ANNUAL REVIEW 2006

BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

ANNUAL REVIEW 2006

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CONTENT

ANNUAL REVIEW
of Activities in Basic Research Areas
2005

BOREKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

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CONTENT

Dear Colleagues,

This issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covers the year 2005 and reflects now more than the ten-year experience of the Institute in publishing such reviews.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and NIS, but also in many western and oriental countries. Since 1960's it has remained the largest Russian chemical research institution in the Asian part of Russia and had 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 reflect Russia entering into the market economy. BIC belongs to the Siberian branch of the Russian Academy of Sciences. However, according to new realities of Russia, a lot deal of activity of BIC is devoted not only to basic research, but also to numerous industrially oriented topics. The intensity and quality of the research and engineering activity at the Institute became at the new period of the Russian history even higher as before. Fortunately, the Institute gained in research in catalysis fundamentals, thus continuing the old traditions originated from the beginning of the Institute due to a very powerful starting impulse of its creator and first director Academician Georgii K. Boreskov, as well as the master ideas of the second director Academician Kirill I. Zamaraev. Hope, the readers will feel that themselves, when comparing the materials of this and previous issues of the Annual Review.

The year 2005, the same as all previous years, was very important for the life of BIC in many aspects. First of all, BIC has nearly finished his work on the largest innovation project of new Russia in the field of application of catalysis in large scale oil refinery. All the technical targets of that project, which is sponsored by the Russian Ministry of Industry and Energetics, have been fulfilled: Russia was offered two excellent industrial catalysts and one principally new industrial chemical technology. The economic efficiency of the project is also large: the Russian oil refineries received already an additional profit in amount more than $200 million. Also, BIC started working actively in development of new efficient catalysts for olefin polymerization, including production of the polyethylene with the superhigh molecular weight, as well as of aromatization of low alkanes, which are the main constituent of the oil associated gases. The strategic collaboration with the Russian industries is nowadays, undoubtedly, a very important feature of the scientific activity of the Boreskov Institute, as well as of many other academic institutes of RAS.

CONTENT

Since 1998 the Institute is 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.

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

Hope this issue of the Annual Review of the Boreskov Institute of Catalysis is exhibiting many sides of the current Institute potentialities in basic research on catalysis, catalysts and catalytic technologies. As to the activity of the Institute in the applied areas, which is now much more active than ever in the past, we publish special leaflets or are inviting to visit the Institute's website.

Valentin N. Parmon

CONTENT

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.

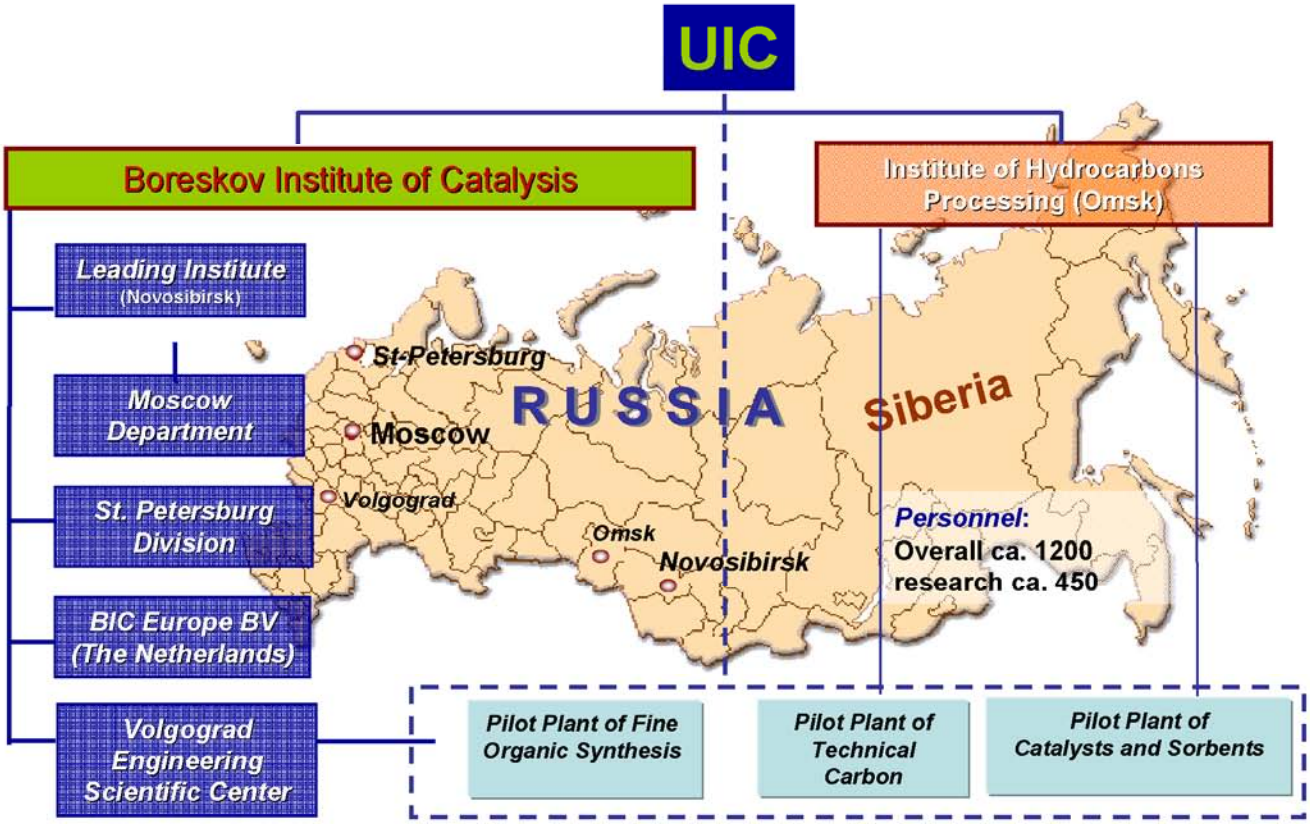
In 1984 Professor Zamaraev became the Director of the Institute of Catalysis, and since that time he was the real leader of all research and development activity of this huge (up to 1000 people in staff) Institute. K.I. Zamaraev, the former President of the International Union of Pure and Applied Chemistry, 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 St. Petersburg Division, Volgograd Scientific-Engineering Center, Moscow Department, BIC Europe BV (The Netherlands) and the Institute of Hydrocarbons Processing in Omsk.

CONTENT

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



UIC

Boreskov Institute of Catalysis

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

Institute of Hydrocarbons Processing (Omsk)

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

Personnel:
Overall ca. 1200
research ca. 450

CONTENT

STRUCTURE OF THE INSTITUTE

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

The structure of the Institute incorporates 6 Scientific-Research Departments, Technological Support and Supply Divisions, Technical Units and Assisting Units.

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.

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 client’s 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.

Organization of different events is essential part of business life of the Institute. The **Scientific Organizing Group** of the Institute has great experience in organization of conferences, seminars, congresses, presentations, symposia and other events in Russia and abroad. **Information Analytical Center** of the Institute is active in competence, perfect service in the field of organization of exhibitions of the new inventions and successive achievements of the Institute.

CONTENT

STRUCTURE OF THE INSTITUTE

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

DIRECTOR

Directorate

Scientific Council

Research Departments

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
Head: Prof. Valerii I. Bukhtiyarov

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

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

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

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

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

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

VOLGOGRAD ENGINEERING SCIENTIFIC CENTER OF THE BORESKOV INSTITUTE OF CATALYSIS
Director Dr. Andrey P. Kovalenko

Scientific-Supportive Units

Manufacturing Facilities

Administration and Services

CONTENT

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

HEAD OF THE DEPARTMENT PROF. VALERII I. BUKHTIYAROV

Surface Science Laboratory
Head: Prof. Valerii I. Bukhtiyarov

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

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

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

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

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

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

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

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

CONTENT

Group of Solid-State NMR Spectroscopy

Head: Prof. Olga B. Lapina

Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion

Head: Prof. Alexander G. Stepanov

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES

HEAD OF THE DEPARTMENT ACADEMICIAN VALENTIN N. PARMON

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

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

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

Laboratory of Adsorption
Head: Dr. Oleg N. Martyanov

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

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

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

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

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

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

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

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

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

Group of Biocatalysis
Head: Dr. Galina A. Kovalenko

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

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

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

Division of Advanced Developments and Technologies
Head: Dr. Sergey A. Shakhov

Group of Small Angle Scattering
Head: Prof. Fedor V. Tuzikov

CONTENT

DEPARTMENT OF HETEROGENEOUS CATALYSIS

HEAD OF THE DEPARTMENT PROF. VLADIMIR A. SOBYANIN

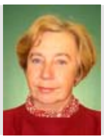
Laboratory of Catalytic Processes in Fuel Cells
Head: Prof. Vladimir A. Sobyanin

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

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

Laboratory of Dehydrogenation
Head: Prof. Viktor V. Molchanov

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



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

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

Group of Noble Metal Based Heterogeneous Catalysts
Head: Prof. Anatolii V. Romanenko

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

CONTENT

Group of Synthesis of Nanodispersed Materials

Head: Prof. Oleg P. Krivoruchko

Group of Selective Oxidation over Metal Oxides

Head: Dr. Vladimir I. Sobolev

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS

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

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

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

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

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

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

Department for Developing Relations with Industry
Head: Dr. Ilya A. Zolotarskii

Analytical Center
Head: Dr. Dmitrii A. Arendarskii

CONTENT

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING

HEAD OF THE DEPARTMENT PROF. ALEKSANDR S. NOSKOV

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

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

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

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

Laboratory of Catalytic Conversion of Carbon Oxides
Head: Prof. Aleksandr A. Khassin

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

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

Group of Catalytic Technologies for Carbon Materials Synthesis
Head: Dr. Vadim A. Yakovlev

CONTENT

Group of Kinetics of Catalytic Processes

Head: Dr. Sergei I. Reshetnikov

Group of Mathematical Methods for Catalytic and Adsorption Processes Modeling

Head: Dr. Natalia A. Chumakova

DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS

HEAD OF THE DEPARTMENT PROF. ZINAIDA P. PAI

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

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

ST. PETERSBURG DIVISION OF THE BORESKOV INSTITUTE OF CATALYSIS

DIRECTOR AND SCIENTIFIC MANAGER
PROF. SERGEY S. IVANCHEV

VICE-DIRECTOR DR. VALERY P. TULMANKOV

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

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

VOLGOGRAD ENGINEERING SCIENTIFIC CENTER OF THE BORESKOV INSTITUTE OF CATALYSIS

DIRECTOR DR. ANDREY P. KOVALENKO

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 **Academician 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 **Academician Kirill I. Zamaraev** came from Moscow. The flow of these specialists significantly enlivened the atomic-molecular studies of catalytic reaction mechanisms and catalytic properties of heterogeneous catalysis by physicochemical methods.

CONTENT

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

— Development of theory of electron tunneling in condensed media;

— Coordination chemistry of metal-complexes solutions;

— Step-wise description of homogeneous catalytic reactions;

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

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

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 of school by **Academician 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

Basic research

- *Determination of general regularities of catalysis*
- *Development of the scientific basis for molecular design the catalysts and materials*
- *Development of the theoretical basis to design the catalytic processes*
- *In-situ methods to study catalyst and mechanism of important catalytic reactions*
- *Methods and algorithms to predict the catalytic action*
- *Methods and facilities for the catalysts testing*
- *Nanotechnological approach to design the catalysts with predictable properties*

Applied catalysis

- *Design of highly efficient catalysts for production of key chemicals; oil & gas processing*
- *Design of the catalytic composites and technologies for applied purposes*
- *Catalysts and catalytic technologies for polymers production with specified properties*
- *Design of sorbents, catalysts and technologies for detoxication of hazardous man-caused wastes*
- *Selective oxidation of light* C_1*-*C_4 *paraffins by molecular oxygen*
- *Gas-phase propylene epoxidation by molecular oxygen*
- *Reactors and new processes based on membrane catalysts. Microchannel catalytic reactors*
- *Catalysts and processes related to hydrogen energy technologies*
- *Catalysis concerned to the environmental and energy problems*
- *New directions and opportunities of catalysis in utilization of renewable natural resources*

Some catalytic technologies owned by BIC

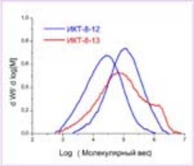
- **Reverse process** for catalytic gas purification
- **Zeoforming processes** for synthesis of gasoline
- **Alphox technology** for the one step phenol form benzene production
- **Adsoroption-catalytic purification** of industrial wastewaters
- **Nitric acid** production with the use of honeycomb catalysts
- **One-step** technology for the **nicotinic acid** production
- New technology of **loading the reactors** with catalysts
- **BIMT technology** for production of gasoline and diesel fuel without preliminary rectifying the hydrocarbon feedstock
- Reburning of Klaus **tail gases**
- The **BICYCLAR** technology for production of aromatic hydrocarbons with methane involvement
- Direct catalytic **oxidation of** H_2S to elemental sulfur
- Treating of mixed **radioactive organic wastes**

CONTENT

- Liquid-phase oxidative **treating of industrial wastewater**
- Technology for **formaldehyde** production
- Technology for **one step formic acid** production
- Technology for **reducing atmospheres** production
- Technique for preparation of **emulsifiers and water-bitumen emulsions**

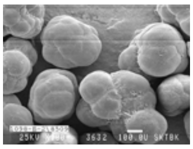
Some industrial catalysts by BIC

Vanadium pentoxide catalysts for sulfuric acid production



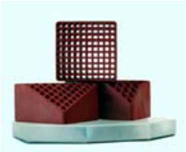
Supported catalysts ICT-8-12 and ICT-8-13 for polyethylene production

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



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

Microspherical zeolite-containing cracking catalysts



Non-platinum catalyst IC-42-1 for nitrogen acid production

Gasoline reforming catalysts of PR series

High silica zeolite catalysts

Hydrogenation catalysts for manufacture of medical products
and edible fats

CONTENT

Catalytic Processes from Molecular Level to Industrial Plants

2005 Cracking catalyst LUKS and reforming catalyst PR-71

2004 Reburning of Klaus tail gases, Russia

2003 BIMT technology for production of gasoline and diesel fuel

2002 Selective water sorbents, Russia

2000 New technology of loading the reactors with catalysts, Russia

1999 Catalyst for hydro purification of terephthalic acid
Developed in cooperation with Samsung Chemicals, 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 + $[N_2O] \rightarrow$ phenol)
Developed in cooperation with Solutia, 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

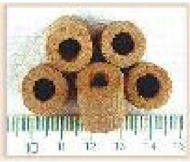
1988 Catalysts for polypropylene polymerization, Russia
DSM, 1995, the Netherlands

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

1978 Vanadium catalysts for sulfuric acid production, Russia

1958

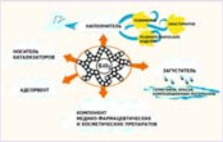
CONTENT



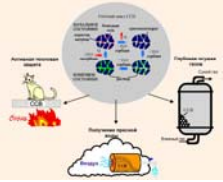
Thermostable catalyst ICT-12-40 for gas purification

Catalyst for hydropurification of terephthalic acid

Some catalyst supports by BIC



Superfine silica gels IC-01-2



Composite selective water sorbents SWS

Mesoporous carbonaceous material SIBUNIT

INSTRUMENTATION 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

CONTENT

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 the information and appropriate materials, exchanging research fellows, visiting scientific centers, and participating in congresses and symposia on theoretical and applied catalysis.

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

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

Visits of the specialists from the Boreskov Institute of Catalysis to foreign institutions in 2005

Azerbaijan	1	India	3	Slovenia	4
Belarus	2	Ireland	1	South Korea	4
Belgium	4	Israel	4	Spain	2
Bulgaria	15	Italy	13	Switzerland	3
China	13	Kazakhstan	1	Turkey	9
Czechia	5	Netherlands	21	Ukraine	20
Egypt	1	Japan	10	United Arab Emirates	1
France	14	Poland	7	United Kingdom	4
Germany	37	Portugal	2	USA	12

Visits of foreign specialists to the Boreskov Institute of Catalysis in 2005

Belgium	1	Germany	14	Poland	12
China	4	India	2	Sought Korea	1
Czechia	1	Italy	2	United Kingdom	3
Finland	1	Japan	9	USA	25
France	2	Netherlands	11		

CONTENT

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

ITALY

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

- *Istituto di Trasformazione e Accumulazione d'Energia* (CNR Institute for Transformation and Storage of Energy), Messina – *BIC*, Novosibirsk on the Programme ***"Catalysis for Solving the Energy Problem"***, Project ***"Adsorption and Catalysis for Advanced Power Technologies"***. Coordinators: **Prof. Yu. Aristov** (*BIC*) and **Prof. G. Cacciola** (*Istituto di Trasformazione e Accumulazione d'Energia*).
- *Istituto di Scienze e Tecnologie Molecolari* (Institute of Molecular Science and Technologies), Milano – *BIC*, Novosibirsk on the Project ***"Methods for Homo- and Heteronuclear Bonds Formation and Opening in Stoichiometric Reactions and Catalytic Reactions Using Transition Metal Complexes"***. Coordinators: **Prof. N. Ustynyuk**, *Institute of General and Inorganic Chemistry* and **Prof. R. Psaro**, *Istituto di Scienze e Tecnologie Molecolari*. The Project theme in 2005 was ***"Process Development for Catalytic Stereoselective Methanol Synthesis"*** (**Dr. I. Simakova**, *BIC*).

FRANCE

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

- *Institute de Recherches sur la Catalyse* (Research Institute on Catalysis), Villeurbanne in the frame of the Russian-French European associated Laboratory on Catalysis which was established by an agreement signed December 6, 2004 in Moscow by RAS and CNRS. Four areas of research were identified:

- ***Catalysis and Energy: Production of Syngas and Hydrogen***
- ***Catalysis and Environment: Treatment of Waste Waters***
- ***Catalysis and Fine Organic Chemistry*: *Selective Oxidation with Hydrogen Peroxide***
- ***Development of Spectroscopic Methods: Mobility of Molecules in Porous Media***.

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

- *Université Pierre et Marie Curie*, Paris, *Université des Sciences et Technologies de Lille* (*Lille University of Science and Technology*) on the Project ***"Development of Novel Method of Quadrupole Nuclei to Study Vanadium Systems".*** Coordinators: **Prof. O. Lapina** (*BIC*) and **Prof. J. Fraissard** (*Université Pierre et Marie Curie*).
- *Université des Sciences et Technologies de Lille* and *Laboratoire de Physique Quantique, Ecole Supéireure de Physique et de Chimie Industrielles* (Laboratory of Quantum Physics, Industrial Physics and Chemistry Higher Educational Institution), Paris on the themes:

CONTENT

- ***Oxidative Ammonolysis of Light Paraffines (Ethane and Propane)***
- ***Studying the Structure of Supported on Various Carbon Supports Bimetal Catalysts by Modern NMR Spectroscopy***

Coordinators: **Prof. O. Lapina** (*BIC*), **Prof. J.-F. Bodart** (*Université des Sciences et Technologies de Lille*), **Prof. Jean-Baptiste d'Espinose de la Caillerie** (*Ecole Supéireure de Physique et de Chimie Industrielles*).

INDIA

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

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

POLAND

In the frame of **RAS-PAS** agreement BIC cooperates with the

- *Instytut Inżynierii Chemicznej PAN* (Institute of Chemical Engineering), Gliwice on the Project ***"Synthesis and Utilization of Hyperporous Solids".*** Coordinators: **Prof. Yu. Aristov** (*BIC*), **Acad. V. Parmon** (*BIC*) and **Prof. A. Burghardt** (*Instytut Inżynierii Chemicznej*).
- *Akademia Medyczna w Warszawie* (Warsaw Medical University), Warsaw on the Project "***Studying of Porous Structures***". Coordinator: **Prof. O. Lapina** (*BIC*).

GERMANY

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

- *Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin on the Projects
- ***"Study of the Catalysts for Partial Oxidation"***. Coordinators: **Prof. V. Bukhtiyarov** (*BIC*) and **Prof. R. Schlögel** (*Fritz-Haber-Institut der MPG*).
- ***"Development of in situ Methods for Study of Solid Surfaces"***. Coordinators: **Prof. V. Bukhtiyarov** (*BIC*) and **Dr. H.-J. Freund** (*Fritz-Haber-Institut der MPG*).
- *Institut für Mineralogie, Kristallographie und Materialwirtschaft, Universität Leipzig* (*Institute for Mineralogy, Crystallography and Material Science at Leipzig University*) on the Project ***"Novel Nanomaterials of Complex Sulphides in*** $PdS\text{-}Bi_2S_3$ ***and*** $CuPdBiS_3\text{-}Bi_2S_3$ ***Systems"***. Coordinators: **Prof. S. Tsybulya** (*BIC*) and **Prof. Dr. K. Bente** (*Leipzig University*).

CONTENT

YUGOSLAVIA

The cooperation in the frame of the agreement between **RAS** and **Serbian Academy of Sciences and Arts** on the Project ***"Novel Catalytic Materials and Technologies".*** Coordinators: **Acad. V. Parmon** (BIC), **Acad. P. Putanov**, **Prof. B. Anadzievic**.

SPAIN

The cooperation with the *Instituto de Catálisis y Petroleoquímica, CSIC* (*Institute of Catalysis and Petrochemistry*), Madrid – ***"Fundamental and Technical Aspects of in situ Spectroscopy of Oxide Catalysts"***. Coordinators: **Prof. O. Lapina** (*BIC*), **Dr. M. Banares** (*Instituto de Catálisis y Petroleoquímica*).

COOPERATION IN THE FRAME OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

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

Participants:

Istituto di Tecnologie Avanzate per L'energia "Nicola Giordano", CNR (Institute for Advanced Energy Technologies "Nicola Giordano"), Messina, Italy
Technische Universität Aachen, RWTH-Aachen, Germany
Boreskov Institute of Catalysis, Novosibirsk, Russia **(Prof. Yu. Aristov)**
Institute for High Temperatures, Moscow, Russia
Moscow Lomonosov State University, Moscow, Russia
Institute of Engineering Thermophysics, Kiev, Ukraine.

II. Transformation of LPG into Gasoline: Elucidation of the Mechanism and Catalytic Design

Project Coordinator:

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

Participants:

Prof. I. Ivanova, Moscow Lomonosov State University, Moscow, Russia
Acad. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. E. Derouane, Universidade to Algarve Faculdade de Ciencias e Technologia (University of the Algarves, Faculty of Sciences and Technology), Faro, Portugal
Dr. Ya. Khimyak, University of Liverpool, Liverpool, United Kingdom.

CONTENT

NATO PROGRAMME: SCIENCE FOR PEACE

I. Solid Oxide Fuel Cells for Energy Security

NATO Country Project Director:

Prof. N. Orlovskaya, Drexel University, Philadelphia, United States

Partner Country Project Director:

Prof. O. Vasiliev, Frantcevych Institute for Problems of Material Science, Kiev, Ukraine

Project Co-Directors:

Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. J. Irvine, University of St. Andrews, St. Andrews, United Kingdom
Prof. N. Sammes, University of Connecticut, Storrs, United States
Prof. R. Hasanov, Azerbaijan State Oil Academy, Baku, Azerbaijan
Dr. A. Schokin, State Committee for Energy Saving of Ukraine, Kiev, Ukraine
Prof. John Kilner, Imperial College, London, United Kingdom.

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

NATO Country Project Director:

Prof. J. Frade, Departamento de Engenharia Cerâmica e do Vidro, Universidade de Aveiro (Department of Ceramics and Glass Engineering, University of Aveiro), Aveiro, Portugal

Partner Country Project Director:

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

Project Co-Directors:

Dr. J. Irvine, School of Chemistry, University of St. Andreas, Scotland, United Kingdom
Dr. T. Norby, SMN, Universitetet i Oslo, Oslo, Norway
Dr. J. Jurado, Instituto de Cerámica y Vidrio, CSIC (Institute of Ceramics and Glass), Madrid, Spain
Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Kozhevnikov, Institute of Solid State Chemistry, Yekaterinburg, Russia
Dr. L. Boginsky, Institute for Personal Development and Staff Retraining in New Areas of Techniques, Technologies and Economics of the Belarus Ministry of Education, Minsk, Belarus.

NATO Linkage Collaborative Grant

I. Investigation of the Structure of Sulfated Catalysts Based on TiO_2 Obtained by Sol-Gel and Microemulsion Methods

Project Coordinators:

Dr. C. Gerardo, Instituto de Ciencia de Materiales de Sevilla (Institute of Materials Science), Sevilla, Spain

Dr. V. Kriventsov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

CONTENT

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 from BIC: **Prof. V. Anikeev**.

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

Project Manager from BIC: **Prof. V. Kirillov**.

III. New Method to Obtain Catalytic Coatings for the Catalysts for Gas Turbine Combustion

Project Manager from BIC: **Dr. O. Podyacheva**.

NWO–RFBR

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

Project Coordinators:

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

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

Project Coordinators:

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

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

Project Coordinators:

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

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

Project Coordinators:

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

CONTENT

V. Microstructured Catalytic Reactors for Oxidation of Unsymmetrical Dimethylhydrazine

Project Coordinators:

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

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

Project Coordinators:

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

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

Project Coordinators:

Prof. J.A. Mouljin, Technische Universiteit Delft, Delft, The Netherlands
Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

CONTENT

CONFERENCE AND EXHIBITION ACTIVITIES

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

In 2005, the most important BIC's achievements in the area of applied Catalysis were presented at the Exhibitions:

- ***Regular Exhibition*** of Novosibirsk in Taejon, January 15-24, Taejon, Korea
- ***V Moscow International Salon of Innovations and Investments***, February 15-18, Moscow, Russia
  Golden Medal and **Diploma** for the project **"Polymers for Extremal Conditions"**;
  Golden Medal and **Diploma** for the project **"Technology for Nicotinic Acid Production"**
- ***VI Regional Exhibition-Fair "North-Russia – 2005. Siberia: Export-Import"***, March 29-31, Novosibirsk, Russia
  Minor Golden Medal and **Diploma** for the project **"BIMF – One-Stage Technology for Motor Fuel Production"**
- ***Exhibition "Russian Academy of Science for Medicine and Man's Health"***, March 26-April 1, Novosibirsk, Russia
- ***VII International Specialized Exhibitions-Fairs "'Khimmash", "Khimprodukt"*** *and* ***"Khimkomplektsnab"***, May 10-13, Kemerovo, Russia.
  Golden Medal and **Diploma** for **"Non-Platinum Catalysts for Nitric Acid Production"**
- ***"Scientific-Technical Exhibition of Sinczyan-Uigursk Autonomous Region of China"***, May 10-15, Novosibirsk, Russia
- ***Exhibition "FEC. Current Technologies and Equipment. Siberia-2005"***, June 7-8, Novosibirsk, Russia
- ***Ninth St. Petersburg International Economic Forum***, June 14-16, St. Petersburg, Russia
- ***XVI Harbin Trade and Economic Fair***, June 15-19, Harbin, China
- ***Fair-Exhibition "Scientific and Technical Achievements of North-Eastern Asia"***, September 21-24, Shenyang, China
- ***4th International Exhibition "TechnoMart-IV"***, October 26-28, Novosibirsk, Russia
  Diploma for the most interesting reciprocal project "**Technologies of Hydrogen Power"**
- ***International Industrial Exhibition "SIBPOLYTECH": "Science of Siberia"***, October 26-28, Novosibirsk, Russia
  Big Golden Medal and **Diploma** for the project **"Polymerization Catalysts".**

CONTENT

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

EXTENSION COURSES IN THE FIELD OF CATALYSTS AND CATALYTIC PROCESSES-III

March 22-23, Severodonetsk, Ukraine

The organizers of the Courses were Boreskov Institute of Catalysis, Novosibirsk, Russia and LLC Research and Production Company "Alvigo-KS", Severodonetsk, Ukraine.

The Programme included 9 lectures by the leading specialists – 1 from the Institute of Hydrocarbons Processing, Omsk, and 8 from the Boreskov Institute of Catalysis, Novosibirsk.

Institute of Hydrocarbons Processing, Omsk, Russia

Likholobov V.A. - *"Catalysis. Introduction and Basic Concepts"*

Boreskov Institute of Catalysis, Novosibirsk, Russia

Kochubey D.I. - *"Catalysis and Physico-Chemical Methods of Investigation"*

Fenelonov V.B. – *"Fundamentals of Adsorption and Theory of Catalysts Texture Control"*

Bobrov N.N. – *"Experimental Methods to Study Catalysts Properties"*

Zagoruiko A.N. – *"Bases for Catalytic Reactors Design. Processes of Heat (Mass) Transfer in Catalytic Reactors"*

Sobyanin V.A. – *"Catalysts and Processes for Syn-Gas and Hydrogen Production"*

Zolotarskii I.A. – *"Modern Trends in Development of Catalytic Process for Nitrogen Industry"*

Klenov O.P. – *"Aerodynamics of Catalytic Reactors and Methods of their Loading"*

Noskov A.S. – *"Novel Catalysts and Catalytic Processes"*

About 250 employees of LLC Research and Production Company "Alvigo-KS" and 50 faculty members, students and post-graduates of Severodonetsk Technological Institute passed training at the Courses.

MEMORIAL Yu.I. YERMAKOV CONFERENCE "MOLECULAR DESIGN OF CATALYSTS AND CATALYSIS FOR HYDROCARBON PROCESSING AND POLYMERIZATION"

June 15-17, Omsk, Russia

The Conference was scheduled to 70th anniversary of Professor Yurii I. Yermakov (1935–2005).

Yu.I. Yermakov was among the first to come to the Institute. In 1963 he became the Head of the Laboratory of Catalytic Polymerization, in 1972 – the Head of the Department of Homogeneous and Coordination Catalysis. Yu.I. Yermakov is the founder of new scientific direction in heterogeneous catalysis – catalysis by anchored metal complexes, the main idea of which is purposeful synthesis of anchored organometallic, cluster and metal catalysts. Theoretical and experimental researches conducted by the school by Professor Yu. Yermakov involves design of supported catalysts, establishing on molecular level the mechanism of their action in selective oxidation and olefin carbonylation, and development of novel efficient catalysts. He made a considerable contribution to the creation of the Omsk Department of Catalytic Hydrocarbon Conversion in Omsk in 1978 (now the Institute of Hydrocarbons Processing). We remember him as an extraordinary organizer, talented scientist and a very interesting person.

The event was organized by

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Hydrocarbons Processing, Omsk, Russia
- Omsk Scientific Center SB RAS, Omsk, Russia
- Scientific Council on Catalysis, Moscow, Russia
- Federal Agency for Science and Innovations of Russian Federation, Moscow, Russia
- Russian Foundation for Basic Research, Moscow, Russia

80 specialists from Russian Academic Institutes and Universities, 8 foreign scientists (from Brazil, Hungary, USA and Kazakhstan) took part in the Conference.

The scientific program of the Seminar comprised 6 key lectures, 30 oral presentation and 21 posters in the following topics:

- Molecular Design in Preparation and Investigation of Supported Catalysts
- Catalysis in Hydrocarbon Raw Processing
- Catalytic Olefin Polymerization (New Catalytic Systems, Composition and Structure of Catalysts, Kinetics of Polymerization and Polymer Structure).

CONTENT

Key lectures**:**

A.T. Bell (Department of Chemical Engineering, University of California, Berkeley, USA) – *"Single Site Catalysts – Ideal Models for Understanding Structure-Function Relationships"*
V.A. Likholobov (Institute of Hydrocarbons Processing, Omsk, Russia) – *"Modern Aspects of Molecular Design of Catalyst Active Centers"*
V.K. Duplyakin (Institute of Hydrocarbons Processing, Omsk, Russia) – *"Studying of the Mechanism of Metal Complexes Anchoring on the Supports as an Approach to Formation of Molecular Structure of Active Component Precursor of the Catalysts of Hydrocarbon Conversion"*
G.V. Echevsky (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"BIMF – Single-Stage Technology for High-Quality Motor Fuels Production from Hydrocarbon Long Distillates"*
V.A. Zakharov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Role of Supports in Formation of Active Component of Supported Catalysts for Olefin Polymerization"*
N.M. Bravaya, A.N. Panin, O.M. Chukanova, E.E. Faingold, E.A. Sanginov (Institute of Problems of Chemical Physics, Chernogolovka, Russia) – *"Triisobutylaluminium and Lewis Bases as Modifiers of Properties of Homogeneous Metallocene Catalysts for Olefin Polymerization"*.

CONTENT

2nd INTERNATIONAL SCHOOL-CONFERENCE ON CATALYSIS FOR YOUNG SCIENTISTS “CATALYST DESIGN”

July 25-29, Altai Mountains, Russia

The Republic of Altai is a whole world that is unexplored and free of smog, haste, and business rhythm of the big city. Full of mystery and inscrutability, the mountain country Altai since olden times is surrounded with legends, myths, heroic legends, and folk songs. The Conference was held at the tourist center STIK situated at the heart of the Altai Mountains, in the banks of the quick mountain river Katun.

Financial support was given by:

Russian Foundation for Basic Research, Moscow, Russia
Presidium of Siberian Branch of the Russian Academy of Sciences
Hiden Analytical Limited, UK

Organizers:

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Council of Young Scientists of Boreskov Institute of Catalysis
- Russian Mendeleev Chemical Society (Novosibirsk Department)
- Novosibirsk State University, Novosibirsk, Russia
- Scientific Council on Catalysis RAS.

The whole number of participants was 165 from 6 countries (Russia, Germany, Poland, The Netherlands, USA, Norway). The leading scientists presented 23 lectures and the young scientists presented 37 oral and 62 poster presentations covering the next main directions:

- Catalysis for Hydrogen Energy, Electrocatalysis
- Catalysis for Petroleum Refining and Petrochemistry
- Catalyst Preparation, Fine Organic Synthesis in Catalysis
- Mechanisms of Heterogeneous Catalysis, Methods of Catalyst Characterization
- Kinetics and Modeling of Catalytic Reactions and Reactors
- Catalysis for Environmental Protection
- The Ways of Technologies Transfer.

The Conference intended to bring together leading experts of the field and the best young researchers, to discuss new results and developments, exchange ideas and new insights, stimulate promising future research projects and promote both existing and new collaborations.

Practical works were an important component of the School-Conference and were conducted by:

- **N.V. Vernikovskaya, Yu.V. Malozemov, S.A. Pokrovskaya -** *"Computer Course: Processes in a Fixed Catalyst Bed".*

The training computer course is developed on the basis of software "Reactor". It includes analysis of the processes occurring in different types of catalytic fixed bed reactors: adiabatic fixed bed reactor (single and multi-stage), tubular and combined ones. Computer course permits students to learn the features of the particular process performance in catalytic fixed bed reactors of different design and to understand how one or another specific process parameter influences on process characteristics.

The course software has modern and ergonomic interface, which supports both Russian and English languages. It provides users with visual presentation of results in form of various graphs and tables.

- **L.S. Poleschuk –** *"Strategy of the Use of Intellectual Property in Commercial Activity. Examples".*

Goals and objectives which can be achieved by patenting, relation of useful model and patent for an invention, relations of author of patent and patentee are discussed. Practical recommendations on preparation for patent specification and claims for invention with connection to strategy of intellectual property application are presented.

A Round Table Discussion on Councils of Young Scientists' activities, and companies' presentations was organized within the Conference framework.

CONTENT

INTERNATIONAL WORKSHOP “BIOSPHERE ORIGIN AND EVOLUTION”

June 26-29, Novosibirsk, Russia

Financial support:

Russian Foundation for Basic Research, Moscow
Presidium of Russian Academy of Sciences

Organizers:

- Trofimuk United Institute of Geology, Geophysics & Mineralogy, Novosibirsk, Russia
- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Cytology and Genetics, Novosibirsk, Russia
- Paleontological Institute, Moscow, Russia

The Workshop comprises 24 plenary lectures, 29 oral presentations and 80 posters in the following sections:

- Problem of Abiogenic Synthesis and Chemical Evolution of Substance under Conditions of Pregeological Stages of Earth Formation to the Beginning Archaean
- Problem of Non-Template Synthesis of Organic Compounds in Biomineral Systems
- “The RNA World”: Problem of Simplest Self-Reproducing Systems on RNA Templates
- Problem of Archaean–Proterozoic Biological Systems
- Problem of Biogeoaromorphosis and Co-Evolution of Abiotic and Biotic Events
- Ecosystem and Biocenosis Organization and Development of Life on Earth
- Problem of Genetic Mechanisms of Progressive Biological Evolution
- Problem of Molecular Genetic Mechanisms of Anthropogenesis.

About 200 participants, among them 19 academicians, have gathered to discuss the problems of biosphere functioning since its origin till now: facts, hypotheses, the newest scientific results.

CONTENT

The workshop was held in the frame of **Program of RAS BIOSPHERE ORIGIN and EVOLUTION**. Nevertheless, foreign colleagues from USA, France, Germany, Norway and Kazakhstan also took part in the meeting.

Chairman of the SB RAS **Academician N. Dobretsov** opened the Workshop with the Lecture "*Origin and Evolution of the Biosphere*". Attention attracted the lectures by **Academician A. Spirin** "*RNA World and its Evolution*" (Institute of Protein Research, Puschino, Russia); **Academician G. Zavarzin** "*Formation of Biosphere*" (Winogradski Institute of Microbiology, Moscow, Russia); **Academician N. Yushkin** *"Mineral Predecessors of Biosystems and Concept of Hydrocarbons Organismobiosis"* (Institute of Geology, Syktyvkar, Russia); **Corresponding Member of RAS A. Rozanov** *"Geobiological Events in the Precambrian"* (Paleontological Institute, Moscow, Russia) and lectures by the team of **Academician V. Parmon** – *"Selective Formation of Ribose from Formaldehyde and Simplest Carbohydrates* C_2-C_3 *in Aqueous Neutral Medium"*, *"Influence of UV Irradiation on the Primary Stages of Butlerov's Reaction"*, *"Putative Mechanism of the Sugar Formation on Prebiotic Earth Initiated by UV-Radiation*".

Academician V. Parmon considered this event as an opportunity for more close cooperation of biologists, geologists, chemists, physicists and philosophers.

Academician G. Zavarzin stated that nowadays the disunity of academic science makes difficult the communication between some main directions. The key point is to establish the contacts between the Earth Science and Life Science. The Workshop provides the base for further developing of collaboration.

Corresponding Member RAS A. Rozanov said: "So many high-level scientists of different specialties have gathered for the first time. There are ideal conditions for discussions".

Scientific Secretary of the Workshop Dr. V. Snytnikov considered that the special feature of the meeting is understands of the fact that natural science is the united area of knowledge and its problems can be solved only at the complex approach to its decision by the experts of a various specialist in the more narrow fields.

Chairman of the SB RAS Academician N. Dobretsov noted the breadth of themes and high level of the lectures.

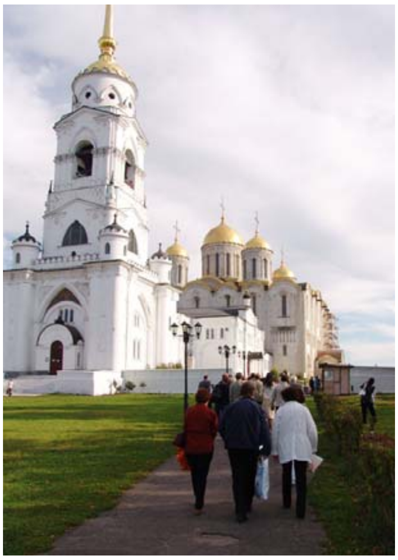
RUSSIAN FOUNDATION FOR BASIC RESEARCH CONFERENCE "FUNDAMENTAL SCIENCE FOR CRITICAL TECHNOLOGIES DEVELOPMENT" with international participation

September 12-14, Vladimir, Russia

The Conference was held in city-museum Vladimir. Vladimir is one of the cities that played the major role in the emergence of the Russian state. The history of the city goes back over one thousand years. Vladimir is famous for its rich and diverse museum expositions which reveal the ancient culture, heroic history and modern life in this fascinating town. Nowadays Vladimir is a big industrial and scientific-technical center with 8 scientific-research institutes.

Conference organizers:

- Russian Foundation for Basic Research, Moscow
- Federal Agency for Science and Innovations, Moscow
- Scientific Council on Catalysis RAS, Moscow
- Boreskov Institute of Catalysis, Novosibirsk
- Uncommercial Partnership "Chemico-Technological Scientific Center", Moscow
- ZAO STC "Vladipor", Vladimir
- JSC "Membranes", Vladimir



CONTENT

Among 130 participants of the Conference – 105 scientists from academic and applied-research institutes and institutes of higher education and 25 – specialists and representatives of industrial enterprises. The lectures were presented by specialists from Russia, Belarus, Ukraine, Kazakhstan, Azerbaijan and Finland.

10 Plenary Lecturers review the latest achievements in the fields of their research.

40 Oral and 58 Poster Presentations were presented in 4 sections:

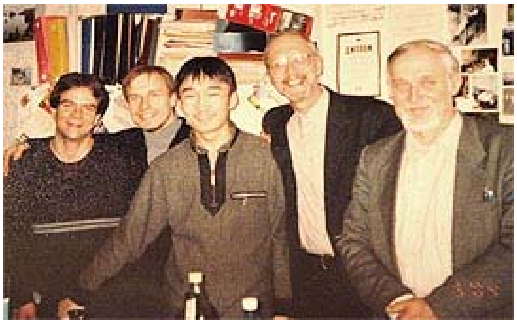
- Catalysts, Membranes and Processes on their Base
- Production, Processing and Investigation of Polymers, Elastomers and Rubbers
- Chemical Products for Medicine, Agriculture, Residential and Special Use
- Energy Saving and Ecology

The section of Young Scientists included 8 presentations on the theme “Membrane and Catalysis”.

Discussions and Round Tables on all themes were organized to held wide contacts between scientists and representatives of the industrial enterprises. One of the purposes of a Conference was acquainting the participants with advanced technologies and processes.

Scientific Social Life

🟩 Last year **Holger Borchert,** a researcher of the Institute of Physical Chemistry of the University of Hamburg engaged in the studies on colloidal nanocrystallites with various physical methods (XPS, electron microscopy, secondary ion mass-spectrometry, X-Ray, IR-spectroscopy of adsorbed CO molecules-probes) and kinetic methods (thermally programmed reduction with methane or hydrogen, thermally programmed reactions of selective methane oxidation, methane steam conversion), had a post-dock training at the Institute of Catalysis after his PhD thesis defense in Germany under the direction of **Prof. V. Bukhtiyarov** and **Prof. V. Sadykov.**



🟩 **Dr. Oleg Martyanov** has got the **prize after Academician K.I. Zamaraev** for the work ***"Development of New Approach to Application of Ferromagnetic Resonance for Physico-Chemical Investigations"*** and **Dr. Ilya Mishakov** has got the **prize after Academician G.K. Boreskov** for the work ***"Study of Chemical and Catalytic Properties of Nanostructured MgO and Catalysts on its Base"*** according to Resolution of the Presidium of the SB RAS on the awarding young scientist with the prizes after the names of outstanding scientists of the SB RAS.

🟩 **"The fame of you will spread across all Russia the Great..."**

May, 20, 2005, annual scientific seminar in memory of Academician Kirill Ilyich Zamaraev has been opened at the conference hall of the Boreskov Institute of Catalysis.

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

The evidence of this were four brilliant lectures, presented by the young scientists, followers of K. Zamaraev scientific school.

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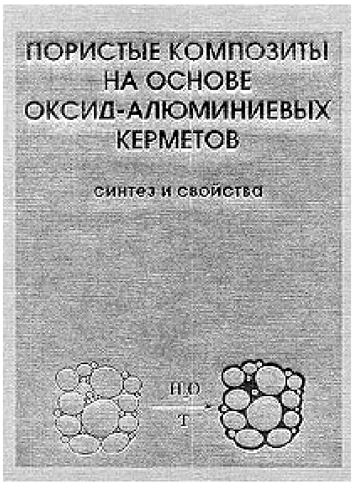
The prize named after Academician V.A. Koptyug is established with the purpose of encouragement of the researchers of the Republic of Belarus and Russian Federation for achievement of outstanding results with performance of joint scientific research within the framework of the interstate programs, and also for the joint works, scientific discoveries and inventions important for a science and practice. It is awarded for the best joint work, discoveries or invention, and also for a series of joint scientific works on uniform subjects having large scientific or practical importance executed within the framework of priority directions approved by the Agreement on Scientific Cooperation between National Academy of Sciences of Belarus and Siberian Branch of Russian Academy of Sciences. The session of the SB RAS Presidium of June, 10 began with a solemn delivery by Chairman of the Branch Academician N. Dobretsov of **Academician V.A. Koptyug prize** to Siberian chemists and Belorussian material scientists.

Results of joint investigations were used as the basis for collective Monograph by **S. Tikhov, V. Sadykov, V. Parmon** (BIC), **V. Romanenkov** (Belarusian National Technical University), **A. Rat'ko** (Institute of General and Inorganic Chemistry NAS Belarusi) *"Porous Composites Based on Oxide-Aluminum Cermets. Synthesis and Properties"* (Publishing House of SB RAS, "Geo" Branch, Novosibirsk, 2004, 205 pp.).

CONTENT



ПОРИСТЫЕ КОМПОЗИТЫ НА ОСНОВЕ ОКСИД-АЛЮМИНИЕВЫХ КЕРМЕТОВ

синтез и свойства

The Monograph is devoted to the physicochemical fundamentals of synthesis of porous ceramometals (cermets): Al_2O_3/Al, $Me/Al_2O_3/Al$, $MeO_x/Al_2O_3/Al$, as well as ceramic composites on their bases, prepared through hydrothermal oxidation of powdered aluminum followed by calcination. The manuscript includes a detailed description of all stages of the preparation and the main properties of the composites (mechanical, textural, thermophysical, and catalytic). Special attention was paid to the relation between the parameters of synthesis and properties of cermets. A series of kinetic and balance equations has been obtained, which permit one to predict the properties of composite materials.

V. Romanenkov
and V. Parmon

The Monograph has no analogs in Russia and abroad as it is based upon the authors’ results obtained for the last 15 years. The Monograph is partially a reference book as it includes summarizing figures, diagrams, and tables. It is useful for specialists in the field of the preparation of porous materials as well as for engineers and students.

V. Sadykov, N. Dobretsov, S. Tikhov

Academician Valentin Parmon was granted the Johnson Matthey sponsored “Innovation in Catalysis” award at the EUROPACAT VII Meeting for “his fundamental contribution to the development of catalytic and photocatalytic solutions to sustainable processes and energy”. The award is managed and administered by the European Federation of Catalyst Societies.

The Presidium of the RAS has awarded the **V.A. Koptyug Prize** for 2005 to **Dr. Andrei Zagoruiko, Prof. Zinfer Ismagilov** (Boreskov Institute of Catalysis) and **Academician Gennadii Sakovich** (Institute of Chemical Power Technologies, Biisk) for the work *"Development and Introduction of New Catalytic Technologies for Preservation of the Environment and Recovery of High-Energy Materials”*.

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

CONTENT

conferences and seminars. In 2005 **S. Arzumanov, I. Glaznev** and **I. Maszov** have got the post-graduate scholarship**; A. Sametova** – incentive post-graduate scholarships.

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

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

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

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

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

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

Boreskov's activity in the area of catalysis was recognized worldwide. He was a foreign member of the National Academy of Sciences of German Democratic Republic, honorary

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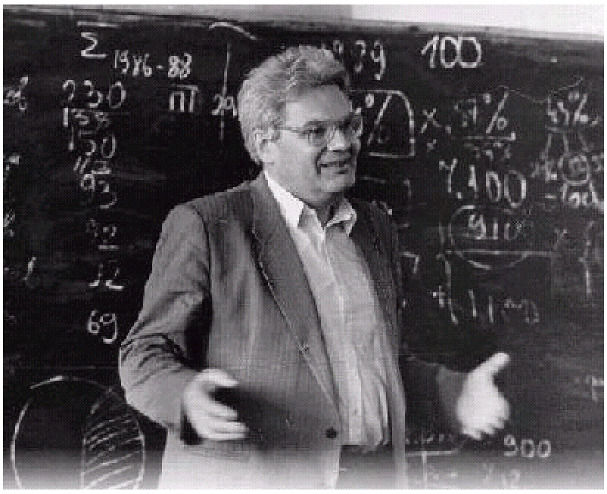
member of the New York Academy of Sciences, Doctor HONORIS CAUSA of the Wroclaw Polytechnic Institute (Poland) and of the Poitiers University (France). Government of Bulgarian Republic awarded the Order of Kirill and Mephodium to G.K. Boreskov. Visitors can see an unusual exposition displaying the full 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.

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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.

CONTENT

RESEARCH ACTIVITY

Quantum-Chemical Studies

MOLECULAR MECHANISM OF DIRECT ALKENE OXIDATION WITH NITROUS OXIDE: DFT ANALYSIS

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

Kinet. Catal., 46(2) (2005) pp. 177-188.

Reaction paths are calculated by the DFT method in the B2LYP/6-31G* approximation for direct oxidation of cyclohexene and butene with nitrous oxide into carbonyl compounds. Two possible reaction channels differing in their intermediate are analyzed. Two-step mechanisms are predicted for these reactions. Both steps are activated reactions. The first step of the first channel is the conversion of the initial reactants into the five-membered heterocycle 1,2,3-oxadiazole, –C–N=N–O–C–, via a transition state. The first step of the second channel leads from the reactants via a transition state to a three-membered heterocycle (epoxide), –C–O–C–. The second step is the decomposition of these intermediates through hydrogen transfer within the hydrocarbon backbone and the formation of the final products. The rate-limiting step in the oxidation of cyclohexene and butene is determined by the electronic structure of the –C–N=N–O–C– heterocycle and is independent of the structure of the other hydrocarbon moieties. The activation energies calculated for separate steps suggest that the first reaction channel, leading to carbonyl compound, is more favorable from the standpoint of energetics. Two reaction pathways are possible for butene-1 oxidation, one leading to a ketone and the other to an aldehyde. The ketone is predicted to dominate in the product.

MODELING OF ACTIVE CENTERS OF SUPPORTED CATALYSTS V_2O_5/SiO_2 AND V_2O_5/TiO_2. THEORETICAL ANALYSIS OF OPTICAL PROPERTIES BY DFT METHOD

V.I. Avdeev, G.M. Zhidomirov

J. Struct. Chem., 46(4) (2005)
pp. 599-612.

Analysis of electron structure of monooxo-, dioxovanadium functional groups in tetrahedral coordination, modeling active centers (AC) of fine supported catalysts V_2O_5/SiO_2 and V_2O_5/TiO have been performed in the frames of the density functional theory (DFT). Optimum structures of three AC are defined as possible models of monomeric and polymer oxyvanadium species over the supports with low vanadium content. Calculations of the energy of excited states of accepted AC models have been performed using modified time-dependent DFT method (TDDFT). Optical absorption spectra in the region 25000—60000 cm^{-1} were reconstructed. Spectrum in this region is caused by $O \rightarrow V$ charge transfer. Characteristic properties of electron spectra with charge transfer are investigated for the catalysts V_2O_5/SiO_2 and V_2O_5/TiO_2, and vibrational spectra for three models of AC centers, corresponding to monomeric and dimeric oxyvanadium species of supported catalysts are determined. Detail interpretation of frequencies of normal vibrations is given. The frequencies typical for monomeric and dimeric oxyvanadium species over surface support are identified.

ETHYLENE ADSORPTION ON THE Pt–Cu BIMETALLIC CATALYSTS. DENSITY FUNCTIONAL THEORY CLUSTER STUDY

V.I. Avdeev, V.I. Kovalchuk*, G.M. Zhidomirov, J.L. d'Itri* (**Department of Chemical Engineering, University of Pittsburgh, Pittsburgh, USA*)

Surf. Sci., 583(1) (2005)
pp. 46-59.

The adsorption of ethylene on $Cu_{12}Pt_2$ clusters has been studied within the density functional theory (DFT) approach to understand the high ethylene selectivity of Cu-rich Pt–Cu catalyst particles in the reaction of hydrogen-assisted 1,2-dichloroethane dechlorination. The structural parameters for $Cu_{12}Pt_2$ clusters with D_{4h}, D_{2d}, and C_{3v} symmetry have been calculated. The relative stability of the isomeric $Cu_{12}Pt_2$ clusters follows the order: $C_{3v} > D_{2d} > D_{4h}$. Each isomer has an active site for ethylene adsorption that consists of a single Pt atom surrounded by Cu atoms. The interaction of ethylene with the active site yields a π-C_2H_4 adsorption complex. The strongest π-C_2H_4 complex forms with the cluster of C_{3v} symmetry; the bonding energy, $\Delta E_\pi(C_2H_4)$, is -15.6 kcal mol^{-1}. The bonding energies for the π-C_2H_4 complex with Cu_{14} and Pt_{14} clusters are -6.5 and -18.8 kcal mol^{-1}, respectively.

ADSORPTION OF CARBON ON Pd CLUSTERS OF NANOMETER SIZE: A FIRST-PRINCIPLES THEORETICAL STUDY

K.M. Neyman*, C. Inntam, A.B. Gordienko**, I.V. Yudanov, N. Roesch**** (**Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain; **Department Chemie, Technische Universität München, Garching, Germany)*

J. Chem. Phys., 122(17) (2005) pp. 174705 (9 pages).

Adsorbed atomic C species can be formed in the course of surface reactions and commonly decorate metal catalysts. C adsorption on Pd nanoclusters was studied computationally using an all-electron scalar relativistic density functional method. The metal particles under investigation, Pd_{55}, Pd_{79}, Pd_{85}, Pd_{116}, Pd_{140}, and Pd_{146}, were chosen as fragments of bulk Pd in the form of three-dimensional octahedral or cuboctahedral crystallites, exposing (111) and (100) facets as well as edge sites. These cluster models are shown to yield size-converged adsorption energies. It was examined which surface sites of these clusters are preferentially occupied by adsorbed C. According to calculations, surface C atoms form strongly adsorbed carbide species (with adsorption energies of more than 600 kJ mol^{-1}) bearing a significant negative charge. Surface sites allowing high, fourfold coordination of carbon are overall favored. To avoid effects of adsorbate-adsorbate interaction in the cluster models for carbon species in the vicinity of cluster edges, the authors reduced the *local* symmetry of selected adsorption complexes on the nanoclusters by lowering the *global* symmetry of the nanocluster models from point group O_h to D_{4h}. On (111) facets, threefold hollow sites in the center are energetically preferred; adsorbed C is calculated to be slightly less stable when displaced to the facet borders.

ADSORPTION OF Cu_4, Ag_4 AND Au_4 PARTICLES ON REGULAR MgO(001) SURFACE: A DENSITY FUNCTIONAL STUDY USING EMBEDDED CLUSTER MODELS

C. Inntam*, L.V. Moskaleva*, I.V. Yudanov, K.M. Neyman,***, N. Roesch*** (**Department Chemie, Technische Universität München, Garching, Germany; **Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain; ***Departament de Química Física, Universitat de Barcelona, Barcelona, Spain*)

Chem. Phys. Lett., 417(4-6) (2005) pp. 515-520.

Cu_4, Ag_4, and Au_4 species adsorbed on the regular MgO(001) surface are studied using a density functional method and cluster models embedded in an elastic polarizable environment. The structure of the coinage metal tetramers is only slightly distorted by adsorption on the oxide surface compared to the rhombic-planar arrangement in the gas phase. The most stable adsorption complexes of all three systems feature upright metal planar particles with the M_4 moiety orthogonal to the surface and two metal atoms attached to surface oxygen anions. Au_4 and Cu_4 exhibit substantially stronger binding to the surface than Ag_4.

ELECTRON STRUCTURE OF OXYGEN COMPLEXES OF FERROUS ION CENTER

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

Chem. Phys. Lett., 414(4-6) (2005) pp. 434-437.

The electron structure of ferryl ion $[FeO]^{2+}$ active in oxidation of hydrocarbons is studied using CASSCF theory followed by ISA-MRMP correction. $[FeO]^{2+}$ is modeled by the $OFe(OH)_2$ species. The $^5A_1$ and $^5B_2$ states are predicted to be low-lying states for the $[FeO]^{2+}$ unit. At the decreased (H)O–Fe–O(H) angles $^5B_2$ becomes the ground state. The $^5B_2$ state appears to be a mixture of configurations with quite large weight of the split-electron-pair configuration. This state can be considered as anion-radical state of oxygen which seems to be responsible for the activity of the $[FeO]^{2+}$ moiety toward the activation of the C–H bond.

SPECTROSCOPIC IDENTIFICATION OF ADSORPTION PROPERTIES OF Zn^{2+} IONS AT CATIONIC POSITIONS OF HIGH-SILICA ZEOLITES WITH DISTANT PLACING OF ALUMINIUM IONS

G.M. Zhidomirov, A.A. Shubin, V.B. Kazansky*, R.A. van Santen** (**Zelinsky Institute of Organic Chemistry, Moscow, Russia; **Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands*)

Theoret. Chem. Acc., 114(1-3) (2005) pp. 90-96.

For Zn^{2+} cations in ZnZSM-5 zeolite unusual type of cationic positions, formed by two distantly placed framework aluminium atoms, is considered. Some extent of structural destabilization of cations in these cationic positions in comparison with traditional localization should result in promoted Lewis activity and adsorption activity of these sites. The last ones are manifested in the significantly increased IR low frequency shifts for adsorbed molecules and in their ability for heterolytic dissociation at elevating temperature. DFT cluster quantum chemical modeling

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of light alkane adsorption on Zn^{2+} in ZnZSM-5 zeolites confirms these conjectures in full agreement with recent experiments. Similar to the previously considered dihydrogen and methane molecule adsorption, here are presented the calculations of ethane molecular and dissociative adsorption on these sites. It is shown that the unusually large ethane IR frequency shift recently observed in ZnZSM-5 zeolite can result from adsorptive interaction of C_2H_6 with Zn^{2+} stabilized in a cationic position with distantly placed aluminium ions. The dissociative adsorption of ethane molecules with the formation of bridged hydroxyl group and Zn–C_2H_5 structure is considered and an activation energy of ethylene formation from the alkyl fragment is evaluated.

ON THE POSITION OF THE NITROGEN 2p ENERGY LEVEL IN ENDOHEDRAL N@C$_{60}$ (I$_h$)

**B.N. Plakhutin, N.N. Breslavskaya*,
E.V. Gorelik**, A.V. Arbuznikov****** (**Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia; **International Tomography Center, Novosibirsk, Russia; ***Nikolaev Institute of Inorganic Chemistry, University of Wuerzburg, Wuerzburg, Germany*)

J. Molec. Struct.: THEOCHEM,
727(1-3) (2005) pp. 149-157.

The work presents results of nonempirical ROHF, UHF, and DFT calculations of endohedral N@C$_{60}$ (I_h) and of its constituents, C$_{60}$ (I_h) and the free N atom, in their neutral and charged forms. Based on these results, a detailed discussion is presented on the position of the nitrogen 2*p* energy level in N@C$_{60}$. The main purpose of this work is to reveal the source of essential discrepancies in previous ROHF and DFT calculations on N@C$_{60}$ (I_h). It is first demonstrated the limited validity of the Koopmans' theorem exploited in previous works. It is shown that the one-electron energies in N@C$_{60}$ derived at the same ROHF/6-31G* level with different quantum chemical programs (Gamess, Gaussian-98, Monstergauss, Turbomole) are not constant and vary over wide limits. The value of the ionization potential from the 2*p* level of the encapsulated N atom was estimated in the present work by both a ΔSCF method and the Koopmans' theorem and was compared with previously reported values. It is also shown that ROHF and DFT methods give in fact the very similar results for N@C$_{60}$ (i.e. the same ground electronic configuration and the same localization of the spin density) and discuss the known opposing conclusion on this point.

ANOMALOUS VALUES $\langle \hat{S}^2 \rangle$ BEFORE AND AFTER ANNIHILATION OF THE FIRST SPIN CONTAMINANT IN UHF WAVE FUNCTION

**B.N. Plakhutin, E.V. Gorelik*,
N.N. Breslavskaya**, M.A. Milov,
A.A. Fokeev***, A.V. Novikov****,
T.E. Prokhorov, N.E. Polygalova****,
S.P. Dolin**, L.I. Trakhtenberg***** (**International Tomography Center, Novosibirsk, Russia; **Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia; ***Karpov Institute of Physical Chemistry, Moscow, Russia; ****Novosibirsk State University, Novosibirsk, Russia*)

J. Struct. Chem., 46(2) (2005) pp. 195-203.

A number of molecular systems for which the average values $\langle \hat{S}^2 \rangle$ before and after annihilation of the first spin contaminant in the wave function of the unrestricted Hartree-Fock method are anomalously large (they substantially exceed the expected value $S(S+1)$) is presenred. An example of such systems is N@C$_{20}$, for the doublet state of which the $\langle \hat{S}^2 \rangle$ values are equal to 4.2595 before and 13.1390 after annihilation, respectively (calculated by UHF/6-31G* method). It is shown that four, at the least, spin multiplets ($S' = S$, $S+1$, $S+2$, $S+3$) contribute comparatively to the wave function of such systems. The relations are derived allowing one to estimate the contributions of the highest multiplets basing on the average values of $\langle \hat{S}^2 \rangle$ before and after annihilation of the first spin contaminant.

SPLITTING OF ATOMIC d^N TERMS IN 3*d*-METAL-ENDOFULLERENES M@C$_{60}$ OF ICOSAHEDRAL SYMMETRY

E.B. Gorelik*, B.N. Plakhutin (**International Tomography Center, Novosibirsk, Russia*)

J. Struct. Chem., 46(5) (2005) pp. 799-812.

Group-theoretical and quantum-chemical investigation of low-lying exited states of 3*d*-metal-endofullerens M@C$_{60}$ (M = Mn, Cr, Fe) in their different charge states were carried out using ROHF and FCI-RAS (Full CI in Restricted Active Space) methods. The studies were mainly aimed at a quantum-chemical examination of the anomalous (non-Bethe's) nature of d^N atomic terms splitting in an electrostatic field with icosahedral symmetry predicted earlier within the framework of the theory of integral invariants. Relationships between the integral invariant theory and quantum-chemical methods used in the work are discussed in detail. The calculations revealed that atomic d^N terms in the icosahedral field generated by fullerene C$_{60}$ (I_h) cage at the metal atom (ion) remain non-split at different charge states of a metal and C$_{60}$. The reasons of the predicted phenomenon and possible approaches to check it are also discussed. It was demonstrated that d^N terms of an encapsulated metal in the icosahedral 3*d*-MEF are only split at a very strong compression of these structures.

THE POSSIBLE ROLE OF INTERMEDIATE NH SPECIES IN OSCILLATIONS OF THE NO+H_2 REACTION ON NOBLE METAL SURFACES

A.R. Cholach, N.N. Bulgakov, B.E. Nieuwenhuys*
(**Leiden Institute of Chemistry, Leiden,*
The Netherlands)

Surf. Sci., 573(2) (2004) pp. 264-271.

A comparative study of the thermodynamic properties of adsorbed NH_n species ($n = 0, 1, 2, 3$) on transition metal surfaces is performed by using the semi-empirical method of interacting bonds. The principal difference between single crystal surfaces exhibiting oscillatory behavior in the NO+H_2 reaction, and those surfaces which do not show such a behavior is that the combination reaction of NH species can easily proceed in the former case, whereas it is substantially endothermic on the latter surfaces.

A trigger-like route for the oscillatory behavior is considered where the combination reaction of NH species operates as a temporary reaction pathway. This pathway practically does not contribute to the N_2 formation until the nitrogen coverage reaches some critical value, which ensures a sufficiently close distance between adjacent NH particles. The trigger pathway starts upon reaching that *stage* initiating the surface wave propagation, and stops immediately when the wave propagation is completed. The surface becomes then nearly clean and ready for the next oscillatory cycle. In this way, the feedback mechanism and the critical point of the regular wave initiation can be understood without any further assumptions. An alternative key reaction is also considered.

TRANSFORMATION OF BLOCH REPRESENTATION INTO ATOMIC ORBITAL REPRESENTATION AND COMBINED MATRIX ELEMENT CALCULATION TECHNIQUE FOR SPATIALLY BOUNDED BASIS FUNCTIONS IN CRYSTALS

V.M. Tapilin

J. Struct. Chem., 46(1) (2005) pp. 1-8.

A method is proposed for transforming the Hamiltonian from Bloch to atomic function representation. For spatially bounded functions, this is a rigorous method based on solution of a certain algebraic system of equations. Unlike the conventional procedure based on integration over the Brillouin zone, the new method requires knowledge of the matrix elements of the Bloch representation only at several points of the Brillouin zone. The number of these points is determined by the trimming radius for the spatially bounded functions and by the lattice constant. The method can be used for calculating matrix elements in a basis of atomic functions and for reducing computations in matrix element calculations of the Bloch representation for procedures using numerical integration.

CORRUGATED SINGLE-LAYER GRAPHITE SHEET AS A MODEL OF STEPPED SURFACE OF A CRYSTAL

V.M. Tapilin

J. Struct. Chem., 46(1) (2005)
pp. 9-15.

Electronic structure calculations have been performed for flat graphite sheets and periodically distorted sheets with different values of deformation angle and hydrogen adsorption. These characteristics do not all behave monotonically with increasing deformation angle. At small deformation angles, the electrons pass from the atoms of terraces to those of edges, while at larger angles the reverse pattern is observed. The position of the Fermi level also varies nonmonotonically. The binding energy of hydrogen depends significantly on the adsorption site, and the difference can be doubled. Based on the ata obtained, it was concluded that a priori statements derived from the “general concepts” on the difference in the physicochemical properties of, for example, terrace and edge atoms on high-index facets are unreliable.

AB INITIO CALCULATION OF NITROGEN OXIDE DIMER STRUCTURE AND ITS ANION-RADICAL

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J. Struct. Chem., 46(2) (2005) pp. 213-219.

A comparative quantum chemical analysis has been made for the most stable dimer of nitrogen oxide with the structure *cis*-ONNO in a singlet state $^1A_1$ by *ab initio* method of SCF MO LCAO, allowing for electron correlation according to Meller-Plesset perturbation theory of the second order (MP2), and density functional technique (DFT). The computations by MP2 method show anion-radical (ONNO)$^-$ to have a strong bond between nitrogen atoms (N-N 1.44 Å) in contrast to molecular weakly bound *cis*-dimer with equilibrium distance N-N 2.23 Å. Molecular orbital structure of the dimer and its anions was examined that made it possible to suggest a reason of preferable stabilization of nitrogen oxide dimer in the *cis*-form. Calculated high affinity to electron (E_a= −1.55 - −1.69 eV) for the molecular dimer ONNO ($^1A_1$) explains an intense strengthening of N-N bond in anion-radical and confirms the experimental data on a possibility of surface anion-π-radical formation on electron donor centers. The DFT computations indicate that this technique poorly reproduces the experimental geometry and electron structure of the *cis*-dimer ONNO having predicted a triplet ground state with the equilibrium distance N-N ≈2 Å instead of a singlet one with N-N 2.26 Å. The comparison between MP2 and DFT calculations for complex dimer ONNO with copper cation reveals the energy state of the complex $(Cu\text{-}O_2N_2)^+$ corresponding to stabilization of anion-π-radical $(N_2O_2)^-$ {term-$^3A_2$, Cu(d)^9-(ONNO)$^{-1}$} to be highly overestimated by DFT.

STRUCTURE OF IRRADIATED POLYTETRAFLUOROETHYLENE ACCORDING TO DFT CALCULATIONS OF NMR CHEMICAL SHIFTS

V.M. Buznik, S.P. Gabuda*, S.G. Kozlova*, L.N. Ignatieva** *(*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia; **Institute of Chemistry, Far East Branch, Vladivostok, Russia)*

J. Struct. Chem., 46(1) (2005) pp. 87-92.

Methods of density functional theory were used to calculate ^{1}H, ^{13}C, and ^{19}F magnetic shielding tensors for $C_7F_nH_mO_l$ model molecules, which can arise as fragments from radiation exposure of polytetrafluoroethylene.

Monte-Carlo Simulations to Study Physicochemical Processes

SIMULATION OF THERMAL DESORPTION SPECTRA OF N$_2$ OBSERVED DURING N$_2$O DECOMPOSITION ON Rh(110)

V.P. Zhdanov, T. Matsushima* (**Catalysis Research Center, Hokkaido University, Sapporo, Japan*)

Surf. Sci., 583(2-3) (2005) pp. 253-264.

Under temperature-programmed conditions, N_2O decomposition occurs on Rh(110) between 60 and 190 K and results in N_2 desorption. Experimental studies of the angular distribution of the flux of the reaction products indicate that N_2 molecules leave the surface both during and after N_2O dissociation events. The N_2 TPD spectra observed are complex. In particular, there are four peaks, registered between 60 and 150 K and related to N_2 desorption accompanying N_2O-dissociation acts, and a peak recorded at 160 K and attributed to desorption of adsorbed N_2 molecules. Monte Carlo simulations of these spectra are presented. The model takes into account both channels of N_2 desorption and also N_2O–O lateral interactions stabilizing N_2O adsorption. With these relatively simple ingredients, the model reproduces the main features of the measured TPD kinetics, including the positions and intensities of all the peaks.

ANALYSIS OF THE KINETICS OF N$_2$O–CO REACTION ON Pd(110)

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Surf. Sci., 583(1) (2005) pp. 36-45.

Experimental studies indicate that the N_2O–CO reaction occurring on Pd(110) under UHV conditions exhibits a first-order kinetic phase transition in the steady-state case and also transient kinetics strongly dependent on the initial state of the system. A mean-field kinetic model describing these phenomena is constructed. With a minimal number of the fitting parameters, the model reasonably reproduces the special features of the reaction kinetics.

SIMULATIONS OF TEMPERATURE DEPENDENCE OF THE FORMATION OF A SUPPORTED LIPID BILAYER VIA VESICLE ADSORPTION

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Coll. Surf. B., 39(1-2) (2004) pp. 77-86.

Recent experimental investigations of the kinetics of vesicle adsorption in solution on SiO_2 demonstrate a thermally activated transition from adsorbed intact vesicles to a supported lipid bilayer. Monte Carlo simulations clarify the mechanism of this process. The model employed is an extension of the model used earlier to describe vesicle adsorption at room temperature. Specifically, it includes limitations of the adsorption rate by vesicle diffusion in the solution, and adsorption- and lipid-membrane-induced rupture of arriving and already adsorbed vesicles. Vesicles and lipid molecules, formed after rupture of vesicles, are considered immobile. With these ingredients, the model is able to quantitatively reproduce the temperature-dependent adsorption kinetics, including a higher critical surface concentration of intact vesicles for lower temperatures, and the apparent activation energy for the vesicle-to-bilayer transition $E_a \simeq 5$ kcal/mol.

FLUCTUATIONS IN KINETIC OSCILLATIONS ON nm-SIZED CATALYST PARTICLES

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Surf. Sci., 588(1-3) (2005) L220-L226.

For adsorption–desorption equilibrium at nm-sized supported catalyst particles, the fluctuations of the number of adsorbates are given by the grand canonical distribution. To clarify what may happen far from equilibrium during chemical oscillations on such particles, Monte Carlo simulations of the kinetics of CO oxidation accompanied by the formation of surface oxide have been executed. The fluctuations were analyzed locally, i.e. inside each oscillation period, and globally by comparing the coverages at different oscillation periods. In both cases, the fluctuations are found to often deviate from those corresponding to equilibrium. In particular, the locally defined fluctuations depend on the phase and may be nearly equal to and/or appreciably larger or smaller than those at equilibrium.

BISTABLE MEAN-FIELD KINETICS OF CO OXIDATION ON Pt WITH OXIDE FORMATION

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Appl. Surf. Sci., 239(3-4) (2005) pp. 424-431.

The bistability of the kinetics of CO oxidation on Pt at sub-atmospheric pressures can be complicated by surface-oxide formation. A simple mean-field model is presented making it possible to describe a transition from the low reactive reaction regime occurring via the conventional mechanism of CO oxidation at CO excess, to the high reactive regime including CO interaction with a fully developed surface-oxide overlayer at O_2 excess. In the latter case, the oxide is assumed to form islands, the CO_2 formation may run primarily on oxide, and in agreement with recent experiments the reaction rate may be several orders of magnitude lower than the CO adsorption rate on a bare metal surface.

TWO-VARIABLE PERIODIC PERTURBATION OF KINETIC OSCILLATIONS

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Catal. Lett., 99(3-4) (2005) pp. 199-202.

Using one of the generic models (CO oxidation on Pt with surface-oxide formation) predicting kinetic oscillations in heterogeneous catalytic reactions, it was shown that the efficiency of two-variable periodic perturbations with respect to converting natural period-1 oscillations to period-l oscillations at the forcing frequency is remarkably sensitive to the kind of perturbations used. “Counter-phase” perturbations are much more effective compared to “in-phase” perturbations. The physics underlying these findings is suggestive of their applicability to many other models and/or real systems exhibiting kinetic oscillations.

MONTE CARLO SIMULATION OF BIFURCATION IN THE INTRACELLULAR VIRAL KINETICS

V.P. Zhdanov

Phys. Biolog., 2 (2005) pp. 46-50.

Intracellular viral kinetics are of especial interest because the virion population inside an infected cell is well known to tend to grow exponentially and the corresponding kinetics may be unstable. To clarify the special features of such kinetics, Monte Carlo simulations are presented taking into account the key steps of virion formation and competition of the host and viral mRNA for the host translation apparatus. Asymptotically, the model employed predicts either a stable steady state or 'ignition' with the unlimited viral growth. Under steady-state conditions, the mean square fluctuations of the viral genome and virion numbers are found to be appreciably larger than those expected on the basis of the Poissonian distribution. In the case of unstable kinetics, the simulations show the type of deviations from the corresponding mean-field results.

DYNAMICS OF SURFACE REACTIONS: FROM "HOT" PRECURSORS TO CONVENTIONAL THERMAL ACTIVATION

V.P. Zhdanov

Surf. Sci., 575(3) (2005) pp. 313-320.

Heterogeneous catalytic reactions usually contain steps, e.g., adsorption, generating energy-rich ("hot") precursors for other steps. With increasing the rate of energy relaxation one can observe a transition from the reaction regime dominated by "hot" precursors to conventional thermal activation. To illustrate this transition in detail and to show what may happen in various situations, an analytical model based on the Fokker–Planck equation for energy relaxation is presented.

PATTERN FORMATION IN HETEROGENEOUS CATALYTIC REACTIONS WITH PROMOTERS AND POISONS

V.P. Zhdanov

Phys. Chem. Chem. Phys.,
7(11) (2005) pp. 2399-2402.

Using one of the simplest models of heterogeneous catalytic reactions occurring on a single-crystal surface and including promoters or poisons, generic Monte Carlo simulations of the growth of islands composed of reactants and promoters or poisons in the case when the lateral interaction between these species is attractive have been performed. The results obtained indicate that in reaction with promoters the islands are traveling and their growth is eventually terminated. These two features are rationalized taking into account that the reaction primarily occurs inside islands and under chemically reactive conditions the balance of adsorbate diffusion there and outside islands can hardly be maintained if the islands are frozen or grow asymptotically. In reaction with poison, in contrast, the model predicts asymptotic power-law island-size growth, because in this case the situation inside islands is kinetically stable and accordingly the conditions in the overlayer are close to those occurring during the Ostwald ripening. The growth exponent obtained for this regime is however somewhat smaller than that expected for the Ostwald ripening.

SIMULATION OF THE GROWTH OF NEUROSPHERES

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Europhys. Lett., 68(1) (2004) pp. 134-140.

Under appropriate conditions, the neural stem cells are able to proliferate and to form suspended neurospheres containing stem cells and neuronal and glial progenitors in different stages of differentiation. Suggested lattice Monte Carlo simulations, taking into account the effect of spatial constraints and cell-cell adhesion on cell diffusion and division, show that i) the neurosphere-size distribution is very broad and ii) the spatial distribution of various cells inside neurospheres is heterogeneous.

SIMULATION OF PROLIFERATION OF NEURAL STEM CELLS ON A SURFACE WITH EMPHASIS ON SPATIAL CONSTRAINTS ON CELL DIVISION

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Phys. Chem. Chem. Phys.,
7(19) (2005) pp. 3496-3500.

Monte Carlo lattice simulations of proliferation of cells on a surface is presented in the situation when the cell–cell adhesion is relatively strong and the cells may form islands and/or flattened hemispheres. The model parameters were chosen to mimic proliferation of adult rat neural stem cells (or, more specifically, adult hippocampal progenitor cells) deposited on polyornithine and laminin coated polystyrene. The results obtained show that the spatial constraints on cell division may result in slowdown of the exponential growth. Depending on the rules used for cell division, this effect may be either nearly negligible or appreciable. In the latter case, the scale of the deviations from the exponential growth is comparable with that observed in experiments. In the simulations, the slowdown of the growth starts however somewhat earlier and occurs in a less abrupt manner. This seems to indicate that the spatial constraints on division of cells are not the main factor behind the experimentally observed termination of the growth.

MODELS OF $(ZrO_2)_n$ COMPLEXES INTERCALATED INTO MONTMORILLONITE

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J. Phys. Chem. B, 109(15) (2005) pp. 7451-7459.

The article discusses the properties of several model zirconium dioxide complexes $(ZrO_2)_n$ intercalated into the interlayer space of montmorillonite clay. Grand canonical Monte Carlo simulation was used in a series of numerical experiments during analysis of the low-temperature nitrogen adsorption in the micropores thus generated. The goal of such experiments was to determine the

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geometrical parameters of introduced molecular complexes of different types inside micropores of various widths. The obtained information was used to characterize textural and structural properties of three pillared interlayer materials prepared by using pillaring species synthesized via aging of zirconyl chloride solutions containing as additives chlorides of Ca, Sr, or Ba. It was found that in the cases of Ba and Ca the interlayer micropores are filled with isolated tetramers $(ZrO_2)_4$. Meanwhile, the presence of Sr in the pillaring solution, most likely, favors the preservation of larger sheetlike complexes $(ZrO_2)_8$.

MODELING OF CRYSTALLIZATION PROCESS IN CONFINED MELT OF SULFURIC ACID CATALYST

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J. Phys. Chem. B,
109(43) (2005) pp. 20051-20054.

Metropolis Monte Carlo technique has been applied to simulate the crystallization process in the melt of vanadium sulfuric acid supported catalysts. The melt is a lattice binary compound consisting of $(V^{4+})_2$ and $(V^{5+})_2$ binuclear complexes (dimers) confined by pore walls of cylindrical or slitlike shape. It has been shown that the crystallization process retards significantly as the pore size decreases. This result is in good agreement with the experimental data obtained earlier. The effect of the energy properties of pore walls (attractive, repulsive, or inert) on the crystallization features has been studied as well.

CLAYS PILLARED BY ZIRCONIA NANOPARTICLES: SPECIFICITY OF STRUCTURE AND ADSORPTION PROPERTIES AS RELATED TO CATALYSIS OF NO_x SELECTIVE REDUCTION BY HYDROCARBONS IN THE EXCESS OF OXYGEN

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Mater. Res. Soc. Symp. Proc.,
Vol. 876E (2005) R8.21.1.-R8.21.6.

Modeling of high resolution nitrogen adsorption isotherms by Grand Canonical Monte Carlo (GCMC) for zirconia-pillared clays containing 20 wt.% of ZrO_2 revealed that pillars are comprised of separate $Zr_4(\mu\text{-}OH)_8(OH)_m (H_2O)_n$ tetramers and Zr_8 dimers as sheets or loose 3D structures. This agrees with the results of modeling of condensation process in solution by DFT approach and semiempirical PM3 method. Bridging and terminal hydroxyls strongly bound with Zr cations are involved in anchoring supported Cu cations and Pt. This nanostructure of the active component as well as developed micro- and mesoporosity are responsible for the high performance of Pt+Cu/ZrPILC catalysts in NO_x selective reduction by propylene and decane in realistic feeds.

ATOMIC SCALE IMAGING OF OSCILLATIONS AND CHEMICAL WAVES AT CATALYTIC SURFACE REACTIONS: EXPERIMENTAL AND STATISTICAL LATTICE MODELS

V.I. Elokhin, V.V. Gorodetskii

In "*Finely Dispersed Particles: Micro-, Nano-, and Atto-Engineering*".
Surf. Sci., Eds. A.M. Spasic, J.-P. Hsu,
Taylor & Francis, CRS Press: New York, 2005,
vol. 130. Chapter 7, pp. 159-189.

The reaction between CO and O_2 on Pd(110) and Pt(100) surfaces and the mechanism of surface wave generation in the oscillating regime of this reaction on Pd and Pt tip surfaces was investigated using different macroscopic (MB, TPR, HREELS, WF) and microscopic (FEM, FIM) analytical tools to learn about the details of the reaction dynamics at those catalyst surfaces.

The principal result of this work is that the non-linear reaction kinetics is not restricted to macroscopic planes since: (i) the planes ~ 200 Å in diameter show the same non-linear kinetics; (ii) the regular waves appear under the reaction rate oscillations; (iii) the propagation of reaction-diffusion waves includes the participation of the different crystal *nano*planes and indicates an effective coupling of adjacent planes.

Chemical wave patterns corresponding to moving surface concentration patches are the result of coupling of surface diffusion, surface reconstruction and surface reaction. Depending on the reaction condition, such spatio-temporal phenomena can also lead to an oscillatory behavior of the overall reaction rate. It becomes possible to study the catalysis on an atomic level which is necessary for understanding of the mechanism of the action of the high-dispersion supported metal catalysts having the metal microcrystallites ~ 100-300 Å in size as an active part of the catalyst. This result opens new fields for the development of theoretical concepts of heterogeneous catalysis.

Statistical lattice models that describe the oscillation and wave dynamics in the adsorbed layer for the reaction of CO oxidation over the Pt(100) and Pd(110) single crystal surfaces were constructed and studied. These models differ in the mechanisms of formation of oscillations: a mechanism involving the phase transition of planes (Pt(100): (hex) → (1×1)) and a mechanism with the formation of surface oxides (Pd(110)). The models demonstrate the oscillations of the rate of CO_2 formation and the concentrations of adsorbed reactants. These oscillations are accompanied by various wave processes on the lattice that models single crystalline surfaces. The effects of the size of the model lattice and the intensity of CO_{ads} diffusion on the synchronization and the form of oscillations and surface waves are studied. It was shown the presence of a narrow zone of the reaction when the wave front propagates along the metal surface. This is supported by the results obtained by FEM and FIM methods. It was found that the inclusion of CO_{ads} diffusion anisotropy, which reflects the real symmetry of the single crystal Pd(110) surface does not affect the dynamics of oscillations of the integral characteristics of the reaction (the rate and the surface coverage), but it leads to the formation of ellipsoid spatio-temporal structures on the surface, which were observed experimentally with modern physical methods for surface science studies. It is possible to obtain a wide spectrum of chemical waves (cellular and turbulent structures and spiral and ellipsoid waves) using the lattice models developed. These waves have been observed in experimental studies of oscillatory dynamics of catalytic reactions.

Finally, the character of the $CO+O_2$ oscillating reaction on Pd differs remarkably from that on Pt because: (a) different subsurface oxygen (Pd) and (hex)↔(1×1) phase transition (Pt) mechanisms apply; and (b) the oxygen front in $CO+O_2$ waves travel in reverse directions: on Pd it goes from (110) to (100) surface, on Pt it travels in the opposite direction.

FIELD ELECTRON AND FIELD ION MICROSCOPY STUDIES OF CHEMICAL WAVE PROPAGATION IN OSCILLATORY REACTIONS ON PLATINUM GROUP METALS

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Catal. Today, 105(2) (2005) pp. 183-205.

The present paper reviews investigations, concerning the reactions of $CO + O_2$, $H_2 + O_2$, $NO + H_2$ on Pt, Pd, Rh and Ir tip surfaces studied on an atomic level. The main goal of the study was to obtain more detailed information on the mechanism of spatio-temporal oscillations on nanoplane surfaces with the help of field electron microscopy (FEM) and field ion microscopy (FIM). Sharp tips in size up to several hundreds of Angstroms have been used to carry out *in situ* investigations of real dynamic surface processes where different crystallographic nanoplanes of the tip are simultaneously exposed to the reacting gas and for which it is possible to study the interaction and the coupling of adjacent planes. The sustained temporal oscillations are associated with the appearance of propagation waves, which are generated by coupling of oscillations on adjacent crystal planes. Three fundamentally different feedback mechanisms generating kinetic oscillations have been identified: periodic changes in surface structure (Pt tip: $CO + O_2$, $H_2 + O_2$), subsurface oxygen formation (Pd tip: $CO + O_2$) and a strongly non-linear interaction between adsorbed species (Rh and Ir tips: $NO + H_2$). Based on experimental results, a model for the carbon monoxide-oxygen reaction on Pt(100) and Pd(110) surfaces is proposed for mathematical Monte Carlo modeling.

TURBULENT AND STRIPES WAVE PATTERNS CAUSED BY LIMITED CO_{ads} DIFFUSION DURING CO OXIDATION OVER Pd(110) SURFACE: KINETIC MONTE-CARLO STUDIES

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Chem. Eng. J., 107 (2005)
pp. 181-189.

The dynamic behaviour of the CO oxidation reaction over Pd(110) has been studied by means of kinetic Monte-Carlo modelling. The influence of the internal parameters on the shapes of surface concentration waves obtained in simulations under the limited surface diffusion intensity conditions has been studied. The hysteresis in oscillatory behaviour has been found under step-by-step variation of oxygen partial pressure. Two different oscillatory regimes could exist at one and the same parameters of the reaction. The parameters of oscillations (amplitude, period and the shape of spatio-temporal patterns on the surface) depend on the kinetic prehistory of the system. The possibility for the appearance of the cellular and turbulent patterns, spiral, ring and stripe oxygen waves on the surface in the cases under study has been shown.

Physico-Chemical Methods to Study Active Sites, Mechanism and Reaction Kinetics

X-RAY PHOTOELECTRON SPECTROSCOPY AS A TOOL FOR *IN-SITU* STUDY OF THE MECHANISMS OF HETEROGENEOUS CATALYTIC REACTIONS

V.I. Bukhtiyarov, V.V. Kaichev, I.P. Prosvirin

Top. Catal., 32(1-2) (2005) pp. 3-15.

An ESCALAB High Pressure photoelectron spectrometer specially designed by Vacuum Generators Co. (UK) for *in-situ* measurements at high pressures has been modified for adsorption and catalytic experiments. New construction of a gas cell, which serves to create a high-pressure zone, allows to measure photoemission spectra *in situ* at pressures up to 0.2–0.5 mbar and to use a sample holder with independent heating of a sample. This makes it possible to measure temperature programmed desorption and reaction spectra and, as a consequence, to characterize the catalytic properties simultaneously with the acquisition of X-ray photoelectron spectroscopy (XPS) data. Capabilities of the modified spectrometer are demonstrated by the examples of studies of CO and methanol adsorption on Pd(111) single crystal and methanol oxidation over Cu_{poly}.

The XPS study of high-pressure adsorption of CO on perfect and sputtered Pd(111) showed that raising the pressure has the same effect as decreasing the temperature. The CO coverage is increased due to adsorption of CO to weakly bound (on-top) state, which appears in addition to more strongly bound three-fold and bridged species. No indications of CO dissociation or carbonyl formation were found under the given experimental conditions (high pressure and sputtering-induced defects), provided that the CO gas was sufficiently clean.

Two pathways of methanol decomposition to $CH_{x,\ ads}$ ($x \leq 3$) and to CO_{ads} were unambiguously identified, with their contribution being dependent on *P* and *T*. The decomposition to carbon-originated species had a small contribution in UHV conditions at room temperature, but became more significant at higher pressures and temperatures.

Analysis of the distribution of the reaction products and surface species during methanol oxidation over copper in the sub-millibar pressure range showed that an increase in catalytic activity observed on heating the sample from 420 to 670 K is accompanied by transformation of the adlayer composition. At low temperatures, the surface is covered by methoxy- and, to a lesser extent, formate-groups. The active surface (T>520 K) is metallic copper with two adsorbed oxygen species. The possible nature of these species is discussed.

ACTIVATION OF THE C-O BOND ON THE SURFACE OF PALLADIUM: AN *IN SITU* STUDY BY X-RAY PHOTOELECTRON SPECTROSCOPY AND SUM FREQUENCY GENERATION

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Kinet. Catal., 46(2) (2005) pp. 269-281.

An *in situ* study of the adsorption of CO on atomically smooth and defect Pd(111) surfaces was performed over wide ranges of temperatures (200-400 K) and pressures (10^{-6}–1 mbar) by X-ray photoelectron spectroscopy and sum frequency generation. Both of the techniques indicated that CO was adsorbed as threefold hollow, bridging, and terminal species to form well-known ordered structures on the surface. In the course of the *in situ* experiments, no signs of CO dissociation or of the formation of carbonyl structures ($Pd(CO)_n$, n>1) were detected. The mechanism of C–O bond activation in the course of methanol decomposition on the surface of palladium was considered. It was found that the adsorption of methanol on the surface of palladium essentially depends on pressure. Along with the well-known reaction path of methanol dehydrogenation to CO and hydrogen, a slow process of methanol decomposition with C–O bond cleavage was observed at elevated pressures. In this case, the formation of carbon deposits finally resulted in the carbonization and complete deactivation of the surface. A mechanism for C–O bond activation on the surface of palladium was proposed; the geometry of adsorption complexes plays an important role in this mechanism.

AN XPS STUDY OF THE PROMOTION OF Ru-Cs/SIBUNIT CATALYSTS FOR AMMONIA SYNTHESIS

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Kinet. Catal., 46(4) (2005) pp. 597-602.

The nature of surface cesium compounds in cesium-modified ruthenium–Sibunit catalysts for ammonia

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synthesis was studied by X-ray photoelectron spectroscopy (XPS). It was found that, on the reduction of promoted catalysts, cesium was incorporated into the micropores of Sibunit to form quasi-intercalation cesium–carbon bonds. In this case, the chemical state of cesium was close to its state in cesium suboxides. The subsequent interaction with atmospheric oxygen resulted in the oxidation of cesium, which occurred as cesium peroxide and cesium superoxide in the oxidized samples. Ruthenium occurred in a metallic state in the reduced samples. The activity of a Ru–Cs^+/C(1) sample was higher than that of inactive Ru–Cs^+/C(2). This is a consequence of the higher surface concentration of ruthenium, which is most likely due to an increase in the dispersity of metal particles, as well as of the higher probability of the interaction between the promoter and the active component due to a symbatic increase in the surface concentrations of both ruthenium and cesium.

INTERACTION OF Al_2O_3 AND CeO_2 SURFACES WITH SO_2 AND $SO_2 + O_2$ STUDIED BY X-RAY PHOTOELECTRON SPECTROSCOPY

M.Yu. Smirnov, A.V. Kalinkin, A.V. Pashis,
A.M. Sorokin, A.S. Noskov, K.C. Kharas*,
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J. Phys. Chem. B, 109(23) (2005) pp. 11712 -11719.

The interaction of Al_2O_3 and CeO_2 thin films with sulfur dioxide (2.5 mbar) or with mixtures of SO_2 with O_2 (5 mbar) at various temperatures (30-400°C) was studied by X-ray photoelectron spectroscopy (XPS). The analysis of temperature-induced transformations of S2p spectra allowed to identify sulfite and sulfate species and determine the conditions of their formation on the oxide surfaces. Sulfite ions, SO_3^{2-}, which are characterized by the $S2p_{3/2}$ binding energy (BE) of ~167.5 eV, were shown to be formed during the interaction of the oxide films with pure SO_2 at temperatures ≤200°C, whereas sulfate ions, SO_4^{2-}, with BE ($S2p_{3/2}$) ~169 eV were produced at temperatures ≥300°C. The formation of both the sulfite and sulfate species proceeds more efficiently in the case of CeO_2. The addition of oxygen to SO_2 suppresses the formation of the sulfite species on both oxides and facilitates the formation of the sulfate species. Again, this enhancement is more significant for the CeO_2 film than for the Al_2O_3 one. The sulfation of the CeO_2 film is accompanied by a reduction of Ce(IV) ions to Ce(III) ones, both in the absence and in the presence of oxygen. It has been concluded that the amount of the sulfates on the CeO_2 surface treated with the $SO_2 + O_2$ mixture at ≥300°C corresponds to the formation of a 3D phase of the Ce(III) sulfate. The sulfation of Al_2O_3 is limited by the surface of the oxide film.

EFFECT OF THE SUPPORT ON THE NATURE OF METAL–PROMOTER INTERACTIONS IN Ru–Cs^+/MgO AND Ru–Cs^+–Al_2O_3 CATALYSTS FOR AMMONIA SYNTHESIS

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Kinet. Catal.,
46(6) (2005) pp. 898-899.

The Ru-Cs^+/MgO and Ru-Cs^+/ν-Al_2O_3 catalysts, which were prepared by an impregnation method using $RuOHCl_3$ and Cs_2CO_3 as precursor compounds and reduced with H_2 at 450°C, are characterized by X-ray diffraction, high-resolution transmission electron microscopy (with X-ray microanalysis), and X-ray photoelectron spectroscopy (XPS). The Cs^+/MgO(Al_2O_3) systems, Ru-Cs^+ black, and model systems prepared by cesium sputtering onto polycrystalline ruthenium foil are studied as reference samples. It is found that, in the Ru-Cs^+/MgO sample, cesium is present as a $Cs_{2+x}O$ cesium suboxide, which weakly interacts with the support, localized on the surface of Ru particles or near them. In the case of Ru-Cs^+/ν-Al_2O_3, cesium occurs as a species that is tightly bound to the support; this is likely surface cesium aluminate, which prevents promoter migration to Ru particles. The Ru-Cs^+/MgO sample exhibits a considerable shift of the Ru3*d* line in the XPS spectra toward lower binding energies, as compared to the bulk metal. It is hypothesized that this shift is due to a decrease in the electron work function from the surface of ruthenium because of the polarizing effect of Cs^+ ions in contact with Ru particles. Based on the experimental results, the great difference between the catalytic activities of the Ru-Cs^+/MgO and Ru-Cs^+/ν-Al_2O_3 systems in ammonia synthesis at 250-400 °C and atmospheric pressure is explained.

ROLE OF PHOSPHATES IN THE PROMOTION OF SILVER CATALYSTS FOR PARTIAL OXIDATION. I. STRUCTURE AND PROPERTIES OF PHOSPHATES ON THE SURFACE OF POLYCRYSTALLINE SILVER

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Kinet. Catal., 46(1) (2005) pp. 144-150.

The chemical composition, structure, and properties of an H_3PO_4-promoted polycrystalline silver foil are studied by XPS. The surface of the doped sample contains oxygen in two states with binding energies of 531.1 and 533.0 eV. Heat treatment results in silver clusters distributed in the polyphosphate matrix. It follows from TDS data that the surface of the promoted catalyst contains a strongly bound oxygen species that desorbs at ~900 K. It is believed that the silver clusters stabilized by the phosphate matrix are active sites on the surface of the phosphorus-promoted catalyst.

ROLE OF PHOSPHATES IN PROMOTION OF SILVER CATALYSTS FOR PARTIAL OXIDATION. II. FORMATION OF ACTIVE SITES IN THE STRUCTURE OF SILVER PHOSPHATE UNDER THE ACTION OF A REDUCTIVE MEDIUM

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Kinet. Catal., 46(1) (2005) pp. 151-156.

The morphology and chemical composition of the surface of silver phosphate are studied. The qualitative and quantitative compositions of silver phosphate are quite the same as those of the surface of the phosphorus-promoted silver catalyst. Silver particles surrounded by silver phosphate form in the subsurface region upon treatment of the sample with hydrogen. As a result, a complex catalytic system is formed in which silver phosphate is both the precursor of the reactive component (metallic silver particles) and the stabilizing matrix for this component. The system obtained is stable toward high temperature and redox reaction media.

IN SITU IR SPECTROSCOPIC AND XPS STUDY OF SURFACE COMPLEXES AND THEIR TRANSFORMATIONS DURING AMMONIA OXIDATION TO NITROUS OXIDE OVER AN Mn–Bi–O/α-Al_2O_3 CATALYST

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Kinet. Catal., 46(4) (2005) pp. 555-564.

Surface complexes resulting from the interaction between ammonia and a manganese–bismuth oxide catalyst were studied by IR spectroscopy and XPS. At the first stage, ammonia reacts with the catalyst to form the surface complexes [NH] and [NH_2] via abstraction of hydrogen atoms even at room temperature. Bringing the catalyst into contact with flowing air at room temperature or with helium under heating results in further hydrogen abstraction and simultaneous formation of [N] from [NH_2] and [NH]. The nitrogen atoms are localized on both reduced (Mn^{2+}) and oxidized ($Mn^{\delta+}$, $2 < \delta < 3$) sites. Atomic nitrogen is highly mobile and reacts readily with the weakly bound oxygen of the oxidized ($Mn^{\delta+}$–N) active site. The nitrogen atoms localized on oxidized sites play the key role in N_2O formation. Nitrous oxide is readily formed through the interaction between two $Mn^{\delta+}$–N species. N_2 molecules result from the recombination of nitrogen atoms localized on reduced (Mn^{2+}–N) sites.

TDS AND XPS STUDY OF OXYGEN DIFFUSION INTO SUBSURFACE LAYERS OF Pd(110)

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React. Kinet. Catal. Lett., 86(2) (2005) pp. 371-380.

The interaction of O_2 with Pd(110) has been studied by TDS and XPS at T = 400 K and at pressures P_{O2} from $2.6x10^{-6}$ to 10 Pa. At low exposures in O_2 (e≤1-5 L), an adsorption layer with q of *ca.* 0.5 and with the O1s peak at BE = 529.3 eV has been found to form on the surface. When e grows from 5 to 10^8 L, the position and intensity of the oxygen O1s peak remain practically constant. At the same time, as much as 5 mL of oxygen is absorbed according to the TDS data. The results obtained by TDS and XPS indicate that oxygen penetrates deep into the subsurface layers of palladium (≥15-20 Å) and is distributed in its bulk in a low concentration.

REACTION OF NANOCRYSTALLINE MgO WITH 1-IODOBUTANE

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J. Catal., 229(2) (2005) pp. 344-351.

The dehydroiodination of 1-iodobutane has been investigated over two different nanocrystalline MgO samples. The reaction with clean MgO takes place at temperatures as low as 100°C. However, a temperature of 300°C or higher is required for catalytic dehydroiodination to take place. At lower temperatures the reaction stops after the maximum degree of surface modification with iodine is reached. It was found by XPS that at all temperatures iodination is limited to the surface and no bulk MgI_2 is formed. The weight gain never exceeds 22%, which corresponds to 3.7% MgO conversion. In accordance with this conclusion, the textures of the samples after reaction are similar to those of the initial MgO. The surface iodination leads to a change in reaction mechanism: from concerted E2 elimination on initial MgO to stage E1 elimination. The secondary process of 2-iodobutane formation over iodinated samples was also established.

INFLUENCE OF MODIFYING ADDITIVES ON FORMATION OF SUPPORTED COPPER NANOPARTICLES

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European Phys. J. D, 34(1-3) (2005) pp. 55-58.

The influence of modifying additives of Ce, Zr, La and Cs oxides on changes of electronic state of supported copper during the catalytic reaction of butane complete oxidation has been studied by the methods of IR-spectroscopy of adsorbed CO, XPS, EXAFS and XRD. The modifying additions of cerium and zirconium oxides stabilize the ionic state of copper, while lanthanum and cesium oxides decrease the effective charge of copper ions. The observed effects are caused by variation in metal dispersivity in the modified samples and by electron donor-acceptor interaction of the surface atoms and ions of copper with the modifier.

STUDY OF THE LOW-TEMPERATURE REACTION BETWEEN CO AND O_2 OVER Pd AND Pt SURFACES

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Top. Catal., 32(1-2) (2005) pp. 17-28.

Field electron microscopy (FEM), high-resolution electron energy loss spectroscopy (HREELS), molecular beams (MB) and temperature-programmed reaction (TPR) have been applied to the study of the kinetics of CO oxidation at low temperature, and to determine the roles of subsurface atomic oxygen (O_{sub}) and surface reconstruction in self-oscillatory phenomena, on Pd(111), Pd(110) and Pt(100) single crystals and on Pd and Pt tip surfaces. It was found that high local concentrations of adsorbed CO during the transition from a Pt(100)-hex reconstructed surface to the unreconstructed 1×1 phase apparently prevents oxygen atoms from occupying hollow sites on the surface, and leads to the appearance of a weakly bound active adsorbed atomic oxygen (O_{ads}) state in an on-top or bridge position. It was also inferred that subsurface oxygen O_{sub} on the Pd(110) surface may play an important role in the formation of new active sites for the weakly bound O_{ads} atoms. Experiments with ^{18}O isotope labeling clearly show that the weakly bound atomic oxygen is the active form of oxygen that reacts with CO to form CO_2 at $T \sim 140–160$ K. Sharp tips of Pd and Pt, several hundreds angstroms in diameter, were used to perform *in situ* investigations of dynamic surface processes. The principal conclusion from those studies was that non–linear reaction kinetics is not restricted to macroscopic planes since: (i) planes as small as ~200 Å in diameter show the same non-linear kinetics as larger flat surfaces; (ii) regular waves appear under conditions leading to reaction rate oscillations; (iii) the propagation of reaction–diffusion waves involves the participation of different crystal nanoplanes via an effective coupling between adjacent planes.

KINETIC PECULIARITIES OF *CIS*/*TRANS* METHYL OLEATE FORMATION DURING HYDROGENATION OF METHYL LINOLEATE OVER Pd/MgO

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Appl. Catal., A, 279(1-2) (2005) pp. 99-107.

Kinetic peculiarities of *cis* and *trans* methyl oleate formation in the course of methyl linoleate hydrogenation over Pd/MgO were studied. Liquid phase hydrogenation was carried out in temperature range of 303–323 K and under hydrogen pressure within 1–10 bar. Gas–liquid chromatography, IR and ^{13}C NMR techniques were employed to characterize the reaction products. Effects of hydrogen pressure and reaction temperature on *cis* and *trans* methyl oleate formation were studied. The general kinetic scheme and reaction mechanism of methyl linoleate hydrogenation and *cis–trans* methyl oleate isomerization have been proposed.

MECHANISM OF CARBOXYLIC ACID FORMATION ON VANADIUM-CONTAINING OXIDE CATALYSTS

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Kinet. Catal., 46(2) (2005) pp. 217-226.

The surface intermediates in acrolein oxidation into acrylic acid on a V–Mo oxide catalyst, formaldehyde oxidation into formic acid on a V–Ti catalyst, and

3-pyridinecarboxaldehyde and β-picoline oxidation into nicotinic acid on a V–Ti catalyst are identified by *in situ* IR spectroscopy. The acids are found to form by similar mechanisms. The intermediates in acid formation are saltlike surface compounds (formates, acrylates, and nicotinates) stabilized on vanadium ions. The role of vanadium in acid formation is discussed in terms of the mechanisms suggested.

n-BUTANE CONVERSION ON SULFATED ZIRCONIA: *IN SITU* ^{13}C MAS NMR MONITORING OF THE KINETICS OF THE ^{13}C-LABEL SCRAMBLING AND ISOMERIZATION

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Catal. Lett., 101(3-4) (2005) pp. 181-185.

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

IN SITU MONITORING OF *n*-BUTENE CONVERSION ON H-FERRIERITE BY ^{1}H, ^{2}H AND ^{13}C MAS NMR. KINETICS OF A DOUBLE-BOND-SHIFT REACTION, HYDROGEN EXCHANGE AND THE ^{13}C-LABEL SCRAMBLING

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J. Catal., 229(1) (2005) pp. 243-251.

Kinetics of a double-bond-shift reaction, hydrogen exchange and ^{13}C-label scrambling were monitored *in situ* by ^{2}H, ^{1}H and ^{13}C MAS NMR for *n*-but-1-ene adsorbed on the zeolite ferrierite under batch reactor conditions at 290-373 K. A double-bond-shift reaction, the fastest among the three reactions studied, can be monitored provided that 97% of Brønsted acid sites are substituted by Na cations. The activation energy for this reaction was found to be 9.8 kcal·mol^{-1}. Hydrogen exchange with protons from the zeolite is observed for both methene and methyl groups of *n*-but-2-ene, formed from the initial *n*-but-1-ene. The terminal olefinic =CH_2 group of *n*-but-1-ene is involved in the exchange, providing the pathway for the exchange into the methyl group of the *n*-but-2-ene, mainly observed in the spectrum in accordance with thermodynamic equilibrium between *n*-but-1-ene and *n*-but-2-ene. This offers similar apparent activation energies of about 7 kcal·mol$^{-1.}$ for the exchange into methene and methyl groups of *n*-but-2-ene. The ^{13}C-label scrambling in *n*-but-2-ene is indicative of *sec*-butyl cation formation from the olefin in the zeolite framework, which can be formed as a small quantity transient species not detectable by NMR but providing the label scrambling. The apparent activation energy for the ^{13}C-label scrambling was found to be 21±2 kcal·mol^{-1}, which is three times higher compared to the activation energy for the label scrambling in *sec*-butyl cation in a superacidic solution.

MECHANISM OF THE CONVERSION OF ^{13}C-LABELED n-BUTANE ON ZEOLITE H-ZSM-5 STUDIED BY ^{13}C MAS NMR SPECTROSCOPY AND GC-MS ANALYSIS

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Chem. Eur. J., 11(1) (2005) pp. 100-105.

^{13}C MAS NMR spectroscopy shows that the conversion of the selectively ^{13}C-labeled *n*-butane on zeolite H-ZSM-5 proceeds at 430-470 K via two pathways: (i) a scrambling of the selective ^{13}C-label in the *n*-butane molecule and (ii) oligomerization-cracking and a conjunct polymerization. The latter two processes produce isobutane and propane simultaneously with the alkyl-substituted cyclopentenyl cations (CPC) and condensed aromatics. *In situ* ^{13}C MAS NMR and complementary *ex situ* GC-MS data provide evidence for a monomolecular mechanism of the ^{13}C-label scrambling, whereas both isobutane and propane are formed via an intermolecular pathways of oligomerization-cracking and a conjunct polymerization. According to ^{13}C MAS NMR kinetic measurements, the ^{13}C-label scrambling as well as the formation of isobutane and propane proceed with nearly the same activation energies (E_a = 75 kJ·mol^{-1} for the scrambling and 71 kJ·mol^{-1} for isobutane and propane formation). This can be rationalized in terms of an intermolecular hydride transfer between primarily initiated carbenium ion and *n*-butane to be the rate-determining stage of the *n*-butane conversion on zeolite H-ZSM-5.

IN SITU ^{1}H AND ^{13}C MAS NMR STUDY OF THE MECHANISM OF H/D EXCHANGE FOR DEUTERATED PROPANE ADSORBED ON HZSM-5

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J. Catal., 235(1) (2005) pp. 221-228.

The kinetics of the hydrogen exchange between the molecules of propane-d_8, propane-1,1,1,3,3,3-d_6, propane-2,2-d_2 and Brönsted acid sites of the zeolite H-ZSM-5 have been monitored *in situ* by ^{1}H MAS NMR spectroscopy in the temperature range of 230-280°C. The intramolecular hydrogen transfer was estimated by *in situ* ^{13}C MAS NMR spectroscopy of the kinetics of ^{13}C-label scrambling in the adsorbed propane-*2*-^{13}C. The hydrogen exchange has been concluded to occur directly between methyl or methylene groups of the alkane and the zeolite acid sites via a pentacoordinated carbonium ion. The exchange with the methyl groups is faster compared to that with the methylene group. This accounts for the earlier observed regioselectivity of the hydrogen exchange for propane on acidic zeolites (J. Am. Chem. Soc., 117 (1995) 1135). The intramolecular hydrogen transfer between methyl and methylene groups is one order of magnitude slower compared to the hydrogen exchange of the both groups with the zeolite acid sites.

^{1}H AND ^{13}C MAS NMR KINETIC STUDY OF THE MECHANISM OF H/D EXCHANGE FOR PROPANE ON ZEOLITE H-ZSM-5

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J. Phys. Chem. B, 109 (2005) pp. 19748 -19757.

The kinetics of hydrogen (H/D) exchange between Brønsted acid sites of zeolite H-ZSM-5 and variously deuterated propane (propane-d_8, propane-1,1,1,3,3,3-d_6, propane-2,2-d_2) have been monitored *in situ* by ^{1}H MAS NMR spectroscopy within the temperature range of 503-556 K. The contribution of intramolecular hydrogen transfer to the H/D exchange in the adsorbed propane was estimated by monitoring the kinetics of ^{13}C-labeled carbon scrambling in propane-*2*-^{13}C *in situ* with ^{13}C MAS NMR at 543-573 K. Possible mechanisms of the exchange have been verified on the basis of the analysis of the variation of protium concentration in both the methyl and the methylene groups of propane in dependence of the reaction time. The main route of the exchange consists of a direct exchange of the acidic OH groups of the zeolite with either the methyl groups or the methylene group presumably with pentacoordinated carbonium ion intermediacy. The assumption that the intramolecular H-scrambling between the methyl groups and the methylene group of propane via carbenium-ion-type intermediates is the fastest process among the other possible routes (*J. Catal.*, 215 (2003) 122) does not account for the experimental kinetics of H/D exchange for propane with different initial content and location of deuterium in a propane molecule. The rate constant (k_3) for intramolecular H/D exchange between the methyl and the methylene groups is 4-5 times lower compared to the direct exchange of both the methyl (k_1) and the methylene (k_2) groups with Brønsted acid sites of the zeolite, the k_1 being *ca.* 1.5 times higher than k_2. At lower temperature (473 K) the exchange is slower, and the expected difference between k_1 and k_2 is more essential, $k_1 \approx 3k_2$. This accounts for earlier observed regioselectivity of the exchange for propane on H-ZSM-5 at 473 K (*J. Am. Chem. Soc.*, 117 (1995) 1135). Faster direct exchange with the methyl groups compared to that with the methylene groups was attributed to a possible, more spatial accessibility of the methyl groups for the exchange. Similar activation energies for H- and C-scramblings with a 2 times more rapid rate of H-scrambling was rationalization by the proceeding of these two processes through an isopropyl cation intermediate, as in classical carbenium ion chemistry.

CONTENT

ansa-TITANOCENE CATALYSTS FOR α-OLEFIN POLYMERIZATION. SYNTHESES, STRUCTURES, AND REACTIONS WITH METHYLALUMINOXANE AND BORON-BASED ACTIVATORS

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Organometallics, 24(5) (2005) pp. 894-904.

The racemic isomers of $C_2H_4(1\text{-Ind})_2TiCl_2$ and $Me_2Si(2\text{-Me-Benzind})_2TiMe_2$ were synthesized and structurally characterized. Reactions of these and related *ansa*-titanocene complexes with methylaluminoxane or with the cationizing reagent $[CPh_3]^+[B(C_6F_5)_4]^-/Al_2Me_6$ were monitored by UV/vis, ^1H NMR, and EPR methods. Under conditions approaching those typically used in olefin polymerizations, heterobinuclear cations of the type $[DianTi^{IV}(\mu\text{-Me})_2AlMe_2]^+$ (with Dian = bridged ligand dianion) dominate in each of these reaction systems, which catalyze the polymerization of propene at temperatures below ambient. Above 0°C, these cations are reduced, mainly to neutral heterobinuclear species $DianTi^{III}(\mu\text{-Me})_2AlMe_2$, which appear to be inactive with regard to polymerization catalysis. In the absence of monomer, the main reducing agent appears to be ethyl aluminum admixtures in Al_2Me_6. Addition of monomer increases the rate of reduction rather drastically, probably via formation of titanium hydrides.

ACTIVE INTERMEDIATES IN ETHYLENE POLYMERIZATION OVER TITANIUM *BIS*(PHENOXYIMINE) CATALYSTS

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Organometallics, 24(23) (2005) pp. 5660-5664.

Reactive intermediates in living olefin polymerization over homogeneous catalysts based on bis[*N*-(3-*tert*-butylsalicylidene)-2,3,4,5,6-pentafluoroanilinato]titanium(IV) dichloride (L_2TiCl_2) have been studied. Outer sphere ion pairs $[L_2TiMe(S)]^+[Me\text{-MAO}]^-$ and $[L_2TiMe(S)]^+[B(C_6F_5)_4]^-$ (S = solvent molecule), formed by activation of L_2TiCl_2 with MAO or with $AlMe_3/[CPh_3]^+[B(C_6F_5)_4]^-$, and reactions of these ion pairs with ethene to afford chain-propagating species $[L_2TiP]^+[Me\text{-MAO}]^-$ and $[L_2TiP]^+[B(C_6F_5)_4]^-$ (P = growing polymeryl chain) have been characterized by ^1H, ^{13}C, and ^{19}F NMR spectroscopy.

RAC-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe^+$: AN ALKYL ZIRCONOCENIUM CATION STABILIZED BY STERIC SHIELDING AGAINST INTERACTION WITH ANCILLARY LIGANDS

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Organometallics, 24(5) (2005) pp. 867-871.

The sterically shielded cation *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe^+$, generated by reaction of *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe_2$ with methylalumoxane (MAO) or with dimethylanilinium or trityl perfluorotetraphenylborate, differs from other, more open zirconocene methyl cations in that it does not form the symmetric $AlMe_3$ adduct *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2Zr(\mu\text{-Me})_2AlMe_2^+$.

Instead, the unsymmetric ternary adduct *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe(\mu\text{-Me})AlMe_3\text{-}NMe_2Ph^+$ is formed in the presence of dimethylaniline and trimethylaluminum. UV/vis and ^1H NMR characteristics of hydrocarbon solutions containing *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe^+\cdots B(C_6F_5)_4^-$ or *rac*-$Me_2Si(2\text{-Me-4-}t\text{-Bu-}C_5H_2)_2ZrMe^+\cdots MAOMe^-$ indicate that cation-anion association in these ion pairs is unusually weak.

THE NATURE OF THE SPIN-STATE VARIATION OF $[Fe^{II}(BPMEN)(CH_3CN)_2](ClO_4)_2$ IN SOLUTION

K.P. Bryliakov, E.A. Duban, E.P. Talsi

European J. Inorg. Chem., 1 (2005) pp. 72-76.Thermally-induced spin variation behavior of $[Fe^{II}(BPMEN)(CH_3CN)_2](ClO_4)_2$ in CD_3CN solution [low spin (LS)-high spin (HS)] was investigated. Variable temperature solution magnetic susceptibility measurements gave $\Delta H°_{LS\text{-}HS} = 39.7 \pm 2.0$ kJ·mol^{-1} and $\Delta S°_{LS\text{-}HS} = 135 \pm 9$ J·mol^{-1} K^{-1} values. These values are too high for a pure spin transition and reflect a significant contribution of chemical processes to the spin transition, namely, the detected dissociation of one bound acetonitrile molecule. Thus, LS-HS conversion should be regarded as a chemical equilibrium overlapped with a thermal spin crossover. The thermodynamic parameters

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for the overall process estimated from the variation of the NMR shifts with temperature ($\Delta H° = 40 \pm 3$ kJ·mol^{-1}, $\Delta S° = 137 \pm 10$ J·mol^{-1} K^{-1}) are in perfect agreement with those obtained by magnetic susceptibility measurements.

CHARACTERIZATION OF LOW-SPIN FERRIC HYDROPEROXO COMPLEXES WITH *N,N′*-DIMETHYL-*N,N′-BIS* (2-PYRIDYLMETHYL)-1,2-DIAMINOETHANE

E.A. Duban, **K.P. Bryliakov**, **E.P. Talsi**

Mendeleev Commun., 15(1) (2005) pp. 12-14.

Hydroperoxo intermediates formed by the interaction of [Fe^{II}(BPMEN)(MeCN)$_2$](ClO$_4$)$_2$ [BPMEN = *N,N′*-dimethyl-*N,N′-bis*(2-pyridylmethyl)-1,2-diaminoethane] with H_2O_2 in a CH_2Cl_2–MeCN mixture were characterised using EPR spectroscopy.

LIQUID-PHASE NONCATALYTIC BUTENE OXIDATION WITH NITROUS OXIDE

S.V. Semikolenov, K.A. Dubkov, E.V. Starokon, D.E. Babushkin, G.I. Panov

Russ. Chem. Bull., 55(4) (2005) pp. 948-956.

The kinetics and mechanism of noncatalytic liquid-phase oxidation of but-1-ene and but-2-ene with nitrous oxide in a benzene solution in the temperature range from 180 to 240°C were studied. Oxidation proceeds via the 1,3-dipolar cycloaddition mechanism to form carbonyl compounds. Both of these reactions occur with close rates and activation energies and have the first orders with respect to the alkene and N_2O. A considerable fraction (39%) of but-1-ene involved in oxidation undergoes cleavage at the double bond yielding propanal and an equivalent amount of methylene, the latter producing ethylcyclopropane and cycloheptatriene. The oxidation of but-2-ene proceeds with a minimum bond cleavage and affords methyl ethyl ketone with 84% selectivity. Regularities of the oxidation of terminal and internal alkenes C2-C8 with nitrous oxide were analyzed using the previously published data.

CYCLOHEXANONE PREPARATION VIA THE GAS PHASE CARBOXIDATION OF CYCLOHEXENE BY NITROUS OXIDE

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

React. Kinet. Catal. Lett., 84(2) (2005) pp. 383-388.

Nitrous oxide is known to provide non-catalytic liquid phase oxidation of alkenes to carbonyl compounds (the carboxidation reaction). This paper shows that carboxidation of cyclohexene can be successfully conducted in the gas phase, too. The gas phase carboxidation is a second order reaction proceeding at 325-450°C under 3-16 bar pressure with an activation energy of 26 kcal/mol. The reaction mechanism does not involve free radical steps and leads to cyclohexanone as a main product.

SPIN DESIGN OF IRON COMPLEXES ON Fe-ZSM-5 ZEOLITES

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Catal. Today,
110(3-4) (2005) pp. 247-254.

The spin state of iron ions in Fe-ZSM-5 zeolites can be purposefully varied by adsorption of gaseous probe molecules. The resulting Fe complexes with half-integer spin (S=1/2, S=3/2 and S=5/2) can be reliably identified by electron paramagnetic resonance (EPR). A good correlation has been found between the concentration of surface sites active in low-temperature nitrous oxide decomposition and the concentration of low-spin (S+1/2) nitrosyl complexes of Fe formed after adsorption of NO molecules. Based on the analysis of the formation of such complexes under varying conditions, it was concluded that these active sites contain a binuclear iron complex with $S = 0$ and three adsorbed NO molecules. An approach to investigate various Fe-containing sites in oxidation catalysts is discussed.

PUTATIVE MECHANISM OF THE SUGAR FORMATION ON PREBIOTIC EARTH INITIATED BY UV-RADIATION

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Adv. Space Res., 36(2) (2005)
pp. 214-219.

UV-irradiation of neutral aqueous formaldehyde solutions leads to the formation of a number of products. CO, CH_4, CO_2 and H_2 are the main products detected in the gas phase over the solutions. In the liquid phase, glycolaldehyde and glyceraldehyde are among the products with the maximum yields of 4.2% and 0.18%, respectively. These aldehydes are shown to be the most active initiators of the formose reaction in the dark to synthesize monosaccharides from formaldehyde. The amounts of the photolytically formed initiators are sufficient for the initiating the formose reaction.

MICROFACETING AND THERMODYNAMIC STABILITY OF THE SURFACE UNDER CHEMISORPTION CONDITIONS

V.N. Parmon, V.I. Bukhtiyarov

Kinet. Catal., 46(2) (2005)
pp. 295-299.

The effect of the adsorption of simple molecules on the excess surface energy of a pure metal surface is evaluated. Even analysis in the framework of simple ideal models of adsorption demonstrates that thermodynamic driving forces resulting from chemisorption can cause surface reconstruction with the formation of microfacets. The validity of this approach for description of real adsorption processes, especially at high adsorbate coverages, is confirmed by the fact that the minimum standard enthalpy of adsorption at which metal surface can lose thermodynamic stability, $(\Delta H^\circ_{ads})_{cr}$, is similar to the typical experimental data available on the heat of chemisorption of reactive molecules (CO, H_2, and O_2) on the surface of transition metals (Ag, Pt, Ni, Pd, and Fe).

CF_2Cl_2 DECOMPOSITION OVER NANOCRYSTALLINE MgO: EVIDENCE FOR LONG INDUCTION PERIODS

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J. Phys. Chem. B, 109(15) (2005)
pp. 6982-6989.

CF_2Cl_2 has been found to react with nanoscale MgO at 325°C and higher temperatures. In excess of the halocarbon, the reaction results in the formation of MgF_2 as a predominant solid product, with CCl_4, and CO_2 formed as the main gaseous products. The kinetics of the process is characterized by a prolonged induction period, which is as long as 8.5 h at 325°C. The length of the induction period decreases with temperature increase and becomes negligible at 500°C. Complete CF_2Cl_2 mineralization has been achieved in an excess of MgO at 450°C. Detailed HRTEM and EDX analysis has shown that the induction period involves the formation of small amounts of magnesium halides on the oxide surface and results in its reconstruction leading to initial oriental ordering of the nanocrystals followed by substantial changes in the bulk composition of the nanoparticles. The reaction proved to be structurally sensitive. It has been found that deep fluoridation is possible only for nanoscale MgO samples. The use of samples with lower surface areas results in lengthening of the induction period and decrease of the reaction depth. The MgO transformation to MgF_2 has been found to result in a surface area decrease by more that an order of magnitude as a result of intense sintering of magnesium fluoride under the reaction conditions.

STRUCTURAL AND CATALYTIC PROPERTIES OF ULTRA-DISPERSED SILVER POWDERS PREPARED BY METAL EVAPORATION WITH HIGH-POWER ELECTRON BEAM. I. STRUCTURAL PROPERTIES

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React. Kinet. Catal. Lett., 86(1) (2005)
pp. 179-185.

Structural properties of ultra-dispersed silver powders synthesized via high-temperature electron-beam evaporation of silver in different gases (Ar, N_2, He) were studied with XRD, TEM, EDX and XRF. The formation of specific oxide-like species on the particle surface of an Ag(Ar) powder was found. It was shown that these particles can contain argon atoms.

STRUCTURAL AND CATALYTIC PROPERTIES OF ULTRA-DISPERSED SILVER POWDERS PREPARED BY METAL EVAPORATION WITH HIGH-POWER ELECTRON BEAM. II. CATALYTIC PROPERTIES IN ETHYLENE EPOXIDATION WITH MOLECULAR OXYGEN

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React. Kinet. Catal. Lett.,
86(1) (2005) pp. 187-193.

Catalytic properties of ultra-dispersed silver powders synthesized via electron-beam silver evaporation in Ar, N_2 and He were studied in the reaction of ethylene epoxidation. The highest selectivity was observed on Ag(Ar) sample that was associated with a formation of specific oxide-like species on the silver surface formed in the presence of argon. The nature of these species was also studied with UV-vis and XPS spectroscopy as well as with TPD.

CONTENT

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

FERROMAGNETIC RESONANCE INVESTIGATION OF COLLECTIVE PHENOMENA IN TWO-DIMENSIONAL PERIODIC ARRAYS OF Co PARTICLES

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Appl. Phys. A, 81(4) (2005)
pp. 679-683.

The ferromagnetic resonance (FMR) method is used to study the collective phenomena in two-dimensional periodic arrays of disk-shaped Co particles. A study of geometrically similar structures with different periods reveals a broadening of the FMR resonance lines due to the excitation of additional size-dependent non-uniform spin waves. It is shown that these collective spin-wave modes are based on dipole–dipole interactions between the ferromagnetic particles in the array. Qualitative and quantitative data on magnetic interparticle interactions can thus be obtained from FMR spectra for two-dimensional periodic arrays of ferromagnetic particles.

MAGNETIC RESONANCE AND STRUCTURAL INVESTIGATIONS OF MONO-OXO-OCTAETHYLCHLORINATOIRON(III) CHLORIDE AND ITS *BIS*-IMIDAZOLE COMPLEX

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Inorg. Chem., 44 (2005)
pp. 1882-1889.

(Monooxooctaethylchlorinato)iron(III) chloride, (oxo-OEC)FeCl, **1**, has been investigated by X-ray crystallography and by ^{1}H NMR spectroscopy. Its *bis*(imidazole-d_4) complex has been studied by multidimensional ^{1}H NMR and EPR spectroscopies, and the results are compared to those for the *bis*(Im-d_4) complex of (octaethylchlorinato)iron(III) chloride, (OEC)FeCl, **2**. EPR and NMR results show that both [(oxo-OEC)Fe(Im-d_4)$_2$]Cl and [(OEC)Fe(Im-d_4)$_2$]Cl are low-spin Fe(III) complexes with $(d_{xy})^2(d_{xz},d_{yz})^3$ electronic ground states, both at 4.2 K (EPR spectra) and at ambient temperatures utilized for solution NMR studies. The pattern of chemical shifts of the pyrrole-CH_2 and *meso* protons are similar, with the 8,17-carbons having the largest and the 12,13-carbons having the smallest spin densities in each case, except that [(OEC)Fe(Im-d_4)$_2$]Cl has a slightly wider range of pyrrole-CH_2 chemical shifts and more resonances are observed for [(oxo-OEC)Fe(Im-d_4)$_2$]Cl due to its lower symmetry. Full proton resonance assignments for both complexes have been made from COSY, NOESY, and NOE difference experiments.

NONINVASIVE *IN SITU* VISUALIZATION OF SUPPORTED CATALYST PREPARATIONS USING MULTINUCLEAR MAGNETIC RESONANCE IMAGING

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J. Am. Chem. Soc.,
127(34) (2005) pp. 11916-11917.

Multinuclear magnetic resonance imaging (MRI) is employed as a new noninvasive tool for monitoring supported catalyst preparation by visualizing precursor transport within the porous support. In particular, liquid phase ^{31}P MRI experiments were used to visualize the dynamics of H_3PO_4 penetration into an alumina pellet and have revealed a strong interaction of H_3PO_4 with the support. Solid state ^{31}P MRI was applied to map the distribution of the adsorbed phosphate inside the support after its drying. Comparison of the liquid phase and solid phase MRI results confirms the correlation of the phosphate distribution in the liquid phase during impregnation and the phosphate adsorbed on the support. The possibility to monitor the transport of metal atoms within the support by a direct detection of their NMR signal is demonstrated for ^{195}Pt nucleus during impregnation of an alumina pellet with an aqueous solution of H_2PtCl_6. Other possible strategies for the utilization of MRI to characterize *in situ* the preparation of supported catalysts and other supported materials are briefly discussed.

CONTENT

^{129}Xe NMR STUDY OF Xe ADSORPTION ON MULTIWALL CARBON NANOTUBES

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Solid State Nucl. Magn. Reson.,
28(2-4) (2005) pp. 135-141.

^{129}Xe NMR spectroscopy has been used to study the adsorption of Xe on multi-wall carbon nanotubes (MWCNT). The results obtained have shown the ^{129}Xe NMR ability to probe the intercrystalline (aggregate) and the inner porosity of CNT. In particular, the effects on porosity of tubes openings by hydrogen exposure and of ball milling were examined. Dramatic changes observed in the ^{129}Xe NMR spectra after moderate ball milling of MWCNTs were attributed to the destruction of the initial intercrystalline pore structure and to the Xe access inside the nanotubes. To examine the exchange dynamics the mixture of as-made and milled MWCNTs was studied with one- and two-dimensional (1D and 2D) ^{129}Xe NMR. The exchange between the interior of milled nanotubes and the aggregate pores of as-made MWCNTs was fast on the NMR acquisition time scale. The Xenon exchange between the interior of the as-made MWCNTs and the large aggregate pores occurred on a longer time scale of 10 ms, as was established by 2D ^{129}Xe NMR exchange spectroscopy. Variable temperature ^{129}Xe NMR data were also discussed and analyzed in terms of the fast exchange approximation.

^{129}Xe NMR INVESTIGATION OF CATALYTIC FILAMENTOUS CARBON

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Micropor. Mesopor. Mater.,
81(1-3) (2005) pp. 41-48.

A series of catalytic filamentous carbons (CFC) obtained from gas phase reaction on iron subgroup metal catalysts was studied by ^{129}Xe NMR. A connection between ^{129}Xe NMR parameters and structural, textural and paramagnetic properties of CFC was discussed. The chemical shift (δ) was shown to depend on the structure of the CFC surface formed by edge, basal or both (edge and basal) graphite faces. This dependence follows a general trend of the chemical shift to increase with adsorption potential of a surface. The term describing Xe–Xe interaction ($\delta_{\text{Xe-Xe}}$) in confined space decreased with the average pore size of CFC granule. For hollow multi-wall carbon nanotubes two ^{129}Xe NMR signals were attributed to voids inside nanotubes and to interstices between the interlaced nanotubes. However, analysis of experimental data is complicated due to the presence of paramagnetic metal particles necessary to the filament growth. Therefore, ESR data are given and correlated with ^{129}Xe NMR results.

^{95}Mo MAGIC ANGLE SPINNING NMR AT HIGH FIELD: IMPROVED MEASUREMENTS AND STRUCTURAL ANALYSIS OF THE QUADRUPOLE INTERACTION IN MONOMOLYBDATES AND ISOPOLYMOLYBDATES

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J. Phys. Chem. B,
109(29) (2005) pp. 14033-14042.

In this study, ^{95}Mo quadrupole couplings in various molydbates were measured easily and accurately with magic angle spinning (MAS) NMR under a directing field of 19.6 T. The resonance frequency of 54 MHz was sufficiently high to remove acoustic ringing artifacts, and the spectra could be analyzed in the usual terms of chemical shift and quadrupolar line shapes. For monomolybdates and molybdite, the quadrupole coupling dominated the NMR response, and the quadrupole parameters could be measured with better accuracy than in previous lower field studies. Moreover, despite the low symmetry of the molybdenum coordination, the usefulness of such measurements to probe molybdenum environments was established by *ab initio* density functional theory (DFT) calculations of the electric field gradient from known structures. The experimental NMR data correlated perfectly with the refined structures. In isopolymolybdates, the resonances were shapeless and DFT calculations were impossible because of the large and low symmetry unit cells. Nevertheless, empirical but clear NMR signatures were obtained from the spinning sidebands analysis or the MQMAS spectra. This was possible for the first time thanks to the improved baseline and sensitivity at high fields. With the generalization of NMR spectrometers operating above 17 T, it was predicted that ^{95}Mo MAS NMR could evolve as a routine characterization tool for ill-defined structures such as supported molybdates in catalysis.

^{93}Nb NMR CHEMICAL SHIFT SCALE FOR NIOBIA SYSTEMS

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Solid State Nucl. Magn. Reson.,
28(2-4) (2005) pp. 204-224.

^{93}Nb solid-state NMR spectra of a series of inorganic niobates with Nb in different oxygen coordination environments were measured. For all studied compounds the chemical shielding and quadrupole tensor parameters were determined using conventional and ultrahigh field NMR facilities, ultrahigh speed MAS, DQ STMAS, solid-echo and computer modeling. It has been demonstrated that the ^{93}Nb isotropic chemical shift is sensitive to the coordination number of Nb sites. For the first time the ^{93}Nb NMR chemical shift scale for NbO$_x$ polyhedra in solid materials has been proposed: for four-coordinated Nb sites, the isotropic shifts occur from −650 to −950 ppm; five-coordinated Nb sites have the isotropic shifts in the range of –900 to –980 ppm; for six-coordinated Nb sites the isotropic shifts vary from −900 to −1360 ppm; the shifts from −1200 to −1600 ppm are typical for seven-coordinated Nb sites; for eight-coordinated Nb sites the shifts are higher than −1400 ppm. The possible correlation between the value of the isotropic chemical shift and the ionic character of the NbO_x–MO_y polyhedra association has been suggested. The magnitude of the ^{93}Nb quadrupole coupling constant depends on the local symmetry of Nb sites and may vary from hundreds of kHz to hundreds of MHz.

^{93}Nb NMR CHEMICAL SHIFT SCALE FOR NIOBIA COMPOUNDS

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2004 Annual Report of the National High Magnetic Field Laboratory

Nb-containing mixed metal oxide catalysts exhibit high activity and selectivity in light alkane conversion. At the present time, however, there is a lack of fundamental structure-activity relationships wich could be critical for development of efficient catalysts. Solid state ^{93}Nb NMR spectroscopy is expected to be effective tool for characterization of Nb-containg catalysts since ^{93}Nb (I=9/2) is the one of the most sensitive quadrupolar nuclei (0.482 relative sensetivity to ^{1}H respectively) with sufficiently favorable qudrupole moment (-0.28×10^{-28} m^2). The lack ^{93}Nb NMR studies is partly a result of a relatively large value of quadrupolar constant and relatively small value of chemical shielding anisotropy. Herein, using ultra high magnetic field facility and convenient SATRAS technique it is proposed the chemical shift and the quadrupolar tensor parameters for a considerable number of Nb compounds with known structure. According to these data and the previous ^{93}Nb NMR studies the chemical shift scale for Nb-O compounds was proposed.

^{14}N AND ^{195}Pt NMR OF POLYNUCLEAR PLATINUM ACETAMIDATE COMPLEXES

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Russ. J. Inorg. Chem., 50(5) (2005)
pp. 747-754.

The platinum(III) acetamidate complexes $[Pt_2Py_2(\mu\text{-}Acam)_4]Cl_2$ (**I**) and $[En(Acam)Pt(\mu\text{-}Acam)_2Pt(Acam)En]Cl_2$ (**II**) and the platinum blue $[PtBipy(Acam)_2(NO_3)$ (**III**), as well as the platinum(II) complex $[EnPt(\mu\text{-}Acam)_2PtEn](NO_3)_2$ (**IV**) and the platinum blue $[PtBipy(Acam)](CF_3SO_3)$ (**V**), where Acam = $CH_3C(O)NH$, were studied by ^{14}N and ^{195}Pt NMR. Based on available X-ray crystallographic data on the iodide analogues of complexes **I** and **II** and compounds **IV** and **V** and on analysis of NMR data for these complexes, a correlation was established between the ^{14}N NMR chemical shift of the acetamide ligand and its coordination mode (N (or O)-monodentate or (N,O)-bidentate bridging coordination) and *trans* partner at the Acam–Pt–L coordinate. The coordinate shifts were used in the analysis of the geometric structure of the platinum acetamidates studied.

CONTENT

NMR SPECTRA OF CYCLIC NITRONES. VII. EFFECT OF SUBSTITUENTS AND HYDROGEN BONDING ON N^{14} AND O^{17} CHEMICAL SHIFTS IN 3-IMIDAZOLINE 3-OXIDE DERIVATIVES

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Chem. Heterocycl. Compd.,
41(9) (2005) pp. 1134-1138.

Derivatives of 3-imidazoline 3-oxide have been studied by ^{14}N and ^{17}O NMR methods. Regularities of the influence of substituents and of a hydrogen bond on chemical shifts have been made apparent. The range of changes of the chemical shifts of the nitrogen and oxygen nuclei of the nitrone group has been determined. Both in the ^{17}O and in the ^{14}N NMR spectra the signals of the amino derivatives are the highest field signals for the nitrone group, and the lowest field signals are the signals of the cyano derivatives in the series of derivatives investigated. Depending on the substituent (from amino to cyano group) the ^{17}O chemical shifts varied over a range ~155 ppm, but the interval of change of the ^{14}N chemical shifts for the same substituents was ~110 ppm.

WATER CONCENTRATION PROFILES IN MEMBRANES MEASURED BY ESEEM OF SPIN-LABELED LIPIDS

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J. Phys. Chem. B,
109(24) (2005) pp. 12003-12013.

Electron spin-echo envelope modulation (ESEEM) spectroscopy of phospholipids spin-labeled systematically down the sn-2 chain was used to detect the penetration of water (D_2O) into bilayer membranes of dipalmitoyl phosphatidylcholine with and without 50 mol % cholesterol. Three-pulse stimulated echoes allow the resolution of two superimposed H-2-ESEEM spectral components of different widths, for spin labels located in the upper part of the lipid chains. Quantum chemical calculations (DFT) and ESEEM simulations assign the broad spectral component to one or two D_2O molecules that are directly hydrogen bonded to the N-O group of the spin label. Classical ESEEM simulations establish that the narrow spectral component arises from nonbonded water (D_2O) molecules that are free in the hydrocarbon chain region of the bilayer membrane. The amplitudes of the broad H-2-ESEEM spectral component correlate directly with those of the narrow component for spin labels at different positions down the lipid chain, reflecting the local H-bonding equilibria. The D_2O-ESEEM amplitudes decrease with position down the chain toward the bilayer center, displaying a sigmoidal dependence on position that is characteristic of transmembrane polarity profiles established by other less direct spin-labeling methods. The midpoint of the sigmoidal profile is shifted toward the membrane center for membranes without cholesterol, relative to those with cholesterol, and the D_2O-ESEEM amplitude in the outer regions of the chain is greater in the presence of cholesterol than in its absence. For both membrane types, the D_2O amplitude is almost vanishingly small at the bilayer center. The water-penetration profiles reverse correlate with the lipid-chain packing density, as reflected by H-1-ESEEM intensities from protons of the membrane matrix. An analysis of the H-bonding equilibria provides essential information on the binding of water molecules to H-bond acceptors within the hydrophobic interior of membranes. For membranes containing cholesterol, approximately 40% of the nitroxides in the region adjacent to the lipid headgroups are H bonded to water, of which ca. 15% are doubly H bonded. Corresponding H-bonded populations in membranes without cholesterol are ca. 20%, of which ca. 6% are doubly bonded.

SUPEROXIDE RADICAL ANIONS ON THE SURFACE OF ZIRCONIA AND SULFATED ZIRCONIA: FORMATION MECHANISMS, PROPERTIES AND STRUCTURE

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Phys. Chem. Chem. Phys.,
7(16) (2005) pp. 3059-3069.

In situ ESR spectroscopy has been used for direct comparison of different thermal and light-induced processes leading to generation of superoxide radical anions on the surface of various zirconia and sulfated zirconia materials. For materials of both types the magnetic resonance parameters of the radical anions were found to be practically independent of the generation method, except for oxygen coadsorption with NO that yields radicals with somewhat smaller g_z values. The parameters appear to depend mostly on the state of the surface zirconia cations stabilizing the radical anions, so that the g tensor anisotropy is significantly smaller over sulfated zirconia. It is shown that light-induced formation of superoxide

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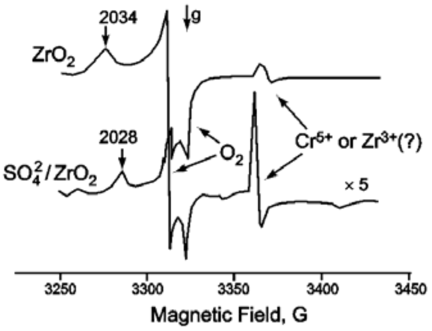
radical anions in the presence of coadsorbed hydrocarbons can be initiated with visible light. Original SIET reaction mechanisms are suggested for the formation of superoxide radical anions by coadsorption with hydrocarbons and illumination after such coadsorption to extend the previously known ones to account for the observed phenomena. Cluster model DFT calculations of magnetic resonance parameters of O_2^- radical anions stabilized on the surface of zirconium dioxide showed that the adsorption complexes have a T-shape rather than linear structure. The magnetic resonance parameters obtained by calculations practically match experimental data and adequately describe their changes after the surface modification with sulfates.



INTERACTION BETWEEN CRYSTAL LATTICE AND MOBILE IONS IN COPPER SELENIDES STUDIED BY EXAFS SPECTROSCOPY

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Nucl. Instrum. Methods Phys. Res., Sect. A, 543(1) (2005) pp. 194-195.

Interaction between crystal lattice and mobile Cu ions has been studied in $Cu_{2-x}Se$ in superionic and in normal state using EXAFS-spectroscopy. It has been found that the transition from normal to superionic state and change of mobile Cu ion concentration practically do not have an influence on local state of Cu atoms, but change of both these parameters is accompanied by a change of Se-sublattice state.

THE EVOLUTION OF THE Cu/ZnO METHANOL SYNTHESIS CATALYST DURING ITS REDUCTION AND RE-OXIDATION

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React. Kinet. Catal. Lett., 86 (2) (2005) pp. 307-314.

Cu K EXAFS studies of the structure of Cu-Zn oxide catalyst were performed for the as prepared samples, those after activation by hydrogen and further reoxidation. During the primary formation of the CuZnO solid solution the copper ions are dissolved in the extended stacking faults of the ZnO lattice as ultra-small oxide clusters. The most of copper cations is reduced to Cu^0 by hydrogen at 473 K, forming the nanoparticles with the characteristic size of *ca.* 1.6 nm. Copper metal particles are reoxidized to Cu^{2+} at 523 K in the helium flow containing 0.05 vol. % oxygen. The re-oxidized cations don't form the CuO phase, however return back to the extended stacking faults of ZnO. This time, they form the stripe-like clusters of flat-square coordinated copper cation.

THE INFLUENCE OF BISMUTH ADDITION ON THE LOCAL STRUCTURE OF CeO_2

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Nucl. Instrum. Methods Phys. Res., Sect. A, 543(1) (2005) pp. 127-130.

The local structure of mixed oxides with the composition $Ce_{1-x}Bi_xO_y$, where x=0.1–0.5, y<2 was studied by EXAFS and X-ray radial distribution of electronic density method. It is shown, that samples represent single-phase systems of solid solutions with the structure close to that of CeO_2. The unit cell parameter increases and disorder of the structure takes place with bismuth content increasing: modification of interatomic distances, distortion in the cation sublattice, and arising of oxygen vacancies in anion sublattice.

EXAFS STUDY OF Nb DOPED $SrCoFeO_{3x}$ PEROVSKITES

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Phys. Scr., T115 (2005) pp. 740-743.

The local structure of the Fe, Co and Nb surroundings of niobium doped $SrCoFeO_{3x}$ perovskites was studied by EXAFS spectroscopy. The samples were prepared by ceramic method at T 1250C. In order to vary the oxygen content, the samples were i) slowly cooled in the furnace, ii) quenched in liquid N_2 and electrochemically oxidised. According to EXAFS data, the Nb and Fe cations occupy octahedral positions even at low oxygen content. At the same time, the Co cations seemingly occupy highly distorted octahedral positions. It should

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be noted that the mean CoO distance 1.84 is much shorter than the mean FeO 1.92 distance in this case. It was assumed that oxygen vacancies are mainly located near cobalt cation positions

EXAFS STUDY OF Fe(3+) INTERACTION WITH ZrO_2 AND TiO_2 OXIDES

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Phys. Scr., T115 (2005) pp.736-739.

The forms of Fe(3+) ions stabilization on TiO_2, ZrO_2 oxide nanoparticles and their composition were studied by EXAFS spectroscopy. The structure of the iron local surrounding was investigated with respect to preparation method, coverage, support crystal modification, acidity of oxide surface and way of iron introduction into oxide matrix. For all oxides, it was shown that Fe(3+) ions stabilized mainly on the nanoparticle surfaces as isolated ions at low coverage. The location of these ions on the oxide surface depends on the correlation between FeO bond length and interatomic distances of oxide carriers. The increase of surface coverage results in formation of two dimension layer structures. For the ZrO_2-TiO_2 composition, it should be noted that the iron cations interact mainly with zirconia. A few structural models of different iron locations were discussed.

CHANGE IN THE COORDINATION MODE OF NITROSYL GROUPS: TRANSFORMATION OF $Pd_4(\mu\text{-}NO)_4(\mu\text{-}OCOCF_3)_4$ INTO $Pd_3(NO)_2(\mu\text{-}OCOCF_3)_4(C_6H_5Me)_2$

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Russ. J. Inorg. Chem., 50(3) (2005) pp. 365-371.

The reaction of the tetranuclear complex of composition $Pd_4(CO)_4(CF_3COO)_4$ (**I**) with nitrogen monoxide (NO) was studied. The reaction involves the replacement of all the coordinated carbonyl groups with nitrosyl groups accompanied by redox transformations to give the tetranuclear complex $Pd_4(NO)_4(CF_3COO)_4$ (**II**). Complex **II** is structurally similar to the starting complex **I**, which was confirmed by elemental analysis, IR spectroscopy, and EXAFS. Complex **II** is unstable in aromatic solvents (benzene and toluene) and decomposes to form the trinuclear complex $Pd_3(NO)_2(CF_3COO)_4(TolH)_2$ (**III**) and metallic palladium. X-ray diffraction analysis showed that the metal atoms in complex **III** form a linear chain in which each terminal atom is linked to the central atom via two bridging trifluoroacetate groups. The nitrosyl ligands are coordinated to the terminal palladium atoms in a bent end-on fashion. The scheme of the transformation of tetranuclear complex **II** into trinuclear complex **III** is proposed. This scheme was confirmed by quantum-chemical calculations.

SPECTROSCOPIC INVESTIGATIONS OF SMOOTH HYDROCARBON DEUTERATED EROSION FLAKES DEPOSITED FROM TOKAMAK T-10 DEUTERIUM PLASMA DISCHARGE

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Nucl. Instrum. Methods Phys. Res., Sect. A, 543(1) (2005) pp. 225-228.

Investigations of smooth deuterated carbon erosion films co-deposited from deuterium plasma discharges inside the tokamak T-10 vacuum chamber were carried out using UV–VIS and X-ray photoluminescence, UV reflection, EXAFS, EPR, and temperature measurements. The influence of defective states on photoluminescence and its temperature quenching are discussed.

CHEMICAL COMPOSITION OF SURFACE LAYERS OF THE PARTICLES OF ATMOSPHERIC AEROSOLS (NOVOSIBIRSK AND IRKUTSK REGION)

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Chem. Sustain. Devel., 13(1) (2005) pp. 51-63.

An elemental analysis of surface layers of the particles of atmospheric aerosols (AA) in Novosibirsk

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Region and the Baikal region has been performed with the technique of Secondary Ion Mass Spectrometry. It has been found that surface layers (one-two) of monolayer of all aerosols are covered by adsorbed hydrocarbons, nitrogen-containing compounds, other more complex compounds, and water. It has been demonstrated that an erosion of aluminosilicate soils with admixtures of iron, titanium, alkaline and alkali-earth metals provides the basic source for AA formation. Action of water results in Na and Ca "washing out" from surface layers and formation of hydroaluminosilicates. XANES technique was used to study the phase and charge state of iron in AA samples taken in Irkutsk. With the aim of analysing the composition of gases adsorbed on the surface, an attempt has been made to apply a technique of temperature-programmed desorption.

SYNTHETIC $Cu_{0.507(5)}Pb_{8.73(9)}Sb_{8.15(8)}I_{1.6}S_{20.0(2)}$ NANOWIRES

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J. Solid State Chem., 178(1) (2005)
pp. 376-381.

Nanowires of an iodine containing Pb–Sb-sulfosalt have been synthesized by chemical vapor transport. Their structure was studied using high-resolution transmission electron microscopy and X-ray powder diffraction. The lattice parameters show values equal to a=4.9801(4) nm, b=0.41132(8) nm (with two-fold superstructure), c=2.1989(1) nm and β=99.918(6)°. These parameters and the results of a multislice simulation are in good agreement with the mineral pillaite, $Cu_{0.10}Pb_{9.16}Sb_{9.84}S_{22.94}Cl_{1.06}O_{0.5}$ (space group $C2/m$, a=4.949(1) nm, b=0.41259(8) nm, c=2.1828(4) nm, and β=99.62(3)°). Microprobe and EDX analyses yielded a chemical composition of $Cu_{0.507(5)}Pb_{8.73(9)}Sb_{8.15(8)}I_{1.6}S_{20.0(2)}$ which is close to natural pillaite but contains no oxygen and iodine instead of chlorine. The structure of the investigated material is based on chains of M–S polyhedra (M=Pb or Sb) typical for the architecture of sulfosalts implying iodine atoms in trigonal prismatic coordination with Pb atoms from the M–S polyhedra of neighboring chains. The [010] superstructure of the specimen was found to be unstable under electron beam irradiation with a rapid decrease of the b lattice parameter from 0.8 to 0.4 nm within 5 min.

STRUCTURAL TRANSFORMATIONS OF QUARTZ AND APATITE UPON MECHANICAL ACTIVATION

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J. Struct. Chem.,
45(supplement) (2004) pp. 122-127.

Transmission Electron Microscopy (TEM) and Microdifraction Technique, X-ray and IR spectroscopy were used to study structural transformations of quartz and apatite in dependence of intensity and conditions of mechanical treatment. The value of mechanical stress, separating the processes of grinding and activation of solids, equal to theoretical breaking point causing structural and chemical transformations, is determined. Nanoparticles with “liquid-crystalline”, “onion” structure and in amorphous state with sizes from 1 to 100 nm are identified in mechanically activated quartz by TEM method. According to electron-diffraction pattern and X-ray, lattice parameters of initial matrix in “liquid-crystalline” quartz samples remain in one crystallographic direction. At the same time IR-spectra of the samples are characteristic for amorphous silicic acid. The identity of structural transformations after indentation of monocrystals of apatite and quartz and activation of these minerals in planetary-type mill is revealed.

SYNTHESIS OF INTERCALATION COMPOUNDS OF MOLYBDENUM DISULFIDE WITH NITROGEN-CONTAINING ORGANIC MOLECULES AND STUDY OF THEIR MICROSTRUCTURE

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Russ. Chem. Bull., 54(9) (2005) pp. 1914-1923.

Reactions of single-layer dispersions of molybdenum disulfide with 2,2′-bipyridyl, paraphenylenediamine, and hexamethylenetetramine afford intercalation compounds consisting of alternating MoS_2 layers and layers formed by organic molecules. The structures of the intercalation compounds were characterized by X-ray powder diffraction and electron microscopy data. The influence of pH on the composition of resulting compounds and the packing of the intercalant was examined.

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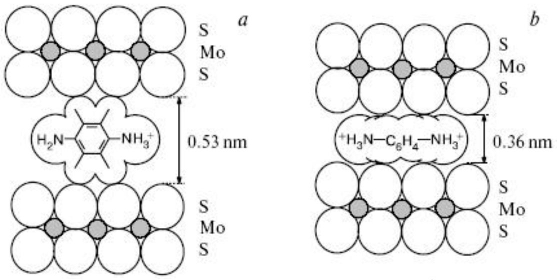

Perpendicular (a) and parallel (b) orientations of the bpyH $^+$ cations relative to the matrix layers in MoS_2 compounds intercalated with bipyridyl.

AN ATTEMPT OF IN VIVO X-RAY DIFFRACTION ANALYSIS OF KIDNEY STONES WITH THE USE OF SYNCHROTRON RADIATION

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Nucl. Instrum. Methods Phys. Res., Sect. A,
543(1) (2005) pp. 302-305.

The paper presents estimation of opportunities of the direct analysis of phase structure kidney stones directly in an organism of the patient with the use of synchrotron radiations (SR), carrying out of experiments on special modelled object “phantom” and estimation of the radiation dose.

X-RAY DIFFRACTION STRUCTURE ANALYSIS OF MCM-48 MESOPOROUS SILICA

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J. Phys. Chem. B, 109(8) (2005) pp. 3233-3237.

The structure of MCM-48 mesoporous silicate materials has been fully characterized from X-ray diffraction data by applying recently developed methods of mesostructure analysis and full-profile refinement. The pore wall thickness of both as-made and calcined MCM-48 was determined with high precision to be 8.0(1) Å. No regular variations of the wall thickness were detected, but its density was found to be ca. 10% higher in the low-curvature regions. The surfactant density in the pores was assessed around 0.6-0.7 g/cm^3 and was found to have a distinct minimum in the pore center similar to that detected previously in MCM-41. A new extended model function of the density distribution in MCM-48 is proposed on the basis of the structural features that were revealed.

ACTUAL TEMPERATURE OF THE ACTIVE COMPONENT OF THE Pt/SiO$_2$ CATALYST IN CO OXIDATION

L.M. Plyasova, V.V. Averyanov, A.A. Khassin, A.V. Kulikova, V.N. Parmon

Doklady Phys. Chem.,
401(1) (2005) pp. 23-27.

In situ X-ray diffraction method is applied to study superheat value of metal Pt in Pt/SiO$_2$ catalyst relatively to mean temperature of catalyst layer, measured with thermocouple, in conditions of reaction of CO oxidation. The range of observed superheat corresponds to the overheating of the whole catalyst sample (particles of the active metal and support).

DEVELOPMENT OF CONTACTLESS METHODS FOR DIRECTLY MEASURING THE TEMPERATURE OF NANOPARTICLES OF THE ACTIVE COMPONENT IN OPERATING SUPPORTED CATALYSTS

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Kinet. Catal., 46(2) (2005) pp. 282-294.

In situ X-ray diffraction and spectroscopic methods for direct contactless measurement of the temperature of nanoparticles of the active component in operating supported catalysts are considered. These methods have provided convincing evidence that the temperature of nanoparticles of the active component may differ significantly from the support temperature during a very exothermic reaction.

SOLID STATE FEATURES OF ELECTROCRYSTALLIZED TUNGSTATE FILMS

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J. Solid State Electrochem.,
9(5) (2005) pp. 371-379.

X-ray diffraction, scanning electron microscopy, and infra-red spectroscopy are applied to study the evolution of films electrodeposited from acidic tungstate solutions. Structural inhomogeneity is found to be responsible for the difference in rechargeability of films of different thickness. Voltammetric responses demonstrate pronounced sensitivity to the nature of crystalline phases, thus throwing light on the defects of the lattice features of nonstoichiometric W(V)–W(VI) oxides. One crystalline phase observed

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in the films under study and attributed to the layered nonstoichiometric oxohydroxide was never reported for oxotungstate films fabricated by other techniques. This phase is believed to be special to electrocrystallized films and to keep some structural features of dissolved isopolytungstate molecular precursors.

ELECTROCHROMIC BEHAVIOR OF OXOTUNGSTATES FABRICATED BY MEANS OF CATHODIC ELECTROCRYSTALLIZATION

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Solid State Ionics, 176(19-22) (2005) pp. 1681-1686.

The electrochromic and voltammetric features of electrocrystallized tungsten oxide films in aqueous medium are compared in two potential regions corresponding to partial W(VI/V) reduction and deep reduction with formation of W(IV). Assignment of certain features to the crystalline components of different structures is presented.

VARIABLE-TEMPERATURE AND VARIABLE-PRESSURE STUDIES OF SMALL-MOLECULE ORGANIC CRYSTALS

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ARKIVOC, Free Online J. Org. Chem., Volume 2004, Part (xii), pp. 128-155.

Several examples of the comparative variable-temperature and variable-pressure studies of the small-molecule organic crystals are discussed. Selected systems represent the crystals with non-spherical flexible molecules/molecular fragments and with different types of intermolecular interactions, ranging from van der Waals interactions to hydrogen bonds of various types (OH…O, NH…OH, NH…O=C). A special attention is paid to the studies of solid drugs (polymorphs of paracetamol), amino acids (polymorphs of glycine, L-serine, D,L-serine), and dipeptides (glycilglycine and glycilglycine hydrate) by structural, spectroscopic and calorimetric techniques. The anisotropy of structural distortion within the range of stability of the same phase, as well as the phase transitions induced by changes in temperature or pressure is discussed.

A NEW, ^{13}C-BASED MATERIAL FOR NEUTRON TARGETS

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Inorganic Mater., 41(5) (2005) pp. 451-460.

A ^{13}C-based neutron-target material is investigated using X-ray diffraction, IR absorption and Raman scattering spectroscopies, transmission electron microscopy, and electrical (conductivity, magnetoresistance, and Hall effect) measurements before and after high-power electron irradiation for various lengths of time.

PROTON CONDUCTIVITY AND STRUCTURAL DYNAMICS IN $Cs_5H_3(SO_4)_4/SiO_2$ COMPOSITES

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Solid State Ionics, 176 (7-8) (2005) pp. 767-771.

$Cs_5H_3(SO_4)_4{\cdot}yH_2O$ and $(1-x)Cs_5H_3(SO_4)_4/xSiO_2$ composite electrolytes (x=0.3–0.9) have been investigated by means of impedance, IR and Raman spectroscopy, differential scanning calorimetry and X-ray analysis. $Cs_5H_3(SO_4)_4{\cdot}yH_2O$ has a phase transition to a high-conductive disordered state ($\sigma \sim 10^{-2}$ S cm^{-1}) at T_{tr}=418 K induced by changes in the structural-water content. This phase transition is shown to be reversible yet the converse transition from the high-temperature phase is slow. Although heterogeneous doping causes only a moderate increase in the low-temperature conductivity of the ionic salt, it stabilizes the high-conductive disordered state. The vibration spectroscopy data confirm the formation of the $Cs_5H_3(SO_4)_4$ disordered state in composites. The composite conductivity does not depend on the composition up to x=0.7 and decreases at $x \geq 0.8$ due to the percolation effect. The structural dynamics of SO_4 tetrahedra is shown to correlate with the proton conductivity.

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FORMATION OF COMPOSITES BASED ON $CsHSO_4$ AND $Cs_5H_3(SO_4)_4$ AND MECHANISM OF THEIR PROTONIC CONDUCTION

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(**Institute of Solid-State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Russ. J. Electrochem., 41(5) (2005) pp. 562-567.

Vibrational spectra of finely divided amorphous $CsHSO_4$, $Cs_5H_3(SO_4)_4{\cdot}H_2O$, and composites based on these are measured and analyzed. An analysis of the spectra indicates the occurrence of substantial changes in the system of hydrogen bonds and in the spectral range of the sulfate group of acid sulfates in the composites. Structural dynamics of the SO_4 tetrahedrons is in full conformance with protonic conduction and the data of X-ray diffraction analyses accompanied by differential scanning calorimetry. It is shown that mobility of protons in the composites increases. A mechanism of the formation of the composites and their conduction is proposed.

SPECTROSCOPIC STUDY OF THE STRUCTURE AND MECHANISM OF PROTON CONDUCTIVITY OF $CsHSO_4$ AND COMPOSITES $CsHSO_4/SiO_2$

E.B. Burgina, V.G. Ponomareva*,
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J. Struct. Chem., 46(4) (2005)
pp. 630-640.

IR and Raman spectra, structural, thermodynamic and transfer properties of $CsHSO_4$ and composites $CsHSO_4/SiO_2$ have been studied. It was shown, that in $CsHSO_4$ composites the phase II (monoclinic modification) is stabilized. This phase transforms into amorphous state upon increasing of SiO_2 content. High-conductive disordered state of $CsHSO_4$ in composites at temperatures significantly lower than that of the superionic phase transition is confirmed. In these high-conductive state equalization of bond length in sulphate-ions, weakening in the system of hydrogen bonds and as a result an increasing of proton mobility in composites in comparison with pure salt occurs. Mechanism of composites formation and their proton conductivity is suggested.

CATIONIC COMPLEXES Eu(III) AND Sr(II) WITH DIPHOSPHINE DIOXIDES IN ORGANIC EXTRACTS

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(**Khlopin Radium Institute, St Petersburg, Russia*)

J. Struct. Chem., 46(5) (2005) pp. 859-868

IR spectroscopy was used to study composition and structure of Eu(III) and Sr(II) complexes formed upon cation-exchange extraction of these metals from aqueous nitrate solutions with dichloroethane solutions of mixture superacid – chlorinated cobalt(III) dicarbollide (CCD) with diphenyl diphosphine dioxides, containing methyl (Me-DPDD), ethyl (Et-DPDD) or polyoxoethylene chains linking two phosphorus atoms of phosphine oxide groups. It was established, that complexes $[Eu(H_2O)_nL_4]^{3+}$ where L = Me- and Et-DPDD are formed in organic phases at molar ratio DPDD/CCD≤1. Polyoxoethylene diphosphine dioxide forms anhydrous complexes of composition Eu:L = 1:1 and 1:2 with Eu(III), and outer-sphere complexes of composition 1:1 and 1:2 with Sr(II), in which molecules of organic ligand cover the hydrated cation $Sr(H_2O)_n^{2+}$. The peculiarities of complexes extraction are explained based on data of their composition and structure.

PROTON SOLVATES, $H^+{\cdot}nH_2O{\cdot}mL$, FORMED BY DIPHOSPHINE DIOXIDES WITH CHLORINATED COBALT(III) DICARBOLLIDE ACID

E.S. Stoyanov, I.V. Smirnov* (**Khlopin Radium Institute, St Petersburg, Russia*)

J. Mol. Struct., 740(1-3) (2005) pp. 9-16.

Interaction of hydrated proton, $H_5O_2^+{\cdot}(H_2O)_4$, in dichloroethane solutions with diphosphine dioxides (L) having methyl (Ph_4Me), ethyl (Ph_4Et) and polyoxyethylene chains (Ph_4PEG) linking two diphenyl phosphine oxide groups has been investigated. A bulky counter ion: chlorinated cobalt(III) *bis*(dicarbollide), $[Co(C_2B_9H_8Cl_3)_2]^-$, minimizes perturbation of the cation. At low concentrations, Ph_4Et and Ph_4PEG form anhydrous 1:1 complexes with $(P{=})O{-}H^+{-}O({=}P)$ fragment having very strong symmetrical H-bonds. At these conditions Ph_4Me form another compound, $H_5O_2^+{\cdot}L(H_2O)_2$, due to lower P═O basicity and optimal geometry of the chelate cycle. At higher concentrations, Ph_4Me and Ph_4Et form isostructural complexes $H_5O_2^+{\cdot}L_2$, whereas Ph_4PEG forms only a 1:1 complex with proton dihydrate, $H_3O^+{\cdot}H_2O$. In excess of free Ph_4Me and Ph_4Et a water molecule is introduced to the first coordination sphere of $H_5O_2^+$ and the average molar ratio $L/H_5O_2^+$ of the complexes exceeds 2. The

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composition of these complexes as a function of L and its concentration is discussed.

SILICA-SUPPORTED ZIRCONOCENE/(PERFLUOROPHENYL)BORATE CATALYST FOR PROPYLENE POLYMERIZATION. DRIFTS STUDY OF THE CATALYST FORMATION AND SURFACE SPECIES

V.N. Panchenko, I.G. Danilova, V.A. Zakharov, E.A. Paukshtis

J. Mol. Catal. A: Chem., 225(2) (2005) pp. 271-277.

IR spectroscopy has been used to study the interaction of silica with $PhNEt_2$ (N) and $B(C_6F_5)_3$ (B) and subsequent interaction of the support $SiO_2/[N + B]$ with dimethylzirconocene $Me_2Si(2\text{-}Me\text{-}Ind)_2ZrMe_2$ ("Zr"). The data were obtained on the composition of the surface compounds appeared at both stages of catalyst synthesis.

It has been shown that (B) and (N) interact with OH groups of silica to form ionic pair $[H—NR_3]^+[(C_6F_5)_3B—O—Si\equiv]^-$ (IP-1). Cation fragment of this pair contains highly reactive N—H bond with a.b. at 3230 cm^{-1}. It has been found that N—H groups in a part of IP-1 complexes react with neighboring OH groups of silica by hydrogen bonding that gives complexes IP-2. It has been shown that "Zr" complexes interact both with complexes IP-1 and IP-2. As "Zr" reacts with IP-1, zirconium ionic complexes IP-3 containing Zr—Me bond are formed on silica. These complexes are suggested to be the precursor of the polymerization active sites. The reaction of "Zr" with IP-2, most likely, produces surface zirconium compound containing no Zr—Me bonds and inactive for propylene polymerization.

N_2 AND CO AS PROBE MOLECULES FOR DETERMINING THE PROPERTIES OF ACID SITES ON THE SURFACE OF ZEOLITES

M.E. Malyshev, E.A. Paukshtis, L.V. Malysheva, A.V. Toktarev, L.A. Vostrikova

Kinet. Catal., 46(1) (2005) pp. 100-106.

The applicability of molecular nitrogen as a probe for the Brønsted and Lewis acid sites of HNaY and HZSM-5 zeolites was studied by Fourier transform IR spectroscopy. The integrated absorption coefficients of bands due to N–N vibrations in complexes with Brønsted and Lewis acid sites were determined. The correlation between the integrated absorption coefficients and the positions of bands due to N–N vibrations in nitrogen interacting with the acid sites of test samples is discussed. It was proposed to use the low-temperature adsorption of nitrogen to express determination of the concentrations of strong Lewis and Brønsted acid sites in zeolites.

INTERACTION OF N_2 WITH THE ACID SITES OF OXIDES

M.E. Malyshev, E.A. Paukshtis, L.V. Malysheva

Kinet. Catal., 46(1) (2005) pp. 107-113.

Nitrogen adsorption on SiO_2, ν-Al_2O_3, TiO_2, and sulphated zircona (SO_4^{2-}/ZrO_2) is studied by Fourier transform IR spectroscopy. Integrated absorption coefficients for the bands due to the N–N vibrations in nitrogen complexes with Brønsted and Lewis acid sites are determined. A general correlation between integrated absorption coefficients and the positions of N–N bands of nitrogen interacting with the above sites in zeolites and oxides is discussed. The orientation of a nitrogen molecule relative to Brønsted and Lewis acid sites is calculated *ab initio* using a 6-31G** basis set.

REVERSIBLE TRANSFORMATIONS OF GOLD NANOPARTICLE MORPHOLOGY

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Langmuir, 21(23) (2005) pp. 10280-10283.

Herein is reported a metamorphosis taking place in a gold nanosized system. The observed phenomenon of shape and size transformations was found to be completely reversible. Unlike most procedures in the literature where shape and size control occur in the synthetic step by adding growth- and shape-controlling agents such as surfactants or polymers, in this system postsynthetic changes in shape and size can be carried out simply by changing the ratio of reactive, competing reagents, more specifically, alkylthiols versus tetraalkylammonium salts. Interestingly, the transfer of gold metal occurs (large prismatic particles to small particles and vice versa) under the influence of reagents that do not cause such interactions with bulk gold. All intermediate steps of the morphology change were observed using HRTEM and electron diffraction. The processes of breaking down and "welding back" solid metal nanoparticles occur under mild conditions and are remarkable examples of the unique chemical properties of nanomaterials. The described process is expected to be relevant to other nanoscale systems where similar structural circumstances could occur.

ATOMIC AND ELECTRONIC STRUCTURES OF AMORPHOUS ZrO_2 AND HfO_2 FILMS

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Microelectron. Eng., 81(2-4) (2005) pp. 524-529.

Atomic and electronic structures of ZrO_2 and HfO_2 films deposited using sputtering technique were studied by X-ray diffraction (XRD), EXAFS spectroscopy, photoemission (with X-ray and ultraviolet excitation sources) and electron energy loss spectroscopy (EELS). XRD results indicated that the as-deposited films were amorphous and a monoclinic phase was detected after annealing them in ambient at 800°C. Photoemission results indicated that the ZrO_2 valence band consists of two bands separated by an ionic gap of 6 eV. The lower band of 10 eV width is occupied mainly by O 2s states. EELS results indicated that the bandgap of ZrO_2 and HfO_2 films are 4.7 and 5.7 eV, respectively.

EFFECT OF MECHANICAL TREATMENT ON THE REACTIVITY OF COPPER POWDER TOWARD ACETIC ACID

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Kinet. Catal., 46(4) (2005) pp. 565-571.

The mechanism of the mechanical activation of copper powder is studied by calorimetry, XPS, and X-ray diffraction. The increase in the heat of copper–acetic acid reaction caused by mechanical treatment is due to the activation of dioxygen involved in this reaction. This activation is due to the presence of suboxide oxygen with an increased electron binding energy in mechanically treated copper.

PRODUCTION OF SILVER NANO-POWDERS BY ELECTRON BEAM EVAPORATION

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Vacuum, 77(4) (2005) pp. 485-491.

Evaporation of metallic silver was performed in Ar, N_2 and He using the ELV-6 electron accelerator. The obtained ultra-dispersed powders with a particle size of 70–80 nm were investigated by XRD, HREM and UV–Vis spectroscopy. The structure of Ag(Ar) powder was shown to differ substantially from that of Ag(N_2) by the presence of small oxide-like species of 10–20 nm on the particle surface. Catalytic activity of the powders in the reaction of ethylene epoxidation was also studied.

LUMINESCENCE OF Al_2O_3 CRYSTAL MODIFICATIONS EXCITED BY THE ArF EXCIMER LASER

V.N. Snytnikov, V.O. Stoyanovsky, V.A. Ushakov, V.N. Parmon

Kinet. Catal., 46(2) (2005) pp. 260-268.

Luminescence spectra induced by a high-power UV laser pulse in the excitation range of extraneous ions in alumina can provide valuable information on this compound. The laser-induced luminescence (LIL) technique markedly extends the capabilities and the area of application of photoluminescence spectroscopy. Luminescence measurements in the red spectral region enable one to detect octahedrally coordinated Cr^{3+} ions at concentrations down to 10^{-7} wt % in metastable alumina modifications. The fact that the Cr^{3+} luminescence line occurs in different positions in the α- and θ-alumina allows LIL spectroscopy to be used in phase and elemental analysis of thin surface layers and in surface temperature measurements when studying the microstructure of heterogeneous catalysts under real pressures and in a real gas medium, including *in situ* measurements.

ADSORPTION OF NITROGEN, OXYGEN, AND ARGON VAPORS ON FINE-PORE OXIDE MATERIALS

V.Yu. Gavrilov

Kinet. Catal., 46(3) (2005)
pp. 403-406.

A comparative study of the adsorption of N_2, O_2, and Ar vapors on supermicroporous and fine-mesopore silica at 77 K is carried out. The oxygen sorption properties of these silica materials, like those of tin oxide and zirconia (earlier studied materials), are affected by supermicropores. Argon sorption is insensitive to the presence of supermicropores. Fine mesopores also have an effect on the oxygen sorption properties of silica.

ADSORPTION OF DIHYDROGEN ON MESOPOROUS MATERIALS AT 77 K

V.Yu. Gavrilov

Kinet. Catal., 46(4) (2005)
pp. 603-608.

The adsorption of dihydrogen at 77 K is studied on a series of oxide materials including silica, pure titania and alumina, and mixed oxides. The experimental data obtained suggest that the sorption properties per unit area of mesopore surface depend on both the texture and chemical composition of the sample. A comparative procedure for the analysis of dihydrogen adsorption isotherms is considered.

APPLICATION OF HETEROPLYCOMPOUNDS FOR DETERMINATION OF CHEMICAL FORMS OF ARSENIC IN NATURAL WATERS

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Chem. Sustain. Devel., 13(3) (2005)
pp. 469-477.

Procedure is developed for determination of arsenate-, arsenite-, monomethylarsonate- and dimethylarsenite-ions in water by method of capillary electrophoresis with spectrophotometric detection of defined derivatives of arsenic chemical forms. Isopolymolybdate was taken as a reagent for derivatization. Stoichiometry was studied and extinction coefficient were determined for detectible heteropolycomplexes. Optimal conditions of their generation and electrophoretic separation were revealed. Upon concentration by electrostacking method the developed procedure provide detection limits ~0.01 mcg/ml.

$CsLiB_6O_{10}$ CRYSTALS WITH Cs DEFICIT: STRUCTURE AND PROPERTIES

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J. Cryst. Growth, 282(3-4) (2005)
pp. 407-413.

Cs–Li borate crystals (CLBO) grown from melts have been examined by chemical and thermal analysis and IR spectroscopy. Evaporation of cesium oxides from melt during growing resulted in crystals with Cs deficit. The defect structure of these crystals has been refined by means of single-crystal X-ray diffraction analysis, while two non equivalent Cs positions have been revealed. Using the close-packed spheres model, the volumes of the structural vacant spaces have been estimated, and the proof of their occupation by one or several water molecules has been given. The behavior of the defect CLBO crystals exposed to dry and moist atmospheres has been considered.

INORGANIC COMPONENTS OF THE UNIQUE SAMPLES OF ARCHAEOLOGICAL TEXTILE FROM "FROZEN GRAVES" OF MOUNTAIN ALTAI (IV-III CENTURIES B.C.)

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

In "*Costume and Textile of Pazyryktsev from Altai (IV-III Centuries B.C.)*",
INFOLIO, 2005, Novosibirsk,
pp. 198-201.

New highly sensitive etalon-free method of differential dissolution was applied for identification and determination of quantitative phase (mineral) composition of inorganic compounds from old textile. This method allows direct determination of phase (mineral) composition of unknown substances. As a whole, analysis of more than 100 different pieces of clothing was conducted.

CONTENT

DEVELOPMENT OF AEROGEL CHERENKOV DETECTORS AT NOVOSIBIRSK

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Nucl. Instrum. Meth. Phys. Res., Sect. A,
A553(1-2) (2005) pp. 125-129.

The development of aerogel Cherenkov counters with the light collection using a wavelength shifter is described. 80 counters of this type are working in the KEDR detector. A project of similar counters for the SND detector based on "heavy" aerogel with n=1.13 has been developed. Aerogel with a refractive index of 1.006–1.13 and dimensions of blocks up to 200×200×50 mm^3 is produced by the Novosibirsk group for use in Cherenkov counters of different types. The Novosibirsk group is participating in the development of LHCb RICH as well as a beam diagnostics for a photo-injector test facility at DESY–Zeuthen. Recently it was started development of RICH based on focusing aerogel (FARICH) for the endcap of the SuperBaBar. For the first time in the world the focusing aerogel with layers of different refractive indices has been produced.

FOCUSING AEROGEL RICH (FARICH)

A.Yu. Barnyakov*, M.Yu. Barnyakov*, V.S. Bobrovnikov*, A.R. Buzykaev*, A.F. Danilyuk, V.L. Kirillov, S.A. Kononov*, E.A. Kravchenko*, A.P. Onuchin* (**Budker Institute of Nuclear Physics, Novosibirsk, Russia*)

Nucl. Instrum. Meth. Phys. Res., Sect. A,
553(1-2) (2005) pp. 70-75.

In this work it was investigated a Ring Imaging Cherenkov detector based on "focusing" aerogel (FARICH). In the proximity focusing RICH, one of the main factors determining precision of ring radius measurements is a finite thickness of a radiator. FARICH development aims at the reduction of this effect by means of using multilayer aerogel. Two options have been considered.

Single ring: refraction index and thickness of each layer are adjusted in such a way that Cherenkov rings from different layers are superimposed on each other.

Multi-ring: refraction index and thickness of each layer are adjusted so that ring images from different layers have different radii and are clearly separated from each other.

For the first time in the world it has been developed a technique for production of multilayer aerogels (SAN-MULTI). A few samples consisting of four aerogel layers with indices from 1.022 to 1.030 have been produced.

A GEANT4 based simulation program has been developed. Velocity resolution was investigated for different momenta and particle incidence angles. It was shown that velocity resolution of 5×10^{-4} is achievable. This permits us to have π/K separation at the level of more than 3σ up to momentum 8.0 GeV/c, π/μ separation up to momentum 1.6 GeV/c.

STATUS OF THE SIBERIAN SYNCHROTRON RADIATION CENTER

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Nucl. Instrum. Methods Phys. Res., Sect. A,
543(1) (2005) pp. 1-13.

Synchrotron radiation (SR) experiments at the Budker Institute of Nuclear Physics had been started in 1973, and from 1981 the Siberian Synchrotron Radiation Center (SSRC) had an official status as Research Center of the Russian Academy of Sciences. SSRC is the research center, which is open and free of tax for the research teams from Russia and abroad.

ELECTRONIC STRUCTURE OF THE Pt(100) SINGLE CRYSTAL SURFACE AFFECTED BY OXYGEN ADSORPTION

A.R. Cholach, V.M. Tapilin

React. Kinet. Catal. Lett., 86(2) (2005)
pp. 315-322.

Disappearance Potential Spectroscopy study of the oxygen adsorption on the Pt(100)-(1×1) single crystal surface revealed a regular set of spectral satellites designated as the platinum bulk plasmons.

Fundamental and Practical Approaches to Catalyst Preparation

INTRODUCTION INTO PHYSICAL CHEMISTRY OF HETEROGENEOUS CATALYSTS TEXTURE FORMATION

V.B. Fenelonov, V.N. Parmon

In "*Industrial Catalysis, Lectures*", Ed. A.S. Noskov,
Moscow, Kalvis, 2005,
Part 1, pp. 36-86.

The molecular (atomic) and supramolecular (texture) level problems should be distinguished in studying fundamentals of heterogeneous catalysts preparation. The term 'texture' means a set of structural and geometric characteristics of particles, pores and their ensembles including the morphology, specific surface areas of phases and components, porosity, spatial arrangement, size distribution. The main problems are the control of catalytic activity on the molecular level and optimization of catalyst efficiency on the texture level. The first group of problems is solved by modern chemical methods. Theoretical bases for the decision of the problems of the second group is physical supramolecular chemistry (or texturology), including the laws of surface-capillary phenomena, geometry of porous and dispersed systems and other specific approaches. At the same time the laws of physical supramolecular chemistry are universal enough and may be applied for deliberate texture control in systems of various chemical compositions at different stages of their synthesis.

INTRODUCTION INTO PHYSICAL CHEMISTRY OF HETEROGENEOUS CATALYSTS TEXTURE FORMATION

V.B. Fenelonov, V.N. Parmon

In "*Industrial Catalysis, Lectures*", Ed. A.S. Noskov,
Moscow, Kalvis, 2005,
Part 2, pp. 9-80.

An approach to the theory of formation of heterogeneous catalyst textures is developed. It is based on the individual analysis of chemical and physical factors. Six series of principal mechanisms of texture formation are specified, and the systematic approach to structure modeling at various hierarchical levels as single module is justified. Molecular level modeling of the structure and mechanisms of ordered structures formation are considered, illustrated with the silica systems formation as an example.

FORMATION OF TEXTURAL AND MECHANICAL PROPERTIES OF EXTRUDED CERAMIC HONEYCOMB MONOLITHS: AN ^{1}H NMR IMAGING STUDY

S.A. Yashnik, Z.R. Ismagilov, I.V. Koptyug*, I.P. Andrievskaya, A.V. Matveev*, J.A. Moulijn** (**International Tomography Center, Novosibirsk, Russia; **Technical University of Delft, The Netherlands*)

Catal. Today, 105(3-4) (2005) pp. 507-515.

The effects of the nature of oxide component and binder, and thermal treatment temperature (100°C and from 600 to 1300°C) on textural and physicochemical properties of honeycomb monoliths based on alumina, titania and aluminosilicates have been studied.

The main regularities of the texture formation have been revealed using ^{1}H NMR imaging, SEM, XRD, adsorption technique and others. It has been shown that the textural changes of monolith samples at different preparation stages from extrusion to thermal treatment are mostly caused by removal of capillary water (20–100 °C), sintering of small pores and consolidation of oxide particles (100–700 °C), and phase transformation of the oxide component or the binder (900–1300°C).

CHARACTERISTICS OF DRYING AND ACTIVE COMPONENT DISTRIBUTION IN ALUMINA MONOLITHS USING ^{1}H-NMR IMAGING

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Catal. Today, 105(3-4) (2005) pp. 484-491.

The distribution of water in the impregnated monolithic substrates was visualized by ^{1}H-NMR imaging. The two-dimensional water content maps along the axial and radial directions have been collected for different monoliths at variation of the drying conditions. Using the blow-through air for drying of the substrate with coated external walls and with free access of air to external walls leads to the parabolic profile of water concentration along the axial direction of the sample. Drying of the monoliths with open external walls proceeds more uniformly in the radial and axial directions of the substrate. Characteristics of drying of alumina monoliths, calcined at 600, 900 and 1200 °C having differences in the pore structure and pore distribution, are studied.

During drying of the impregnated washcoated monolith the certain part of the introduced active component precursor (H_2PtCl_6 or H_2PdCl_4) is transported from the substrate macropores to the mesoporous washcoated layer which leads to enrichment of the washcoat of the final catalyst by active component. The non-destructive character of ^{1}H-NMR microimaging demonstrated its capability to visualize the water content maps in monoliths in the presence of Pt and Pd.

NEW CATALYSTS OF THE METAL-FILAMENTARY CARBON TYPE: FROM FUNDAMENTAL RESEARCH TO TECHNOLOGY

V.V. Molchanov, V.V. Chesnokov, R.A. Buyanov, N.A. Zaitsev, V.I. Zaikovskii

Kinet. Catal., 46(5) (2005) pp. 660-668.

A principally new basic catalytic system is developed. The system is based on dispersed metal particles incorporated into carbon filaments by the catalytic decomposition of hydrocarbons on these particles. The basic system enables one to synthesize a series of catalysts for different processes. Mechanisms and methods for controlling the catalytic properties of this system are studied. The role of the crystal faces of the metal particles and of chemisorbed hydrogen species in selective hydrogenation is established. The chemical composition of the active component is optimized for the removal of acetylene from ethylene and of butadiene from butenes. A technology for catalyst precursor preparation is developed, which includes a mechanochemical activation stage and the shaping of the resulting powder. Optimum conditions are found for hydrocarbon decomposition in order to obtain metal–carbon catalysts for selective hydrogenation.

MECHANOCHEMICAL SYNTHESIS OF INTERMETALLIC HYDRIDES AT ELEVATED HYDROGEN PRESSURES

V.V. Goidin, V.V. Molchanov, R.A. Buyanov

Inorg. Mater., 40(11) (2004) pp. 1328-1332.

An apparatus is described for producing gas pressures of up to 10 MPa in the grinding vessels of a planetary mill. Mechanochemical reactions are carried out for the first time at gas pressures above 1 MPa. A novel approach to the synthesis of intermetallic hydrides is proposed which involves mechanical activation of a metal mixture at a high hydrogen pressure. Using this approach, two new hydrides are synthesized: Mg_2NiH_6 and a magnesium copper hydride with the approximate composition $MgCuH_2$.

MECHANOSYNTHESIS OF COMPLEX OXIDES AND PREPARATION OF MIXED CONDUCTING NANOCOMPOSITES FOR CATALYTIC MEMBRANE REACTORS

V.V. Zyryanov*, N.F. Uvarov*, V.A. Sadykov, Yu.V. Frolova, G.M. Alikina, A.I. Lukashevich, M.I. Ivanovskaya, J.M. Criado***, S. Neophytides****** (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Research Institute for Physical Chemical Problems of the Belarus State University, Minsk, Belarus; ***Institute de Ciencias de Materiales, Sevilla, Spain; ****Institute of Chemical Engineering and High Temperature Processes, Patras, Greece*)

Catal. Today, 104(2-4) (2005) pp. 114-119.

Nanopowders of $LaGaO_3$- and $LaMnO_3$-based complex perovskites (P) and ceria-based fluorites (F) were prepared by mechanosynthesis. Compatible nanocomposites F + P and P + P with mixed ion and electron conducting (MIEC) properties were prepared and sintered at moderate temperatures up to dense ceramics. The obtained materials were studied by means of XRD, SEM, TEM, electrical conductivity measurements, temperature programmed (TP) reduction/oxidation and preliminary estimations of permeability were obtained. A new strategy based on the advantages of the mechanochemical ceramic approach is proposed to design multilayer ceramic membranes for CMR. Casting technology and one-step sintering were used for the production of thin film membranes with MIEC properties on porous substrates. The coarse fraction of as-milled powders from agglomerates with density ~70% was used for the porous substrate, and fine fractions of aggregates with sizes <1 μm were used in preparation of composites for thin dense films. Ceria-based composites prepared by the Pechini route and/or mechanochemical method are proposed as materials for protecting thin films.

MECHANOSYNTHESIS OF COMPLEX OXIDES WITH FLUORITE AND PEROVSKITE-RELATED STRUCTURES AND THEIR SINTERING INTO NANOCOMPOSITES WITH MIXED IONIC–ELECTRONIC CONDUCTIVITY

V.V. Zyryanov*, V.A. Sadykov, N.F. Uvarov*, G.M. Alikina, A.I. Lukashevich, S. Neophytides, J.M. Criado***** (**Institute of Solid State Chemistry, Novosibirsk, Russia; **Institute of Chemical Engineering and High Temperature Processes, Patras, Greece; ***Institute of Materials Science, Sevilla, Spain*)

Solid State Ionics,
176(37-38) (2005) pp. 2813-2818.

It is shown that mechanochemical approach allows fast synthesis of individual phases with fluorite and perovskite structures and preparation of dual-phase nanocomposites with mixed ionic–electronic conductivity. Binary oxides obtained by mechanosynthesis are frequently metastable compounds which decompose at moderate temperatures before sintering into the dense ceramics. Complex doping provides kinetic stabilization of perovskites and fluorites and allows their sintering into dense ceramics. Moreover, complex doping of structurally different phases makes possible a preparation of compatible compounds for nanocomposites. In all 10 nanocomposites considered, the chemical interaction (interdiffusion) was found to occur in some degree. Rules are formulated for preparation of composites from compatible compounds. All perovskites and ceria-based composites are likely to be more promising as membrane materials.

CHARGE AND COORDINATION STATES OF IRON CATIONS IN $La_{1-x}Me_xFeO_{3-y}$ (Me=Ca, Sr, Ba) PREPARED BY MECHANOCHEMICAL ROUTE AS RELATED TO OXYGEN REACTIVITY

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Solid State Chemistry of Inorganic Materials V,
MRS Symposium Proceeding,
Eds. J. Li, N. Brese, M. Kanatzidis, M. Jansen, MRS,
Warrendale, Pensylvania,
Vol. 848, 2005, pp. 511-516.

This studies aimed at elucidation of the effect of the type and content of dopant (Ca,Sr, Ba) on the coordination and charge states of the iron cation as well as on the formation of new oxygen forms in lanthanum ferrite prepared by mechanochemical route. According to X-ray analysis homogeneous solid solutions (with Orthorhombic and Cubic structures) were formed in the samples in the case of Sr and Ba substituted perovskites and two-phase samples (composed of $LaFeO_3$ and $Ca_2Fe_2O_5$) were revealed for all Ca substituted perovskites. Formation of Fe^{+4} cations in O coordinations was determined by Moessbauer investigation in Sr and Ba substituted perovskites. Formation of Fe^{+3} in P coordination is not excluded only for samples with x>0.6. No Fe^{+4} cation was detected in Ca-substituted perovskites, only Fe^{+3} cations in O_1, O_2, P and T coordinations were revealed.

A formation of new low-bounded oxygen forms was detected by TPR in H_2. Fe^{+4} content calculated from TPR data was higher than that obtained from Moessbauer data, that may be a result of formation not only Fe^{+4} or oxygen vacancy to maintain the eleconeutrality of substituted with Me perovskites, but of the low charge oxygen anion as well. Probably such low charge oxygen anions are formed during reoxidation of vacancy high-temperature solid solutions under cooling in the air.

REACTIVITY OF $La_{1-x}Sr_xFeO_{3-y}$ (x = 0–1) PEROVSKITES IN OXIDATION REACTIONS

L.A. Isupova, I.S. Yakovleva, G.M. Alikina, V.A. Rogov, V.A. Sadykov

Kinet. Catal., 46(5) (2005) pp. 729-735.

Oxygen species and their reactivity in $La_{1-x}Sr_xFeO_{3-y}$ perovskites prepared using mechanochemical activation were studied by temperature-programmed reduction (TPR) with hydrogen and methane. The experimental data were compared with data on the catalytic activity in oxidation reactions. It was found that the rates of CO and methane oxidation on the perovskites in the presence of gas-phase oxygen correlated (k = 0.8) with the amount of reactive surface oxygen species that were removed by TPR with hydrogen up to 250°C. Maximum amounts of this oxygen species were released from two-phase samples (x = 0.3, 0.4, and 0.8), which exhibited an enhanced activity in the reaction of CO oxidation. In the absence of oxygen in the gas phase, methane is oxidized by lattice oxygen. In this case, the process activity and selectivity depend on the mobility of lattice oxygen, which is determined by the temperature, the degree of substitution, the degree of reduction, and the microstructure of the oxide. Thus, the high mobility of oxygen, which is reached at high concentrations of point defects or interphase/domain boundaries, is of importance for the process of deep oxidation. However, the process of partial oxidation occurs in single-phase samples at low degrees of substitution (x = 0.1–0.2).

SELF-PROPAGATING SYNTHESIS OF SUPPORTED OXIDE CATALYSTS FOR DEEP OXIDATION OF CO AND HYDROCARBONS

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Kinet. Catal., 46(5) (2005) pp. 752-757.

The surface self-propagating thermal synthesis (SSTS) of supported oxide catalysts is reported, which is a new modification of self-propagating high-temperature synthesis. The propagation of the combustion front on a variety of supports differing in nature and shape is studied. A group of catalysts based on simple and mixed oxides of cobalt, copper, and manganese are prepared by SSTS, and their physicochemical properties are determined. The dependence of synthesis parameters on catalyst preparation conditions is studied. The activity of the resulting catalysts is estimated in deep CO and methane oxidations as model reactions.

EFFECT OF THERMAL TREATMENT ON STATES OF MOLYBDENUM IN Mo/H–ZSM-5 CATALYST FOR METHANE DEHYDROAROMATIZATION: ESR AND UV–VIS STUDY

N.T. Vasenin, V.F. Anufrienko, I.Z. Ismagilov, T.V. Larina, E.A. Paukshtis, E.V. Matus, L.T. Tsykoza, M.A. Kerzhentsev, Z.R. Ismagilov

Top. Catal., 32(1-2) (2005) pp. 61-70.

Valence and coordination states of molybdenum ions formed upon thermal treatment of Mo/H–ZSM-5 catalyst for methane dehydroaromatization in Ar and Ar/CH_4 media at 573–973 K have been studied by ESR and UV–VIS spectroscopy. For comparison, the characteristic ESR spectra of thermolyzed bulk ammonium heptamolybdate have been studied and analyzed in detail. The nature of earlier observed Mo^{5+} ions has been verified, and new paramagnetic states of molybdenum in Mo/H–ZSM-5 catalysts have been detected: Mo^{3+} ions, and Mo^{5+} ions in tetrahedral coordination with delocalization of unpaired electron to Al and H or Al and N atoms.

PHYSICOCHEMICAL PRINCIPLES OF THE SYNTHESIS OF POROUS COMPOSITE MATERIALS THROUGH THE HYDROTHERMAL OXIDATION OF ALUMINUM POWDER

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Kinet. Catal., 46(5) (2005) pp. 641-659.

The main versions of the synthesis of a new class of porous cermet materials such as Al_2O_3/Al, $MO_x/Al_2O_3/Al$, and $M^1/MO_x/Al_2O_3/Al$ and ceramic composites on their basis were analyzed. These ceramic composites were prepared through the stage of the hydrothermal oxidation of aluminum powder and were designed for catalytic and adsorption processes. Equations that express the dependence of the apparent density of the resulting composite on the density of the initial powder mixture, on the concentration of the powdered active component, and on the conversion of aluminum are given. It was found that the formal kinetics of aluminum oxidation with water at 100°C can be described by the Kolmogorov–Erofeev equation. The results were compared with data obtained in an autoclave at higher temperatures and steam pressures. The synthesis parameters that affect the total pore volume and the specific surface area of aluminum oxide obtained from aluminum powder were determined. For the case of the transfer of soluble components from an autoclave to a press mold, the molar coefficients of this process were calculated. The texture peculiarities of composites were analyzed. The texture exhibited a polymodal character with developed micropore, mesopore, and ultramacropore structures, which are responsible for the high permeability of granulated composites. Factors affecting the mechanical properties of metal ceramics were studied. The catalysts and products of composite materials were exemplified.

SYNTHESIS OF ALUMINA THROUGH HYDROTHERMAL OXIDATION OF ALUMINUM POWDER CONJUGATED WITH SURFACTANT-DIRECTED ORIENTED GROWTH

S.F. Tikhov, Yu.V. Potapova, V.A. Sadykov, V.B. Fenelonov, I.V. Yudaev, O.B. Lapina, A.N. Salanov, V.I. Zaikovskii, G.S. Litvak

Mater. Res. Innov., 9(3-1) 2005 pp. 431-446.

The hydrothermal oxidation of powder aluminum in the presence of alcohols was found to be leading to an interaction of HTO products with the surfactants. An increase of the number of OH-groups in the alcohols and, consequently, their boiling temperature and density, results in their greater influence on the aluminum reactivity, the degree of their interaction with the HTO products, structural and textural characteristics of alumina formed from the products of aluminum oxidation in the Al_2O_3/Al composites. This method yields a slit-like alumina porous structure that is thermally stable up to 540°C and can be varied as a function of the composition of reactants and dopants (surfactants) as well as, apparently, temperature and HTO reaction time. The structure of obtained aluminum oxide is significantly different from those known earlier.

CURRENT TRENDS IN THE IMPROVEMENT AND DEVELOPMENT OF CATALYST PREPARATION METHODS

N.A. Pakhomov, R.A. Buyanov

Kinet. Catal., 46(5) (2005)
pp. 669-683.

The state of the art in the scientific foundations of catalyst preparation is analyzed. New lines and trends in the development of conventional catalyst preparation methods that have appeared in the last 10-15 years are discussed. The theoretical and experimental foundations of the syntheses of porous materials by the sol–gel processing of alkoxides are considered. The synthesis of fine MgO aerogel, which is a unique destructive sorbent and catalyst, is described as one of the numerous examples of the use of this method in combination with supercritical drying. The synthesis of complex oxide and supported metallic catalysts by the sol–gel method is analyzed. Some new approaches to active catalyst deposition are considered, including the deposition–precipitation method. Unconventional methods of catalyst preparation are classified. Tasks are formulated for the development of the scientific basis of these methods.

HONEYCOMB SUPPORTED PEROVSKITE CATALYSTS FOR AMMONIA OXIDATION PROCESSES

L.A. Isupova, E.F. Sutormina, N.A. Kulikovskaya, L.M. Plyasova, N.A. Rudina, I.A. Ovsyannikova, I.A. Zolotarskii, V.A. Sadykov

Catal. Today, 105(3-4) (2005)
pp. 429-435.

Pechini route (M.P. Pechini. U.S. Patent no. 3,330,697 (1967)) was used for supporting perovskite–like systems $LaBO_3$ (B = Mn, Fe, Co, Ni, Cu) on thin-wall (0.35 mm) cordierite honeycomb support with low thermal expansion coefficient to prepare stable to thermal shocks supported catalysts for high-temperature processes of ammonia oxidation into NO in nitric acid production. In this preparation route, perovskites (2–6%) have nearly uniform distribution in the walls as well as form surface grainy perovskite layer 2–3 μm thick that may be also important for the high temperature processes occurring at short contact times. Cordierite supported lanthanum manganite and cobaltite are the most active in the reaction of ammonia oxidation into NO especially when supported twice or on a secondary sublayer (Ln_2O_3, ZrO_2, MeO, $LaBO_3$).

THE FORMATION OF STRUCTURAL DEFECTS IN THE Ce–Sm–O AND Ce–Sm–O/Ru NANOSYSTEMS SYNTHESIZED BY THE SOL-GEL METHOD

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Russ. J. Phys. Chem.,
79(8) (2005) pp. 1187-1192.

The structure of Ce–Sm–O and Ce–Sm–O/Ru samples with 5, 10, and 15 at % Sm synthesized by the inorganic sol–gel method was characterized by EPR, X-ray diffraction, and electron microscopy. The thermal dehydration of xerogels of the products of cohydrolysis of Ce(IV) and Sm(III) at 600-800°C results in the formation of a structure on the basis of cubic CeO_2 with particle sizes less than 10 nm. The EPR spectra of Ce–Sm–O contain signals of the Ce^{3+} ($g_{\perp} = 1.966$ and $g_{||} = 1.947$) and [SmO_n-V_O] ($g_{||} = 1.996–1.998$ and $g_{\perp}=1.973–1.974$) centers with different coordination environment symmetries. The introduction of Sm(III) decreases the concentration of volume Ce^{3+} centers to a greater degree the higher the content of Sm(III). After deposition of Ru(IV), the concentration of Ce^{3+} increases substantially, by one to two orders of magnitude, and surface Ce^{3+} ions appear ($g_{\perp}=1.966$ and $g_{||}=1.940$). Synthesis through the step of sol formation ensures homogeneous distribution of 10% Sm in the crystal lattice of CeO_2.

DEVELOPMENT OF Fe-BASED CATALYSTS FOR PURIFICATION OF COKE OVEN GASES

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Eurasian Chem.-Techn. J.,
6(3) (2004) pp. 213-219.

Fe-based catalysts of different geometry are developed for the purification of coke oven gases: bulk, supported on alumina and supported on alumina silicate monoliths. Adsorption and decomposition of H_2S on the catalysts developed are studied. Influence of active component content, type of support material and modification by Mn and Mo on the catalyst activity in de-H_2S process is elucidated. Supported monolith catalysts show superior activity over bulk and supported spherical catalysts in H_2S decomposition reaction and demonstrate stable operation in ammonia decomposition process during 2 hours at 900°C giving 100% ammonia conversion.

CORRELATION BETWEEN THE Cu/Al VALUE AND ACTIVITY OF Cu-ZSM-5 CATALYSTS AND THE CHEMICAL NATURE OF THE STARTING COPPER SALT

L.T. Tsykoza, E.V. Matus, Z.R. Ismagilov, V.A. Sazonov, V.V. Kuznetsov

Kinet. Catal., 46(4) (2005) pp. 613-615.

Cu-ZSM-5 catalysts for the selective reduction of NO with propane were obtained by ion exchange between H-ZSM-5 zeolite and an aqueous or aqueous ammonia solution of a copper salt (acetate or nitrate). Their Cu/Al values (%) defined as 2 × 100 (Cu : Al), where Cu : Al is the copper-to-aluminum atomic ratio, were determined as a function of ion exchange pH, which was varied by changing the copper salt and solution concentration. Cu/Al is primarily determined by the chemical nature of the starting copper salt. For a given salt, it is governed by the salt concentration in the solution. At a fixed salt concentration, Cu/Al is always larger for copper acetate than for copper nitrate. It can be raised to >>100% by using an aqueous ammonia solution of a copper salt. Furthermore, it increases with increasing Si/Al in the starting zeolite if the other ion exchange conditions are equal. Irrespective of preparation conditions, the catalytic activity of Cu-ZSM-5 grows in proportion to Cu/Al. It peaks at Cu/Al ~ 100% and then remains constant up to Cu/Al ~ 400%. In order to achieve Cu/Al ~ 100%, it is most appropriate to use a copper acetate solution.

THE SPECIAL FEATURES OF THE ELECTRONIC STATE OF COPPER AND THE STRUCTURE OF COPPER-CONTAINING FRAGMENTS IN CuO-ZrO$_2$ CATALYSTS SYNTHESIZED IN MOLTEN AMMONIUM NITRATE

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Russ. J. Phys. Chem., 79(8) (2005) pp. 1249-1255.

The formation of copper oxide cluster structures starting with copper concentrations of 0.5 at % in CuO-ZrO$_2$ catalysts synthesized using ammonium nitrate melts was proved by electronic paramagnetic resonance and diffuse reflectance electron spectroscopy (DRES) measurements. Formations of disperse CuO phase particles appear in samples with copper concentrations above 20 at %. The formation of the volume CuO phase in the CuO-ZrO$_2$ system was observed in samples containing more than 40 at % copper. The DRE spectra were independent of the temperature of calcining, which led to conclusion that copper ions were stabilized in the form of an anomalous solid solution. DRES measurements showed the occurrence of intervalent $Cu^{2+}\cdots Cu^{+}$ transitions related to the ease of copper ion reduction in oxide cluster structures.

HEAT-CONDUCTING CATALYSTS FOR THE REACTIONS AT MEDIUM TEMPERATURES

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Catal. Today, 105(3-4) (2005) pp. 697-700.

Highly active composite catalysts having good thermal technical and mechanical properties were developed for the reactions at middle temperatures. These composite catalysts consist of the catalytic active component, metal powder and loosening material. These composites have excellent heat conductivity (above 10 W $(m\cdot K)^{-1}$) and strength. The catalyst loading to composite is as high as 1 - 1.2 g/cm^3. At that, catalysts retain their activities, while the effectiveness factors of the catalyst usage are even higher than for the traditional pellets in the tubular fixed bed reactor (e.g. 50% versus 35% for the water gas shift reaction). The scheme of catalyst layer design is proposed, having effective mass- and heat-exchange and low resistance to the reaction gas flow.

MOLECULAR DESIGN AND CHARACTERIZATION OF CATALYSTS FOR NO$_x$ SELECTIVE REDUCTION BY HYDROCARBONS IN THE OXYGEN EXCESS BASED UPON ULTRAMICROPOROUS ZIRCONIA PILLARED CLAYS

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Top. Catal., 32(1-2) (2005) pp. 29-38.

Approaches to design of zirconia pillared clays via control of the properties of pillaring species in

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solutions were elaborated. Structural features of pillars and Pt + Cu active components fixed at these nanoparticles were shown to determine catalytic properties of pillared clays in NO_x selective reduction by hydrocarbons in the oxygen excess.

STRUCTURAL FEATURES OF MAGNESIUM OXIDES DERIVED FROM VARIOUS PRECURSORS

L.M. Plyasova, N.A. Vasilieva, I.Yu. Molina, G.V. Odegova

Russ. J. Inorg. Chem., 50(8) (2005) pp. 1131-1135.

A comparative study of the structural features of magnesium oxides derived from various precursors was carried out. The compositions and structures of the starting compounds were found to substantially influence the character and degree of modification of MgO microcrystals. Magnesium oxide, which was prepared by thermal decomposition starting from $MgCO_3$ as a precursor, has standard unit-cell parameters. Thermal decomposition of $Mg(OH)_2 \cdot MgCO_3 \cdot 2H_2O$ yielded a highly dispersed two-phase system with different degrees of modification of the oxide. Hydration of magnesium oxide in an $MgAc_2$ solution afforded imperfect MgO as an individual compound (a substitution solution), which has high thermal stability and activity in catalytic reactions.

STRUCTURE, TEXTURE, AND ACID-BASE PROPERTIES OF ALKALINE EARTH OXIDES, RARE EARTH OXIDES, AND BINARY OXIDE SYSTEMS

A.S. Ivanova

Kinet. Catal., 46(5) (2005) pp. 620-633.

The effect of synthesis conditions on the formation of the phase composition, dispersity, pore structure, and acid–base properties of alkaline earth oxides, rare earth oxides, and the Mg–M–O (M = Y, La, or Ce) and Y(La)–M–O (M = Ca, Sr, or Ba) binary systems was studied. It was found that the nature of the system was responsible for the character of phase transformations: the Mg–M–O samples were a mixture of either MgO with Y_2O_3 or MgO with a solid solution based on rare earth oxides ($(LaMg)_2O_3$ or $(CeMg)O_2$); the Y(La)–M–O samples (M = Ca, Sr, or Ba) contained the $M_2Y_2O_5$, MY_2O_4, and MLa_2O_4 compounds, which differ in chemical stability, in addition to La_2O_3 and Y_2O_3 phases. According to XPS data, the M/Mg atomic ratios were much higher than the bulk values; this is indicative of an enrichment of the surface of samples in the second component. An increase in the concentration of M_2O_3 from 5 to 25 mol % resulted in a decrease in the S_{sp} of the MgM–O samples from 220 ±10 to 110 ±10 m^2/g; the S_{sp} of samples calcined at 750°C was lower by a factor of ~1.5–2. The S_{sp} of the Y(La)–M–O samples was higher than the S_{sp} of individual La_2O_3 and Y_2O_3. The samples were characterized by a biporous texture. The concentrations and strength distributions of surface OH groups, Lewis acid sites, and Lewis base sites depend on the nature and concentration of rare earth elements in the binary samples. The activity of the Mg–M–O samples in the oxidative dehydrogenation reaction of propionitrile correlated with the acid–base surface sites. Among the Ru/Y(La)–M–O catalysts for ammonia synthesis, Ru/Y–Ba–O was the most active; this catalyst provided a higher yield of NH_3 at 250-300°C, as compared with catalysts prepared with the use of other supports (Sibunit, KVU-1, and C/MgO).

NEW BINARY SYSTEMS Mg–*M*–O (*M*=Y, La, Ce): SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERIZATION

A.S. Ivanova, B.L. Moroz, E.M. Moroz, Yu.V. Larichev, E.A. Paukshtis, V.I. Bukhtiyarov

J. Solid State Chem.,
178(11) (2005) pp. 3265-3274.

New binary oxide Mg–*M*–O (*M*=Y, La, Ce) systems are obtained by co-precipitation and characterized by adsorption methods, X-ray diffraction method (XRD), X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared (FTIR) spectroscopy of adsorbed probe molecules (CO and $CDCl_3$). It is shown that Mg–Y–O systems after calcination at 450–750°C represent the physical mixtures of MgO and Y_2O_3, while the components of Mg–La(Ce)–O systems interact to form La_2MgO_x and $(Ce,Mg)O_2$ solid solutions, respectively. From XPS data, the surface of the binary systems is enriched with lanthanide ions. Addition of ≈5 mol% M_2O_3 to MgO results in an increase in concentrations of strong and weak Lewis acidic sites, the content of the latter being much higher and changing in the series: MgO<Mg–Ce–O<Mg–La–O<Mg–Y–O. At the same time basic sites become stronger in the binary systems but their total content decreases in comparison to that in individual MgO. Mg–*M*–O samples containing ≈5 mol% M_2O_3 are highly-dispersed and characterized by bimodal porous texture.

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CARBONIZATION OF ALUMINA-BASED CATALYSTS IN PROPIONITRILE AMMONOLYSIS

A.S. Ivanova, V.M. Bondareva, A.S. Bobrin, G.S. Litvak, E.A. Paukshtis, A.L. Chuvilin, A.S. Noskov

React. Kinet. Catal. Lett., 84(1) (2005) pp. 143-150.

Carbonization of the surface of alumina-based catalysts has been studied with respect to the composition of the catalysts and conditions of the propionitrile ammonolysis. It was shown that the surface concentration of carbon increases with the increase in temperature and with time of the reaction and depends on the catalysts nature in the order: Al-Zr(5)-O < Al-Zr(40)-O < Al-O < Al-Mg-O. The surface concentration of the Brönsted acidic sites follows the same sequence.

ACID-BASE PROPERTIES OF SINGLE-PHASE ALUMINUM OXIDES

E.V. Kulko, A.S. Ivanova, A.A. Budneva, E.A. Paukshtis

Kinet. Catal., 46(1) (2005) pp. 132-137.

It was found that the surface of single-phase aluminum oxides contains terminal, bridging, and hydrogen-bonded hydroxyl groups, which differ in both concentration and position of related absorption bands. A transition from η-Al_2O_3 to θ-Al_2O_3 does not change the number of absorption bands, but the intensities of these bands decrease. The total concentration of Lewis acid sites in single-phase oxides increases from 2.5 to 5.34 μmol/m^2 for ν-Al_2O_3 and θ-Al_2O_3, respectively. As distinct from other species, η-Al_2O_3 contains strong Lewis acid sites (ν (CO) = 2238 cm^{-1}). The total concentration of basic sites in aluminum oxides prepared by boehmite dehydration at 600, 800, and 1000°C decreases from 4.86 to 3.72 μmol/m^2.

SYNTHESIS AND CHARACTERIZATION OF FLUORITE-LIKE Ce–Zr–Y–La–O SYSTEMS

G.A. Turko, A.S. Ivanova, L.M. Plyasova, G.S. Litvak, V.A. Rogov

Kinet. Catal., 46(6) (2005) pp. 884-890.

Ce–Zr–O and Ce–Zr–Y–La–O materials obtained under various conditions and at varying component ratios are characterized. At Ce/Zr ≈1, a tetragonal phase that can hardly be distinguished from a cubic phase by X-ray diffraction forms in the ternary system. Raising the precipitation temperature favors the formation of two-phase systems. Promoting the Ce/Zr = 0.26–0.62 materials with both yttrium and lanthanum favors the formation of a single-phase specimen, namely, a $(Ce,Zr,Y,La)O_2$ fluorite-like solid solution at 600°C. This structure persists up to 1150°C. The specific surface area of the $(Ce,Zr,Y,La)O_2$ materials is primarily determined by their calcination temperature: S_{sp} = 50–80 m^2/g at 600°C and 0.6–0.8 m^2/g at 1150°C. The specimens calcined at 600°C are mesoporous, with uniformly sized pores of mean diameter 32 ± 2 Å, and have no micropores. According to TPR data, the specimens calcined at 600°C are reduced with hydrogen in two steps that can apparently be interpreted as surface and bulk reduction. The Ce/Zr = 0.26 and 0.40 specimens calcined at 1150°C are reduced in a single step, giving rise to TPR peaks at 707 and 686°C, respectively, and their degree of reduction increases with decreasing Ce/Zr.

EFFECT OF METAL LOADING AND CARBON SUPPORT MICROSTRUCTURE ON THE DISPERSION OF Pt/C CATALYSTS PREPARED VIA ADSORPTION OF CHLOROPLATINIC ACID

A.N. Kholodovich, P.A. Simonov

React. Kinet. Catal. Lett.,
86(2) (2005) pp. 381-388.

Adsorption of H_2PtCl_6 onto a carbon support followed by reduction of the adsorbed platinum species with H_2 at 250°C leads to Pt/C catalysts which show universal volcano-like dependence of platinum dispersion on the metal loading in the range from 0.01 to 0.55 μmol (Pt)/m^2 (S_{BET}) when highly disordered carbons, namely, active carbons and carbon blacks, are used as supports. The maximal dispersion Pt = 0.8 is attained at 0.18 μmol (Pt)/m^2 (S_{BET}). With other factors being equal, the dispersion of platinum supported on carbons with a more regular crystal structure, especially Sibunit-type supports, proves to be the highest and independent of the metal loading. The differences between the two groups of carbon supports are explained by the differences in the state of the adsorbed platinum precursors.

MECHANISM OF THE GROWTH OF MONODISPERSED SPHERICAL SILICA PARTICLES TO THE SUBMICRON SIZE

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React. Kinet. Catal. Lett.,
84(2) (2005) pp. 389-394.

Monodispersed spherical submicron silica particles were obtained by the precipitation of soluble silica on the surface of preliminary obtained smaller particles. Silica was added into the system at low concentrations to prevent both its polymerization in the solution and the formation of new particles. The kinetics of the particle growth is controlled by the diffusion of soluble silica through the double diffusion layer.

OPTIMIZATION OF ANODIC OXIDATION AND Cu–Cr OXIDE CATALYST PREPARATION ON STRUCTURED ALUMINUM PLATES PROCESSED BY ELECTRO DISCHARGE MACHINING

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Catal. Today, 105(3-4) (2005) pp. 516-528.

This paper describes the optimization of three processes applied in fabrication of a microstructured reactor for complete oxidation of volatile organic compounds. The first process involves the optimization of the electro discharge machining (EDM) method to produce a set of microchannels with a high length to diameter ratio of 100, with a standard deviation from the average diameter below 0.2%, and with a surface roughness not higher than 2.0 µm. To satisfy these criteria, fabrication of microchannels must be carried out with two machining passes in the Al51st alloy. Then, the effect of several parameters on the anodization current efficiency with respect to oxide formation was studied. The best process conditions to get a 30 µm porous alumina layer in a 0.4 M oxalic acid electrolyte, were found to be a temperature of 1 °C, an anodic current density of 5 mA/cm^2, and 23 h oxidation time. At last, the resulting coatings were impregnated with an aqueous solution of copper dichromate followed by drying and calcination at 450 °C to produce active catalysts. The effect of a copper dichromate concentration, number of impregnation cycles (1 or 2), and different after-treatments on catalytic activity and stability in complete oxidation of n-butane were studied. The catalytic activity of the obtained coatings is superior to that of alumina supported pelletized catalysts even at much lower loadings of active metals.

SYNTHESIS OF NEW CHIRAL PHOSPHOROUS- AND NITROGEN-CONTAINING LIGANDS FROM RESIN ACIDS

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Chirality,
16(Suppl S) (2004) pp. S40-S50.

Starting from the phytogenic diterpenes, chiral phosphine, urea, and thiourea derivatives were synthesized. Using these new chiral ligands, Rh(I) and Ru(II) complexes were prepared and used as catalysts for the catalytic asymmetric hydrogenation of unsaturated carboxylic acids and asymmetric hydrogen-transfer reduction of carbonyl compounds. Although the enantiopurity of the products obtained was not high, it was demonstrated that chiral ligands derived from diterpenes could be used for asymmetric reduction.

Carbon and Carbon Related Processes

PHOTOEMISSION STUDY OF ONIONLIKE CARBONS PRODUCED BY ANNEALING NANODIAMONDS

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Physical Review B, 71(7) (2005) 075420 (10 pages).

Photoelectron spectroscopy has been used to study the products resulting from high temperature phase transformation of nanodiamonds (ND). Depending on the temperature of annealing various particles with a diamond core covered by nanometer sized fullerene-like shells and onionlike carbon (OLC) were formed. Analysis of the C1*s* photoemission lines of the intermediates of ND transformation, prepared at temperatures of 1420 and 1600 K and then exposed to atmosphere, reveals the presence of oxygen-containing groups and both sp^2 and sp^3 carbon. The sp^2 component for these samples has binding energies of 284.70±0.05 eV (for the sample prepared at 1420 K) and 284.50±0.05 eV (for the sample prepared at 1600 K). A difference of 1.3±0.1 eV in the binding energy of the sp^3 and sp^2 components was observed. The sp^2 component for OLC prepared at 1800, 1900, and 2140 K has a binding energy of 284.45±0.05 eV. The shift towards higher binding energies of the sp^2 component of the samples prepared at lower temperatures is explained by significant curvature of graphite layers formed in the initial stages of graphitization. The observed increase in density of states at the Fermi level for the samples prepared at 1600, 1800, and 1900 K is associated with an accumulation of different types of defects in the curved graphite layers during graphitization of diamond. The Lorentzian widths of C1*s* photoemission lines from OLC are large compared with those of HOPG. The possible reasons for this broadening are discussed.

NANODIAMOND GRAPHITIZATION AND PROPERTIES OF ONION-LIKE CARBON

V.L. Kuznetsov, Yu.V. Butenko

In *"Synthesis and Applications of Ultrananocrystalline Diamond"*,
Eds. D.M. Gruen et al., Springer, The Netherlands,
Vol. 192, 2005, pp. 199-216.

The comparative study data on the wide set of diamond and diamond containing samples graphitization with a special effort on low temperature graphitization (1370-1870 K) are presented. The graphitization products were characterized using HRTEM, XPS, XRD, Raman spectroscopy and other techniques. It was found that onion-like carbon (OLC) is formed during the annealing of nanodiamond (ND) while the annealing of micron size diamond produces closed curved graphite like structures (nanotubes, nanofolds etc.). Theoretical consideration based on molecular modeling using combination of molecular mechanics, molecular dynamics and HF methods allows to propose that their formation has features of self-assembling processes. Comparison of graphitization kinetics data with the 'classical' data of Evans and Davies for the high temperature region (>2000 K) leads to conclusion that there are at least two temperature regions in which the diamond graphitization occurs by different mechanisms. The Debye temperature for diamond, 1910 K, appears to serve as the boundary between these regions. At and above this temperature all oscillating freedom degrees are excited and the graphitization involves the displacements of individual atoms. In the low temperature regime, the graphitization starts on surface defects and proceeds via a 'concert' mechanism where the energy required for breaking the C-C bonds is simultaneously compensated by the formation of new bonds. The knowledge of the kinetics of ND graphitization provides with the possibility to produce the diamond/nanographite composites with variable ratio of decreasing in size diamond core and defective curved graphitic shells (*sp2/sp3* nanocomposites). Small size of curved graphitic shells, the presence of interface between nanosize diamond cores and graphitic shells and probably high concentration of open graphitic edges can cause the unusual electronic properties of these composites and OLC.

COMMON FEATURES OF THE FORMATION MECHANISM OF CARBON NANOSTRUCTURES AND SILICON CARBIDE WHISKERS ON METAL CATALYSTS

V.L. Kuznetsov, A.N. Usoltseva, I.N. Mazov

Russ. Chem. J.,
48(5) (2004) pp. 37-45.

Common features of the formation mechanism of carbon nanostructures and silicon carbide whiskers on metal catalysts are considered. The data obtained indicate that in spite of different nature of carbon nanotubes, fibers and silicon carbide whiskers, the scenarios of their growth over metal catalysts have common regularities.

COMMON FEATURES OF THE FORMATION MECHANISM OF CARBON FILAMENTS, NANOTUBES, AND SILICON CARBIDE WHISKERS ON METAL CATALYSTS

V.L. Kuznetsov, A.N. Usoltseva, I.N. Mazov

Fullerenes, Nanotubes Carbon Nanostruct.,
13(s1) (2005) pp. 121-129.

The formation mechanisms of carbon deposits and silicon carbide whiskers on metal surface catalysts have some common steps. The most important are: (1) the formation of metal particle alloys oversaturated with carbon or silicon and carbon atoms, and (2) the nucleation of corresponding deposits on the metal catalyst surface. A thermodynamic analysis of the carbon and/or silicon carbide nucleation on the metal surface was performed. The master equations for the dependence of critical radius of carbon or SiC nucleus on reaction parameters, such as reaction temperature, supersaturation degree of catalyst particles with C (or Si and C), work of adhesion of metal to carbon (or metal to SiC) were obtained. These equations combined with the phase diagram approach can be used for the description of different scenarios of carbon and/or SiC deposits formation and for the development of the main principles of catalyst and promoters design.

ELECTRONIC STATE OF NANODIAMOND/GRAPHITE INTERFACES

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Appl. Phys. A,
81(2) (2005) pp. 393-398.

The electronic state of nanodiamond/graphite interfaces in samples prepared by annealing of nanodiamonds (ND) at 1150–1600 K has been probed

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using X-ray fluorescence spectroscopy and field-emission measurements. Comparison between $[_{\mathrm{C}}]K_{\alpha}$ spectra of ND before and after annealing revealed an enhancement of density of high-energy occupied states in the products. A quantum-chemical calculation using a carbon model showed that the observed states could originate from the electrons of dangling bonds produced by peeling of a graphitic shell from the (111) surface of a diamond particle. The developed graphitic layers screen the weakly bonding electrons, which results in a lowering of the efficiency of field-electron emission from the samples with an increase of annealing temperature.

CATALYTIC FILAMENTOUS CARBONS-SUPPORTED Ni FOR LOW-TEMPERATURE METHANE DECOMPOSITION

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Catal. Today, 102-103 (2005) pp. 115-120.

Ni/CFC catalysts were shown to have sufficient efficiency in secondary carbon formation in low-temperature methane decomposition (525°C). The highest yield of secondary carbon was found to reach 268.5 g/gNi on Ni/CFC (Fe-Ni) catalyst. The catalytic properties of Ni/CFCs may be explained by formation of active Ni particles (ca. 50 nm in size), which are optimal for growth of filament with "herring-bone" structure. The large Ni particles are preferably localized in the pores formed by interlaced filaments and the interaction of metal particles with graphene basal planes occurs mainly through weak dispersive forces. The accumulation of carbon on Ni/CFC catalysts is also influenced by textural properties of the used supports. The carbon supports with high value of the meso- and macropore volume are likely to be more suitable for development of Ni/CFC catalysts for low-temperature methane decomposition. The modification of the textural properties of catalytic filamentous carbon (CFC) by their activation with H_2 or CO_2 opens up interesting possibilities of its application as support in heterogeneous catalysis.

NEW GENERATION OF POROUS CARBON MATERIALS FROM PETROLEUM COKE AND COMPOUNDS MODELING ITS STRUCTURE

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Petroleum Chem., 44(6) (2004) pp. 403-406.

The results of a study on new highly porous carbon materials obtained from petroleum coke and aromatic compounds are presented. These materials are characterized by a high specific surface area and a high micropore volume. It was shown that they adsorb up to 180 mg of methane per gram of a sample at room temperature and a pressure of 4 MPa.

DEVELOPMENT OF ACTIVE CATALYSTS FOR LOW Pt LOADING CATHODES OF PEMFC BY SURFACE TAILORING OF NANOCARBON MATERIALS

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Catal. Today, 102-103 (2005) pp. 58-66.

The use of novel nanocarbon supports—carbon nanofibers (CNF) and amorphous supermicroporous carbons (ASC) for synthesis of platinum cathode catalysts for proton exchange membrane fuel cells (PEMFC) was investigated. Different types of CNF - with “parallel” and “deck of cards” arrangement of graphitic planes and samples of ASC originating from different organic precursors were synthesized and characterized by XRD, electron microscopy and adsorption methods. Platinum catalysts for PEMFC cathodes on different structural types of CNF and one sample of ASC were synthesized and characterized by XRD, electron microscopy, CO adsorption and by studying characteristics of conventional membrane electrode assembly (MEA) cell with a low Pt loading level of 0.02–0.09 mg/cm^2. The MEA testing showed that the Pt cathode catalysts on CNF exhibit inferior performance in comparison with a catalyst on conventional carbon black support Pt/Vulcan XC-72R. The cathode catalyst prepared on ASC support exhibits considerably better output in MEA, compared with Pt/Vulcan XC-72R even at a lower Pt loading.

DEVELOPMENT OF METHODS OF GROWING CARBON NANOFIBERS ON SILICA GLASS FIBER SUPPORTS

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Catal. Today, 102-103 (2005) pp. 85-93.

Samples of carbon nanofibers (CNF) with different carbon contents (6.5–55 wt.%) are prepared by decomposition of CH_4 on Ni catalysts supported on silica glass fibers (SGF). The incipient wetness impregnation of support, introduction of the active component into alumina washcoat and ion-exchange methods were used to prepare Ni catalysts on SGF. On the optimal catalyst prepared on washcoated SGF, carbon forms as CNF of diameter 20–50 nm, and the carbon capacity is rather high - 55 g_C/g_{Ni}. Diameter of the CNF corresponds to the size of catalyst particles of Ni metal, which have the cuboctahedral form typical for the formation of CNF with conical embedding of graphite layers with respect to the filament axis. The SGF with supported CNF is a mesoporous material with polydisperse pore distribution similar by structural and textural parameters to the granulated bulk CNF obtained in methane decomposition over high-loaded nickel-alumina catalysts.

The XRD, ESR and DTA methods were used for phase and structural analysis and demonstrated that CNF has a uniform graphite-like structure and does not include the amorphous phase.

CATALYSTS Ru-CeO$_2$/SIBUNIT FOR CATALYTIC WET AIR OXIDATION OF ANILINE AND PHENOL

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Top. Catal., 33(1-4) (2005) pp. 69-76.

Catalytic properties of carbon materials Sibunit (commercial samples) and ceria-promoted precious metals (Ru, Pt, Pd) supported on carbon were studied in the processes of catalytic wet air oxidation (CWAO) of aniline and phenol at elevated pressures and temperatures ($T = 433–473$ K, $P_{O2} = 0.3–1.0$ MPa). It was found that the activity increases when the catalyst is pretreated with hydrogen peroxide. An efficiency of Ru–CeO$_2$/Sibunit catalyst with a low ruthenium content (~0.6 Ru) for deep cleaning of polluted waters is demonstrated.

THE INFLUENCE OF CARBON SUPPORT POROSITY ON THE ACTIVITY OF PtRu/SIBUNIT ANODE CATALYSTS FOR METHANOL OXIDATION

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J. Power Sources, 145(2) (2005) pp. 178-187.

In this paper are analyzed the promises of homemade carbon materials of Sibunit family prepared through pyrolysis of natural gases on carbon black surfaces as supports for the anode catalysts of direct methanol fuel cells. Specific surface area (S_{BET}) of the support is varied in the wide range from 6 to 415 $m^2 g^{-1}$ and the implications on the electrocatalytic activity are scrutinized. Sibunit supported PtRu (1:1) catalysts are prepared via chemical route and the preparation conditions are adjusted in such a way that the particle size is constant within ±1 nm in order to separate the influence of support on the (i) catalyst preparation and (ii) fuel cell performance. Comparison of the metal surface area measured by gas phase CO chemisorption and electrochemical CO stripping indicates close to 100% utilisation of nanoparticle surfaces for catalysts supported on low (22–72 $m^2 g^{-1}$) surface area Sibunit carbons. Mass activity and specific activity of PtRu anode catalysts change dramatically with S_{BET} of the support, increasing with the decrease of the latter. 10%PtRu catalyst supported on Sibunit with specific surface area of 72 $m^2 g^{-1}$ shows mass specific activity exceeding that of commercial 20%PtRu/Vulcan XC-72 by nearly a factor of 3.

ON THE PROCESSES OCCURRING IN THE METAL PARTICLES UPON CATALYTIC DECOMPOSITION OF HYDROCARBONS BY "CARBIDE CYCLE" MECHANISM

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Chem. Sustain. Devel., 13(1) (2005) pp. 37-40.

The role of fine metal particles of iron sub group in catalytic hydrocarbon decomposition by "carbide cycle" mechanism is considered. The crucial correlation of their crystallographic characteristics with the structure of resulting carbon composites is revealed. Major factors to control the processes of carbon filaments and fibers formation are determined.

NANOSIZED CARBON FIBERS LOCATED ONTO CERAMICS

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In "*Complex Mediums VI: Light and Complexity*",
Eds. Martin W. McCall, Graeme Dewar,
Mikhail A. Noginov, 2005, Vol. 5924, 592412 (5 pp.)

Nanosized carbon fibers are of great importance due to its numerous technological applications. One of its disadvantages is low mechanical strength. This problem could be solved by incorporation of carbon fibers into cavities or channels of ceramic monoliths with foam or honeycomb structure. In the present work the experience of preparation of uniform carbon layer consisting from nanosized fibers onto ceramic monoliths with different geometry will be presented. Carbon fibers were produced by catalytic pyrolysis of methane over nanosized metal particles supported over ceramic monolith. Variation of preparation conditions permits to obtain carbon fibers with different density and thickness.

NANOSCALED PALLADIUM CATALYSTS ON ACTIVATED CARBON SUPPORT "SIBUNIT" FOR FINE ORGANIC SYNTHESIS

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In "*Complex Mediums VI: Light and Complexity"*,
Eds. M.W. McCall, G. Dewar, M.A. Noginov,
Vol. 5924, 592413 (7 pp.)

The application of nanosized palladium catalysts has gained growing importance over the last few years. Palladium based catalytic methods for fine organic synthesis permits the replacement of traditional labor-consuming techniques in multi-step organic syntheses and provides an improvement from the standpoint of cost and environmental impact. The use of activated carbon "Sibunit" as a substrate for catalysts has been fostered by the substrate's high surface area, chemical inertness both in acidic and basic media, and at the same time by the absence of very strong acidic centers on its surface which could promote undesirable side reactions during the catalytic run. A conversion of alpha-pinene derivatives to commercial biologically active compounds and fragrances as well as sun screens with ultra violet filtering properties, involves a catalytic hydrogenation as a key intermediate step. The aim of the present work is to clarify the factors favoring the dispersion of Pd metal on carbon. The effect of reduction temperature and pretreatment of the carbon surface on metal size during preparation of Pd on "Sibunit" catalysts for selective verbenol conversion was studied. The electron microscopy method (TEM) was used to show the influence on Pd metal dispersion of carbon surface oxidation by the oxidant H_2O_2, HNO_3. The catalytic activity of Pd/C catalyst samples in verbenol hydrogenation reaction was determined. Kinetic peculiarities of verbenol hydrogenation over the most active catalyst sample were obtained.

Catalysis by Metal Complexes and Heteropolycomplexes

SYNTHESIS, CHARACTERIZATION AND CATALYTIC APPLICATION FOR WET OXIDATION OF PHENOL OF IRON-CONTAINING CLAYS

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Appl. Catal., B, 59(3-4) (2005) pp. 243-248.

High-surface-area pillared clays (PILC) were prepared from naturally occurring montmorillonites by exchanging interlayer ions to polyoxocations containing (i) aluminum (Al_{13}-PILC), (ii) iron adsorpted onto Al_{13}-PILC, and (iii) iron and aluminum located within the same complex ($Fe_{0.8}Al_{12.2}$-PILC). The obtained $Fe_{0.8}Al_{12.2}$-PILCs were characterized by DR–UV–vis and IR spectroscopy, XRD, ESR, scanning electron microscopy and low temperature N_2 adsorption measurements. Important factors affecting catalyst activity and phenol removal efficiencies have been studied, i.e. the effect of pH, temperature, catalyst concentration and stability of the catalyst.

SURFACE ACID SITES OF $H_3PW_{12}O_{40}$ AS STUDIED BY THE ADSORPTION OF STABLE NITROXYL RADICALS

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Kinet. Catal., 46(1) (2005) pp. 123-127.

The surface acidity of $H_3PW_{12}O_{40}$ and $Na_xH_{3-x}PW_{12}O_{40}$ (x = 1-3) was studied using the

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adsorption of 2,2',6,6'-tetramethyl-4-oxopiperidine-1-oxyl (TEMPON) and 2,2',6,6'-tetramethyl-4-hydroxypiperidine-1-oxyl (TEMPOL) radicals. It was found that the amount of surface proton sites determined from the adsorption of TEMPON decreased with the degree of substitution of Na^+ cations for protons. A correlation between amount of strong surface proton sites and catalytic activity of $Na_xH_{3-x}PW_{12}O_{40}$ (x = 0-3) in the dealkylation reaction of 2,6-di-*tert*-butyl-4-methylphenol was found.

THE ROLE OF PROTONS IN CYCLOHEXENE OXIDATION WITH H_2O_2 CATALYSED BY Ti(IV)-MONOSUBSTITUTED KEGGIN POLYOXOMETALATE

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J. Mol. Catal. A: Chem., 232(1-2) (2005) pp. 173-178.

The effect of the number of protons in the Ti(IV)-monosubstituted Keggin polyoxometalate $Na_{5-n}H_nPTiW_{11}O_{40}$ (n = 1-5; Ti-POM) on its catalytic behaviour in cyclohexene (CyH) oxidation with aqueous H_2O_2 in MeCN is reported. It has been found that Ti-POMs with n = 2-5 catalyse efficiently CyH oxidation to yield *trans*-cyclohexane-1,2-diol as the main reaction product, while Ti-POM containing only one proton shows lower activity in CyH oxidation and produces allylic oxidation products, 2-cyclohexene-1-ol and 2-cyclohexene-1-one, along with comparable amounts of the corresponding epoxide and diol. The obtained results strongly support homolytic oxidation mechanism for CyH oxidation in the presence of the monoprotonated Ti-POM and heterolytic oxygen-transfer mechanism in the presence of Ti-POMs having two and more protons. The ^{31}P and ^{183}W NMR studies revealed that Ti-POMs are stable towards at least 100-fold excess of H_2O_2 and the high catalytic activity of Ti-POMs with n = 2-5 is not due to the formation of lower nuclearity species. The addition of 1 equiv. of H^+ to the monoprotonated peroxo complex $[Bu_4N]_4[HPTi(O_2)W_{11}O_{39}]$ (**I**, ^{31}P NMR in MeCN: –12.40 ppm) results in the formation of the diprotonated titanium peroxo species $[H_2PTi(O_2)W_{11}O_{39}]^{3-}$ (**II**, ^{31}P NMR in MeCN: –12.14 ppm). This peroxo species can also be obtained by adding an excess of H_2O_2 to $Na_{5-n}H_nPTiW_{11}O_{40}$ (n = 2-5) in MeCN. The presence of the second proton in the peroxo species is a crucial factor determining the capability of **II** to oxidise alkenes *via* heterolytic oxygen transfer mechanism. Both ^{31}P NMR and GC-MS studies corroborated that **II** reacts with CyH producing *trans*-cyclohexane-1,2-diol as the main reaction product, whereas **I** is not reactive towards CyH under stoichiometric conditions.

OXIDATION OF 2-METHYL-1-NAPHTHOL WITH H_2O_2 OVER Ti-MMM-2 CATALYST

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J. Catal., 236(1) (2005) pp. 62-68.

The catalytic oxidation of 2-methyl-1-naphthol (MNL) to 2-methyl-1,4-naphthoquinone (MNQ; menadione; vitamin K_3) using aqueous H_2O_2 as an oxidant and hydrothermally stable mesoporous mesophase titanium silicates Ti-MMM-2 as catalysts has been studied. The effects of mesopore diameter, temperature, solvent nature, reagent concentrations, and catalyst amount on the yield of MNQ were evaluated. Crucial factors affecting the MNQ yield include MNL concentration, H_2O_2/MNL molar ratio, reaction temperature, and the mode of MNL addition to the reaction mixture. Selectivity dramatically decreases with increasing MNL concentration and decreasing temperature. Stepwise addition of the substrate to the reaction mixture improves selectivity. Oxidation in the presence of $^{18}O_2$ provided 96.2±0.1% of unlabeled MNQ, indicating H_2O_2 as an oxygen source. The Ti-MMM-2 catalyst allows one to obtain MNQ with selectivity as high as 78% at complete substrate conversion. The catalyst can be used repeatedly without loss of either activity or selectivity. The proposed method is convenient and environmentally benign.

H_2O_2-BASED ALLYLIC OXIDATION OF *α*-PINENE OVER DIFFERENT SINGLE SITE CATALYSTS

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J. Catal., 235(1) (2005) pp. 175-183.

Catalytic properties of different solids, containing Ti(IV), Zr(IV), and Fe(III) isolated in inorganic matrixes, have been assessed in allylic oxidation of α-pinene with aqueous H_2O_2. Among the catalysts studied were mesostructured metal-silicates Ti-MMM-2 and Fe-MMM-2, TiO_2-SiO_2 mixed oxides, Ti- and Zr-grafted on mesoporous cellular foams (Ti- and Zr-MCF), and a new composite material $H_5PW_{11}TiO_{40}$/silica first prepared by a sol-gel method. The catalysts were characterized by elemental analysis, N_2 adsorption, and DRS-UV. The Ti- and Zr-containing materials showed catalytic properties superior to those of Fe-MMM-2. The reaction selectivity strongly depends on the solvent nature, substrate/oxidant molar ratio, reaction temperature, and α-pinene conversion. In MeCN at 30 °C, the total selectivity toward verbenol/verbenone reaches the maximal value of 80-82% at 8-15% conversion. The $H_5PW_{11}TiO_{40}$/silica catalyst can be used repeatedly without loss of activity and selectivity. No leaching of the active species occurs, and the oxidation is a true heterogeneous process operating via a radical non-chain mechanism.

FTIR SPECTROSCOPIC STUDY OF TITANIUM-CONTAINING MESOPOROUS SILICATE MATERIALS

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Langmuir, 21(22) (2005) pp. 10545-10554.

The surface acidity of different mesoporous titanium-silicates, such as well-organized hexagonally packed Ti-MMM, Ti-MMM-2, Ti-SBA-15, and amorphous TiO_2-SiO_2 mixed oxides (aerogels and xerogels), was studied by means of FTIR spectroscopy of CO adsorbed at 80 K and CD_3CN adsorbed at 293 K. The surface hydroxyl groups of mesoporous titanium-silicates with 2-7 wt % Ti revealed a Bronsted acidity slightly higher to that of pure silicate. TiO_2-SiO_2 xerogels revealed the highest Bronsted acidity among the titanium-silicates studied. CO adsorption revealed two additional sites on the surface in comparison to pure silicate, characterized by υ(CO) from 2185 (high pressure) to 2178 (low pressure) cm^{-1} and from 2174 (high pressure) to 2170 (low pressure) cm^{-1}. These bands are due to CO adsorbed on isolated titanium cations in the silica surrounding or having one Ti^{4+} cation in their second coordination sphere and due to CO interactions with Ti-OH groups, respectively. CD_3CN adsorption similarly revealed the existence of two additional sites, which were not detected for pure silicate: at 2289 cm^{-1} due to CD_3CN interaction with titanol groups and from 2306 (low pressure) to 2300 (high pressure)cm^{-1} due to acetonitrile interaction with isolated framework titanium cations with probably one Ti^{4+} cation in their second coordination shell. The spectroscopic results are compared with computational data obtained on cluster models of titanium-silicate with different titanium content. According to the IR data, the Ti accessibility on the surfaces for mesoporous titanium-silicates with similar Ti loading (2 wt %) was found to fall in the order TiO_2-SiO_2 aerogel ≈ TiO_2-SiO_2 xerogel > Ti-MMM ≈ Ti-MMM-2 > Ti-SBA-15. This order (except TiO_2-SiO_2 xerogel) correlates with the catalytic activity found previously for titanium-silicates in 2,3,6-trimethylphenol oxidation with H_2O_2.

SYNTHESIS, CHARACTERIZATION, AND REACTIVITY OF Ti(IV)-MONOSUBSTITUTED KEGGIN POLYOXOMETALATES

O.A. Kholdeeva, T.A. Trubitsina, G.M. Maksimov, A.V. Golovin, R.I. Maksimovskaya

Inorg. Chem., 44(5) (2005) pp. 1635-1642.

The Ti(IV)-monosubstituted Keggin type polyoxometalates (Ti-POMs), μ-oxo-dimer $[Bu_4N]_8[(PTiW_{11}O_{39})_2O]$ (**1**) and three monomers $[Bu_4N]_4[PTi(L)W_{11}O_{39}]$, where L = OH (**2**), OMe (**3**), and OAr (**4**, ArOH = 2,3,6-trimethylphenol (TMP)), have been prepared and characterized by elemental analysis, IR, UV-vis, and multinuclear (^{31}P, ^{1}H, ^{183}W) NMR. The interaction of **1** and **3-5** with H_2O in MeCN produces **2**. The hydrolysis constants, estimated from ^{31}P and ^{1}H NMR data, are 0.006 and 0.04 for **1** and **3**, respectively. Studies by ^{31}P NMR, IR, potentiometric titration and cyclic voltammetry revealed that **1-3** and **5** afford the same protonated titanium peroxo complex $[Bu_4N]_4[HPTi(O_2)W_{11}O_{39}]$ (**I**) upon interaction with aqueous H_2O_2 in MeCN. The rates of the formation of **I** correlate with the rates of hydrolysis of the Ti-POMs and fall in the order of **5** > **1** > **3**. A two-step mechanism of the reaction of Ti-POMs with H_2O_2, which involves hydrolysis of the Ti–L bonds to yield **2** followed by fast interaction of **2** with hydrogen peroxide producing **I**, is suggested. The equilibrium constant for the reaction of **2** with H_2O_2 to yield **I** and H_2O, estimated using ^{31}P NMR, is 10. The interaction of the Ti-POMs with TMP follows the trends similar to their interaction with H_2O_2 and requires preliminary hydrolysis of the Ti–L bonds**.** All the Ti-POMs catalyze oxidation of TMP with H_2O_2 in MeCN to give 2,3,5-trimethyl-*p*-benzoquinone (TMBQ) and 2,2',3,3',5,5'-hexamethyl-4,4'-biphenol (BP). The product distribution is similar for all the Ti-POMs. The catalytic activities of the Ti-POMs correlate with the rates of the formation of **I** and fall in the order of **2** > **5 > 1** > **3**. The findings lay a basis for a better understanding of the nature of the reactivity of titanium in Ti-catalyzed oxidations.

AEROBIC FORMALDEHYDE OXIDATION UNDER MILD CONDITIONS MEDIATED BY Ce-CONTAINING POLYOXOMETALATES

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In "*Catalysis of Organic Reactions*",
J.R. Sowa, Ed.; Taylor & Francis Group, Boca Raton,
2005, pp. 429-433.

Various Ce-POMs have been synthesized and evaluated as catalysts for the aerobic oxidation of formaldehyde at ambient conditions along with simple Ce-compounds. The most active catalyst was the monosodium acid salt of the Ce(IV)-monosubstituted silicotungstate, $NaH_3SiW_{11}CeO_{39}·7H_2O$ (**1**). Optimization of the reaction conditions led to a system that afforded 30 turnovers of **1** after 5 h. Based on both IR and UV-vis, the Ce-POM retains its structure under the turnover conditions. The formic acid product inhibits the reaction. The kinetic data obtained are consistent with a chain radical mechanism of oxidation. POM **1** can be heterogenized on NH_2-functionalized supports such as xerogels, fibers, etc., and in this form used repeatedly without significant loss of catalytic activity.

AEROBIC OXIDATION OF FORMALDEHYDE MEDIATED BY A Ce-CONTAINING POLYOXOMETALATE UNDER MILD CONDITIONS

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Inorg. Chem., 44(3) (2005) pp. 666-672.

An evaluation of over 50 polyoxometalates (POMs) identified the complex $NaH_3[SiW_{11}Ce^{IV}O_{39}]$ ($NaH_3$1) as a selective and effective catalyst for the aerobic oxidation of formaldehyde to formic acid under very mild (including ambient) conditions. ^{183}W NMR, UV-vis, cyclic voltammetry, and potentiometric titration establish that the catalyst is a monomer (C_s symmetry), **1**, in solution, while X-ray crystallography (a=12.9455(15) Å, b=13.2257(16) Å, c=14.5288(17) Å, α= 81.408(2)°, β=85.618(2)°, γ=80.726(2)°, P1, Z=1, R1=5.79% based on 17244 independent reflections) and IR establish it to be a dimer (Ci symmetry), $\mathbf{1}_2$, in the solid state. Several lines of evidence, including the parabolic kinetic order in **1**, nonlinear Arrhenius plot, independence of the rate on O_2 pressure, presence of titratable H_2O_2 and HCO_3H intermediates, and inhibition by conventional radical scavengers, all indicate the O_2-based oxidations proceed by complex homolytic chemistry (autoxidation and Haber-Weiss radical-chain processes) likely initiated by protonated **1**.

HYDROXYLATION OF BENZENE WITH OXYGEN AND HYDROGEN OVER CATALYSTS CONTAINING GROUP VIII METALS AND HETEROPOLY COMPOUNDS

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Catal. Today, 99(1-2) (2005) pp. 193-198.

The vapor phase hydroxylation of benzene to phenol with a mixture of oxygen and hydrogen over silica supported bi-component catalysts containing Group VIII metals (M) and heteropoly compounds (HPC) was investigated. The productivity of the catalysts was ascertained for various metal and HPC combinations and a range of reaction conditions. The $Pt–PMo_{12}/SiO_2$ and $Pd–PMo_{12}/SiO_2$ catalysts of optimal composition provide up to 380 mol phenol/g-atom Pt or Pd/h. The observed catalysis appears to be associated with an interface between metal particles and those of the heteropoly compound, as illustrated by an HREM image of a $Pt–PMo_{12}/SiO_2$ sample.

OXIDATION OF HYDROCARBONS WITH DIOXYGEN VIA PEROXIDE INTERMEDIATES

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Kinet. Catal., 46(2) (2005) pp. 204-216.

Cyclohexane, cyclohexene, and α-pinene react with dioxygen in the liquid phase in the presence of catalysts based on platinum, heteropoly compounds (HPCs), metal-containing HPCs, and combinations of these components. In cyclohexane and α-pinene oxidations occurring by an autooxidation mechanism at 160-170 and 80-90°C, respectively, the catalysts serve to control free-radical processes. The simultaneous action of a Ru-containing

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phosphotungstate as a hydroperoxide decomposition catalyst and of a V-containing phosphotungstate as a scavenger of hydroxyl and alkoxyl radicals increases the cyclohexanol + cyclohexanone selectivity of cyclohexane oxidation without yielding a hydroperoxide. A Pt/C catalyst affords an increase in α-pinene conversion in a fixed time. In combination with ammonia or tetrahexylammonium chloride admixtures, it retards side reactions and raises the yield of verbenol and verbenone, which are the most valuable products. During cyclohexane, cyclohexene, and α-pinene oxidation with an O_2–H_2 mixture at room temperature, no free-radical chain reaction develops in the Pt–HPC system and reactive intermediates form and interact, involving the HPC, with hydrocarbons on the surface of the platinum catalyst. Analysis of reactivity and of the composition of substrate oxidation products suggests a mechanism for the conjugate oxidation of hydrocarbons in systems with various HPCs. In this mechanism, HPC composition determines, to a large extent, the nature of reactive intermediates, which may be peroxides or radicals bound to platinum or HPC. The properties of catalytic systems in oxidation with O_2–H_2 mixtures can be controlled by selecting an appropriate HPC as the modifying component.

KINETICS OF OXIDATION OF REDUCED PHOSPHORUS-MOLYBDENUM-VANADIUM HETEROPOLY ACID SPECIES WITH DIOXYGEN IN AQUEOUS SOLUTIONS

E.G. Zhizhina, V.F. Odyakov, M.V. Simonova, K.I. Matveev

Kinet. Catal., 46(3) (2005) pp. 354-363.

The kinetics of dioxygen oxidation of the reduced heteropoly acid $H_{7+m}PV_m{}^{IV}V_{4-m}{}^{V}Mo_8O_{40}$ (H_mHPA-4) in aqueous solutions at atmospheric pressure and 313–363 K was studied, and a rate equation was proposed for this reaction. The reaction was of first order with respect to dioxygen. However, the order of the reaction with respect to H_mHPA-4 was close to 1 at [H_mHPA-4] > 0.20 mol/l but increased to ≈2.8 at [H_mHPA-4] < 0.20 mol/l. Variable orders of reaction with respect to H^+ ions with high negative values were observed. The introduction of overstoichiometric VO^{2+} cations into H_mHPA-4 accelerated the oxidation of the solution. The apparent activation energy of the reaction dramatically increased as the degree of reduction of H_mHPA-4 decreased. This can be explained by the fact that the heats of endothermic preequilibrium steps of the disproportionation of weakly reduced heteropoly anions are added to the true activation energy of formation of an active intermediate complex of the heteropoly anion with O_2.

RECOVERY OF Mo-V-PHOSPHOROUS HETEROPOLY ACIDS UNDER OXYGEN PRESSURE

E.G. Zhizhina, M.V. Simonova, V.F. Odyakov, K.I. Matveev

Catal. Ind., 2 (2005) pp. 17-24.

Solutions of Mo-V-phosphorous heteropoly acids of the following composition $H_{3+x}PMo_{12-x}V_xO_{40}$ (HPA-x) are the reversibly acting oxidizers in numerous catalytic processes. Oxidation of their reduced forms by oxygen followed by regeneration of oxidized HPA-x is here the common and hardest stage. The aim of the present work is searching the conditions of the catalyst (HPA-x) regeneration stage acceleration. It is shown that regeneration by oxygen of concentrated (0.1-0.4 M) water solutions of HPA-x ($2 \leq x \leq 4$) can be accelerated when it is carried out at T=353-433 K and $Po_2 \leq 8$ atm. When temperature is rising, the reaction depth increases as well. HPA-4 solutions are regenerated with maximum rate at T=433 K, and at higher temperature they become thermally instable and gradually produce precipitates. HPA-2 solutions are regenerated by oxygen slower but they are thermally stable up to T=463 K. The features of HPA-x solution regeneration mechanisms are considered. It is found that apparent activation energy of this reaction rises when the regeneration depth increases. Capability of HPA-x water solutions to become regenerated quickly and deeply by oxygen permits using them as reversibly acting oxidizers during oxidation of different organic compounds.

REGENERATION OF CATALYSTS ON BASIS OF AQUEOUS SOLUTIONS OF Mo-V-P HETEROPOLY ACIDS UNDER O_2 PRESSURE

E.G. Zhizhina, M.V. Simonova, V.F. Odyakov, K.I. Matveev

Chem. Sustain. Devel., 12(6) (2004) pp. 683-688.

Oxidation of 0.2 M $H_{7+m}PV^{IV}{}_mV^{V}{}_{4-m}Mo_8O_{40}$ solutions (H_mHPA-4) at 373-433 K with dioxygen under 8 atm pressure was studied. The rate maximum was observed at 433 K and at higher temperature solutions of H_mHPA-4 became thermally instable. The apparent activation energy of the reaction increased as the depth of oxidation of H_mHPA-4 increased.

RECOVERY OF SOLUTIONS OF HETEROPOLY ACID $H_5PMo_{10}V_2O_{40}$ UNDER O_2 PRESSURE

E.G. Zhizhina, M.V. Simonova, V.F. Odyakov, K.I. Matveev

Chem. Sustain. Devel., 13(1) (2005) pp. 45-50.

It was shown in principle that concentrated aqueous solutions of heteropoly acid with composition $H_5PV_2Mo_{10}O_{40}$ (HPA-2) can be used as stable reversibly reacting oxidizer. The reduced form of HPA-2 can be successfully oxidized with O_2 at 353-433 K under 8 atm pressure to regenerate HPA-2. It was investigated an influence of temperature and pressure on depth and rate of oxidation reaction. Reduced and oxidized solutions of HPA-2 were stable up to 463 K.

PRODUCTION OF K_3 VITAMIN BY THE REACTION OF DIENE SYNTHESIS IN THE PRESENCE OF THE SOLUTIONS OF MO-V-PHOSPHORIC HETROPOLY ACIDS AS CATALYSTS

M.V. Simonova, E.G. Zhizhina

Chem. Sustain. Devel., 13(3) (2005) pp. 479-482.

The principal opportunity of production of vitamin K_3 (2-methyl-1,4-naphthoquinone) from such accessible substrates as 2-methylphenol (o-cresol) and 2-methylaniline (o-toluidine) was shown. These processes proceed by reaction of diene synthesis. Polyfunctional catalysts of such processes were the solutions of Mo-V-phosphoric hetropoly acids that allowed to carry out oxidation and diene synthesis by one technological stage.

OXIDATION OF ANILINE WITH SOLUTIONS OF Mo-V-PHOSPHORIC HETEROPOLYACIDS

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Russ. Chem. Bull., 6 (2005) pp. 1532-1535.

Mo–V-phosphoric heteropolyacids (HPA) can be used for aniline oxidation to polyaniline or 1,4-benzoquinone. At room temperature and the molar ratio HPA : aniline = 0.67, more than 95% substrate are oxidized to polyaniline. At 90–100 °C and HPA : aniline = 3, the substrate is quantitatively oxidized to 1,4-benzoquinone. Solutions of HPA are regenerated by oxygen in a separate step.

CATALYTIC SYNTHESIS OF 9,10-ANTHRAQUINONE IN PRESENCE OF SOLUTIONS OF Mo-V-PHOSPHORIC HETEROPOLYACIDS

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Catal. Ind., 1 (2005) pp. 12-17.

It was shown that catalytic synthesis of 9,10-anthraquinone can be realized in one processing stage by combining diene synthesis reaction with oxidation of its adducts. Hydroquinone, 1,4-benzoquinone or 1,4-naphthoquinone can serve as staring substrate of such a process. The synthesis proceeds at T=60-80°C in atmosphere of 1,3-butadiene in the presence of Mo-V-phosphoric heteropolyacids (HPA-x, x=4-6) solutions playing the role of polyfunctional (acidic and oxidizing) catalysts. The effect of temperature, HPA-x concentration, substrate:HPA molar ratio has been studied in the process of production of mixture of 9,10-anthraquinone and its derivatives. Upon separating the reaction products, HPA-x is regenerated by oxygen or the air under pressure at T=150–160°C and used repeatedly.

NEW CATALYTIC REACTIONS IN THE PRESENCE OF Mo-V-PHOSPHORIC HETEROPOLY ACID SOLUTIONS

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Russ. J. Appl. Chem., 78(5) (2005) pp. 758-763.

The possibility of performing new catalytic reactions in the presence of solutions of $H_{x+3}PMo_{12-x}V_xO_{40}$ Mo-V-phosphoric heteropoly acids was examined.

A POTENTIOMETRIC STUDY OF PRECIPITATION IN THE (Pb^{2+}–$H_2PO_4^-$-Cl^-) SYSTEM

V.F. Odyakov, E.G. Zhizhina

Russ. J. Inorg. Chem., 50(6) (2005) pp. 969-973.

Interaction of Pb^{2+} and $H_2PO_4^-$ ions in acetate buffer solutions results in the formation of a precipitate with variable composition $Pb_x(PO_4)_yA_z$, where A^- is a monovalent anion. In the presence of excess chloride (the Cl^- : $H_2PO_4^-$ molar ratios from 0.5 to 2.0) in the range $4.10 \leq pH \leq 4.95$, the precipitate composition is approximately formulated as $Pb_5Cl(PO_4)_3$ (Pb : P = 1.667). In the absence of chlorides, the Pb^{2+} : $H_2PO_4^-$ ratio decreases to 1.56–1.62 during precipitation.

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DEVELOPMENT OF NEW TECHNOLOGY OF CATALYTIC SYNTHESIS OF METHYL-ETHYL KETONE BY OXIDATION OF N-BUTYLENES

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Catal. Ind., 5 (2005) pp. 28-35.

A new method of industrial production of methyl-ethyl ketone by direct oxidation of n-butylenes over homogenous catalysts Pd+ GPK-x', where GPK-x' is the Mo-V-phosphoric heteropoly acid was proposed. The process is performed continuously in two reactors. In the first of them, the moving water catalyst solution contacts liquid n-butylenes at T=60°C. The methyl-ethyl ketone formed is stripped from the reduced catalyst form in the stripping column. In the second one, the oxidized catalyst form is generated by atmospheric oxygen at $T \leq 190°C$ and $P \leq 3$ MPa. The regenerated catalyst repeats its cycle. The stripped raw methyl-ethyl ketone is sent to rectification. The new process is characterized by high efficiency and ecological properties.

STUDY OF THE HETEROPOLYACID $H_{21}B_3W_{39}O_{132}$ nH$_2$O

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G.S. Litvak

Russ. J. Inorg. Chem., 50(7) (2005) pp. 1062-1065.

The heteropolyacid $H_{21}B_3W_{39}O_{132}\cdot nH_2O$ (B_3W_{39}) was studied by solid-state IR spectroscopy and differential thermal analysis and by ^{183}W, ^{17}O, and ^{11}B NMR in solution. The NMR spectra of the B_3W_{39} anion, which consists, according to structural data, of three equivalent BW_{13} fragments, confirmed the integrity of the HPA in solutions but revealed the deviation from the C_s and C_{3h} symmetry determined previously, which results in structure chirality. Potentiometric titration showed the nonequivalence of the HPA protons, only 11 of which are strongly acidic. Concentrated (≥0.05 M) solutions of HPA are unstable; after several days, $H_5BW_{12}O_{40}$ and tungstic acid can be isolated from the solutions. On heating, solid B_3W_{39} starts to decompose into the same products below 200°C.

Photocayalytic and Related Processes

PHOTOCATALYTIC OXIDATION OF VX SIMULANT 2-(BUTYLAMINO)ETHANETHIOL

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J. Hazardous Mater. B, 113(1-3) (2004) pp. 89-95.

Photocatalytic oxidation of 2-(butylamino)ethanethiol (BAET) was undertaken in aqueous suspension of TiO_2 Hombikat UV 100 and Degussa P25 under different initial reaction conditions in order to determine the best parameters for the fastest mineralization of the substrate. BAET is considered to be a simulant for the VX chemical warfare agent. The application of ultrasound had only a small positive effect on the BAET photocatalytic degradation. The highest mineralization rate of 0.433 mg/(l min) was found in unbuffered TiO_2 Degussa P25 suspension with initial pH value of about 9.4, TiO_2 concentration 500 mg/l and the initial BAET concentration 1000 mg/l. Decreasing of the initial solution pH to 6.1 or below stops the mineralization of BAET while increasing of pH to about 11 drastically changed the degradation profile. At this initial pH, the first 100 min of reaction led to only oxidation of sulfur moiety and organic intermediates accumulated in the solution. Thereafter, mineralization of the products started. The main detected volatile product was butyl aldehyde and the main polar one was 2-(butylamino) acetic acid. In the case of TiO_2 Hombikat UV 100, conversion of TOC at initial pH 11 exceeded that at initial pH 9.1. For Degussa P25, the starting pH 9.4 was the best for TOC conversion. The results can be used for treatment of water from pollutants with aliphatic nitrogen and sulfur atoms.

PHOTOCATALYTIC DESTRUCTION OF A THIOSULFONATE

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Top. Catal., 35(3-4) (2005) pp. 245-253.

This paper presents experimental and quantum chemical consideration of photocatalytic and photochemical transformations in acetonitrile of $CH_3C_6H_4S(O_2)SCH_2CH_2N(iPr)_2$ (diisopropylaminoethyl 4-methylbenzene-thiosulfonate, DAMT), an imitant of chemical agent VX with close structural properties and ionization energy. Diisopropylaminoethyl disulfide and 4-methylbenzenesulfonic acid were detected as major products of photocatalytic and photochemical degradation. Photocatalytic degradation stopped at about 60% DAMT conversion due to acidification of the system. Photochemical degradation proceeded slower but to a higher conversion since DAMT protonation did not stop

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photolysis completely. $DAMT^{\cdot +}$ forms at the first step of photocatalytic degradation, then it splits into $CH_3C_6H_4SO_2^{\cdot}$ and $SCH_2CH_2N^{+}(iPr)_2$. The former fragment transforms into sulfonic acid and the latter decomposes into SCH_2 and $CH_2N^{+}(iPr)_2$ in the absence of TiO_2, the route observed in mass spectrometry. However it is stable in adsorbed state on the TiO_2 surface and after reduction with photogenerated electron recombines to produce the disulfide product. The results suggest that photocatalytic and photolytic detoxification of VX is possible provided conditions are adjusted for its complete conversion.

TiO_2 PHOTOCATALYTIC OXIDATION. I. PHOTOCATALYSTS FOR LIQUID-PHASE AND GAS-PHASE PROCESSES AND THE PHOTOCATALYTIC DEGRADATION OF CHEMICAL WARFARE AGENT SIMULANTS IN A LIQUID PHASE

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Kinet. Catal., 46(2) (2005) pp. 189-203.

The results of studies on the effect of the preparation procedure on the properties of TiO_2-based photocatalysts and the kinetics and mechanism of the photocatalytic oxidation of organic water pollutants are surveyed. The effects of calcination temperature, surface modification with platinum, and acid–base treatment of the surface of titanium dioxide on its activity in model gas-phase and liquid-phase reactions are considered. Optimal catalyst preparation conditions were found in order to achieve maximum activity, and conceivable reasons for the effects of the above factors on the activity were revealed. The intermediate products and mechanisms of the photocatalytic and dark reactions of solutes that simulated chemical warfare agents in water are considered. All of the test simulants can undergo complete oxidation to form inorganic products in an aqueous TiO_2 suspension under irradiation with UV light. It was found that, in addition to oxidation, the dark steps of hydrolysis also play an important role in the degradation of these substances. The low-frequency ultrasonic treatment (20 kHz) of a photocatalyst suspension in the course of the photocatalytic oxidation of dimethyl methylphosphonate can accelerate the reaction because of the facilitated transport of reactants to the surface of photocatalyst particles.

TiO_2 PHOTOCATALYTIC OXIDATION. II. GAS-PHASE PROCESSES

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Kinet. Catal., 46(3) (2005) pp. 422-436.

The results of studies on the TiO_2 photocatalytic oxidation of model air pollutants are summarized. The kinetics of photocatalytic oxidation of CO and the vapors of a number of simple organic substances was studied in detail. It was found that, in the course of reaction, all of the test substances underwent complete mineralization. Gaseous substrates were converted with the participation of several types of reaction centers. The photocatalytic oxidation of sulfur- and phosphorus-containing substances resulted in gradual deactivation of the photocatalyst; however, its activity can be restored by washing the photocatalyst with water. It was found that, along with oxidation, the steps of hydrolysis play an important role in the photocatalytic degradation of air pollutants, such as dimethyl methylphosphonate and 2-chloroethyl sulfide.

TiO_2 PHOTOCATALYTIC OXIDATION. III. GAS-PHASE REACTORS

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Kinet. Catal., 46(3) (2005) pp. 437-444.

A number of reactor designs for photocatalytic oxidation in the gas phase are considered: cylindrical reactors with photocatalysts supported by various techniques, a reactor with a vibrationally fluidized bed of a photocatalyst, and a coil reactor with the reactivation of a photocatalyst at regular intervals. It was found that the vibrational fluidization of catalyst grains enhanced catalyst activity because of the effect of periodic illumination of different grain sides. The results of testing of two types of domestic photocatalytic air purifiers commercially manufactured in Russia are reported.

PHOTOINDUCED HETEROGENEOUS PROCESSES ON CHEMICAL PHASE COMPONENTS OF SOLID TROPOSPHERIC AEROSOLS

V.S. Zakharenko, A.N. Moseichuk* (**Institute of Petroleum Chemistry, Tomsk, Russia*)

Atmosph. Oceanic Optics, 17(5-6) (2004) pp. 393-395.

Some results are presented on investigation of the photoinduced processes in some metal oxides (In_2O_3, Sc_2O_3, V_2O_5 and MoO_3), which can be the phase

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chemical components of solid tropospheric aerosols. The quantum yield and spectral behavior of the quantum yield of photoadsorption and photocatalytic oxidation in the spectral region that involves the spectrum of solar radiation in the troposphere has been determined.

ADSORPTION OF FREONS BY CALCIUM CARBONATE UNDER ATMOSPHERIC CONDITIONS

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Atmosph. Oceanic Optics,
18(5-6) (2005) pp. 454-458.

The process of interaction of halogen-containing organic compounds (Freons: 134a, 22, and 12) with calcium carbonate surface under illumination and conditions close to the tropospheric ones was studied. It is suggested that the interaction is a destructive photosorption of Freons (134a or 22). This interaction yields the surface calcium fluoride and calcium chloride. The spectral dependence of the effective quantum yield for Freon 134a is determined.

PHOTOSORPTION OF OXYGEN AND NITRIC OXIDE BY ALUMINUM AND SILICON OXIDES UNDER CONDITIONS OF TROPOSPHERE

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High Energy Chem.,
39(3) (2005) pp. 154-157.

The photosorption characteristics of finely divided ν-Al_2O_3 and SiO_2 with the state of the surface formed under long-term action of atmospheric air, were studied. The effective quantum yields and the action spectra of photoinduced adsorption of oxygen and nitric oxide were determined. It has been assumed that the absence of noticeable photoinduced adsorption of halogenated compounds on these powdered aluminum and silicon oxides is due to their low degree of crystallinity.

PHOTOINDUCED HETEROGENEOUS PROCESSES ON CHEMICAL PHASE COMPONENTS OF SOLID TROPOSPHERIC AEROSOLS

V.S. Zakharenko

Top. Catal., 35(3-4) (2005)
pp. 231-236.

This work shows the results of photoinduced process investigations over some metal oxides of the semiconductor type (In_2O_3, Sc_2O_3, V_2O_5 and MoO_3) and insulator type (MgO). These metal oxides can be the chemical phase components of solid tropospheric aerosols. The quantum yields and spectral dependencies of the quantum yields of photoadsorption and photocatalytic oxidation in the spectral region including the spectral region of solar tropospheric irradiation are determined.

SPECIFICS OF SUBSTRATE-MEDIATED PHOTO-INDUCED CHEMICAL PROCESSES ON SUPPORTED nm-SIZED METAL PARTICLES

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J. Phys.: Condens. Matter,
16 (2004) pp. 7131-7141.

Substrate-mediated mechanism of photochemical reactions on metals includes direct and/or plasmon-related excitation of electron–hole pairs in the bulk by photons and subsequent chemical transformation due to interaction of excited (hot) electrons (or holes) with the adsorbate. In nm-sized metal particles, the excited electrons are confined. It is shown in detail that this factor is beneficial for photochemistry under low-intensity steady-state conditions (linear regime) and also during intensive sub-ps laser pulses (non-linear regime). In both cases, the confinement may increase the contribution of secondary hot electrons to the photochemical conversion. In addition, in the non-linear regime the decrease of electron temperature after heating may be much slower than that on the surfaces of bulk samples and accordingly photochemical reactions may be more probable.

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Electrocatalysis and Electrochemical Processes

INFLUENCE OF PARTICLE AGGLOMERATION ON THE CATALYTIC ACTIVITY OF CARBON-SUPPORTED Pt NANOPARTICLES IN CO MONOLAYER OXIDATION

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Phys. Chem. Chem. Phys.,
7(2) (2005) pp. 375-383.

Fuel cell electrocatalysts usually feature high noble metal contents, and these favour particle agglomeration. In this paper a variety of synthetic approaches (wet chemical deposition, electrodeposition and electrodeposition on chemically preformed Pt nuclei) is employed to shed light on the influence of nanoparticle agglomeration on their electrocatalytic properties. Pt loading on model glassy carbon (GC) support is increased systematically from 1.8 to 10.6 μg Pt cm^{-2} and changes in the catalyst structure are followed by transmission electron microscopy. At low metal loadings ($\leq$5.4 μg Pt cm^{-2}) isolated single crystalline Pt nanoparticles are formed on the support surface by wet chemical deposition from H_2PtCl_4 precursor. An increase in the metal loading results, first, in a systematic increase of the average diameter of isolated Pt nanoparticles and, second, in coalescence of nanoparticles and formation of particle agglomerates. This behaviour is in line with the previous observations on carbon-supported noble metal fuel cell electrocatalysts. The catalytic activity of Pt/GC electrodes is tested in CO monolayer oxidation. In agreement with the previous studies (F. Maillard, M. Eikerling, O. V. Cherstiouk, S. Schreier, E. Savinova and U. Stimming, *Faraday Discuss.*, 2004, 125, 357), we find that the reaction is strongly size sensitive, exhibiting an increase of the reaction overpotential as the particle size decreases below *ca.* 3 nm. At larger particle sizes the dependence levels off, the catalytic activity of particles with diameters above 3 nm approaching that of polycrystalline Pt. Meanwhile, Pt agglomerates show remarkably enhanced catalytic activity in comparison to either isolated Pt nanoparticles or polycrystalline Pt foil, catalysing CO monolayer oxidation at *ca.* 90 mV lower overpotential. Enhanced catalytic activity of Pt agglomerates is ascribed to high concentration of surface defects. CO stripping voltammograms from Pt/GC electrodes, comprising Pt agglomerates along with isolated single crystalline Pt nanoparticles from 2 to 6 nm size, feature double voltammetric peaks, the more negative corresponding to CO oxidation on Pt agglomerates, while the more positive to CO oxidation on isolated Pt nanoparticles. It is shown that CO stripping voltammetry provides a fingerprint of the particle size distribution and the extent of particle agglomeration in carbon-supported Pt catalysts.

A COMPARATIVE STUDY OF HYDROXIDE ADSORPTION ON THE (111), (110), AND (100) FACES OF SILVER WITH CYCLIC VOLTAMMETRY, EX SITU ELECTRON DIFFRACTION, AND *IN SITU* SECOND HARMONIC GENERATION

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Langmuir, 20(25) (2004) pp. 10970-10981.

Hydroxide adsorption on the (111), (110), and (100) faces of silver electrodes from mixed NaOH/NaF solution is studied using cyclic voltammetry and *in situ* second harmonic generation (SHG). Cyclic voltammograms for the three low index silver planes in alkaline electrolytes are for the first time compared. They show two pairs of anodic and cathodic peaks in the potential interval below the equilibrium Ag/Ag_2O potential. These are attributed to the specific adsorption of hydroxide ions followed by submonolayer oxide formation. The differences in the cyclic voltammograms for the (111), (110), and (100) planes are attributed to different (i) work functions, (ii) surface atomic densities, and (iii) corrugation potentials for these surfaces. Ex situ low energy electron diffraction (LEED) and reflection high energy electron diffraction (RHEED) show that disordered adlayers are formed on Ag(111) and Ag(100), in contrast to Ag(110), where ordered structures are produced in the region of the first pair of current peaks. In the region of the second pair of peaks, LEED indicates disordered oxide phases on each crystal plane and RHEED shows the presence of small islands of $c(2 \times 2)$ structure at some potentials on (110) and (100). SHG measurements were performed (i) in the potential scan mode at constant rotational angle and (ii) at constant potential as a function of the rotational angle. The isotropic (for the (111), (110), and (100) planes) and anisotropic (for the (110) and (111) planes) contributions to the SHG intensity were calculated by fitting the experimental data and are discussed in terms of their dependence on the charge density at the interface, on hydroxide adsorption, and on submonolayer oxide formation.

Biotechnology and Biology Related Catalysis

ROTOR-INERTIAL BIOREACTOR FOR HETEROGENEOUS BIOCATALYTIC PROCESSES. II. SUCROSE ENZYMATIC INVERSION

G.A. Kovalenko, S.V. Sukhinin, A.V. Simakov, V.V. Khomov, L.V. Perminova, O.V. Komova

Biotechnology, 1 (2005)
pp. 68-72.

It is shown that cellular membranes of autolysated baker's yeasts possess invertase activity and may be used for synthesis of heterogeneous biocatalysts for the process of sucrose enzymatic inversion. The given biocatalyst synthesized by membrane immobilization on foam-like ceramics covered by the layer of catalytic filamentous carbon was tested in rotary-inertial bioreactor (RIB), and bioreactor operating conditions were optimized. Comparison of RIB with conventional fixed-bed bioreactor does not reveal noticeable difference in their efficiency.

CARBON-CONTAINING MACROSTRUCTURED CERAMIC SUPPORTS FOR ENZYMES AND MICROORGANISM ADSORPTIVE IMMOBILIZATION. IV. BIOCATALYTIC PROPERTIES OF IMMOBILIZED YEAST MEMBRANES

G.A. Kovalenko, L.V. Perminova, V.V. Khomov, O.V. Komova, N.V. Chuenko, A.V. Simakov, N.A. Rudina

Biotechnology, 6 (2004)
pp. 34-43.

Heterogeneous biocatalysts for sucrose inversion based on cellular membranes of autolysated baker's yeasts possessing invertase activity and immobilized over carbon-containing macrostructured ceramic supports were developed. Biocatalytic properties of synthesized heterogeneous biocatalysts were studied, and also effect of surface carbon layer morphology and surface chemical properties on activity and stability of immobilized east membranes was revealed. The supports with the surface layer of filamentous carbon were shown to possess optimal morphology and hydrophilic-hydrophobic properties of the surface layer, providing constancy of invertase activity of soluble membranes after immobilization and their maximal stabilization.

IMMOBILIZED YEAST MEMBRANES AS BIOCATALYSTS FOR SUCROSE INVERSION

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Appl. Biochem. Microbiol., 41(4) (2005)
pp. 399-403.

Yeast membranes were obtained by autolysis of various strains with relatively high invertase activity. Heterogeneous biocatalysts for sucrose inversion were made of the yeast membranes and granulated carbon-containing supports made of common natural materials: expanded clay aggregate (ECA), sapropel, and lignin. The properties of these biocatalysts were studied. It was shown that the biocatalyst activity and stability of the immobilized yeast membranes increased with reference to the initial ECA, independent of the morphology of the carbon layer synthesized on the support surface. Heterogeneous biocatalysts prepared by adsorption of yeast membranes on sapropel had the greatest activity and stability, whereas lignin-based biocatalysts were relatively unstable.

BASIC RESEARCH IN THE INTERESTS OF DEVELOPMENT OF THE CHEMICAL-PHARMACEUTICAL INDUSTRY (II Conference)

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(**Institute of Technical Chemistry, Perm, Russia*)

Catal. Ind., 4 (2005) pp. 56-61.

Analytic review of the works presented as 6 plenary lectures, 22 oral reports, and 19 communications on the basic and applied aspects of chemical and biotechnological processes was carried out. It was shown that considerable part of the reports was dedicated to the development of the new original methods and approaches to the synthesis of the biologically active compounds that are of interest as products for medicine purposes or intermediates in their synthesis. It was noted that the conference was successful and useful for the estimation of prospective trends in this area and establishing the new contacts of the researchers of the academic and university science with the representatives of the chemical and pharmaceutical industries.

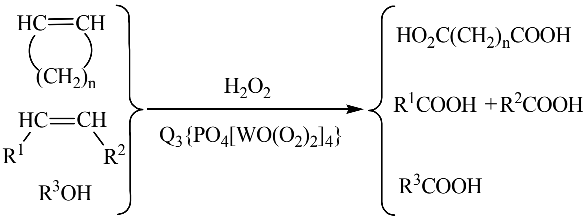
CONTENT

CATALYTIC OXIDATION OF OLEFINS AND ALCOHOLS WITH HYDROGEN PEROXIDE IN A TWO-PHASE SYSTEM GIVING MONO- AND DICARBOXYLIC ACIDS

Z.P. Pai, A.G. Tolstikov, P.V. Berdnikova, G.N. Kustova, T.B. Khlebnikova, N.V. Selivanova, A.B. Shangina, and V.G. Kostrovsky* (**Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

Russ. Chem. Bull., 8 (2005)
pp. 1847-1854.

The investigations in the fields of phase-transfer catalysis were carried out for the purpose of development of the new approaches to the synthesis of commercially important compounds of mono- and dicarboxylic acids.



$R^1 = -(CH_2)_mCH_3$; $R^2 = -(CH_2)_nCOOH$
$R^3 = -(CH_2)_nCH_3$ или Ar

The various factors influencing the catalytic activity of the system based on the tetrakis(oxodiperoxotungsto)phosphate(3-) combined with the quaternary ammonium cations, for example, methyltri-n-octylammonium – $[CH_3(n\text{-}C_8H_{17})_3N]^+$, were studied in the reactions of oxidation of cycloolefins (cyclohexene, cyclooctene), alcohols (1-octanol, phenylmethanol) and fatty acids (cis-9-octadecenic, 12-hydroxyoleinic) by the hydrogen peroxide resulting in carboxylic acids. It is ascertained that the oxidation reactions in the presence of the catalyst proceed in the mild conditions (atmospheric pressure, temperature 80÷90 ^{0}C). Catalytic systems were characterized with the use of the IR and KR spectroscopy methods. The state of systems synthesized with the use of various peroxocomplex precursors and phase-transfer catalyst salts was studied. It is shown first that the anion contained in the quaternary ammonium salt has an impact on the peroxocomplex structure formation. The optimal reactions conditions were determined on the basis of the experimental data.

REACTION OF SOME TERPENOIDS WITH MALONONITRILE IN THE PRESENCE OF HYDROTALCITE

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Russ. J. Org. Chem., 41(6) (2005)
pp. 838-842.

α-Ionone and 5,5,8-trimethyl-3,7-nonadien-2-one react with malononitrile in the presence of specially prepared hydrotalcite to afford the corresponding Knoevenagel condensation products with high yield and selectivity.

NEW BIPHASE SILICON-HYDROGEL POLYMER MATERIAL FOR LONG-TERM SOFT CONTACT LENSES OF CONTINUOUS WEARING

E.V. Boiko*, N.L. Vlasova, B.F. Danilichev, S.S. Ivanchev, S.A. Novikov*, V.N. Pavlyuchenko, N.A. Ushakov*, N.A. Chekina** (**Institute of Military Medicine, St-Petersburg, Russia; **Military Medical Academy, St-Petersburg, Russia*)

Eye, (39) (2004) pp. 2-5.

New silicon-hydrogel material for production of soft contact lenses (SCL) is developed. Method is based on interpenetrating polymer networks (IPN) formation. The hydrophilic polymer network is formed via radical copolymerization of hydrophilic monomers in the presence of cross-linking agents. Silicon network is formed by interaction between two olygosiloxanes with different reaction groups such as hydride and vinyl. Developed material has high hydrophilicity, oxygen permeability and mechanical strength. Soft contact lenses (SCL) were obtained in closed polymer forms. The developed SCL are competitive to existing analogue due to application of inexpensive commercially accessible basic material and simple technology.

A MINIMAL GENERIC MODEL OF BACTERIA-INDUCED INTRACELLULAR Ca^{2+} OSCILLATIONS IN EPITHELIAL CELLS

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Biophys. J., 88 (2005) pp. 2976-2981.

The toxin *α*-hemolysin expressed by uropathogenic *Escherichia coli* bacteria was recently shown as the first pathophysiologically relevant protein to induce oscillations

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of the intracellular Ca^{2+} concentration in target cells. Here, a generic three-variable kinetic model is proposed describing the Ca^{2+} oscillations induced in single rat renal epithelial cells by this toxin. Specifically, the interplay between 1), the cytosolic Ca^{2+} concentration; 2), IP_3-sensitive Ca^{2+} channels located in the membrane separating the cytosol and endoplasmic reticulum; and 3), toxin-related activation of production of IP_3 by phospholipase C was taken into account. With these ingredients, the predicted response of cells exposed to the toxin is in good agreement with the results of experiments.

Olefin Polymerization

AMOUNT OF ACTIVE CENTERS AND PROPAGATION RATE CONSTANT DURING ETHYLENE POLYMERIZATION ON THE 2,6-*BIS*(IMINO)PYRIDINEIRON(II) CHLORIDE + TRIISOBUTYLALUMINUM HOMOGENEOUS CATALYST

A.A. Barabanov, G.D. Bukatov, V.A. Zakharov,
N.V. Semikolenova, L.G. Echevskaya,
M.A. Mats'ko

Polymer Sci., Ser B,
47(11-12) (2005) pp. 349-353.

The amount of active centers c_p and the propagation rate constant k_p during ethylene polymerization over the homogeneous complex $2,6\text{-}(2,6\text{-}(Me)_2C_6H_3N{=}CMe)_2C_5H_3NFeCl_2$ with Al(*i*-Bu)$_3$ as an activator were determined by the method of quenching by radioactive carbon monoxide ^{14}CO. At a rate close to maximum, active centers compose a substantial part of the iron complex (41 mol %). The k_p value for these centers is 26×10^3 l/(mol s) at 35°C. The activity drops with the polymerization time as a result of a decrease in both the amount of active centers (to 0.16 mol/mol Fe) and the k_p value (to 8.2×10^3 l/(mol s)). Data on the influence of polymerization time on the molecular mass and the molecular-mass distribution of the product polyethylene are presented. On the basis of these data, it was assumed that highly reactive but unstable active centers generated in the initial polymerization stage affect the formation of low-molecular-mass polyethylene, while more stable and less active centers mediate the formation of polyethylene with a higher molecular mass.

ANTITURBULENT POWERS OF HIGHER POLYOLEFINS AND OLEFIN TERPOLYMERS

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A.V. Ilyushnikov*, A.N. Ochered'ko*,
V.A. Zakharov, T.B. Mikenas, S.A. Sergeev
(**Institute of Oil Chemistry, Tomsk, Russia*)

Russ. J. Appl. Chem., 77(3) (2004) pp. 449-453.

Terpolymers of ethylene with propylene and higher α-olefins with various compositions and molecular weights were synthesized, as well as copolymers with higher poly-α-olefins with various molecular weights. The possibility of laboratory assessment of the antiturbulent power of polymers and turborheometric determination of the volumes and molecular weights of poly-α-olefin macromolecules was examined.

ETHYLENE POLYMERIZATION OVER SUPPORTED CATALYSTS [2,6-*BIS*(IMINO)PYRIDYL IRON DICHLORIDE/MAGNESIUM DICHLORIDE] WITH AlR_3 AS AN ACTIVATOR

T.B. Mikenas, V.A. Zakharov, L.G. Echevskaya,
M.A. Matsko

J. Polym. Sci., Part A: Polym. Chem.,
43(10) (2005) pp. 2128-2133.

Data on ethylene polymerization over supported $LFeCl_2/MgCl_2$ catalysts {L = 2,6-*bis*[1-(2,6-dimethylphenylimino)ethyl]pyridyl} containing AlR_3 (R = Me, Et, *i*-Bu, or *n*-Oct) as an activator are presented. These catalysts are highly active (100-300 kg of polyethylene/g of Fe h bar of C_2H_4) and stable in ethylene polymerization at 70-80°C. Data on the effects of the iron content, AlR_3 type, Al(*i*-Bu)$_3$ concentration, and hydrogen presence on the catalyst activity are presented. The molecular structure of polyethylene produced with these catalysts (including the molecular masses, molecular mass distribution, branching, and number of C═C bonds) has been studied; data on the effects of AlR_3 and hydrogen on the molecular structure are presented.

MECHANISM OF OLEFIN POLYMERIZATION ON SUPPORTED ZIEGLER-NATTA CATALYSTS BASED ON DATA ON THE NUMBER OF ACTIVE CENTERS AND PROPAGATION RATE CONSTANTS

G.D. Bukatov, V.A. Zakharov, A.A. Barabanov

Kinet. Catal., 46(2) (2005) pp. 166-176.

The number of active centers (C_g) and propagation rate constants (k_g) for the polymerization of propylene and ethylene on highly active titanium–magnesium

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catalysts (TMCs) of different compositions at 70°C were determined using the method of ^{14}CO inhibition of polymerization. In the polymerization of propylene on the $TiCl_4/D_1/MgCl_2\text{-}AlEt_3/D_2$ system (D_1 is dibutyl phthalate or 2,2'-diisobutyl-1,3-dimethoxypropane; D_2 is a silane), the effects of D_1 and D_2 donors on the values of C_g and k_g were studied. It was found that the donors decreased the values of k_g for nonstereospecific centers, had no effect on the values of k_g for stereospecific centers, and increased the fraction of stereospecific centers, as well as the fraction of "sleeping" centers regardless of their stereospecificity. The rate constants of isotactic-chain transfer with C_3H_6, $AlEt_3$, H_2, and $ZnEt_2$ were determined. In the polymerization of ethylene, a number of TMCs exhibited strong diffusion limitations, which manifested themselves in a dramatic decrease in the determined values of k_g. It was demonstrated that diffusion limitations can be removed by decreasing the particle size and the concentration of active centers and by performing prepolymerization with propylene. The values of k_g in ethylene polymerization were similar for stereospecific and nonstereospecific centers.

KINETIC PECULIARITIES OF ETHYLENE POLYMERIZATION OVER HOMOGENEOUS *BIS*(IMINO)PYRIDINE Fe(II) CATALYSTS WITH DIFFERENT ACTIVATORS

A.A. Barabanov, G.D. Bukatov, V.A. Zakharov, N.V. Semikolenova, L.G. Echevskaya, M.A. Matsko

Macromol. Chem. Phys.,
206(22) (2005) pp. 2292-2298.

Method of polymerization inhibition by radioactive carbon monoxide (^{14}CO) has been used to determine the number of active centers (C_P) and propagation rate constant (k_P) for ethylene polymerization with homogeneous complex $2,6\text{-}(2,6\text{-}(Me)_2C_6H_3N{=}CMe)_2C_5H_3NFeCl_2$ ($LFeCl_2$), activated with methylalumoxane (MAO) or $Al(i\text{-}Bu)_3$. With both activators the rate profile of polymerization was unstable: high activity [0.8×10^3 – 1.5×10^3 kg PE per ($mol_{Fe} \cdot h \cdot atm$) at 35 °C] of the initial period sharply decreases (sevenfold in 10 min). In the beginning of polymerization with the catalysts $LFeCl_2$/MAO and $LFeCl_2/Al(i\text{-}Bu)_3$, the C_P values were found to be 8 and 41% of total Fe-complex content in catalysts, respectively, and decreased 1.5-2-fold in 9 min. As polymerization proceeds, the k_P value for $LFeCl_2$/MAO system decreases from 5×10^4 to 1.5×10^4 $L \cdot (mol \cdot s)^{-1}$ $LFeCl_2$/MAO, and for $LFeCl_2/Al(i\text{-}Bu)_3$ system from 2.6×10^4 to 0.82×10^4 $L \cdot (mol \cdot s)^{-1}$. Data on the effect of polymerization time on polyethylene molar mass distribution are presented. Basing on the obtained results it was suggested that highly reactive, but unstable centers, dominating at short polymerization times, produce low-molar-mass polyethylene, while polyethylene with higher molar mass is produced by less active (low k_P) and more stable centers.

SUPPORTED CATALYSTS BASED ON 2,6-*BIS*(IMINO)PYRIDYL COMPLEX OF Fe(II): DRIFTS STUDY OF THE CATALYST FORMATION AND DATA ON ETHYLENE POLYMERIZATION

N.V. Semikolenova, V.A. Zakharov, E.A. Paukshtis, I.G. Danilova

Top. Catal., 32(1-2) (2005) pp. 77-82.

The supported catalysts for ethylene polymerization were prepared by interaction of 2,6-*bis*[1-(2,6-dimetilphenylimino)-ethyl]pyridineiron(II) dichloride ($LFeCl_2$) with silica and alumina. The catalysts exhibit high and stable activity at ethylene polymerization in presence of $Al(i\text{-}Bu)_3$ as co-catalyst. $LFeCl_2$ interaction with surface functional groups of the supports was studied by means of DRIFTS. $LFeCl_2$ adsorbed on the support surface mainly retains its structure. $LFeCl_2$ is strongly bounded to the support due to formation of multiple bonds between $LFeCl_2$ and surface functional groups of the supports. DRIFTS data on the state of the surface iron compounds have been obtained using CO as probe molecule.

STUDY OF THE SUPPORTED ZIRCONOCENE CATALYSTS BY MEANS OF UV/VIS AND DRIFT SPECTROSCOPY

V.N. Panchenko, V.A. Zakharov, E.A. Paukshtis

J. Mol. Catal. A: Chem.,
240(1-2) (2005) pp. 33-39.

UV/vis in diffusion reflection mode (DRS) and DRIFT spectroscopy have been used to study the surface zirconocene species formed at the interaction of $Me_2Si(Ind)_2ZrCl_2$ and $Me_2Si(Ind)_2ZrMe_2$ complexes with the MAO/SiO_2 support. Effect of additional activation of these catalysts with TIBA has been studied as well.

Structure of type $[Me_2Si(Ind)_2ZrMe]^+[MeMAO]^-$ (C) is formed at the reaction of $Me_2Si(Ind)_2ZrMe_2$ complex with MAO/SiO_2 (a.b. at 456 nm in UV/vis spectra). Interaction of this complex with TIBA results in the formation of new structure (D) with a.b. at 496 nm in UV/vis spectra.

The surface species of different composition and structures are formed at interaction of $Me_2Si(Ind)_2ZrCl_2$ complex with MAO/SiO_2. The ratio between these species depends on the zirconium content in the $Me_2Si(Ind)_2ZrCl_2/MAO/SiO_2$ catalysts. According to the DRIFTS data (CO and ethylene adsorption) and ethylene polymerization data these catalysts contain active Zr-Me bonds but activity of these catalysts at ethylene polymerization is low. Interaction of $Me_2Si(Ind)_2ZrCl_2/MAO/SiO_2$ with TIBA leads to the formation of the new cationic structure of type (D) with a.b. at 496 nm in UV/vis spectra and great increasing of activity at ethylene polymerization.

POLYMERIZATION OF ETHYLENE CATALYZED BY SiO_2-SUPPORTED 2,6-*BIS*(ARYLIMINO)PYRIDINE COMPLEXES OF FERROUS CHLORIDE AND 1,2-*BIS*(IMINO)ACENAPHTHYL COMPLEXES OF NICKEL BROMIDE

S.S. Ivanchev, V.K. Badaev, N.I. Ivancheva,
E.V. Sviridova, S.Ya. Khaikin, D.G. Rogozin,
A.S. Abakunchik

Polymer Sci., ser. A, 47(6) (2005) pp. 566-573.

The slurry and gas-phase polymerization of ethylene catalyzed by silica-supported *bis*(imino)pyridine complexes of ferrous chloride with ligands, such as 2,6-*bis*[1-(2-methyl-6-cyclohexylphenylimino)ethyl] pyridine (**I**), 2,6-*bis*[1-(2,4-dimethyl-6-cyclohexylphenylimino)ethyl] pyridine (**II**), 2,6-*bis*[1-(2-methyl-6-cyclooctylphenylimino)ethyl] pyridine (**III**), 2,6-*bis*[1-(2,4-dimethyl-6-cyclooctylphenylimino)ethyl]-pyridine (**IV**), and 2,6-*bis*[1-(2,4-dimethyl-6-cyclododecylphenylimino) ethyl]pyridine (**V**), and bisimines of nickel bromide with ligands, such as 1,2-*bis*(2-cyclopentyl-6-methylphenylimino)acenaphthene] (**VI**), 1,2-*bis* (2-cyclopentyl-4,6-dimethylphenylimino)acenaphthene] (**VII**), and 1,2-*bis*(2-cyclohexyl-6-methylphenylimino) acenaphthene] (**VIII**) was studied. Methylaluminoxane was used as a cocatalyst. In polymerization initiated by supported catalysts **I**–**V**, triisobutylaluminum was employed as an activator, while in the case of catalysts **VI**–**VIII**, polymerization proceeded without any cocatalyst. The studied heterogeneous catalytic systems were found to be close to the analogous homogeneous catalysts with respect to their activity and structure of the resulting polyethylene.

MONODISPERSE CARBOXYLATED POLYSTYRENE PARTICLES: SYNTHESIS, ELECTROKINETIC AND ADSORPTIVE PROPERTIES

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Polymer, 46(4) (2005) pp. 1417-1425.

Effect of conditions of styrene dispersion polymerization initiated by 4,4′-azo-*bis*-(4-cyanopentanoic acid) in ethanol solutions of polyvinylpyrrolidone was investigated. Suitable methods ensuring the control of final particle size, surface structure, and surface concentration of carboxylic groups in the polymerization process are discussed. Particle ability to interact with protein was also studied. Monodisperse particles of diameters up to 4 μm had a complex surface layer containing polyvinylpyrrolidone-*graft*-polystyrene copolymers as well as carboxylic groups of the initiator. The effect of this surface structure on the isotherms of adsorption and chemisorption of bovine serum albumin was revealed. Electrophoretic mobility of the particles and their isoelectric point values before and after protein binding depending on pH and ionic strength were determined. These data depend on conditions of particle preparation as well as on protein coating values.

THE REACTION MECHANISM OF THE TRANSETHERIFICATION AND CROSSLINKING OF MELAMINE RESINS

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Macromol. Symp., 217(1) (2004) pp. 431-443.

Melamine formaldehyde resins (MFR) are well known resins in the wood board and paper coating market. Etherified MFR's are applied as crosslinkers in the automotive coating industry. In Europe the growth of the market and the research activities are relatively small. On the other side in comparison to other polymers outstanding properties are possible to realize. So the development of new melamine ether resins (MER) was started. MER is a partly methylolated and fully etherified resin with a highly stable “thermoplastic” processing range. The MER's themselves are transparent granulates with enough stability for storage and transport. The crosslinking reaction can be started either by thermal or acidic catalytic activation, without losses of formaldehyde. Transetherifications with oligomeric diols can lead to more elastic and higher molecular melamine polyether resin (MPER) structures. The reaction

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mechanism and the crosslinking kinetics of the partly methylolated melamine ethers of methanol in comparison to the fully methylolated hexamethylol melamine ether will be discussed in this paper.

SUBMICRON SIZED HOLLOW POLYMER PARTICLES: PREPARATION AND PROPERTIES

V.N. Pavlyuchenko, O.V. Sorochinskaya, O.N. Primachenko, S.S. Ivanchev

Macromol. Symp., 226(1) (2005) pp. 213-226.

The considered method for obtaining hollow polymer particles is based on the following pathway: (1) preparation of a carboxylated core latex by emulsion copolymerization of acrylic monomers with methacrylic acid, (2) synthesis of a core-shell latex comprising a styrene (co)polymer shell, (3) neutralization of the core carboxylic groups with a base followed by the core ionization and hydration to a high degree, shell expansion and formation of water-filled hollows. A number of approaches to improve the hydrophilic core - hydrophobic shell compatibility and enlarge the hollow volume are considered. The synthesized hollow particles are of a submicron size with the relative hollow volume $V_{hol} : V_{part.} = 0.43 - 0.64$. Methods for cationic hollow particle latex preparation by anionic latex recharging with a cationic surfactant or acidic melamine resin are discussed. Recharging with a melamine resin is shown to afford hollow particles with an external polymer shell providing a high thermal stability of the particles.

PREPARATION OF CATIONIC LATICES COMPRISING HOLLOW THERMOSTABLE PARTICLES

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J. Polym. Sci. Part A: Polymer Chemistry, 42(9) (2004) pp. 2225-2234.

A method is described for the preparation of cationic latices comprising submicron hollow particles for a possible application as a thermally stable polymeric pigment in coatings or pigmented compositions on the basis of thermosetting polymers cured at temperatures up to 170-190°C. The method is based on the deposition of melamine-formaldehyde resin in the form of cationic colloid onto anionic hollow particles resulting in the recharging of anionic hollow particles and the formation of an outer melamine shell, which provides thermal stability of the hollow particles at curing and application of pigmented coatings and compositions.

DESIGN OF SCHIFF BASE-LIKE POSTMETALLOCENE CATALYTIC SYSTEMS FOR POLYMERIZATION OF OLEFINS.

III. SYNTHESIS OF 1,2-*BIS*-(ARYLIMINO)ACENAPHTHENES HAVING CYCLIC SUBSTITUENTS

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Russ. J. Org. Chem., 41(9) (2005) pp. 1329-1332.

Reactions of substituted cycloalkylanilines with acenaphthenequinone in a mixture of methanol with methylene chloride afforded a number of the corresponding 1,2-*bis*(cycloalkylarylimino)-acenaphthenes. The products may be used as ligands for the synthesis of nickel complexes which are capable of catalyzing olefin polymerization at elevated temperature in the presence of methylaluminoxane.

NEW MULTIFUNCTIONAL *BIS*(IMINO)PYRIDINE-IRON CHLORIDE COMPLEXES AND ETHYLENE POLYMERIZATION CATALYSTS ON THEIR BASIS

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Doklady Phys. Chem., 404(1) (2005) pp. 182-185.

Oligomeric *bis*(imino)pyridine ligands are synthesized for the first time and upon their interaction with $FeCl_2$ new multifunctional *bis*(imino)pyridine-iron chloride complexes are obtained. Kinetic peculiarities of ethylene polymerization in temperature region 50-90°C over new catalytic systems in conjunction with activator methylaluminoxane are studied. Polymerization over monofunctional analogues - *bis*(imino)pyridine $FeCl_2$ of the same structure was carried out for comparison. It was shown that new multifunctional *bis*(imino)pyridine $FeCl_2$ are more efficient catalysts for ethylene polymerization at elevated temperature (60-90°C). The catalysts provide not only high reaction rates, but also high molecular weight of polyethylene mass in contrast to analogues monofunctional systems.

CONTENT

STRUCTURE AND CATALYTIC ACTIVITY OF TITANIUM AND ZIRCONIUM PHENOXYIMINE COMPLEXES

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Doklady Phys. Chem., 404(1-3) (2005) pp. 165-168.

5 complexes with general formula *bis*[N-(3-tert-butyl-5R'-saliciliden)-R''-aminato] MCl_2C (M = Ti, Zr; R' = Me, tBu; R''= n-Bu, cyclohexyl, phenyl) were synthesized in order to reveal the correlation between the structure and activity of phenoxy-imine catalysts for olefin polymerization. Ethylene polymerization was studied using these catalysts in the presence of co-catalyst methylaluminoxane. X-ray method was used to study structure and bulk architecture of Zr and Ti complexes in comparison with complexing ligand N-(3-tert-butyl-5-methyl-saliciliden)-aniline.

The conception about "living" mechanism of ethylene polymerization in the presence of catalytic systems based on phenoxy-imine Ti complexes is presented based on the results of kinetics studies and X-ray analysis. A great difference in catalytic activity of Zr and Ti derivatives is attributed not only to atomic (ionic) radiuses of transition metals, but also to their electronic structure.

Composite Sorbents and Catalysts

INVESTIGATION OF THE MOISTURE EXCHANGE IN A STATIONARY ADSORBENT LAYER THROUGH WHICH AIR IS PASSED

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JEPTER, 78(2) (2005) pp. 248-255.

The nonstationary moisture exchange between a stationary adsorbent layer and the air passed through it has been experimentally investigated. It is shown that the air humidity can be effectively regulated at both the stage of water adsorption (air dehumidification) and the stage of water desorption (air humidification) with the use of commercially produced desiccants. The degree of dehumidification and humidification of the air passed through an adsorbent can be varied from 0 to 1 by varying the nature of the adsorbent, the size of its granules, and the time for which it is in contact with the air flow.

SORPTION PROPERTIES OF CALCIUM NITRATE DISPERSED IN SILICA GEL: THE EFFECT OF PORE SIZE

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Russ. J. Phys. Chem., 79(8) (2005) pp. 1307-1311.

New composite $Ca(NO_3)_2$-in-silica gel mesopore sorbents of water were synthesized and analyzed. Sorption isobars at a water vapor pressure of 17 mbar and various sizes of silica gel pores (6, 10, 12, and 15 nm) were measured over a temperature range of 30 to 160°C. It was demonstrated that the composite sorbs water by three mechanisms: (a) heterogeneous adsorption on silica gel, (b) the formation of salt dihydrate, and (c) formation of salt aqueous solution in silica gel pores. The modification of silica gel with the salt increased significantly its sorption capacity for water (from 0.04–0.06 to 0.2–0.3 g/g). The sorption properties of the composite were found to deviate from those predicted by a linear combination of the properties of silica gel and bulk calcium nitrate. The temperature of conversion of the water-free salt into its crystalline dihydrate shifts increases with decreasing size of the pores in the host matrix. Near this transition, a sorption hysteresis was observed, which narrowed with increasing dispersity of $Ca(NO_3)_2$. The properties of a solution in the pores were found to be identical to those of the corresponding bulk solution, with no hysteresis observed. Measurements with the use of differential solvation, X-ray diffraction, and differential scanning calorimetry demonstrated that the properties of the salt change due to its being dispersed into nanosized grains rather than due to its interaction with the matrix.

APPROXIMATION EQUATIONS FOR DESCRIBING THE SORPTION EQUILIBRIUM BETWEEN WATER VAPOR AND A $CaCl_2$-IN-SILICA GEL COMPOSITE SORBENT

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Russ. J. Phys. Chem., 79(9) (2005) pp. 1490-1493.

The Polanyi potential $\Delta F = -RT \ln(p/p_s)$ was demonstrated to adequately describe the sorption equilibrium between water vapor and a $CaCl_2$-in-silica gel composite sorbent. Approximation formulas for calculating the dependence of the value of adsorption of water on ΔF and the dependence of heat of sorption on the adsorption value were derived. A comparison of experimental and theoretical data for a temperature-independent curve and sorption isobars was performed.

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AMMONIA ADSORPTION BY $MgCl_2$, $CaCl_2$ AND $BaCl_2$ CONFINED TO POROUS ALUMINA: THE FIXED BED ADSORBER

V.E. Sharonov, Yu.I. Aristov

React. Kinet. Catal. Lett., 85(1) (2005) pp. 183-188.

New composite sorbents "chlorides of alkaline-earth metals confined to porous alumina" were synthesized and tested for ammonia abatement in a fixed-bed flow adsorber at 25-300°C. It was found that the matrix modification with the salts leads to an increase in its dynamic sorption capacity in the row $BaCl_2 < CaCl_2 < MgCl_2$. This can be caused by a salt-ammonia interaction that results in the formation of ammonia complexes. The dynamic capacity was found to strongly decrease with temperature. The maximal sorption capacity was detected for a sorbent based on $MgCl_2$. It equals 58.6 and 11.6 mg/g at T = 25 and 300°C, respectively, or 3.2 and 0.6 mole of ammonia per 1 mole of the salt. The data obtained can be used for the analysis of the dynamic behavior of the new sorbents in flow systems for the ammonia removal from gas mixtures, which can be of high interest for gas separation, chemical engineering and catalysis.

COMPOSITE WATER SORBENTS OF THE SALT IN SILICA GEL PORES TYPE: THE EFFECT OF THE INTERACTION BETWEEN THE SALT AND THE SILICA GEL SURFACE ON THE CHEMICAL AND PHASE COMPOSITIONS AND SORPTION PROPERTIES

L.G. Gordeeva, A.V. Gubar, L.M. Plyasova, V.V. Malakhov, Yu.I. Aristov

Kinet. Catal., 46(5) (2005) pp. 736-742.

The influence of the inorganic salt–silica gel surface interaction on the chemical and phase compositions and sorption properties of composites of the salt in silica gel pores type is studied. Two possible interaction mechanisms are considered: (1) the ion-exchange adsorption of metal cations on the silica gel surface from a solution of a salt ($CaCl_2$, $CuSO_4$, $MgSO_4$, Na_2SO_4, and LiBr) and (2) the solid-phase spreading of a salt ($CaCl_2$) over the silica gel surface. The adsorption of metal cations on the silica gel surface in the impregnation step affords $\equiv$Si-OM^{n+} surface complexes in the composites. As a result, two salt phases are formed in silica gel pores at the composite drying stage, namely, an amorphous phase on the surface and a crystalline phase in the bulk. The sorption equilibrium between the $CaCl_2/SiO_2$ system and water vapor depends on the ratio of the crystalline phase to the amorphous phase in the composite.

ADSORPTION CHILLER BASED ON COMPOSITE $CaCl_2$ IN SILICA GEL

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Refriger. Engin., 1 (2005) pp. 2-6.

The results of tests of the laboratory prototype of adsorption chiller with two types of adsorber and consolidated layer of sorbent based on ecologically sound working pair "water - SWS-1L adsorbent" are presented. The adsorbent relates to the family of selective water sorbents and is a mesoporous silica gel KSK modified with calcium chloride. The device produces cold water with high coefficient of performance reaching 0.6 for low temperature of water desorption (80-90^{o}C) and specific power P_s=400 J/kg. These indexes prove the prospectivity and advantages of composite sorbent compared to conventional systems for adsorptive cooling.

Catalysis for Petrochemical Industry

DEVELOPMENT OF BIMF-ARKON PROCESS FOR COMPLEX PROCESSING OF HYDROCARBON RAW MATERIAL

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Catal. Ind., 1 (2005) pp. 18-19.

Based on combination of two catalytic processes BIMF (Binary Motor Fuels) and Arkon, a process of complex processing hydrocarbon raw material has been developed. The followings take place according to the method being proposed: first, conversion of hydrocarbon raw material occurs, which boils away at T = 35÷360 °C, into high-octane gasoline, winter diesel fuel, and condensed gas C3–C4 (BIMF); then exhaust gases are supplied in the Arkon process reactor where they are converted into concentrate of aromatic compounds. The new method was tested in a pilot plant of no more than 1.5 thousand ton/year in capacity as to raw material using zeolite catalysts IK-30-BIMF (charge is 150 liters) and IK-17-M for

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Arkon (60 liters) containing no precious metals. The process being proposed allows to increase significantly output of liquid products as compared with the base version of the BIMF process.

ACIDIC AND CATALYTIC PROPERTIES OF Mo-CONTAINING ZEOLITE CATALYSTS FOR NON-OXIDATIVE METHANE CONVERSION

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Eurasian Chem.-Techn. J., 6(3) (2004) pp. 201-206.

The conversion of methane into benzene, toluene and naphthalene at the reaction temperature of 750°C and gas hourly space velocity (GHSV) of 500-1500 h^{-1} over zeolites modified via impregnation with ammonium heptamolybdate and mechanical mixing with Mo oxide and nanopowder is studied under non-oxidative conditions. It has been established that the highest methane conversion per one run and maximal yield of aromatic hydrocarbons are reached for the sample containing 4.0 mass.% of Mo nanopowder. The stability of Mo-containing zeolite catalysts in the process of methane dehydroaromatization at different GHSV has been studied and a characteristic presence of the induction period caused by the formation of active Mo forms both on the external surface and into the zeolite channels has been established. Both the duration of induction period and stable catalyst operation are decreasing with increasing of GHSV. It was demonstrated that acidic properties of a Mo-containing zeolite catalyst depend on Mo concentration and method of its introduction.

DEACTIVATION OF MOLYBDENUM-CONTAINING ZEOLITES IN THE COURSE OF NONOXIDATIVE METHANE CONVERSION

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Kinet. Catal., 46(5) (2005) pp. 724-729.

It was found that the nonoxidative dehydroaromatization of methane occurs over Mo-containing pentasil-type zeolites with various framework compositions at 750°C. This reaction is accompanied by catalyst deactivation because of coke formation. The effects of the space velocity of methane and the composition of the zeolite matrix on the amount and properties of the resulting condensation products were studied. It was found that the lowest amount of coke with a relatively low degree of polycondensation was formed on zeolite with $SiO_2/Al_2O_3 = 40$ containing Mo nanoparticles.

RELATION BETWEEN HYDRO-DEHYDROGENATING AND ACID FUNCTIONS OF ZEOLITE CATALYSTS AND THEIR EFFECTIVENESS IN AROMATIZATION OF LIGHT PARAFFINS

**G.V. Echevsky, E.G. Kodenev, E.A. Paukshtis,
V.V. Molchanov**

React. Kinet. Catal. Lett., 84(2) (2005) pp. 367-373.

Aromatization of light paraffins with Zn-containing catalysts based on the ZSM-5 zeolite is considered. The correlation between acidic and hydro-dehydrogenating functions of the catalysts, on one hand, and their activity and selectivity towards aromatics, on the other hand, is discussed. The modification of external acid sites is shown to influence significantly the catalytic properties of the prepared samples.

PERFORMANCE OF A CATALYTIC MEMBRANE REACTOR FOR THE FISCHER-TROPSCH SYNTHESIS

**A.A. Khassin, A.G. Sipatrov, T.M. Yurieva,
G.K. Chermashentseva, N.A. Rudina, V.N. Parmon**

Catal. Today, 105(3-4) (2005) pp. 362-366.

The study of permeable composite monolith (PCM) membranes for the Fischer-Tropsch synthesis is continued. On the scale of membranes with outer diameter of 42 mm, it is proved that PCM can combine high productivity of hydrocarbons (above 55 $kg_{C5+}\cdot(m_{PCM}^{3}\cdot hr)^{-1}$ at 0.6 MPa, 484 K), high selectivity towards heavy hydrocarbons ($\alpha_{ASF} > 0.85$, C_{5+} up to 0.9), as well as high heat-conductivity and high mechanical strength.

MEMBRANE REACTORS FOR THE FISCHER-TROPSCH SYNTHESIS

A.A. Khassin

In "*Sustainable Strategies for the Upgrading of Natural Gas: Fundamentals, Challenges, and Opportunities*", NATO Sci. Ser. II: Math., Phys. and Chem., Eds. E.G. Derouane, V.N. Parmon, F. Lemos, F.R. Ribeiro, Springer Verlag, Vol. 191, 2005, pp. 249-271.

The analysis of the specific features of the Fischer-Tropsch synthesis helps formulating the most important requirements to the FTS reactor. Membrane reactor designs can be useful for the FTS process application. Semi-permeable hydrogen-selective distributors allow to control the H_2:CO ratio along the catalyst bed and thus enhance the selectivity of the process. Membranes of extractor type can help to improve the FTS performance by selective removing water from the reaction volume. On the other hand, plug-through contactor membrane reactor design (PCM) seems to meet all the other requirements, ensuring the high concentration of the catalyst, isothermicity, high gas-liquid interface area, small effective diffusion length and reasonable hydraulic resistance. Varying the membrane composition and conditions of its preparation leads to the changes in porous structure parameters of the PCM membrane. This allows to weaken the diffusion constrains in a predictable way and, therefore, to control the productivity and selectivity of the Fischer-Tropsch process.

FISCHER–TROPSCH SYNTHESIS USING PLUG-THROUGH CONTACTOR MEMBRANES BASED ON PERMEABLE COMPOSITE MONOLITHS. SELECTIVITY CONTROL BY POROUS STRUCTURE PARAMETERS AND MEMBRANE GEOMETRY

A.A. Khassin, A.G. Sipatrov, G.K. Chermashetseva, T.M. Yurieva, V.N. Parmon

Top. Catal., 32(1-2) (2005) pp. 39-46.

The Fischer–Tropsch synthesis using a contactor membrane reactor was studied varying pore size distribution parameters and membrane geometry. These parameters are responsible for the magnitude of the diffusion constrains and, therefore, correlate with the FTS process productivity and selectivity. The nature of the observed correlations is discussed.

FISCHER-TROPSCH CATALYSTS BASED ON Zr-Fe INTERMETALLIDES ENCAPSULATED IN AN Al_2O_3/Al MATRIX

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Kinet. Catal., 46(5) (2005) pp. 743-751.

Zr-Fe and Zr-Fe_2 intermetallides in an Al_2O_3/Al cermet matrix are reported as catalysts for the fixed-bed Fischer–Tropsch synthesis, and the effects of some preparation conditions on their texture, structural, mechanical, and catalytic properties are discussed. A nonmonotonic dependence of their catalytic activity on the size of intermetallide particles is observed. The selectivity, activity, and mechanical strength of the composites depend on the calcination temperature and on the place of the hydriding step in the catalyst preparation procedure. In terms of volumetric efficiency, the catalysts prepared are comparable with bulk, unencapsulated intermetallides and are among the most efficient iron-containing catalysts known to date.

OXIDATION OF CO, DEEP OXIDATION OF CH_4, AND REDUCTION OF NO_X BY PROPANE ON $CuCo_2O_4$ AND Pd-CeO_2 CATALYSTS SUPPORTED ON RIBBON SUBSTRATES

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Petroleum Chem., 45(4) (2005) pp. 255-260.

The catalytic properties of Co_3O_4, CuO, $CuCo_2O_4$, and Pd–CeO_2 were studied in neutralization reactions of toxic components of exhaust gases: deep oxidation of CH_4, oxidation of CO, and reduction of NO_x by propane. The activity of cobalt–copper oxide catalysts in these reactions was shown to be comparable with that of palladium-containing samples as the result of synergistic effects.

SELECTIVE OXIDATION OF HYDROCARBONS INTO SYNTHESIS GAS AT SHORT CONTACT TIMES: DESIGN OF MONOLITH CATALYSTS AND MAIN PROCESS PARAMETERS

V.A. Sadykov, S.N. Pavlova, R.V. Bunina, G.M. Alikina, S.F. Tikhov, T.G. Kuznetsova, Yu.V. Frolova, A.I. Lukashevich, O.I. Snegurenko, N.N. Sazonova, E.V. Kazantseva, Yu.N. Dyatlova, V.V. Usoltsev, I.A. Zolotarskii, L.N. Bobrova, V.A. Kuzmin, L.L. Gogin, Z.Yu. Vostrikov, Yu.V. Potapova, V.S. Muzykantov, E.A. Paukshtis, E.B. Burgina, V.A. Rogov, V.A. Sobyanin, V.N. Parmon

Kinet. Catal., 46(2) (2005) pp. 227-250.

This review summarizes the main achievements of the Boreskov Institute of Catalysis in the development of efficient and stable monolith catalysts for selective oxidation of hydrocarbons into synthesis gas at short contact times. Research in this field has included (1) design of new types of active component based on metal

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oxides, (2) design of new types of monolith support and development of supporting procedures for active components, and (3) optimization of process parameters for different types of fuel (natural gas, isooctane, and gasoline) and oxidant (air oxygen, including its mixtures with water and carbon dioxide), including the start-up regime. Design of active components (platinum, nickel, or their combination) supported on fluorite-like solid solutions based on cerium dioxide and rare-earth (samarium, gadolinium, and praseodymium) or zirconium cations has been aimed at separating hydrocarbon activation (on metal sites) and oxidation (on the support) and conjugating the separated steps of hydrocarbon oxidation at the metal–oxide interface. Optimization of oxygen mobility in the support lattice by varying the nature and concentration of doping cation along with optimization of hydrocarbon activation on supported metal clusters allow hydrocarbons to be completely converted into synthesis gas by selective oxidation or dry or steam reforming at contact times of a few milliseconds, ruling out undesirable carbon build-up on the catalyst surface. The development of new types of monolith support has targeted the enhancement of thermal shock resistance, including testing of supports based on thermally stable metal foils and composites (cermets). The main steps of the production of these supports have been refined, including unique technologies of blast dusting and hydrothermal treatment. The electric conductivity of these systems allows a quick startup of selective oxidation to be performed by passing electric current, and their thermal conductivity minimizes the temperature gradient arising from heat transfer in the bed. Procedures for loading monolith supports with active components have been developed, including impregnation, washcoating, or encapsulation in cermet matrices. The catalysts produced show a high efficiency and an operational stability adequate to the above tasks in the selective oxidation and steam–air autothermal reforming of natural gas (including processes under pressure), isooctane, and gasoline into synthesis gas.

PARTIAL OXIDATION OF METHANE TO SYNTHESIS GAS OVER CORUNDUM SUPPORTED MIXED OXIDES: ONE CHANNEL STUDIES

S.N. Pavlova, N.N. Sazonova, V.A. Sadykov, S.A. Pokrovskaya, V.A. Kuzmin, G.M. Alikina, A.I. Lukashevich, E.L. Gubanova

Catal. Today, 105(3-4) (2005) pp. 367-371.

Catalytic partial oxidation of methane (POM) over the monolithic catalyst $LaNiO_x/CeO_2–ZrO_2/\alpha\text{-}Al_2O_3$ has been studied. Experiments were conducted with one channel of a monolith at a varied channel length, contact time (~1–6 ms) and temperature using the diluted gas mixture (1% CH_4 + 0.5% O_2 in He). At increasing temperature and contact time, CO selectivity rises within the whole temperature range whereas the contact time dependence of H_2/CO ratio varies with the temperature. These results support the POM reaction scheme including primary formation of CO and H_2 followed by their oxidation in the presence of gas-phase O_2. Steam and dry methane reforming reactions occur in the part of monolithic channel where oxygen is absent, thus increasing syngas yield.

HONEYCOMB SUPPORTED CATALYSTS FOR METHANE OXIDATION

L.A. Isupova, N.A. Kulikovskaya, Yu.I. Amosov, N.F. Saputina, L.M. Plyasova, N.A. Rudina, I.A. Ovsyannikova, V.F. Tretyakov, T.N. Burdeinaya, V.A. Sadykov

In “*Catalytic Combustion*”, Eds. P. Forzatti,
G. Groppi, P. Cisambelli, D. Sannino,
Proceedings of the 6th International Workshop on
Catalytic Combustion,
Vol. 2, 2005, pp. 34-38.

The paper presents data on the catalytic activity in methane oxidation and its autothermal flameless combustion for oxides supported on honeycomb cordierite monoliths by Pechini route and noble metral doped oxide catalysts.

STRUCTURAL FEATURES AND THE LATTICE OXYGEN REACTIVITY OF LOW-TEMPERATURE LANTHANUM MANGANITES DOPED WITH DIFFERENT CATIONS

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React. Kinet. Catal. Lett.,
86(2) (2005) pp. 249-256.

Dispersed samples of $LaMnO_3$ prepared *via* the Pechini route and annealed at 500°C were doped with cations of a different charge and size (Ce, Fe, Bi, Sr+Bi). The effects of doping on the structural features (XRD, IR) and reducibility (H_2TPR) of these samples were considered.

MOBILITY AND REACTIVITY OF LATTICE OXYGEN IN Gd-DOPED CERIA PROMOTED BY Pt

V.A. Sadykov, Yu.V. Frolova, V.V. Kriventsov, D.I. Kochubey, E.M. Moroz, D.A. Zyuzin, Yu.V. Potapova, V.S. Muzykantov, V.I. Zaikovskii, E.B. Burgina, H. Borchert*, S.N. Trukhan, V.P. Ivanov, S. Neophytides, E. Kemnitz***, K. Scheurell***** (**Oldenburg University, Oldenburg, Germany; **Institute of Chemical Engineering & High Temperature Processes, Patras, Greece; ***Institute for Chemistry, Humboldt-University, Berlin, Germany*)

React. Kinet. Catal. Lett., 85(2) (2005) pp. 367-374.

For samples of the $Ce_{1-x}Gd_xO_{2-y}$ system prepared by the Pechini route and promoted with Pt, the mobility and reactivity of lattice oxygen were found to correlate with the density of surface and bulk anion vacancies.

EFFECT OF THE LATTICE OXYGEN MOBILITY ON THE ACTIVITY OF Gd–DOPED CERIA PROMOTED WITH Pt IN SYNGAS GENERATION FROM METHANE AT SHORT CONTACT TIMES

V.A. Sadykov, Yu.V. Frolova, G.M. Alikina, A.I. Lukashevich, S. Neophytides* (**Institute of Chemical Engineering & High Temperature Processes, Patras, Greece*)

React. Kinet. Catal. Lett.,
85(2) (2005) pp. 375-382.

The activity of $Pt/Ce_{1-x}Gd_xO_{2-y}$ samples in steam and dry reforming of methane at short contact times correlates with the lattice oxygen mobility. For the partial oxidation of methane (POM), the oxygen mobility should be optimized to prevent methane combustion.

NANOSTRUCTURED, Gd-DOPED CERIA PROMOTED BY Pt OR Pd: INVESTIGATION OF THE ELECTRONIC AND SURFACE STRUCTURES AND RELATIONS TO CHEMICAL PROPERTIES

H. Borchert*, Yu. Borchert, V.V. Kaichev, I.P. Prosvirin, G.M. Alikina, A.I. Lukashevich, V.I. Zaikovskii, E.M. Moroz, E.A. Paukshtis, V.I. Bukhtiyarov, V.A. Sadykov (**Oldenburg University, Oldenburg, Germany*)

J. Phys. Chem. B,
109(43) (2005) pp. 20077-20086.

Nanostructured ceria doped with other rare earth elements is a good oxygen ion conductor, which gives rise to various catalytic applications such as the construction of membranes for syngas production by partial oxidation of methane. This article focuses on the Gd-doped cerium dioxides, which can be modified with Pt or Pd to enhance the reactivity of the lattice oxygen in interaction with methane. The aim of the work is the elucidation of correlations between the structural, electronic, and chemical properties of these nanomaterials. Detailed studies were performed for a series of samples with and without surface modification by noble metals using a complex combination of physicochemical methods: XRD, TEM, CH_4 TPR, XPS, SIMS, and FTIR spectroscopy of adsorbed CO. XPS and TPR data revealed that surface modification with noble metals enhances the reducibility of the doped ceria support, where the effect is more pronounced for Pd than for Pt. The formation of highly cationic Pd species due to strong metal support interactions provides a possible explanation for this behavior. Furthermore, the results obtained in the present work for the Gd-doped ceria system are compared to those obtained for the Pr-doped ceria system.

MOBILITY AND REACTIVITY OF THE LATTICE OXYGEN OF Pr-DOPED CERIA PROMOTED WITH Pt

V.A. Sadykov, Yu.V. Frolova, G.M. Alikina, A.I. Lukashevich, V.S. Muzykantov, V.A. Rogov, E.M. Moroz, D.A. Zyuzin, V.P. Ivanov, H. Borchert*, E.A. Paukshtis, V.I. Bukhtiyarov, V.V. Kaichev, S. Neophytides, E. Kemnitz***, K. Scheurell***** (**Oldenburg University, Oldenburg, Germany; **Institute of Chemical Engineering & High Temperature Processes, Patras, Greece; ***Institute for Chemistry, Humboldt-University, Berlin, Germany*)

React. Kinet. Catal. Lett.,
86(1) (2005) pp. 21-28.

For Pr-doped ceria $Ce_{1-x}Pr_xO_{2-y}$ prepared by the Pechini route and promoted with Pt, the mobility and reactivity of lattice oxygen were found to depend on the Pr content, which seems to determine the density of surface and bulk anion vacancies and domain boundaries.

PERFORMANCE OF Pr-DOPED CERIA PROMOTED BY Pt IN SYNGAS GENERATION FROM METHANE AT SHORT CONTACT TIMES

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React. Kinet. Catal. Lett.,
86(1) (2005) pp. 29-36.

Effects of the lattice oxygen mobility, Pt dispersion and the surface features of $Pt/Ce_{1-x}Pr_xO_{2-y}$ samples on their performance in the selective oxidation of methane into syngas, in the steam and dry reforming of methane at short contact times are considered.

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STRUCTURE SPECIFICITY OF NANOCRYSTALLINE PRASEODYMIA DOPED CERIA

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Mater. Res. Soc. Symp. Proc.,
848 (2005) pp. 231-236.

The features of the structure of nanorystalline $Ce_{1-x}Pr_xO_{2-y}$ system ($0<x<0.5$) prepared via a complex polymerized precursor (Pechini) route have been elucidated by using a combination of spectroscopic (XANES, XPS) and structural (TEM, neutron diffraction) methods. Within the studied range of composition, the structure of all samples air annealed at 500°C corresponds to single-phase fluorite-like solid solution. The relative content of Pr^{3+} both in the bulk and in the surface layer appears to be as high as 20-50%. The Rietveld refinement revealed non-monotonous variation of structural parameters (lattice parameter, domain size, microstrain density, Ce-O and O-O distances) and residual lattice hydroxyls concentration with Pr content. Clustering of defects along with variation of the mean Pr cation radius/charge state and disordering of the surface layer/domain boundaries appear to be responsible for the observed features.

ELECTRONIC AND CHEMICAL PROPERTIES OF NANOSTRUCTURED CERIUM DIOXIDE DOPED WITH PRASEODYMIUM

H. Borchert*, Yu.V. Frolova,V.V. Kaichev, I.P. Prosvirin, G.M. Alikina, A.I. Lukashevich, V.I. Zaikovskii, E.M. Moroz, S.N. Trukhan, V.P. Ivanov, E.A. Paukshtis, V.I. Bukhtiyarov, V.A. Sadykov (**Oldenburg University, Oldenburg, Germany*)

J. Chem. Phys. B, 109(12) (2005)
pp. 5728-5738.

Nanostructured doped ceria is a prospective material for catalytic applications such as the construction of membranes with mixed electronic and ionic conductivity for effective syngas production. In this article, the surface properties of nanostructured ceria doped with praseodymium have been studied by X-ray photoelectron spectroscopy, secondary ion mass spectrometry, and Fourier transform infrared spectroscopy of adsorbed carbon monoxide. The effects of supporting 1.4 wt % Pt as well as structural changes upon the reduction of the samples with methane have been investigated. While in samples without supported platinum, mainly praseodymium cations are reduced in a methane atmosphere; stronger reduction of cerium cations was found in the case of surface modification with Pt. The structural differences correlate with results from temperature-programmed reaction experiments with methane. Explanations are discussed in terms of different reaction mechanisms.

SPECIFICITY OF THE LOCAL STRUCTURE OF NANOCRYSTALLINE DOPED CERIA SOLID ELECTROLYTES

V.A. Sadykov, Yu.V. Frolova, V.V. Kriventsov, D.I. Kochubey, E.M. Moroz, D.A. Zyuzin, Yu.V. Potapova, V.S. Muzykantov, V.I. Zaikovskii, E.B. Burgina, H. Borchert*, S.N. Trukhan, V.P. Ivanov, S. Neophytides, E. Kemnitz***, K. Scheurell***** (**Oldenburg University, Oldenburg, Germany; **Institute of Chemical Engineering & High Temperature Processes, Patras, Greece; ***Institute for Chemistry, Humboldt-University, Berlin, Germany*)

Mater. Res. Soc. Symp. Proc.,
Vol. 835 (2005) K3.6, pp. 199-204.

This work presents results of studies of the structural features of nanocrystalline doped $Ce_{1-x}Me_xO_{2-y}$ samples (Me = Sm, Bi, Gd; x = 0-0.5) prepared via the polymerised precursor (Pechini) route by using a combination of diffraction (XRD, TEM, WAXS on SR) and spectroscopic (EXAFS, Raman, FTIRS of lattice modes, XPS, SIMS) methods.

FUEL-RICH METHANE COMBUSTION: ROLE OF THE Pt DISPERSION AND OXYGEN MOBILITY IN A FLUORITE-LIKE COMPLEX OXIDE SUPPORT

V.A. Sadykov, T.G. Kuznetsova, Yu.V. Frolova, G.M. Alikina, A.I. Lukashevich, V.A. Rogov, V.S. Muzykantov, L.G. Pinaeva, E.M. Sadovskaya, Yu.A. Ivanova, E.A. Paukshtis, N.V. Mezentseva, V.N. Parmon, S. Neophytides*, E. Kemnitz, K. Scheurel**, C. Mirodatos***, A.C. van Veen***** (**Institute of Chemical Engineering & High Temperature Processes, Patras, Greece; **Institute for Chemistry, Humboldt-University, Berlin, Germany *Institut de Recherches sur la Catalyse, Villeurbanne Cedex, France*)

Proceedings of 6th International Workshop on Catalytic Combustion, Eds. P. Forzatti, G. Groppi,
P. Ciambelli, D. Sannino, Vol. 1, 2005, pp. 94-98.

This work summarizes results of systematic studies of the role of the oxygen mobility in support, Pt dispersion and Pt-support interaction for ceria and ceria-zirconia systems doped with La, Sm, Pr or Gd and promoted with Pt as catalysts of methane selective oxidation into syngas (POM) at short contact times.

CATALYTIC SYNTHESIS OF THIOLS FROM ALCOHOLS AND HYDROGEN SULFIDE

A.V. Mashkina

Petroleum Chem., 45(1) (2005) pp. 44-52.

The basic features of the reaction of thiol synthesis from hydrogen sulfide and methanol, *n*-propanol, *n*-butanol, or *n*-dodecanol in the presence of acid–base catalysts was studied. The catalysts with paired surface sites - weak Lewis acid sites and strong base sites - have a low activity but are selective in thiol formation. The catalysts with strong acid sites exhibited a high activity in the conversion of alcohols but were not selective in the formation of thiols. In the presence of proton-donor catalysts, the thiolation of methanol alone took place; other alcohols underwent only dehydration. The thiolation of methanol on various catalysts yielded dimethyl sulfide along with metanethiol; no dialkyl sulfides was produced in the reaction of hydrogen sulfide with higher alcohols.

HYDROGENOLYSIS OF DIMETHYL DISULFIDE TO METHANETHIOL IN THE PRESENCE OF COBALT SULFIDE CATALYSTS

A.V. Mashkina, L.N. Khairulina

Kinet. Catal., 46(6) (2005) pp. 873-878.

The hydrogenolysis of dimethyl disulfide to methanethiol at T=180–260°C and atmospheric pressure in the presence of supported cobalt sulfide catalysts has been studied. Cobalt sulfide on aluminum oxide exhibits a higher activity than that on a carbon support or silicon dioxide. The maximum reaction rate per gram of a catalyst is observed on an 8% Co/Al_2O_3 catalyst. At temperatures of up to 200°C and conversions up to 90%, methanethiol is formed with nearly 100% selectivity regardless of the cobalt content, whereas the selectivity for methanethiol under more severe conditions decreases because of its condensation to dimethyl sulfide.

CATALYTIC TRANSFORMATIONS OF ALKYLTHIOPHENES

A.V. Mashkina, V.I. Chernov

Petroleum Chem., 45(3) (2005) pp. 209-215.

The transformations of alkylthiophenes in the presence of amorphous aluminosilicate and decationated zeolite HNaY were studied. Substituted thiophenes with R = 2- and 3-Me, 2-Et, and 2-*iso*-Pr undergo dealkylation to thiophene with close rates, migration of the alkyl group from the α- to the β-position of the thiophene ring (or in the opposite direction with an elevated rate), and decomposition with H_2S elimination. The dealkylation rate of 2-substituted thiophenes with a branched-chain radical (R = *iso*-Pr, *tert*-Bu) is much higher and the elimination rate with this radical is lower than those for normal-chain radicals; the isomerization step is virtually absent. Di-, tri-, and tetrasubstituted thiophenes with R = Et and *iso*-Pr undergo stepwise dealkylation, which is facilitated by an increase in the degree of substitution on the thiophene ring. Thiophene and its lower homologues can be obtained by the transformation of a mixture of high-molecular thiophenes.

CATALYST ACTIVITY IN ALKYLTHIOPHENE DEALKYLATION

A.V. Mashkina, V.I. Chernov

Kinet. Catal., 46(1) (2005) pp. 88-95.

The transformations of 2-alkylthiophenes on various catalysts were studied. In the presence of oxide and sulfide catalysts, 2-methylthiophenes and 2-isopropylthiophenes underwent dealkylation to thiophene. The reaction was complicated by isomerization to 3-alkylthiophene and cracking. The dealkylation of 2-ethylthiophene occurred only in the presence of oxide catalysts. Side-chain dehydrogenation resulting in the formation of 2-vinylthiophene primarily occurred under the action of sulfide and some oxide catalysts. Acid catalysts (amorphous aluminosilicate and zeolites in the form of hydrogen) were the most active and selective in the dealkylation of 2-alkylthiophenes. It is believed that the dealkylation reaction of 2-alkylthiophenes on these catalysts occurs by means of a protolytic mechanism.

Mathematical Simulation of Processes and Reactors. Chemical Engineering

MATHEMATICAL MODELING OF STEAM REFORMING TUBES WITH SHAPED PARTICLES

A.P. Kagyrmanova, I.A. Zolotarskii,
N.V. Vernikovskaya, E.I. Smirnov, V.A. Kuzmin

In *"Sustainable Strategies for the Upgrading of Natural Gas: Fundamentals, Challenges, and Opportunities"*, Eds. E.G. Derouane, V. Parmon, F. Lemos, F.R. Ribeiro, *NATO Science Series II: Mathematics, Physics and Chemistry*, 191 (2005) pp. 389-394.

In the present work modeling of steam reformer tubes is performed for different shaped catalysts based on an original two-dimensional pseudo-homogeneous model. The model accounts for the following heat and mass transfer phenomena: heat transfer between the tube wall and catalyst bed, conductivity and diffusivity in the radial direction in the packed bed and intraparticle diffusion.

SIMULATION OF STEAM REFORMING TUBE WITH SHAPED PARTICLES

A.P. Kagyrmanova, N.V. Vernikovskaya,
I.A. Zolotarskii, E.I. Smirnov, V.A. Kuzmin

Eurasian Chem.-Tech. J., 7(1) (2005) pp. 57-66.

Shaped catalysts are widely used in steam reforming. A comprehensive mathematical model able to predict and compare performance of different shaped catalysts is developed. The two-dimensional pseudo-homogeneous model accounts for heat transfer between the tube wall and catalyst bed, diffusivity in the radial direction in the packed bed and intraparticle diffusion. Gas volume changing caused by reaction stoichiometry results in a radial convective mass flux. A verification of the model and simulated performance of different shaped catalyst in steam reforming of natural gas are presented.

THEORETICAL OPTIMIZATION OF THE SHAPE AND DIMENSIONS OF THE STEAM REFORMING CATALYST

A.P. Kagyrmanova, I.A. Zolotarskii,
N.V. Vernikovskaya, E.I. Smirnov

Chem. Ind. Today, 11 (2005) pp. 18-30.

This paper presents theoretical optimization of dimensions of shaped catalyst for steam natural gas conversion and also the comparison of their efficiency. Optimization was performed using the previously elaborated comprehensive mathematical model of the process in catalyst grain and layer with application of novel procedure for prediction of parameters of radial heat and mass transfer in the catalyst layer of complex particles.

THE PARALLEL REALIZATION OF FUNDAMENTAL SOLUTION OF POISSON'S EQUATION

E.A. Kuksheva, V.N. Snytnikov

Comput. Technol., 10(4) (2005) pp. 63-71.

A discrete analogue of the fundamental solution of the Poisson's equation is considered with the emphasis on the parallelization and adequacy of solution.

SUPERCOMPUTER SIMULATION OF SELF-GRAVITATING MEDIA

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Future Gener. Comput. Syst., 21(5) (2005) pp. 749-757.

A numerical 3D-model for investigation of non-stationary processes in a gravitating system with gas has been created. The model is based on the solution of the Poisson equation for gravitational field, the Vlasov–Liouville equation for solids and equations of gas dynamics. For solution of the Poisson equation at each time step an efficient iterational solver is created with extrapolation of the evolutionary processes under study. It provides fast convergence at high precision. Parallelisation technique and load balancing strategy are discussed.

NUMERICAL SOLUTION OF DIRECT CHEMICAL KINETICS PROBLEMS ON THE BASIS OF MODERN INFORMATION TECHNOLOGIES

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Numerical Meth. Progr., 6 (2005) pp. 71-76.

The ChemPAK program package for solving direct chemical kinetics problems with arbitrary number of chemical reactions is considered. The package contains an expandable library of computational modules and provides data transfer to multiprocessor systems. Using the ChemPAK software package, the problem of applicability of kinetic schemes for the C1-C2 hydrocarbon's pyrolysis to modeling the physico-chemical processes in gas-dynamic reactors with emission is solved.

NMR IMAGING OF MASS TRANSPORT PROCESSES AND CATALYTIC REACTIONS

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Top. Catal., 32(1-2) (2005) pp. 83-91.

NMR imaging and spectroscopy techniques are applied to study flow and filtration of liquids, gases and granular solids in various geometries and to the *in situ* studies of the interplay of mass transport and catalytic reactions in porous media. In particular, quantitative spatially resolved maps of flow velocities of liquids and gases in the channels of monoliths have been obtained. A comparative study of the filtration of water and propane through model porous media has revealed that the dispersion coefficients for water are dominated by the holdup effects even in a bed of nonporous glass beads. Similar experiments performed with the gravity driven flow of liquid-containing fine solid particles through a porous bed have yielded the distributions of particle velocities for various flow rates. The NMR imaging technique was employed to visualize the propagation of autocatalytic waves for the Belousov–Zhabotinsky reaction carried out in a model porous medium. It was demonstrated that the wave propagation velocity decreases as the wave crosses the boundary between the bulk liquid and the flooded bead pack. The images detected during the catalytic hydrogenation of α-methylstyrene on a single catalyst pellet at elevated temperatures have revealed that the reaction and the accompanying phase transition alter the distribution of the liquid phase within the pellet.

IN SITU MRI OF THE STRUCTURE AND FUNCTION OF MULTIPHASE CATALYTIC REACTORS

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(**International Tomography Center, Novosibirsk, Russia*)

Catal. Today, 105(3-4) (2005) pp. 464-468.

NMR imaging (MRI) was used to study the distribution of the liquid phase in an operating trickle bed reactor using hydrogenation of α-methylstyrene or *n*-octene-1 as representative examples. In a single pellet reactor, the existence of oscillating regimes under unchanged external conditions was shown. The experiments with packed beds have demonstrated the non-uniform distribution of the liquid phase over the bed, the presence of partially liquid-filled or completely dry catalyst particles in the operating reactor, and the existence of liquid phase transport between liquid-filled and dry catalyst particles. Detection of spatially resolved NMR spectra was used to characterize chemical conversion variations within the operating reactor. Preliminary MRI results for an operating monolithic reactor were obtained. It was found that MRI can be used to directly image solid materials using NMR signal detection of nuclei other than ^{1}H. In particular, imaging of alumina using ^{27}Al NMR signal appears highly promising for the development of novel MRI applications in chemical engineering and catalysis, including spatially resolved NMR thermometry.

SELF-OSCILLATIONS ON A PARTIALLY WETTED CATALYST PELLET IN α-METHYLSTYRENE HYDROGENATION: EXPERIMENT AND MATHEMATICAL MODELING

V.A. Kirillov, I.V. Koptyug*, A.V. Kulikov, N.A. Kuzin, A.A. Lysova*, A.B. Shigarov, V.N. Parmon** (**International Tomographic Center, Novosibirsk, Russia; **Novosibirsk State University, Novosibirsk, Russia*)

Theor. Found. Chem. Eng., 39(1) (2005) pp. 24-35.

Self-oscillation modes on an irrigated porous catalyst pellet in exothermic hydrogenation accompanied by liquid evaporation is studied. By NMR tomography (magnetic resonance microimaging), images of the liquid-phase distribution within the porous object are obtained and the liquid-phase redistribution is monitored immediately during the process without destroying the object and without introducing any probes or molecular labels.

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RADIAL REACTOR-HEAT EXCHANGER FOR NATURAL GAS COMBUSTION IN A STRUCTURED POROUS METAL CATALYST BED

V.A. Kirillov, N.A. Kuzin, V.A. Kuzmin, V.B. Skomorokhov, A.B. Shigarov

Theor. Found. Chem. Eng.,
39(4) (2005) pp. 407-414.

A compact (0.01 m^3 in volume) radial reactor for deep oxidation of methane (with a heat output of 16–30 kW) that is combined with an internal water heat exchanger is designed. The reactor contains the structured porous metal catalyst 5% (0.5% Pt/ν-Al_2O_3) + 65% Ni + 5% Al. The reactor performance at different heat outputs is experimentally studied. It is demonstrated that, if catalytic methane combustion is virtually complete, the fraction of heat transferred to the internal heat exchanger (to the water) is large (31-53%) and allows the reactor to reach a specific heat output up to 130 kW/m^2 (on the outer surface of the catalytic heating element). The coefficients of heat transfer to the internal heat exchanger and the radial thermal conductivity of the catalyst bed are shown to theoretically strongly affect the thermal conditions in the catalyst bed. It is concluded that the proposed mathematical model fits the experimental data well.

AMMONIA OXIDATION INTO NITROUS OXIDE OVER Mn/Bi/Al CATALYST. II. FLUIDIZED BED REACTOR EXPERIMENTS

A.S. Noskov, I.A. Zolotarskii, S.A. Pokrovskaya, V.N. Kashkin, E.M. Slavinskaya, V.V. Mokrinskii, V.N. Korotkikh

Chem. Eng. J., 107(1-3) (2005) pp. 79-87.

The process of synthesis of nitrous oxide by ammonia oxidation in a fluidized catalyst bed reactor was studied using a suite of tools including both hardware and software. Pilot testing of the process was carried out in a fluidized bed reactor with a microspherical Mn/Bi/Al catalyst loaded therein. The experimental runs were guided by kinetic and simulation results. The stable operation regimes were achieved at the inlet ammonia concentration up to 45%; the selectivity for N_2O was 86–88% at the ammonia conversion of 98–99.5% in the optimal temperature range. The catalytic activity and the selectivity remained constant during pilot tests. The modeling data agreed with the experimental results.

Modeling of the large-scale reactor revealed that the catalyst productivity could be improved using the fluidized bed reactor in comparison to that in the tubular reactor due to the much more concentrated inlet flow. The inlet concentrations of ammonia could be much higher than that used in a tubular reactor (35–50 and 7–8%, respectively).

OPTIMIZATION OF THE ACTIVE COMPONENT DISTRIBUTION THROUGH THE CATALYST BED FOR THE CASE OF ADIABATIC REACTOR

V.M. Khanaev, E.S. Borisova, A.S. Noskov

Chem. Eng. Sci., 60(21) (2005) pp. 5792-5802.

This article is the next one in the previous series of publications concerning the optimal active component distribution. The aim of the present work is to extend the optimization problem taking into account the energy balance. The variational problem on searching for the optimal active component distribution profile along the catalyst bed was formulated for the case of an adiabatic reactor at an arbitrary form of reaction rate expression. The Euler differential equation was derived and the existence conditions for the solution of variational problem were obtained. A numerical algorithm was suggested and the optimal profiles of the active component distribution were calculated for the first-order reaction. Under isothermal conditions with linear dependence of the reaction rate on reactant concentration at a constant mass transfer coefficient, the uniform distribution is optimal. As opposed to the case of an isothermal reactor with a first-order catalytic reaction, in an adiabatic reactor considerable economy in the active component loading might be achieved due to optimization of its distribution. It was shown that the optimal active component distribution profiles were axially decreasing for the first-order exothermic reactions and increasing for endothermic reactions. The optimal active component distribution profile was calculated for the case of methane combustion on catalytic monoliths.

OPTIMAL DISTRIBUTION OF THE ACTIVE COMPONENT IN CATALYTIC METHANE OXIDATION

V.M. Khanaev, E.S. Borisova, A.S. Noskov

Theor. Found. Chem. Eng.,
39(5) (2005) pp. 478-486.

A mathematical model for determining the optimal distribution of the active component in catalytic methane oxidation is considered, and necessary conditions for the existence of a solution are obtained. It is shown that, under adiabatic conditions, the optimal distribution is a monotonically decreasing distribution of the active component of the catalyst along the catalytic monolith length. For catalytic methane oxidation on a monolithic catalyst under conditions typical of gas-turbine applications, the optimal distribution of the active component is found.

RESEARCH OF MASS-TRANSFER IN FIBROUS SORPTION-ACTIVE MATERIALS

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Catal. Today, 105(3-4) (2005) pp. 680-688.

The mass-transfer processes in fiberglass were studied in the course of drying the saturated glass fabric sample. Experiments were carried out using an Avance DRX Bruker spectrometer equipped with a micro tomography device. Experimental signal intensities of fluids flowing at different velocities were obtained. A one-dimensional mathematical model was applied to calculate mass-transfer coefficients from experimental data. Dependencies Nu(*Re*) at the Reynolds number varied between 0 and 400 were obtained at different fluid velocities. The data obtained were compared to correlation dependencies for woven Pt/Pd gauzes and for rows of parallel cylinders. Numeric experiments of gas flow filtration at low Reynolds numbers ($Re < 1$) were carried out using the CFD FLUENT software package. Fibrous material was represented as porous system consisting of bunches of parallel cylinders with varied distances between the cylinders. Dependence Nu(*Re*) was calculated at various parameters of system.

DECOMPOSITION AND OXIDATION OF ALIPHATIC NITRO COMPOUNDS IN SUPERCRITICAL WATER

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(**Kumamoto University, Kumamoto, Japan*)

Ind. & Eng. Chem. Res., 43(26) (2004) pp. 8141-8147.

Decomposition and oxidation of nitromethane, nitroethane, and 1-nitropropane in supercritical water (SCW) near the critical point have been studied in a flow reactor. It was found that the rate of aliphatic nitro compounds decomposition in SCW decreased with an increase in the number of carbon atoms, while the rate of their oxidation increased with an increase in the carbon number. Experimental data on the decomposition of the studied nitro compounds showed that the apparent rate constants, calculated on the assumption of first-order reaction, increased exponentially with an increase in the pressure at constant temperature. The transition-state theory has been applied to simulate the effect of pressure on the rate constants. Some ideas on the nature of the activation complex have been suggested. The calculated values of the activation volumes in the decomposition reactions of nitromethane, nitroethane, and 1-nitropropane in SCW were similar, which suggested the same nature of the activation complex in all three cases.

DECOMPOSITION AND OXIDATION REACTIONS OF ALIPHATIC NITRO COMPOUNDS IN SUPERCRITICAL WATER

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(**Kumamoto University, Kumamoto, Japan*)

Kinet. Catal., 46(6) (2005) pp. 821-825.

The reaction kinetics of nitromethane, nitroethane, and 1-nitropropane decomposition and oxidation in supercritical water near the critical point was studied in a flow reactor. The reaction rate constants were calculated assuming first-order reaction. It was found that pressure has a considerable effect on the rates of decomposition of the above nitrogen-containing compounds in supercritical water over a wide pressure range. The reactivity of the above aliphatic nitro compounds in supercritical water in decomposition reactions decreased and in oxidation reactions increased with an increasing number of carbon atoms.

EFFECT OF SUPERCRITICAL WATER DENSITY ON THE RATE CONSTANT OF THE ALIPHATIC NITROCOMPOUNDS DECOMPOSITION

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J. Supercrit. Fluids, 33(3) (2005) pp. 243-246.

It was shown experimentally that the rate of aliphatic nitrocompounds decomposition in supercritical water (SCW) depends on pressure/density at constant temperature. The SCW density dependence of the apparent rate constant of decomposition for each of three compounds under consideration (nitromethane, nitroethane and 1-nitropropane) was found to correlate with the density dependence of the H_3O^+ concentration in dissociated SCW. The rate constant of RNO_2 decomposition in SCW decreased with increasing the length of hydrocarbon radical R.

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ANALYSIS OF THE CSTR WITH TWO-PHASE FLOW UNDER PHASE EQUILIBRIUM CONDITIONS

A. Yermakova, V.I. Anikeev

Chem. Eng. Sci., 60(12) (2005)
pp. 3199-3206.

A mathematical model of the flow gas–liquid continuous stirred tank reactor (CSTR) is presented under the assumption of thermodynamic equilibrium of the two-phase flow. Phase equilibrium was calculated using the Redlich–Kwong–Soave (RKS) equation of state. An efficient algorithm based on homotopy method was used to obtain a numerical solution of the system of nonlinear algebraic equations of the model. By an example of the liquid-phase hydrogenation of benzene, steady states were analyzed in isothermal and adiabatic regimes and at partial removal of heat released as a result of exothermic reaction. It was shown that under certain conditions, a multiplicity of stationary solutions is possible due to nonlinearity of the kinetic reaction, on the one hand, and deviation of the reaction mixture properties from the ideal state, on the other hand.

CALCULATION OF BINODAL LINES FOR A MULTICOMPONENT MIXTURE BY THE HOMOTOPY METHOD

A. Yermakova, O.V. Sazhina, V.I. Anikeev

Theor. Found. Chem. Eng., 39(1) (2005) pp. 85-91.

Equations are proposed for binodal lines of a multicomponent mixture in the T-P and P-V planes. A numerical method for solving the equations of the thermodynamics model is described, which is based on the homotopy method and uses the physical parameters of the system, in particular, temperature and pressure, as parameters of continuation of solution. Calculation results illustrating the features of the phase states of binary and multicomponent mixtures are presented.

THEORETICAL AND EXPERIMENTAL ASPECTS OF USING STRUCTURED CATALYTIC SYSTEMS

A.S. Noskov

Kinet. Catal., 46(3) (2005) pp. 414-421.

Mass transfer in honeycomb monolith catalysts has been theoretically and experimentally studied by methods of computational hydrodynamics and NMR tomography. Theoretical estimates have been obtained for optimum parameters of processes employing honeycomb monolith catalysts. Newly developed catalysts for selective ammonia oxidation have provided a technological basis for nitrous oxide production with a selectivity of 85–88%, and a pilot plant using these catalysts has been designed. Methods of mathematical description have been developed for catalytic processes in fibrous materials, and the potential of these materials in soot aerosol removal from waste gas has been demonstrated. Principles of structuring of granular catalyst beds have been developed through theoretical analysis and experimentation. Results of commercial-scale application of structured beds in tubular and adiabatic reactors are presented.

PERFORMANCE OF SELECTIVE CATALYTIC EXOTHERMIC REACTIONS IN THE "REVERSED HEAT WAVE" MODE: A WAY TO IMPROVE SELECTIVITY

A.N. Zagoruiko

Chem. Eng. J., 107(1-3) (2005) pp. 133-139.

The paper considers the model system of exothermic catalytic selective and complete conversion reactions, occurring according to the scheme $A + m[B] \Rightarrow C + [\cdot]$, $C + [B] \Rightarrow D + [\cdot]$, $B + [\cdot] \Rightarrow [B]$, where A and B - initial reagents, C – desired product (of selective conversion), D – undesirable by-product (of complete conversion), [B] – reagent B, chemisorbed at the catalyst surface, $[\cdot]$ – vacant catalyst active site. Numerical simulation of the system behavior in fixed adiabatic catalyst bed showed that being compared to steady-state regimes it is possible to significantly improve the desired product yield and catalyst unit productivity by application of nonstationary regimes, based on periodical, separated in time, feeding of reagents A and B. The most interesting results were obtained for process performance in "reversed heat wave" mode, when temperature front of reaction is moving upstream the flow of the reaction mixture. Such operation regime is characterized with significant decrease of maximum catalyst temperature, therefore, expanded possibility to increase inlet concentration of reagents and with increased selectivity of conversion into target products.

SELECTIVE EXOTHERMIC CATALYTIC REACTIONS IN A REVERSE HEAT FRONT

A.N. Zagoruiko

Theor. Found. Chem. Eng.,
39(1) (2005) pp. 70-77.

A model system of exothermic reactions of selective and complete catalytic conversion is considered. The system comprises the reactions A + m[B] ⇒C + [ ], C + n[B] ⇒D + [ ], and B + [ ] ⇒[B], where A and B are the initial reactants, C is the desired product (of the selective conversion), D is the undesired side product (of the complete conversion), [B] is the reactant B chemisorbed on the catalyst surface, and [ ] is a free catalytic active site. Numerical study of the system of reactions in an adiabatic catalyst bed shows that the yield of the desired product and the specific performance of the catalyst can be significantly increased if the reactions are performed not under steady-state conditions but in unsteady-state modes involving periodic time-separated introduction of the reactants A and B. Of greatest interest is to carry out the process in a reverse heat front propagating upward the flow of the gaseous reaction mixture, since, in this front, the maximal catalyst temperature is much lower and also the conversion selectivity is high.

DEVELOPMENT OF CATALYTIC PROCESS FOR AFTERBURNING OF WASTE GASES IN THE CLAUS PLANTS

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Catal. Ind., 5 (2005) pp. 52-61.

The catalyst and the process for catalytic afterburning of waste gases at Claus plants are considered. The experimental investigations conducted showed the industrial aluminum-copper-chromium oxide catalyst IKT-12-8 to be optimal. It provides efficient oxidation of toxic impurities (H_2S, CO, COS, CS_2, hydrogen, sulfur vapors) and it is characterized by high stability and resistance to deactivation. The kinetic parameters of the reactions are determined. The mathematical modeling of the process is performed revealing a possibility of reaching the significant degree of impurity conversion (98–100 %) within a very wide range of waste gas composition. The autothermal process (i.e. its conduction at the cost of oxidation reaction heat without using additional fuel) allows to refuse from natural gas utilization at the waste gas afterburning stage. It is important that a small production site is necessary for arrangement of the catalytic plant. The work is made by the example of the elemental sulfur production conditions at the Copper Plant of the «Norilsk Nickel» Mining-and-Metallurgical Integrated Works.

THERMOGRAPHY STUDY OF PROPANE OXIDATION TO SYNTHESIS-GAS OVER NICKEL

A.Yu. Gladky, V.V. Ustugov, A.M. Sorokin, A.I. Nizovskii, V.N. Parmon, V.I. Bukhtiyarov

Chem. Eng. J., 107(1-3) (2005) pp. 33-38.

Propane oxidation to the synthesis-gas over a metallic nickel ribbon in a self-oscillation mode has been studied by mass-spectrometry and *in situ* thermography. The combined application of these methods has shown that the oscillations of the reaction rate are accompanied with periodic changes of the catalyst temperature, with the half-periods of high reaction rate being correspondent to the sufficient rise of the catalyst temperature. It has been concluded that this additional heating of the surface is due to heat evolution during this exothermic reaction. The use of thermography made it possible to detect also the formation of 'hot spots' on the nickel surface during the half-period of high activity. It has been, however, shown that the 'hot spots' are not responsible for the formation of the oscillations. Possible reasons for the 'hot spot' formation in this system are discussed.

PROPANE OXIDATION ON NICKEL IN A SELF-OSCILLATION MODE

A.Yu. Gladky, V.V. Kaichev, V.K. Ermolaev, V.I. Bukhtiyarov, V.N. Parmon

Kinet. Catal., 46(2) (2005) pp. 250-259.

The kinetics of the catalytic oxidation of propane with oxygen on nickel in a self-oscillation mode was studied. A comparative analysis of changes in reaction rate oscillations with time in the presence of nickel wire and foil was performed. It was found that the reaction medium influenced the morphology of the catalyst surface. With the use of X-ray photoelectron spectroscopy, it was demonstrated that a NiO layer no less than 100 nm in thickness was formed on the catalyst surface in the course of the reaction of propane oxidation. The mechanism of the appearance of self-oscillations in the test system is discussed.

VORTEX CENTRIFUGAL BUBBLING REACTOR

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Chem. Eng. J., 107(1-3) (2005) pp. 55-62.

The vortex centrifugal bubbling apparatus is considered as a basis for a new type of multiphase

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vortex centrifugal bubbling reactor. In this device, a highly dispersed gas–liquid mixture is produced in the field of centrifugal forces inside the vortex chamber. The operation of the vortex centrifugal bubbling apparatus is based on the rotation of liquid by the tangential entry of gas flows via the many tangential guiding vanes around the periphery of the vortex chamber. At certain regimes there appears a highly dispersed gas–liquid vortex bubbling layer. Vortex bubbling layer represents the following unique characteristics: low hydrodynamic resistance (1000-2000 Pa); homogeneity and stability over wide range of centrifugal acceleration (10^2 to 10^3 m/s^2); large specific surface with the high renovation rate (of about 5 m^2 per 1 l of water); high gas content (of about 0.5-0.6); high gas throughput (up to 200–300 m^3 of gas per 1 l of liquid per hour) and, consequently, very high rates of heat and mass transfer. The energy consumption for the vortex bubbling layer maintenance is about 50–80 W per 1 l of treated liquid. The design features of the vortex chamber are described in view of the methods of stabilization of the vortex bubbling layer. The data on the hydrodynamic resistance, the structure and the lifetime of the vortex gas–liquid layer are presented. The main advantages and features of the devices of this type are discussed in view of their possible application.

SYNTHESIS GAS CONVERSION INTO HYDROCARBONS (GASOLINE RANGE) OVER BIFUNCTIONAL ZEOLITE-CONTAINING CATALYST: EXPERIMENTAL STUDY AND MATHEMATICAL MODELLING

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Chem. Eng. J., 107(1-3) (2005) pp. 63-71.

Bifunctional catalysts were investigated in the temperature range 320–400 °C, at pressures 40–80 atm, GHSV = 500–20,000 h^{-1}, ratio $H_2/CO = 2–10$. The influence of the Zn–Cr/ZSM-5 catalyst composition on the products distribution and the process productivity with regard to the liquid hydrocarbons (gasoline range) has been studied. It has been shown that the products distribution depends mainly upon the molar ratio H_2/CO and GHSV, while the main factors affecting the process productivity and the yield of the liquid hydrocarbons are pressure and temperature in the reactor.

On the basis of the experimental data, mathematical modelling has been performed for the process flow sheet with the unreacted gas recycled. The influence of various parameters of the process on the catalyst productivity with regard to liquid hydrocarbons was studied.

THE INFLUENCE OF OXYGEN MOBILITY IN SOLID CATALYST ON TRANSIENT REGIMES OF CATALYTIC REACTION

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Chem. Eng. J., 107(1-3) (2005) pp. 141-146.

Mathematical modeling of the influence of oxygen mobility in solid catalyst on transient regimes of catalytic reaction has been carried out. The region of Thiele modulus Ψ in which the diffusion of oxygen in solid catalyst effect on the transient regime of reaction was determined. These values of Ψ lies in the interval of 0.7–7. The diffusion coefficient corresponding to these values of Thiele modulus lies in the interval of 10^{-17}–10^{-13} cm^2/s.

TRANSIENT KINETICS OF TOLUENE INTERACTION WITH V/Ti-OXIDES IN ANAEROBIC CONDITIONS

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Chem. Eng. J., 107(1-3) (2005) pp. 147-155.

Toluene interaction with the catalysts consisting of 0.35, 0.62, 0.75 and 3.7 monolayers (ML) of VO_x supported on anatase–titania, containing potassium, was studied by transient response techniques at 523-673 K. FT-Raman spectroscopy under dehydrated conditions was used to determine the state of vanadia. K-perturbed (1020 cm^{-1}) and K-doped (990 cm^{-1}) monomeric vanadia species as well as “amorphous” KVO_3 (960–940 cm^{-1}) were found at vanadia coverage less than a monolayer. Bulk V_2O_5 (994 cm^{-1}) was present only in the 3.7 ML V/TiO_2 catalyst as a dominant species. Benzaldehyde (BA), total oxidation products and surface carbon-containing species were the main products of the toluene interaction. The proposed reaction network involves five steps and two types of oxygen sites. Both the BA and CO_2 formation increased with the concentration of vanadia. The former is determined mainly by nucleophilic-lattice oxygen that is involved in the monolayer vanadia species. The latter as well as the formation of the main part of surface carbon-containing species increased much more steeply being dependent, probably, from electrophilic oxygen abundant in polymerised vanadia

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species and V_2O_5. The performed kinetic modelling satisfactorily describes the response curves of BA, CO_2 and toluene obtained during the toluene interaction with the pre-oxidised 0.35–0.75 ML V/TiO_2 catalysts. The presence of bulk V_2O_5 in the 3.7 ML V/TiO_2 catalyst seems to provide some change in the reaction mechanism demanding a modification of the reaction scheme.

COMPUTATIONAL SYSTEM FLOCAS FOR CHEMICAL TECHNOLOGICAL SCHEMES CALCULATION

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Chem. Ind.,
82(9) (2005) pp. 446-452.

The application of computer system FLOCAS is considered for solution of various problems of chemical industry concerned with analysis and calculation of chemical-engineering schemes, such as production design, optimization and reconstruction, analysis of technical and improvement suggestions. Main directions of package applicability, its structure and face are shown. Demo examples are used to show the typical task solvable by application of the package.

TSEFLAR™ – THE CENTRIFUGAL FLASH REACTOR FOR RAPID THERMAL TREATMENT OF POWDERED MATERIALS

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Chem. Eng. J., 107(1-3) (2005)
pp. 157-161.

The concept of the centrifugal thermal activation (CTA) of powdered materials on a rotating solid heat carrier is developed. A compact centrifugal flash reactor has been manufactured and tested. The tested set-up provided: the heating of gibbsite powder to the temperature of 400–900 K with the rate more than 10^3 K/s; the duration of the powder thermal treatment less than 1.5 s; the regulation of the treatment duration by changing the speed of the plate rotation and the shape of the rotating heat carrier; the product output up to 40 dm^3/h; the removal of the extracted steam containing gases and rapid quenching of the thermally activated solid products. The device tested has been used for the thermal activation of commercial aluminium hydroxide $Al(OH)_3$ (gibbsite). The obtained thermally activated product possesses a high reactivity and can be used for the preparation of various alumina-based compounds.

PHYSICO-CHEMICAL PROPERTIES OF TSEFLAR™-TREATED GIBBSITE AND ITS REACTIVITY IN THE REHYDRATION PROCESS UNDER MILD CONDITIONS

L.A. Isupova, Yu.Yu. Tanashev, I.V. Kharina, E.M. Moroz, G.S. Litvak, N.N. Boldyreva, E.A. Paukshtis, E.B. Burgina, A.A. Budneva, A.N. Shmakov, N.A. Rudina, V.Yu. Kruglyakov, V.N. Parmon

Chem. Eng. J., 107(1-3) (2005)
pp. 163-169.

Physical and chemical properties of TSEFLAR™-treated gibbsite/hydrargillite (centrifugal thermal activation) CTA HG were studied with X-ray analysis, TA, EM, BET and IRS. CTA HG product obtained at the temperature range of 330–580 °C and contact time ~1 s is the one with a transitional non-equilibrated layered hydroxide structure with partly lost hydroxide groups. The CTA HG structure does not correspond to the produced chemical composition $Al_2O_3{\cdot}(0.4–2)H_2O$ and, therefore, the products reveal a higher reactivity. Such products are already readily hydrated at room temperature in water and aqueous ammonia to form eventually the stable bayerite-like hydroxide structure.

SYNGAS FORMATION BY SELECTIVE CATALYTIC OXIDATION OF LIQUID HYDROCARBONS IN A SHORT CONTACT TIME ADIABATIC REACTOR

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Chem. Eng. J., 107(1-3) (2005)
pp. 171-179.

The research of pilot plant scale explores syngas formation from such liquid fuels like isooctane and gasoline by selective catalytic oxidation at short contact times in nearly adiabatic reactor operating with the representative throughputs. The original monolithic catalysts with different (microchannel ceramics and metallic honeycomb structure) supports have been used in the experiments. The results demonstrated that over the range of the operational parameter $O_2/C = 0.50–0.53$ required for syngas generation, equilibrium synthesis gas was produced over the catalysts employed, thus proving some evidence of their high activity and selectivity. Pre-reforming of fuel with releasing of some chemical energy before the catalytic monolith can occur in reactor. Both feed composition and superficial velocity affect the pre-reforming process. The phenomenon may be favored in syngas production because of a milder catalyst temperature mode is created. In general, axial temperature profile depends on catalytic composition in the frontal part of monolith, while the back-face catalyst temperature controls equilibrium product gas. Minimal both longitudinal and transversal temperature gradients were observed in the metallic catalytic monolith in comparison to the microchannel ceramic one. This helps to decrease deformations and thermal stresses in monolithic catalysts at the process performance.

MODELING OF RELAXATION OSCILLATIONS IN CO OXIDATION ON METALLIC CATALYSTS WITH CONSIDERATION OF RECONSTRUCTIVE HETEROGENEITY OF THE SURFACE

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Chem. Eng. J., 107(1-3) (2005) pp. 191-198.

This paper is devoted to the development of a low-dimensional kinetic model of CO oxidation on a metallic catalyst surface and theoretical study of arising nonlinear phenomena and relaxation oscillations of the reaction rate. Experimental results of studies on the adsorbed oxygen are presented and its significance in the CO oxidation mechanism on Ir catalyst is shown. The authors consider the conventional Langmuir–Hinshelwood mechanism of catalytic CO oxidation and take into account the possibility of a metallic surface modification during reaction due to the oxygen penetration into subsurface layers. It is suggested that when the adsorbed oxygen concentration exceeds some critical value, a surface modification occurs and the reaction capability of adsorbed oxygen changes, so that the activation energy of the interaction between the adsorbed species sharply increases. Construction of bifurcation curves on the parametric plane (P_{CO}, P_{O2}) permits to separate areas of CO and O_2 partial pressures, for which self-oscillations and/or multiplicity of steady states appear. This paper deals with parametric analysis of a new two-variable kinetic model of CO oxidation on Ir catalyst surface, but the approach developed is rather general and can be applied to studies of different catalytic reactions.

POSSIBILITIES FOR OPTIMIZATION OF TECHNOLOGICAL MODES FOR ETHYLENE POLYMERIZATION IN AUTOCLAVE AND TUBULAR REACTORS

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Chem. Eng. J., 107(1-3) (2005) pp. 221-226.

Results of experimental studies on high-pressure ethylene polymerization in industrial autoclave and tubular reactors are considered using various peroxides and their mixtures with oxygen as initiators.

A possibility for the process improvement providing the increase of conversion, productivity and versatility of the obtained polyethylene brands is demonstrated.

According to the experimental data for the processes performed in single- and double-zone mixing mode reactors the initiator consumption, temperature profile stability and possibilities for rapid control over the process are analyzed depending on the type of the used peroxides or their complex mixtures.

Peculiarities of ethylene polymerizations in tubular reactors using the initiators either individually (stepwise initiation) or in a complex (mixed) initiation mode are revealed and discussed.

OPTIMIZATION OF POLYMERIZATION IN AUTOCLAVE AND TUBULAR REACTORS

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Russ. J. Appl. Chem.,
78(1) (2005) pp. 113-119.

The possibilities of improving operation of one-zone autoclave and tubular reactors using appropriate initiating systems without changes in the reactor design and process scheme were analyzed and experimentally tested on pilot and industrial installations for high-pressure polymerization of ethylene.

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METHANE OXIDATION OVER PEROVSKITE-RELATED FERRITES: EFFECTS OF OXYGEN NONSTOICHIOMETRY

V.V. Kharton*,, M.V. Patrakeev*,***, J. C. Waerenborgh****, V.A. Sobyanin, S.A. Veniaminov, A.A. Yaremchenko*, P. Gaszynski****, V.D. Belyaev, G.L. Semin, J.R. Frade*** (**Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, Aveiro, Portugal; **Institute of Physicochemical Problems, Belarus State University, Minsk, Belarus; ***Institute of Solid State Chemistry, Yekaterinburg, Russia; ****Chemistry Department, ITN/CFMC-UL, Sacavém, Portugal*)

Solid State Sci.,
7(11) (2005) pp. 1344-1352.

The oxidation of CH_4 pulses supplied in helium flow over perovskite-related $La_{0.3}Sr_{0.7}Fe_{0.8}M_{0.2}O_{3-\delta}$ (M=Ga, Al) and $SrFe_{0.7}Al_{0.3}O_{3-\delta}$ leads to significant yields of CO and H_2 after achieving a critical level of oxygen deficiency in the ferrite-based mixed conductors. This effect, reproducible under steady-state conditions in the membrane reactors for methane conversion, may be of interest for the development of monolithic ceramic reactors where the dense membrane and porous catalyst at the permeate-side surface are made of similar compositions. The Mössbauer spectroscopy and coulometric titration studies show that the presence of metallic Fe under typical operation conditions can be neglected, whilst most oxygen vacancies in the ferrite lattices are ordered. Increasing selectivity towards the partial oxidation of methane is observed in the vicinity of the state where the iron cations are predominantly trivalent and massive ordering processes in the oxygen sublattice start. The catalytic activity of ferrite-based materials may hence result from the lattice instability characteristic of morphotropic phase transformations. The correlations between catalytic behavior and oxygen ionic transport are briefly discussed.

METHANE OXIDATION OVER Fe-, Co-, Ni- AND V-CONTAINING MIXED CONDUCTORS

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Solid State Ionics,
176(7-8) (2005) pp. 781-791.

The catalytic oxidation of methane over mixed conducting ceramics, including perovskite-type $SrFe_{0.7}Al_{0.3}O_{3-\delta}$ and $La_{0.3}Sr_{0.7}Co_{0.8}Ga_{0.2}O_{3-\delta}$, dual-phase composite $(SrCo)_{0.5}(Sr_2Fe_3)_{0.5}O_{4.75\pm\delta}$, $La_2Ni_{0.9}Co_{0.1}O_{4+\delta}$ with K_2NiF_4-type structure and zircon-type $CeVO_{4+\delta}$, is primarily governed by bonding energy between oxygen and transition metal cations, which leads to general correlations between the catalytic activity, oxygen desorption, oxygen ionic transport, thermal expansion, and, often, phase stability. The steady-state conversion of dry CH_4 either by oxygen permeating through dense oxide ceramics in a membrane reactor or by atmospheric O_2 (methane/air ratio of 30:70) in a fixed bed reactor with membrane material as catalyst results in high CO_2 selectivity, increasing when the oxygen permeability of mixed conductors increases. The prevailing mechanism of total methane combustion makes it necessary to incorporate reforming catalysts in the membrane reactors for natural gas conversion to Synthesis gas (syngas). Dominant CO_2 formation is also observed for the oxidation of CH_4 pulses supplied in helium flow over the mixed conductor powders, except for $SrFe_{0.7}Al_{0.3}O_{3-\delta}$ yielding synthesis gas with the H_2/CO ratio close to 2, characteristic of the partial oxidation process. For a model reactor comprising one disk-shaped membrane and a catalyst both made of $SrFe_{0.7}Al_{0.3}O_{3-\delta}$, the methane conversion and CO selectivity at 1223 K achieved 65% and 48%, respectively.

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DETONATION VELOCITY OF EMULSION EXPLOSIVES CONTAINING CENOSPHERES

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Combust., Explosion, Shock Waves,
41(5) (2005) pp. 591-598.

The detonation velocity of an emulsion explosive containing hollow alumosilicate microspheres (cenospheres) as the sensitizer is measured. The size of the microspheres is 50–250 µm. The relations between the detonation velocity and the charge density and diameter are compared for emulsion explosives containing cenospheres or glass microballoons as the sensitizer. It is shown that for a 55 mm diameter charge, the maximum detonation velocity of the composition with cenospheres of size 70–100 µm is 5.5–5.6 km/sec, as well as for 3M glass microballoons. The critical diameter for the emulsion explosive with cenosphere is 1.5–2 times larger than that for the emulsion explosive with glass microballoons and is 35–40 mm.

MULTICAPILLARY COLUMNS FOR CHROMATOGRAPHY

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American Labor.,
37(6) (2005) pp. 42-46.

The principles and theory of high-speed capillary chromatography have been known since the 1960s. To realize the maximum speed capabilities, it is necessary to use capillaries with a diameter of approx. 5–50 µm. However, capillary columns with a diameter smaller than 100 µm are rarely used because they require very small sample quantities that are difficult to inject and detect. To overcome this problem, multicapillary columns (MCCs) composed of a large number of capillaries were developed. Due to much larger surface and cross-sectional areas, MCCs overcome the flow rate, volume, and sample capacity limitations associated with single-capillary columns. MCCs are compatible with standard chromatographic equipment and work with all common sample sizes and injection techniques. No extensive modifications of the injector and detector are needed.

NITROUS OXIDE IN OXIDATION CHEMISTRY AND CATALYSIS: APPLICATION AND PRODUCTION

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Catal. Today,
100(1-2) (2005) pp. 115-131.

An overview is given on extensive studies, which are targeted to involve N_2O into organic synthesis as an oxidant. Due to unique oxidative properties, nitrous oxide provides remarkable prospects in catalytic and non-catalytic oxidation chemistry in both gas and liquid phases. The interest to new oxidant resulted in appearance of a new technology for the production of inexpensive N_2O too.

ACTIVITY OF CATALYSTS OF KLAUS-CONVERSION OF HUMID GAS

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Catal. Ind., 4 (2005) pp. 23-28.

Comparative laboratory tests of activity of a new domestic industrial alumina catalyst AO-MK2 (Novomichurinsk Catalyst Plant) and its foreign analogue CR-3S («Procatalyse», France) in the Claus model reaction are given. An essential difference in H2S conversion degree in dry and wet gaseous mixtures has been found, therefore the results and practical conclusions of works on comparative testing of catalysts in dry model mixtures cannot be used in the industrial processes. The effect of hydrothermal aging on the catalyst texture characteristics and activity rating was shown. Domestic catalyst AO-MK2 was found not to be inferior to foreign CS-3S in activity and it is more stable to sulfation in the presence of water vapors and oxygen. At present, catalyst AO-MK2 passes experimental-industrial tests (charge is 5 t) in the process of production of elemental sulfur according to the Claus process from industrial gas.

NUCLEATION RESEARCH PROGRESS FOR DESCRIPTION OF ATMOSPHERIC AEROSOL DYNAMICS. I. EXPERIMENT AND SEMIEMPIRICAL APPROACHES

M.P. Anisimov

Optics Atmosph. Ocean,
18(5-6) (2005) pp. 328-337.

Using the experimental and semiempirical approaches, the topology of the nucleation rate surface near the triple point is determined. Some general

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requirements to the vapor nucleation experiments are formulated. The most important problem is now the measurement of a single-channel nucleation rate for two- and higher channel nucleation. Measurements of the single-channel nucleation rate are of key importance as compared with the experimental data on the nucleation rate and single-channel nucleation theory.

NUCLEATION RESEARCH PROGRESS FOR DESCRIPTION OF ATMOSPHERIC AEROSOL DYNAMICS. II. NUCLEATION RATE SURFACE FOR WATER VAPOR

M.P. Anisimov, L.D. Anisimova, P. Turner*, P.K. Hopke* (**Clarkson University, Potsdam, USA*)

Optics Atmosph. Ocean,
18(5-6) (2005) pp. 338-343.

General computer algorithm for constructing the nucleation rate surface is developed. Algorithm is applicable in case of water vapor nucleation. Results can be used in calculations of the water vapor nucleation in atmosphere. An obvious advantage of the computer semi-empirical construction of nucleation rate surfaces is the ability to construct this surface over the whole interval of nucleation parameters that is impossible in experiments. Examples of hard-to-reach conditions include very low temperatures, media with high-pressures and/or very high-temperature (such as stars), etc. It is assumed that the current algorithm can be further developed for semi-empirical construction of nucleation rate surfaces for one- and two-component systems.

AN ALGORITHM FOR SEMI-EMPIRICAL DESIGN OF NUCLEATION RATE SURFACE

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J. Colloid Interface Sci.,
290(1) (2005) pp. 107-116.

During the last half of century, Classical Nucleation Theory (CNT) has been developed and there have been advances in the molecular theory of nucleation. Most of these efforts have been directed towards small molecule system modeling using intermolecular potentials. Summarizing the nucleation theory, it can be concluded that the current theory is far from complete. Agreement is generally not obtained between experimental and theoretical results. In practical applications, parametric theories can be used for the systems of interest. However, experimental measurements are still the best source of information on nucleation. Experiments are labor intensive and costly, and thus, it is useful to extend the value of limited experimental measurements to a broader range of nucleation conditions. The available nucleation parameters represent only small regions of possible nucleation conditions over the range from the critical temperature to absolute zero. Thus, it is useful to develop better tools to use the data to estimate semi-empirical nucleation rate surfaces. The nucleation rate surface for any system can be constructed over its phase diagram. This concept involves using the phase equilibrium diagram to establish lines of zero nucleation rates. Nucleation rate surfaces arise from equilibrium lines and their extensions that are representing unstable equilibria. Only limited experimental data is available for use in normalizing the slopes of the linearized nucleation rate surfaces. The nucleation rate surface is described in terms of steady-state nucleation rates. To design the surfaces of nucleation rates, several assumptions are presented. In the present study, an algorithm for the semi-empirical design of nucleation rate surfaces is introduced. The topology of the nucleation rate surface for a unary system using the example of water vapor nucleation is created semi-empirically. The nucleation of two concurrent (stable and unstable) phase states of critical embryos is considered in the context of multi-surface nucleation rates. Only one phase transition (melting) in the condensed state of water is considered for simplicity. The nucleation rate surface is constructed numerically using the available experimental results for vapor nucleation and phase diagram for water. The nucleation rate for water vapor is developed for the full temperature interval, i.e. from critical point to absolute zero. The results help to suggest a new direction for experimental nucleation research.

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