molecular hydrogen sulfide interacts with the Al_2O_3 surface with formation of sulfur compounds with oxygen, which later transform into the final reaction products - elemental sulfur.

OXIDATION OF UNSYMMETRICAL DIMETHYLHYDRAZINE OVER HETEROGENEOUS CATALYSTS. SOLUTION OF ENVIRONMENTAL PROBLEMS OF PRODUCTION, STORAGE AND DISPOSAL OF HIGHLY TOXIC ROCKET FUEL

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Catal. Today, 75(1-4) (2002) pp. 277-285.

The catalytic oxidation of unsymmetrical dimethylhydrazine (UDMH) by air has been studied in a vibro-fluidized catalyst bed laboratory kinetic setup over catalysts $Cu_xMg_{1-x}Cr_2O_4/\gamma$-$Al_2O_3$, 32.9%$Ir/\gamma$-$Al_2O_3$ and β-Si_3N_4 in a temperature range of 150-400°C. The catalyst $Cu_xMg_{1-x}Cr_2O_4/\gamma$-$Al_2O_3$ was found to be optimal regarding high yields of CO_2 and low yields of NO_x. A probable mechanism of UDMH heterogeneous catalytic oxidation is proposed. Catalyst $Cu_xMg_{1-x}Cr_2O_4/\gamma$-$Al_2O_3$ has been further used in the pilot plant specially designed for the destruction of UDMH. Results of testing the main fluidized bed catalytic reactor for UDMH oxidation and the reactor for selective catalytic reduction of NO_x with NH_3 are presented. These results prove that the developed UDMH destruction technology is highly efficient and environmentally safe.

DETOXICATION OF WATER CONTAINING 1,1-DIMETHYLHYDRAZINE BY CATALYTIC OXIDATION WITH DIOXYGEN AND HYDROGEN PEROXIDE OVER Cu- AND Fe-CONTAINING CATALYSTS

O.P. Pestunova, G.L. Elizarova, Z.R. Ismagilov, M.A. Kerzhentsev, V.N. Parmon

Catal. Today, 75(1-4) (2002) pp. 219-225.

A number of Cu- and Fe-hydroxide containing catalysts, supported on oxide carriers, were prepared to provide the removal of 1,1-dimethylhydrazine from aqueous solutions via its oxidation by hydrogen peroxide and air oxygen. The Cu-containing samples as well as Fe/ZSM-5 are the most active catalysts in the reaction. The reaction products were analyzed by gas chromatography and UV-Vis spectroscopy. The effect of nature of the oxidizer and catalyst, pH and temperature on both the reaction rate and product composition was studied.

CATALYTIC OXIDATION OF VOLATILE ORGANIC COMPOUNDS IN INDUSTRIAL OFF-GASES

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Eurasian ChemTech. J., 4(1) (2002) pp. 31-44.

Processes and apparatuses for catalytic oxidation of VOCs in industrial off-gases are described, including steady state and unsteady state processes, a combined adsorption-catalytic process and an advanced method of ozone induced oxidation for low concentrated exhausts. On the basis of research and development works a series of catalytic incinerators, operating in steady state and unsteady state mode, of various capacity were designed, constructed and tested in the purification of ventilation air and off-gases from VOCs. The principles of operation of different types of catalytic incinerators and possible areas of application are discussed. For VOC concentrations 150-1000 mg/m^3 unsteady state catalytic incinerators of KART type should be used, for concentrations 1000-3000 mg/m^3 steady state KROT apparatuses are recommended, and for concentrations over 3000 mg/m^3 up to 7000 mg/m^3 installations TKM-250. It is shown that for the purification of low concentrated gases with the content of organic vapors below 150 mg/m^3 adsorption-catalytic method or catalytic oxidation with ozone in the installation OKA-3000 are most effective. Main kinetic dependencies of the ozone induced oxidation of toluene and acetone over copper oxide catalyst are given and discussed. It is shown that the efficiency of this method of VOCs removal is based on low operation temperature 313-343 K, by contrast to conventional catalytic incineration by air requiring preliminary heating of the gases to 523-573 K. A special consideration is given to adsorptive damping as an efficient method for leveling the VOCs concentrations in the real industrial exhausts directed to the catalytic treatment. The use of adsorptive dampers filled with carbon allows elimination of large deviations of pollutant concentrations in the gas entering the catalyst bed, thus increasing the VOCs removal efficiency from average values. For calculations of adsorptive dampers, an equation describing the profiles of VOC concentrations in gas phase along the length of the adsorbate bed in the damper was derived.

Mathematical Simulation of Catalytic Processes and Reactors. Chemical Engineering

RAISING THE SELECTIVITY OF THE UNSTEADY-STATE OXIDATIVE DEHYDROGENATION OF *n*-BUTANE IN A TWO-REACTOR SYSTEM WITH A CIRCULATING CATALYST

S.I. Reshetnikov, N.M. Ostrovskii, E.A. Ivanov

Theor. Found. of Chem. Engin., 36(1) (2002) pp. 80-85.

A mathematical model of oxidative dehydrogenation of *n*-butane is proposed. It is based on a kinetic model and takes into consideration two types of catalytic center. Ways of raising the divinyl formation selectivity of the process in a two-reactor system with a circulating catalyst are found.

PHASE TRANSITIONS IN THE ACTIVE COMPONENT OF VANADIUM CATALYSTS FOR SULFUR DIOXIDE OXIDATION: CRYSTAL PHASE DISSOLVING

N.P. Belyaeva, S.I. Reshetnikov, B.S. Bal'zhinimaev

Chem. Engin. J., 88(1-3) (2002) pp. 201-207.

As sulfur dioxide is oxidized on vanadium catalysts, phase transitions may occur in the catalyst active component, which are related to the crystallization of vanadium (IV) compounds resulting in the decrease of catalyst activity. In the present paper the peculiarities of reversal process such as crystal phase dissolving, which is aimed at catalyst regeneration, are reported. It has been studied, how crystal phase dissolving rate depends on dissolving conditions such as temperature, gas mixture composition, as well as on the conditions of crystal phase formation. Dissolving dynamics is described by a mathematical model, which was earlier suggested for the processes of crystal phase generation and growth.

MATHEMATICAL MODELLING OF CLAUS REACTORS UNDERGOING SULFUR CONDENSATION AND EVAPORATION

A.N. Zagoruiko, Yu.Sh. Matros* (*Matros Technology, St.-Louis, USA)

Chemical Engin. J., 87(1) (2002) pp. 73-88.

The paper is dedicated to the mathematical modelling of Claus reaction performance in the packed catalyst bed under conditions of sulfur condensation and evaporation. The proposed mathematical model accounts for heat and mass transfer between reaction gas and solid catalyst, condensation and evaporation of sulfur, reversible catalyst deactivation by liquid sulfur, Claus reaction reversibility, intraparticle diffusion limitations, heat conductivity of the catalyst bed frame. Reverse-flow operation of the catalyst bed have been investigated. The complex process flow-sheets, comprising two and three catalyst beds with intermediate sulfur condensers, have been simulated. It has been shown, that application of the reverse-flow technique provides increase of process efficiency.

CATALYTIC REACTORS FOR FISCHER-TROPSCH PROCESS

A.A. Khasin, V.A. Kirillov

Catalysis in Industry, 2 (2002) pp. 26-37.

The main features of Fischer-Tropsch synthesis and the requirements to the reactors to execute the process are analyzed. The well-known reactor types for Fischer-Tropsch synthesis and the schemes available in the literature but untried out in the industry have been analyzed with relation to correspondence with the criteria formulated. A conclusion is made on necessity of both continuation of the studies on development of known reactor types and search of new solutions to organize a catalyst layer.

ANALYZING BIOMASS CONVERSION INTO LIQUID HYDROCARBONS

V.D. Meshcheryakov, V.A. Kirillov

Theor. Found. of Chem. Engin., 36(5) (2002) pp. 466-471.

Variants of the Fischer–Tropsch producer-gas conversion into liquid hydrocarbons are analyzed under the assumption that thermodynamic equilibrium is attained in the reactions occurring in the biomass gasification. When the raw material is wood waste, the optimum variant of the process involves partial biomass oxidation by atmospheric oxygen with tail-gas recycling after the separation of liquid hydrocarbons. Before mixing with fresh producer gas, the hydrocarbons contained in the tail gas are reformed on a nickel catalyst.

CATALYTIC HEAT-EXCHANGER REACTOR FOR STRONGLY EXOTHERMIC REACTIONS

V.A. Kirillov, N.A. Kuzin, V.D. Mescsheryakov, V.I. Drobyshevich* (*Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russia)

Chem. Eng. Sci., 56(2) (2001) pp. 381-386.

A tubular catalytic apparatus of a new type, in which the heat release and heat-exchange surfaces are not spatially separated, is described. The reactors strongly allow exothermal chemical reactions to be performed with no significant overheating of the catalyst. Potential possibilities of the reactors of this type are illustrated on examples of the strongly exothermic processes of oxidation and hydrogenation.

CATALYTIC HEATING INSTALLATIONS FOR SOLUTION OF ECOLOGICAL AND POWER PROBLEMS

V.N. Parmon, Z.R. Ismagilov, V.A. Kirillov, A.D. Simonov

Catalysis in Industry,
3 (2002) pp. 20-28 (Part 1).
4 (2002) pp. 28-32 (Part 2).

The developments of Boreskov Institute of Catalysis in the field of independent power engineering are presented. Developed by the Institute and applied in the domestic industry, independent heating installations of 1kW to 2 MW in capacity based on ecologically pure catalytic combustion of gaseous, liquid, and solid fuels are discussed. Substantial advantages of the system developed are their environmentally cleanness, small dimensions, and high power effectiveness. The heating installations with a fluidized catalyst bed also prove to be practically «omnivorous» in respect to the nature of the fuel used: from natural gas to low-qualitative coals and even moist sludge and biomass.

PHASE DISEQUILIBRIUM IN THE COURSE OF AN EXOTHERMIC REACTION ACCOMPANIED BY LIQUID EVAPORATION IN A CATALYTIC TRICKLE-BED REACTOR

A.B. Shigarov, N.A. Kuzin, V.A. Kirillov

Theor. Found. of Chem. Engin., 36(2) (2002) pp. 159-165.

α-Methylstyrene hydrogenation in a fixed catalyst bed is studied experimentally and theoretically for a cocurrent downflow of the gas and liquid. Gas-phase hydrogenation on dry catalyst granules disturbs the liquid–vapor phase equilibrium. A dimensionless parameter related to the Raoult–Dalton law for a liquid–vapor mixture is suggested to characterize phase disequilibrium in the system.

TREATMENT OF MASS TRANSFER FOR GAS-PHASE HYDROGENATION/ DEHYDROGENATION OF HEAVY COMPOUNDS

A.B. Shigarov, S.I. Fadeev*, I.A. Mikhailova, A.V. Kulikov, V.K. Korolev*, N.A. Kuzin, V.A. Kirillov (*Institute of Mathematics, Novosibirsk, Russia)

Korean J. Chem. Eng., 19(2) (2002) pp. 252-260.

Gas-phase benzene hydrogenation at normal pressure by thermocouple measurements of gas flow and the pellet center has been experimentally studied using single catalyst pellets (5 mm) 15% Pt/γ-Al_2O_3. A simplified pseudobinary treatment of both multicomponent intrapellet mass transfer and multicomponent external mass transfer is proposed on the basis of the analytical estimation. The simplified approach appears to be quite accurate for reactions $A+nH_2=B$ of hydrogenation ($n>0$) or dehydrogenation ($n<0$) of sufficiently heavy compounds, i.e. if $D_{AH}=D_{BH}>>D_{AB}$.

STUDY OF CRITICAL PHENOMENA IN EXOTHERMIC REACTIONS ON PARTIALLY WETTED POROUS CATALYST GRAIN

V.A. Kirillov, I.A. Mikhailova, S.I. Fadeev*, V.K. Korolev* (*Institute of Mathematics, Novosibirsk, Russia)

Combustion, Explosion and Shock Waves, 38(5) (2002) pp. 22-32.

Mathematical model for analysis of gas-liquid reactions of hydrocarbon hydrogenation, accompanied by liquid evaporation and chemical transformations in liquid and vapour phases on a porous grain is proposed and numerical experiments have been carried out. The adequacy of mathematical model has been proved by the experimental data.

A THERMODYNAMIC THEORY OF AUTOWAVE PROCESSES IN A STATIC CATALYST BED

A.P. Gerasev

Russ. J. Phys. Chem., 76(2) (2002) pp. 161-166.

A static catalyst bed in a reversible reaction was thermodynamically described in the quasihomogeneous model approximation, and the nonequilibrium entropy of fast and slow heat waves was constructed. The total entropy production in a distributed open nonlinear system was shown to be a functional of the autowave solution. The rules governing the production of entropy in fast and slow heat waves were formulated. The existence of a space-time dissipative structure (a fast heat wave) near the thermodynamically equilibrium state was established.

THE EFFECT OF THE CATALYTIC LAYER DESIGN ON OXIDATIVE DEHYDROGENATION OF PROPANE OVER MONOLITHS AT SHORT CONTACT TIMES

S.N. Pavlova, V.A. Sadykov, Yu.V. Frolova, N.F. Saputina, P.M. Vedenikin, I.A. Zolotarskii, V.A. Kuzmin

Chem. Engin. J., 91(2-3) (2002) pp. 227-234.

Main factors determining performance of straight channel corundum monolith supported catalysts in the autothermal reaction of propane oxidative dehydrogenation at short contact times are verified. It was made possible by using a unique design of the catalytic reactor which allows an independent tuning of the gas preheat temperature and the catalyst temperature. It is also equipped with a cooled sampler to cut any homogeneous reactions after the catalyst layer. The effects of the front and back thermal shields, feed rate, relative contact time and the void space between the catalytic monoliths or after them are elucidated. The performance of the monolithic catalyst is compared with that crushed and packed into a granulated layer. A substantial impact of the homogeneous gas-phase reactions on the propane conversion and product selectivities is demonstrated. In turn, their share depends upon the longitudinal temperature gradient within the monolithic layer as determined by the heat generation in the inlet part due to propane combustion by oxygen, its transfer along the monolith layer and consumption in the rear part of the monolith in the absence of oxygen through endothermic reactions of dehydrogenation, cracking and steam reforming. In the autothermal mode of the propane oxidative dehydrogenation at short contact times on monolithic catalysts, the effect of those factors is as important as that of the catalyst and feed chemical composition.

CATALYTIC DEHYDRATION IN THE PRODUCTION OF SYNTHETIC RUBBER MONOMERS

E.A. Taraban, V.I. Simagina

Catalysis in Industry, 4 (2002) pp. 14-19.

Current developments of the national industrial production and consumption of dehydrogenation catalysts for producing synthetic rubber (SR) monomers have been considered. The main trends of evolution in production of SR monomers are identified, e.g., implementation of modern energy and resource saving technologies (production of butadiene by extraction from pyrolized C4 fraction, production of isoprene from C4 fraction and formaldehyde by one-stage method).

SCIENTIFIC PUBLICATIONS

JOURNAL PUBLICATIONS AND MONOGRAPHS

1. **(N. Alonso-Vante), I.V. Malakhov, S.G. Nikitenko, E.R. Savinova, D.I. Kochubey,**
   The Structure Analysis of the Active Centers of Ru-Containing Electrocatalysts for the Oxygen Reduction. An *in situ* EXAFS Study,
   Electrochim Acta, 47 (22-23) (2002) pp. 3807-3814.
2. **(A.I. Ancharov, T.F. Grigorieva), S.G. Nikitenko, (M.R. Sharafutdinov),**
   X-Ray Diffraction and EXAFS Spectroscopy Study of Reactions in Diffusion-Hardening Alloys on the Base of the Cu-Ga System,
   Surface Investigation.: X-Ray, Synchrotron and Neutron Techniques, 7 (2002) pp. 25-28 (in Russian).
3. **V.I. Anikeev, A. Yermakova, (D. Manion, R. Hugh),**
   Reaction Kinetics of 2-Propanol Dehydration in Supercritical Water,
   Kinetics & Catalysis, 43(2) (2002) pp. 189-194 (English language translation).
4. **M.P. Anisimov, (P.K. Hopke),**
   Nucleation Rate Surface Topologies for Binary Systems,
   J. Phys. Chem. B, 105(47) (2001) pp. 11817-11822.
5. **V.F. Anufrienko, N.N. Bulgakov, (N.T. Vasenin), S.A. Yashnik, L.T. Tsykoza, (S.V. Vosel), Z.R. Ismagilov,**
   Detection of O^- Radical Anions in Cu-ZSM-5 Zeolites After Heat Treatment,
   Doklady Chemistry, 386(4-6) (2002) pp. 273-276 (English language translation).
6. **Yu.I. Aristov, (G. Restuccia, G. Cacciola), V.N. Parmon,**
   A Family of New Working Materials for Solid Sorption Air Conditioning Systems,
   Appl. Therm. Engin., 22(2) (2002) pp.191-204.
7. **V.I. Avdeev, A.I. Boronin, G.M. Zhidomirov,**
   Properties of the Adsorbed Oxygen Forms on a Defective Surfaces Ag(111). The Theoretical Analysis by DFT Method,
   J. Struct. Chem., 43(1) (2002) pp. 26-32 (in Russian).
8. **L.B. Avdeeva, T.V. Reshetenko, Z.R. Ismagilov, V.A. Likholobov,**
   Iron Containing Catalysts of Methane Decomposition: Accumulation of Filamentous Carbon,
   Applied Catal. A: General, 228(1-2) (2002) pp. 53-63.
9. **D.E. Babushkin, (H.-H. Brintzinger),**
   Activation of Dimethyl Zirconocene by Methylaluminoxane (MAO) - Size Estimate for $Me\text{-}MAO^-$ Anions by Pulsed Field-Gradient NMR,
   J. Amer. Chem. Soc., 124 (2002) pp. 12869-12873.
10. **B.S. Bal'zhinimaev, (V.V. Barelko), A.P. Suknev, E.A. Paukshtis, L.G. Simonova, V.B. Goncharov, V.L. Kirillov, A.V. Toktarev,**
    Catalysts Based on Fiberglass Supports:
    5. Absorption and Catalytic Properties of Palladium Catalysts Based on a Leached Silica-Fiberglass Support in the Selective Hydrogenation of an Ethylene-Acetylene Mixture,
    Kinetics & Catalysis, 43(4) (2002) pp. 542-549 (English language translation).
11. **B.S. Bal'zhinimaev, L.G. Simonova, (V.V. Barelko), A.V. Toktarev, D.A. Arendarskii, E.A. Paukshtis, (V.A. Chumachenko),**
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