



# BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

# ANNUAL REVIEW 2007

<http://catalysis.ru>

**ANNUAL REVIEW**  
**of Activities in Basic Research Areas**  
**2006**



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

**Novosibirsk**



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Dear Colleagues,

This issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covers the year 2006 and reflects 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 the fSU countries, 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 2006, the same as all previous years, was very important for the life of BIC in many aspects. First of all, BIC has 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 three 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. BIC has transferred to the Russian Industry new efficient catalysts and technologies for olefin polymerization, including the production of polyethylene with the superhigh molecular weight. Also, the first Russian technology of the aromatization of low alkanes, which are the main constituent of the oil associated gases, has been developed by BIC and successfully tested at the semi-industrial level. The strategic collaboration with the Russian industries is nowadays,

undoubtedly, the very important feature of the scientific activity of the Boreskov Institute, as well as of many other academic institutes of RAS.

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 a new legal entity, the Institute of Hydrocarbons Processing (IHP), and the Volgograd Scientific center with a large flexible pilot facilities for fine organic synthesis has joined BIC as its Volgograd Division. Thus, now UIC consists of two large legal entities: BIC and IHP. The facilities of the UIC include three flexible and powerful semi-industrial plants capable of manufacturing the first industrial batches of various catalysts and specialty chemicals. Thus, BIC together with UIC is now one of the most powerful Russian specialized R&D organizations in the industry-oriented chemistry with unique facilities for scaling up numerous innovations for that industry. Indeed, the current management of the Institute realizes the existing problems of the large R&D structure operation and tries to take care of the maintenance of high R&D activity and productivity of BIC and UIC in both fundamental and applied areas as the goal of the highest priority.

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



Valentin N. Parmon

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

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

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

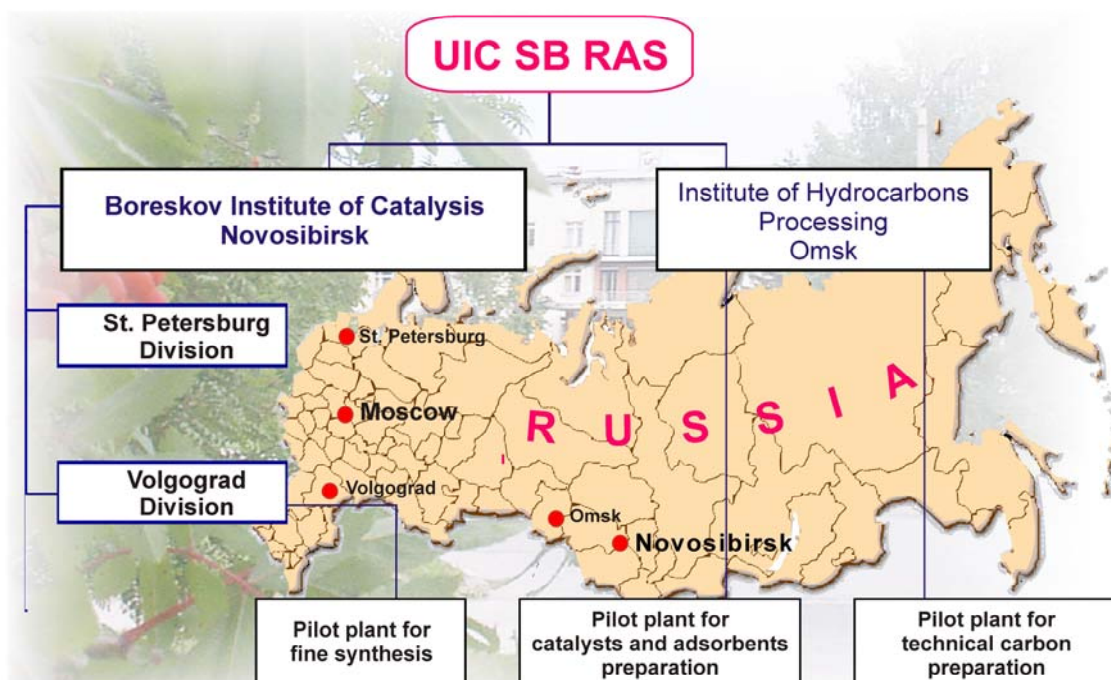
In 1976 Professor Kirill I. Zamaraev has been invited by Academician G.K. Borekov to join the Institute of Catalysis as a Deputy Director. Kirill Ilyich has come to Novosibirsk at early 1977 together with a large team of young chemical physicists, thus largely widening the studies of elementary catalytic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

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

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

Since 1998 the Institute has been united with some other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a new R&D association: the United Institute of Catalysis headed by the director of the Borekov Institute of Catalysis. Now the United Institute of Catalysis (UIC) includes the Borekov Institute of Catalysis with its St. Petersburg Division, Volgograd Engineering Scientific Center and the Institute of Hydrocarbons Processing in Omsk.

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



Structure of the United Institute of Catalysis

## 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 catalysis problems, able to solve any questions related to phenomena of catalysis, from theoretical problems like quantum-chemical calculations up to designing of industrial catalysis 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 catalysis, 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.



## DIRECTORATE



V.N. Parmon



A.S. Noskov



V.I. Bukhtiyarov



V.A. Sobyenin



B.S. Bal'zhinimaev

## STRUCTURE OF THE INSTITUTE



O.N. Martyanov



S.P. Kildyashev



S.E. Glaznev



I.A. Kamolkin



V.N. Novikov

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#### Directorate

#### Scientific Council

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#### 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. Sobyenin



#### 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

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Scientific Director Dr. Aleksandr M. Beskopylnyi



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#### Manufacturing Facilities



#### Administration and Services

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**Group of Surface Compounds Synthesis**

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**Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion**

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## **DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES**

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Head: Academician Valentin N. Parmon



**Laboratory of Adsorption**  
Head: Dr. Oleg N. Martyanov



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



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



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



**Division of Advanced Developments and Technologies**  
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**Group of Adsorption-Catalytic Processes for Fuel Cells**  
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**Group of Aerosol Catalysis**  
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**Group of Biocatalysis**  
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## **DEPARTMENT OF HETEROGENEOUS CATALYSIS**

Head of the Department Prof. Vladimir A. Sobyenin



**Laboratory of Catalytic Processes in Fuel Cells**  
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**Head: Dr. Vladimir I. Sobolev**



**Laboratory of Catalysts for Deep Oxidation**  
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**Head: Prof. Gennadii I. Panov**



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



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



**Group of Synthesis of Nanodispersed Materials**  
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**Laboratory of Unsteady-State Catalytic Methods for Gas Purification**

**Head: Prof. Aleksandr S. Noskov**



**Laboratory of Multiphase Processes Modeling**

**Head: Prof. Valerii A. Kirillov**



**Laboratory of Catalytic Conversion of Carbon Oxides**

**Head: Prof. Aleksandr A. Khassin**



**Laboratory of Catalytic Hydrocarbon Conversion**

**Head: Prof. Gennadii V. Echevsky**



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**Head: Prof. Vladimir A. Zakharov**



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**Head: Prof. Andrey N. Zagoruiko**



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



**Group of Development and Optimization of Catalytic Processes with Catalyst Deactivation**  
**Head: Dr. Vitalii N. Kashkin**



**Group of Processes in Fixed Catalyst Layer**  
**Head: Dr. Ilya A. Zolotarsky**



**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. Eugenio 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 OF CATALYTIC PROCESSES OF FINE  
ORGANIC AND BIOORGANIC SYNTHESIS**

Head of the Department Prof. Zinaida P. Pai



**Laboratory of Liquid-Phase Catalytic Oxidation of Organic  
Compounds**

**Head: Prof. Zinaida P. Pai**



**Group of Catalysts and Processes Based on Heteropoly Acids**

**Head: Prof. Elena G. Zhizhina**



**Group of Heterogeneous Catalysts for Selective Liquid-Phase  
Oxidation**

**Head: Prof. Oxana A. Kholdeeva**

**ST. PETERSBURG DIVISION  
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**Vice-Director Dr. Valery P. Tulmankov**



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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**



**Scientific Director Dr. Aleksandr M. Beskopylnyi**

## SCHOOLS OF THE BORESKOV INSTITUTE OF CATALYSIS

The Borekov 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. Borekov** 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 60–70<sup>th</sup> 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.

*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.*

# Nanotechnologies in Catalysis

## From molecular level to industrial plants



1958

1978 • Vanadium catalysts for sulfuric acid production, USSR

1982 • REVERS-Process, USSR  
Enviro - Chem Systems, Inc. (A Monsanto - Company), USA, 1992

1988 • Catalysts for propylene polymerization, USSR  
DSM, the Netherlands, 1995

1992 • ZEOFORMING process for synthesis of gasoline.  
In cooperation with SEC "ZEOSIT", Russia  
Lurgi, Germany, 1997

1993 • SIBUNIT® - carbonaceous material, Russia  
Sibunit for phosgene synthesis, Du Pont, USA, 1994

1995 • Catalysts for FCC (oil cracking), Russia

1996 • AlphOx™ technology (benzene + [N<sub>2</sub>O] → phenol)  
Developed in cooperation with Solutia Inc., USA, 1996

1997 • Non-platinum catalysts for production  
of nitric acid, Russia

1998 • One-step technology for production  
of nicotinic acid, Russia  
Degussa, Germany, 2000

1999 • Catalysts for hydro purification of  
terephthalic acid  
Developed in cooperation with Samsung,  
Korea, 2000

2000 • New technology of loading the reactors  
with catalysts, Russia

2002 • Selective water sorbents, Russia

2003 • BIMT® technology for production of  
gasoline and diesel fuel, Russia

2004 • New generation of catalysts LUKS and  
reforming catalysts of PR and RU series.  
In cooperation with the Institute for Hydrocarbons  
Processing (Omsk), Russia

2006 • Supported catalysts for olefines polymerization.  
Ultrahigh molecular weight polyethylene, Russia

2007

## 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<sub>1</sub>-C<sub>4</sub> 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*

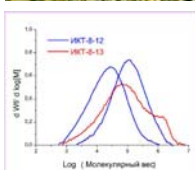
- **Reverse process** for catalytic gas purification
- **Zeoforming processes** for synthesis of gasoline
- **Alphox technology** for the one step phenol form benzene production
- **Adsorption-catalytic purification** of industrial wastewaters
- **Nitric acid** production with the use of honeycomb catalysts
- **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<sub>2</sub>S** to elemental sulfur

- Treating of mixed **radioactive organic wastes**
- 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*



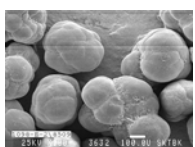
Vanadium pentoxide catalysts for sulfuric acid production



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



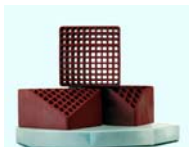
Catalyst ICT-8-20 for production of ultrahigh molecular weight polyethylene



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



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. The Boreskov Institute of Catalysis has specialized groups united into Department of Physicochemical Methods for Catalyst Investigation oriented at analytical and scientific studies. At the Department there are many specialists of high qualification specializing in the investigation of catalysts and nanomaterials.

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

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

**Analytical** (composition of catalysts and catalytic reaction products)

***Bulk composition***

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

***Phase analysis***

- X-Ray diffraction, including *in situ* diffraction
- Differential dissolution



Thermally programmed reduction, oxidation, desorption  
X-Ray diffraction 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 2006

|         |    |              |    |                |   |
|---------|----|--------------|----|----------------|---|
| Bahrein | 1  | India        | 2  | South Korea    | 1 |
| Belarus | 2  | Ireland      | 1  | Spain          | 9 |
| Belgium | 5  | Israel       | 6  | Singapore      | 4 |
| China   | 16 | Italy        | 8  | Switzerland    | 4 |
| Czechia | 4  | Japan        | 8  | Thailand       | 1 |
| Egypt   | 1  | Montenegro   | 4  | Turkey         | 2 |
| Finland | 2  | Netherlands  | 15 | Ukraine        | 3 |
| France  | 10 | Poland       | 6  | United Kingdom | 8 |
| Germany | 28 | Saudi Arabia | 4  | USA            | 6 |
| Greece  | 32 |              |    |                |   |

### Visits of foreign specialists to the Boreskov Institute of Catalysis in 2006

|         |    |             |    |             |    |
|---------|----|-------------|----|-------------|----|
| Canada  | 1  | Germany     | 17 | South Korea | 7  |
| China   | 9  | Italy       | 4  | Spain       | 1  |
| DPRK    | 5  | Japan       | 10 | Turkey      | 1  |
| Estonia | 1  | Netherlands | 3  | USA         | 13 |
| France  | 10 |             |    |             |    |

**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, Moscow*) and **Prof. R. Psaro** (*Istituto di Scienze e Tecnologie Molecolari*). The Project theme is “**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**
  - **Advanced 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 Supérieure de Physique et de Chimie Industrielles* (Laboratory of Quantum Physics, Industrial Physics and Chemistry Higher Educational Institution), Paris on the themes:
  - **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 Supérieure 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:

- *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 Project “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-Bi<sub>2</sub>S<sub>3</sub> and CuPdBiS<sub>3</sub>-Bi<sub>2</sub>S<sub>3</sub> Systems”.* Coordinators: **Prof. S. Tsybulya** (BIC) and **Prof. Dr. K. Bente** (Leipzig University).

## 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. Anadzivic** (Serbian Academy of Sciences and Arts).

## CZECH REPUBLIC

The cooperation with *J. Heyrovského Ústav Fyzikální Chemie AV ČR* (J. Heyrovsky Institute of Physical Chemistry ASCR) on the Projects

- “*Study of Cation Distribution in Zeolites*”. Coordinators: **Prof. Z. Sobalik** (*J. Heyrovského Ústav Fyzikální Chemi*) and **Prof. O. Lapina** (BIC).
- “*Electron Spectroscopy to Study Catalyst Surface*”. Coordinators: **Prof. P. Carsky**, **Prof. Z. Bastl** (*J. Heyrovského Ústav Fyzikální Chemi*), **Prof. A. Boronin** (BIC).

## CHINA

The cooperation in the frame of **Associated Research Laboratory** which was established by an agreement signed December 4, 2004 by the Borekov Institute of Catalysis and Heilundzyan University, Harbin. Chief Executive officers of Laboratory are: **Prof. V. Bukhtiyarov** (BIC) and **Fu Hong-Gang** (*Heilundzyan University*). Project “*Synthesis and Modification of ZSM-12 Zeolites. Zeolite ZSM-12 in Reaction of Naphthalene Alkylation with Methanol*”. Coordinators: **Prof. G.J. Sheng** (*Heilundzyan University*), **Prof. G. Echevsky** (BIC).

## 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, Messina, Italy  
*Technische Universität Aachen*, RWTH-Aachen, Germany  
*The Borekov 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 Supérieure de Chimie de Montpellier*, France

Participants:

**Prof. I. Ivanova**, *Moscow Lomonosov State University*, Moscow, Russia  
**Acad. V. Parmon**, *The Borekov Institute of Catalysis*, Novosibirsk, Russia  
**Prof. E. Derouane**, *Universidade to Algarve Faculdade de Ciências e Tecnologia*, Faro, Portugal  
**Dr. Ya. Khimyak**, *University of Liverpool*, Liverpool, United Kingdom.

#### III. Novel Catalytic Process for Industrial Waste Water Treatment

Project Coordinator:

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



Participants:

**Acad. V. Parmon**, *The Boreskov Institute of Catalysis*, Novosibirsk, Russia  
**Prof. B. Laskin**, *Research Scientific Center for Applied Chemistry*, St. Petersburg, Russia.

#### **IV. Competitive Hydrogen from Agro-Forestry Residues**

Project Coordinator:

**Prof. G. Grassi**, *European Biomass Industry Association (EUBIA)*, Brussels, Belgium

Participants:

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

#### **V. Sustainable Route to the Generation of Synfuels via Syngas Derived from Biomass**

Project Coordinator:

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

Participants:

**Dr. K. Seshan**, *Universiteit Twente*, Enschede, The Netherlands

**Dr. O. Hazewinkel**, *Techno Invent Ingenieursbureau voor Milieutechniek b.v.*, Zoetermeer, The Netherlands

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

**Prof. A. Rozovskii**, *Topchiev Institute of Petrochemical Synthesis*, Moscow, Russia.

#### **INTAS - SB RAS Supported Project**

##### **Electromagnetic Response Properties of Carbon Onions and Carbon Onion-Based Composites**

Project Coordinator:

**Dr. Ph. Lambin**, *Facultes Universitaires Notre-Dame de la Paix*, Namur, Belgium

Participants:

*Belarus State University*, Minsk, Belarus; *University of Joensuu*, Finland; *Institute for Technical Physics and Materials Science*, Budapest, Hungary; *The Boreskov Institute of Catalysis*, Novosibirsk, Russia (**Dr. V. Kuznetsov**), *Nikolaev Institute of Inorganic Chemistry*, Novosibirsk, Russia.

#### **CRDF Project**

##### **The Utilization of Ortho/Para-Hydrogen Induced Nuclear Spin Polarization for New NMR Application in Catalysis and Chemical Engineering and the Exploration of Ultra-Low Field MRI**

Project Directors:

**Prof. I. Koptug**, *International Tomography Center*, Novosibirsk, Russia

**Prof. A. Pines**, *University of California*, Berkeley, United States

Project Coordinator from BIC **Prof. V. Kirillov**.

#### **EUROPEAN COMMUNITY SIXTH FRAMEWORK PROGRAM**

##### **I. International Partnership for a Hydrogen Economy for Generation of New Ionomer Membranes**

Coordinator: **Dr. R. Mallant**, *Energy Research Centre of The Netherlands*, Petten, The Netherlands

Partners:

*Daimler Chrysler; FuMA-Tech GmbH; CNRS Montpellier; Dohgyue Chenzhou New Materials Company; Shanghai Jiao Tong University, Shanghai, China; The Boreskov Institute of Catalysis, Novosibirsk, Russia (Prof. V. Bukhtiyarov).*

## **II. Co-Processing of Upgraded Bio-Liquids in Standard Refinery Units**

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

Partners:

*Rijksuniversiteit Groningen, The Netherlands; The Boreskov Institute of Catalysis, Novosibirsk, Russia (Prof. V. Kirillov); Uhde Hochdrucktechnik GmbH, Germany; BTG Biomass Technology Group BV, The Netherlands; University of Twente, The Netherlands; STFI-PACKFORSK AG, Sweden; Institute of Wood Chemistry, Hamburg, Germany; Slovenian Institute of Chemistry, Slovenia; Arkema SA, France; Helsinki University of Technology, Finland; ALMA Consulting Group SAS, France; Centre National de la Recherche Scientifique, France; Chimar Hellas SA, Greece; Albermarle Catalysts Company BV, The Netherlands; Metabolic Explorer, France; Shell Global Solutions International, The Netherlands.*

## **III. Non-Noble Catalysts for Proton Exchange Membrane Fuel Cell Anodes**

Coordinator:

**Dr. G. Tsotridis**, *Institute for Energy, Joint Research Centre*, Petten, The Netherlands

Partners:

*Technical University of Denmark, Lyngby, Denmark; The Boreskov Institute of Catalysis, Novosibirsk, Russia (Prof. E. Savinova); Southampton University, United Kingdom; Technical University of Munich, Germany; Bavarian Center for Applied Energy Research; Umicore, AG & Co KG, Germany.*

## **IV. Novel Materials for Silicate-Based Fuel Cells**

Coordinator: **Dr. Ch. Arguirusis**, *Technische Universität Clausthal*, Clausthal, Germany

Partners:

*University of Aveiro, Aveiro, Portugal; Foundation of Research and Technology Hellas, Greece; Katholieke University of Leuven, Belgium; Max-Planck Institute of Colloids and Interfaces, Munchen, Germany; The Boreskov Institute of Catalysis, Novosibirsk, Russia (Prof. V. Sadykov); Ceramics and Refractories Technological Development Company, Greece; Ceramiques Techniques et Industrielles, France.*

## **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**, *Frantcevykh Institute for Problems of Material Science*, Kiev, Ukraine

Project Co-Directors:

**Prof. V. Sadykov**, *The 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*, 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*, Madrid, Spain

**Prof. V. Sobyenin**, *The Boreskov Institute of Catalysis*, Novosibirsk, Russia

Prof. V. Kozhevnikov, *Institute of Solid State Chemistry*, Ekaterinburg, Russia

Dr. L. Boginsky, *Institute for Personal Development and Staff Retraining in New Areas of Techniques, Technologies and Economics of the Belarus Ministry of Education*, Minsk, Belarus.

## **NATO PROGRAMME: SCIENCE FOR PEACE AND SECURITY**

### **Capture and Decontamination of Chemical & Biological Agents by Novel Catalysts and Millisecond Jet Reactors**

Project Coordinator from a NATO Country:

**Prof. P. Smirniotis**, *University of Cincinnati*, Cincinnati, United States.

Project Coordinator from a Partner Country:

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

## **NATO COLLABORATIVE LINKAGE GRANTS**

### **I. Structural Study of TiO<sub>2</sub> Sulfated Catalysts Prepared by Sol-Gel and Microemulsion Methods**

Project Coordinator from a NATO Country:

**Dr. C. Gerardo**, *Instituto de Ciencia de Materiales de Sevilla*, Sevilla, Spain

Project Coordinator from a Partner country:

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

### **II. Oxide Catalysts for Air and Water Quality Control Ammonia Removal**

Project Coordinator from a NATO Country:

**Dr. M. Banares**, *Instituto de Catalisis y Petroleoquimica*, Madrid, Spain

Project Coordinator from a Partner Country:

**Prof. O. Lapina**, *The Boreskov Institute of Catalysis*, Novosibirsk, Russia.

## **INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)**

### **I. Development of Fundamental Basics and Principles of Designing a Universal Mobile Plant for Oxidation of Toxic, Hazardous Organic Wastes and Energetic Materials in Supercritical Water**

Project Manager from BIC **Prof. V. Anikeev**.

### **II. Environmentally Friendly Small Capacity Power Plants Based on Fuel Cells for Stationary Application**

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

### **III. Development of an Efficient, Inexpensive Nanocomposite Catalyst and Elaboration of a Flexible Technology to Produce Syn-Gas for Fuel Cells**

Project Manager from BIC **Prof. V. Sadykov**.

### **IV. Development of High-Performance Oxygen-Containing Membranes and Compact Syn-Gas Generators on their Base**

Project Manager from BIC **Prof. V. Sadykov**.

### **V. Development of a Compact and Economic Apparatus of Gas Conditioning for Proton Exchange Membrane Fuel Cells**

Project Manager from BIC **Prof. T. Yurieva**.

### **VI. Development of an Integrated Separator for Direct Reforming of Hydrocarbons in High-Temperature Fuel Cells**

Project Manager from BIC **Prof. Z. Ismagilov**.

## NWO–RFBR

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

Project Coordinators:

**Prof. R.A. Santen**, *Technische Universiteit Eindhoven*, Eindhoven, The Netherlands

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

### II. Experimental and Theoretical Studies of Non-Linear Phenomena in Catalytic Oxidation of NH<sub>3</sub> and Reduction of N<sub>2</sub>O over Platinum Metal Surfaces

Project Coordinators:

**Prof. B. Nieuwenhuys**, *Universiteit Leiden*, Leiden, The Netherlands

**Prof. V. Gorodetskii**, *The 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*, Leiden, The Netherlands

**Prof. V. Bukhtiyarov**, *The 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. Blik**, *Universiteit Amsterdam*, Amsterdam, The Netherlands

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

### V. Microstructured Catalytic Reactors for Oxidation of Unsymmetrical Dimethylhydrazine

Project Coordinators:

**Prof. J. Schouten**, *Universiteit Amsterdam*, Amsterdam, The Netherlands

**Dr. S. Khairulin**, *The 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*, Enschede, The Netherlands

**Acad. V. Parmon**, *The 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**, *The Boreskov Institute of Catalysis*, Novosibirsk, Russia.

## CONFERENCE AND EXHIBITION ACTIVITIES

Participation in exhibitions, discussion of commercial prospects of the displayed innovations illustrates the research and social activities of an institution and promotes an increase in its rating, 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 2006, the most important BIC's achievements in the area of applied catalysis were presented at the Exhibitions:

- ❖ *Exhibition "Hydrogen Technologies for Energy Production"*, February 7-10, Moscow, Russia  
**Diploma and Cup** for development of "**Portable Sodium Borohydride-Based Hydrogen Generator**"
- ❖ *VI Moscow International Salon of Innovations and Investments*, February 15-18, Moscow, Russia  
**Golden Medal and Diploma** for the project "**New Efficient Method for Catalyst Loading**"
- ❖ *Permanent Exhibition of Complete Developments of SB RAS*, March 27-April 3, Barnaul, Russia
- ❖ *International Exhibition "Sibnedra. Mining. Sibneftegas. Metals of Siberia. Foundry, Metal Working, Welding"*, March 22-24, Novosibirsk, Russia
- ❖ *Permanent Exhibition of Complete Developments of SB RAS*, May 30-June 1, Omsk, Russia
- ❖ *Permanent Exhibition of Complete Developments of SB RAS*, June 26-28, Komsomolsk-na-Amure, Russia
- ❖ *Exhibition of Scientific and Technical Achievements*, September 19-21, Shenyang, China
- ❖ *Seminar-Presentation of New Developments, Technologies and Equipment for Medicine*, October 9, Novosibirsk, Russia
- ❖ *International Industrial Exhibition "SIBPOLYTECH: Science of Siberia"*, October 24-26, Novosibirsk, Russia
- ❖ *International Exhibition of Russian Federation*, November 8-13, Pekin, China

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



**XVII INTERNATIONAL CONFERENCE ON CHEMICAL REACTORS  
“CHEMREACTOR-17”**

**Post-Symposium “Catalytic Processing of Renewable Sources:  
Fuel, Energy, Chemicals”**

May 15-19, Athens-Crete, Greece



The Conference was organized by

- ◆ The Boreskov Institute of Catalysis, Novosibirsk, Russia
- ◆ Russian Scientific and Cultural Center in Athens
- ◆ Russian Center of International Scientific and Cultural Cooperation under RF Government
- ◆ Ministry of Education and Science of the Russian Federation
- ◆ European Federation on Chemical Engineering
- ◆ Scientific Council on Theoretical Bases of Chemical Technology RAS
- ◆ Scientific Council on Catalysis RAS
- ◆ with assistance of the General Secretariat for Research and Technology of the Ministry of Development, Greece.

Three-day scientific program of CHEMREACTOR-17 comprised plenary invited lectures, oral presentations and posters on the following topics:

- Kinetics of Catalytic Reactions
- Physico-Chemical and Mathematical Bases of the Processes in Chemical Reactors
- Catalytic Processes and Reactors Development: Modeling, Optimization and Catalyst Design
- Catalytic Technologies in Fuel and Energy Production
  - *Hydrogen Production*
  - *Production of Environmentally Safe Fuel*
  - *Environmentally Friendly Energetics.*



200 scientists took part in the Conference. Among them 120 participants from 41 foreign countries – USA, Germany, UK, The Netherlands, France, Italy, Spain, Japan, China, Singapore, Colombia, Saudi Arabia and others.

The Conference program included 8 plenary lectures, 61 oral presentations and 130 posters. 35% of all scientific reports were given by Russian participants.

***Plenary Lectures:***

**G.F. Froment** (Artie Mc Ferrin Department of Chemical Engineering Texas A & M University, Texas, USA) – *“Fundamental Kinetic Modeling for Reactor Design and Simulation”*

**B.S. Bal’zhinimaev** (The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Woven Fiber Glass Materials as a New Generation of Structured Catalysts”*

**D.Yu. Murzin** (Åbo Akademi University, Åbo/Turku, Finland) – *“Is It Worth Doing Kinetic Modelling in Asymmetric Heterogeneous Catalysis of Fine Chemicals?”*

**J. Hanika\*\*\***, V. Jiricny\*, J. Kolena\*\*\*, J. Lederer\*\*\*, V. Stanek\*, V. Tukac\*\* (\*Institute of Chemical Process Fundamentals, Prague; \*\*Institute of Chemical Technology, Prague; \*\*\*Unipetrol, a.s., div. VUANCH, Litvinov, Czech Republic) – *“Trickle Bed Reactor Operation under Forced Liquid Feed Rate Modulation”*

**C.G. Vayenas** (University of Patras, Patras, Greece) – *“Monolithic Electropromoted Reactors: From Fundamentals to Practical Devices”*

**V.A. Kirillov**, V.A. Sobyenin (The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Hydrogen Production for Fuel Cells”*

**A.A. Lemonidou** (Aristotle University of Thessaloniki, Thessaloniki, Greece) – *“Alternative Catalytic Processes for Light Olefins Production: From Lab to Practice”*

**J.-C. Charpentier** (CNRS, Paris, France) – *“In the Frame of Globalisation and Sustainability, Some Tracks for the Future of Chemical and Catalytic Process Engineering”*.

Representatives of industrial enterprises and companies engaged in chemical technology took part in the Conference and in the Exhibition *“Chemical and Catalytic Technologies for Ecologically Save Production”* organized on behalf of Russian Science and Innovation Agency (Rosnauka) as part of the Conference.

## Post-Symposium “Catalytic Processing of Renewable Sources: Fuel, Energy, Chemicals”



Post-Symposium was organized by

- The Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia
- European Federation on Chemical Engineering
- Russian Centre for International Scientific and Cultural Cooperation, ROSZARUBEZHCENTR, Moscow
- European Thyroid Association, ETA, Italy.

150 participants from 38 countries participated in the Post-Symposium. Two-day scientific program of the Post-Symposium comprised plenary invited lectures and oral presentations. Plenary lectures were given by **B.N. Kuznetsov** (Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia) – “*Present Trends in Catalytic Processing of Renewable Plant Biomass into Valuable Products*”, and G. Grassi, **N.N. Vassen\***, L. Conti \*\*, S. Mascia\*\* (European Biomass Association, Brussels, Belgium; \*ETA – Renewable Energies, Florence, Italy; \*\*University of Sassari, Sassari, Italy) – “*Low Cost Production of Bio-Hydrogen from Agri-Pellets*”.

An emphasis of the oral topics was made on catalytic methods for solution of energy problems, mainly for energy production from renewable sources, processes for natural resources processing.

The **Round Table** on the international cooperation in the field of chemical engineering for energy problems solving was organized.

## VII CONFERENCE “MECHANISMS OF CATALYTIC REACTIONS”

July 3-8, St. Petersburg, Russia



The Conference was held at the St. Petersburg Scientific Center.

### Organizers:

- ◆ St. Petersburg Scientific Center RAS, St. Petersburg
- ◆ Scientific Council on Catalysis RAS
- ◆ Ministry of Education and Science of the Russian Federation, Moscow
- ◆ The Boreskov Institute of Catalysis SB RAS, Novosibirsk
- ◆ Lomonosov Moscow State University, Moscow
- ◆ Russian Foundation for Basic Research, Moscow
- ◆ St. Petersburg State University, St. Petersburg
- ◆ International Science and Technology Center, Moscow
- ◆ Russian Mendeleev Chemical Society, St. Petersburg Department
- ◆ JSC “Spectroscopy Systems”, Moscow

220 scientists from Russia and fSU countries (Azerbaijan, Kazakhstan, Ukraine, and Belarus) and 34 representatives from western countries (Austria, Bulgaria, Finland, France, Germany, Hungary, Ireland, Israel, The Netherlands, Poland, UK, and USA) were among the participants. The six-day Conference program consisted of 6 plenary and 19 keynote invited lectures, 93 oral presentations and 96 posters. The keynote sectional and oral presentations were scheduled in the following parallel sessions:

- *Heterogeneous Catalysis of Redox Reactions*
- *Acid-Base Heterogeneous and Homogeneous Catalysis*
- *Methods of Investigation of the Mechanism of Catalytic Reactions.*



### ***Plenary lectures***

**S.D. Varfolomeyev** (Emanuel Institute of Biochemical Physics, RAS; Lomonosov Moscow State University, Moscow, Russia) – *“Enzyme Catalytic Centers: Bioinformatics, Structure and Modes of Action”*

**I.V. Koptuyug** (International Tomography Center, Novosibirsk, Russia) – *“Multinuclear NMR Imaging in Catalytic Research: Recent Developments and Future Prospects”*

**C. Mirodatos**, V.A. Sadykov\* (Institut de Recherches sur la Catalyse, Villeurbanne, France; \*The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Investigation of Redox Reactions Mechanism: Potential Impact on Catalyst Design. Case Study of Hydrogen Production and Purification on Ceria-Based Materials”*

**D.Yu. Murzin** (Åbo Akademi University, Åbo/Turku, Finland) – *“Kinetics and Mechanism of Selective Catalytic Reduction of NO<sub>x</sub> with Hydrocarbons under Lean Conditions”*

**C. Hardacre** (The Queen's University Belfast (Belfast, Northern Ireland) – *“Catalysis in Ionic Liquids”*

S. Damyanova, **L. Petrov** (Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria) – *“Nobel Metals Containing Catalysts for Hydrogen Production”*.

The Section of Young Scientists was organized for the first time in the frames of Conference Program. The Council of Young Scientists of the Boreskov Institute of Catalysis selected 12 best oral presentations for this Section. Two lectures: *“N-Pentane Isomerization at the Supercritical Conditions”* by **A.E. Koklin**, Zelinsky Institute of Organic Chemistry, Moscow, Russia, and *“Photocatalytic Oxidation of Natural and Synthetic Estrogens in Aqueous Solutions”* by **T. Malygina**, Lappeenranta University of Technology, Lappeenranta, Finland were awarded with the Prize of Organizing Committee for the most interesting results.

The Conference program included the International Science and Technology Center (ISTC) Workshop *“Catalysis in Solving the Problems of Hydrogen Energetics and Environment Protection”*. 45 participants discussed the results and prospects of successful research collaboration in the frame of the ISTC program.

## II INTERNATIONAL SYMPOSIUM ON CARBON FOR CATALYSIS

July 11-13, St. Petersburg, Russia



The Symposium on Carbon for Catalysis followed the VII Conference “*Mechanisms of Catalytic Reactions*”.

The Symposium was organized by:

- The Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia
  - Institute of Hydrocarbons Processing SB RAS, Omsk, Russia
  - Swiss Federal Institute of Technology, Lausanne, Switzerland
- under the auspices of the St. Petersburg Scientific Center of RAS, St. Petersburg, Russia.

105 scientists participated in the Symposium including 45 participants from Russia, 4 – from Ukraine and 56 participants from western countries (Belgium, China, Finland, France, Germany, Hungary, Italy, Norway, The Netherlands, Poland, Portugal, Spain, Switzerland, Turkey, UK, USA).

3 plenary and 7 key lectures, 32 oral presentations and 62 posters were presented at the Symposium.

### *Plenary Lectures*

**V.A. Likholobov** (Institute of Hydrocarbons Processing, Omsk, Russia) – “*Catalysts on Carbon Materials Basis: Technological Aspects*”

**E. Ustinov** (Scientific and Production Company “Provita”, St. Petersburg, Russia) – *“Characterization of Porous Structure of Carbonaceous Materials by Means of Density Functional Theory”*

**S. Tennison** (MAST Carbon Technology Ltd, Henley Park, England) – *“Preparation of Carbon Thin Films on Ceramic Supports”*.

### **Key Lectures**

**V.B. Felonov**, E.A. Ustinov\*, V. Yakovlev\*, Ch.N. Barnakov (The Boreskov Institute of Catalysis, Novosibirsk, Russia; \*Scientific and Production Company “Provita”, St Petersburg, Russia) – *“Is It Possible to Solve the Hydrogen Storage Problem with Activated Carbons?”*

**Z.R. Ismagilov**, A.E. Shalagina, O.Yu. Podyacheva, N.V. Shikina, Ch.N. Barnakov, (The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Nitrogen Doped Carbon Nanofibers and Amorphous Carbons for PEMFC Cathode Catalyst Preparation”*

**L. Kiwi-Minsker** (Swiss Federal Institute of Technology, Lausanne, Switzerland) - *“Carbon Based Structured Catalysts for Process Intensification: Opportunities and Limitations”*

**B.N. Kuznetsov** (Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia) – *“Synthesis and Properties of Carbon Supports and Palladium-Carbon Catalysts from Natural Organic Raw Materials”*

**S. Perathoner**, M. Gangeri, G. Centi (University of Messina, Messina, Italy) – *“Nanostructured Carbons for the Development of Advanced Electrocatalysts”*

**A.I. Rusanov** (St. Petersburg State University, St. Petersburg, Russia) – *“Theory of Mechanical Behavior of Microporous Carbon Catalysts”*

**V.V. Strelko** (Institute for Sorption and Problems of Endoecology, National Academy of Sciences of Ukraine, Kiev, Ukraine) – *“Molecular Structure Effect of Carbons on Their Catalytic Activity in the Electron and Proton Transfer Reactions”*.

Oral presentations and posters were scheduled in the following sessions:

- I - *Novel Carbon Based Catalysts and Supports: Synthesis, Characterization, Application*
- II - *New Trends in Carbon Technologies for Adsorption and Catalysis.*

Presentations by the Institute of Hydrocarbons Processing (Omsk, Russia); State Unitary Enterprise “Elektrostal’ Research-and-Production Association “Neorganika” (Elektrostal, Moscow reg., Russia) and Buchi AG (Uster, Switzerland) took place in the frame of the Symposium.



**4<sup>th</sup> EFCATS SCHOOL ON CATALYSIS**  
September 20-24, Tsars Village, St. Petersburg suburb, Russia



The EFCATS School was held in the Education & Conference Center ("Mansion of Duke Kochubey") in a beautiful suburb of St. Petersburg Tsars Village (now named as city of Pushkin).

**Organizers:**

- The Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
- European Federation of Catalysis Societies (EFCATS)
- Scientific Council on Catalysis RAS
- Russian Mendeleev Chemical Society
- St. Petersburg Scientific Center RAS

It was a great honor for the Boreskov Institute of Catalysis to organize the 4<sup>th</sup> EFCATS School in Russia. 180 participants, among them 122 from 26 foreign countries took part in the event.

16 leading European specialists in the field of catalysis from 11 countries were invited as lecturers. Young scientists obtained 62 Grants by Organizing Committee for participation in the School.



***Plenary lectures***

***I. New Approaches for Testing and Characterization of Catalysts***

**V.N. Parmon, N.N. Bobrov, I.I. Bobrova, I.Yu. Pakharukov, M.M. Matrosova**  
(The Boreskov Institute of Catalysis, Novosibirsk, Russia) – “*Modern Techniques for Testing the Catalytic Activity and Kinetics of Catalytic Reactions*”

**H.W. Zanthoff, R.W. Mayer, T. Riermeier** (Degussa, Germany) - “*Fast Development of Innovative Catalysts Applying High-Throughput Kinetic Screening Methods*”

**C. Mirodatos** (Institut de Recherches sur la Catalyse, Villeurbanne, France) – *“Isotopic Studies of the Kinetics and Mechanisms of Heterogeneous Catalytic Reactions”*

**I.I. Ivanova** (Lomonosov Moscow State University, Moscow, Russia) – *“In situ and Operando MAS NMR Spectroscopy in Heterogeneous Catalysis: Advances and Perspectives”*

## **II. Fundamental Aspects of Catalysis on Atomic-Molecular Level**

**V.I. Bukhtiyarov** (The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Studies on Mechanisms of Catalytic Reactions”*

**E.J. Baerends, P.H.T. Philipsen** (Free University, Amsterdam, The Netherlands) – *“The Role of the Fermi Surface in Adsorbate-Metal Interactions: An Energy Decomposition Analysis”*

**G. Rupprechter** (Institute of Materials Chemistry, Vienna University of Technology, Austria) – *“In situ Methods for the Surface Characterization of Catalysts”*

## **III. Catalyst Preparation and Catalytic Processes**

**I.V. Kozhevnikov** (University of Liverpool, UK) – *“Polyoxometalates as Catalysts for Fine Chemical Synthesis”*

**S. Hermans, P. Ruiz, M. Devillers, E.M. Gaigneaux** (Universite Catholique de Louvain, Belgium) – *“Recent Trends in Catalysts Preparation”*

**J. Santamaria** (University of Zaragoza, Spain) – *“Development of Catalytic Reactors Containing Zeolite Films and Coatings”*

**D. Sanfilippo** (Snamprogetti S.p.A., San Donato Milanese, Italy) – *“Routes to Olefins and Derivatives from the Natural Gas Wet Fraction: Catalysis and Reactor Engineering Aspects”*

**J.K. Norskov** (Technical University of Denmark, Lyngby, Denmark) – *“Catalytic Hydrocarbon Production”*

**V. Hessel\*\***, **M. de Croon\*\***, **G. Guan\***, **G. Kolb\***, **H. Lowe\*\*\*\*\***, **E. Rebrov\*\***, **J. Schouten\*\***, **R. Zapf\*** (\*Institut für Mikrotechnik Mainz GmbH (IMM), Mainz, Germany; \*\*Eindhoven University of Technology, Eindhoven, The Netherlands; \*\*\*Johannes-Gutenberg-Universität Mainz, Mainz, Germany) – *“Microchannel Reactors in Chemistry and Catalysis”*

## **IV. Catalysis for Environmental Protection**

**Z.R. Ismagilov** (The Boreskov Institute of Catalysis, Novosibirsk, Russia) – *“Catalytic Combustion for Advanced Energy Generation Technologies and Environmental Protection”*

**D. Murzin** (Åbo Akademi University, Åbo/Turku, Finland) – *“Chemicals from Renewables and Biomass: Role of Catalysis”*

The young scientists presented 31 oral presentations and 104 posters on urgent problems of fundamental and applied present catalysis – mechanism of heterogeneous reactions, up-to-date methods for catalysts investigation, novel equipment for precision tests of catalytic activity of nanomaterials and kinetic studies, combinatorial catalysis, quantum-chemical approaches in catalysis, role of catalysis for fine organic synthesis and environmental protection, fundamentals of catalytic conversion of renewables.

## EDUCATIONAL ACTIVITIES

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

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

More than 50 scientists combine teaching and their job at the Research Institute. They present lectures, give seminars and practical classes; participate in the organization and renovation of the educational process.

From the first years, the strategy of the training of students was built up by leading scientists of BIC and harmonically combines two aspects: on the one hand, curricula provide the students with deep theoretical and practical knowledge in catalysis, i.e. theory of the prevision of the catalytic action of substances, kinetics of catalytic reactions, scientific bases of the preparation of catalysts, bases of the technology of catalytic processes, application of modern physical and mathematical methods for investigation of catalysts and catalysis; on the other hand, the educational process arrangement allows to wide significantly the sphere of the postgraduate activity of the students. They can work as technologists, production managers, researchers at various research organizations, teach at universities.

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

### ***BIC – NSU***

Novosibirsk State University was established as an essential part of the Siberian Branch of the Academy of Sciences; it embodies the idea of the close integration of education and science.

The chief mission of the University is to train professionals for scientific institutions of the country.

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

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

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

*Courses of lectures:*

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

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

*Courses of lectures:*

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

***BIC – NSTU***

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

*Courses of lectures:*

- ◆ Technology Bases for Environmental Protection
- ◆ Processes and Apparatuses for Environmental Protection
- ◆ Catalytic Methods for Environment Protection
- ◆ Methods and Devices for Environmental Control, Ecological Monitoring
- ◆ Mathematical Modeling of Chemical Processes and Reactors
- ◆ Organic Chemistry
- ◆ Industrial Ecology
- ◆ Technologies for Utilization of Industrial Wastes
- ◆ Oil-Gas Branch
- ◆ Analytic Chemistry and Physical-Chemical Methods of Analysis

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

***Dissertation Council Activities***

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

in chemical kinetics and catalysis, physical chemistry, chemical engineering in the BIC laboratories.

Dissertation Council D 002.13.01 was organized at the Boreskov Institute of Catalysis in 1991. It was confirmed by Supreme Certifying Commission (SCC) of Russia on December 8, 2000, order number D 003.012.01. Dissertation Council is allowed to uphold a thesis to receive an academic degree Doctor of Science on specialties: 02.00.15 "Catalysis" within chemical and technical sciences and 02.00.04 "Physical Chemistry" within chemical sciences. Head of the Dissertation Council is the director of the Institute – Academician V. Parmon.

Dissertation Council K 003.012.01 was organized at the Boreskov Institute of Catalysis on December 8, 2000. Dissertation Council is allowed to uphold a thesis to receive an academic degree on specialties 02.00.15 "Catalysis" within chemical sciences and 05.17.08 "Processes and Apparatuses in Chemical Technology" within technical sciences. Head of the Dissertation Council is deputy director of the Institute Prof. Vladimir A. Sobyenin.

6 Doctoral theses and 5 Ph.D. theses have been defended in 2006.

Doctoral theses:

**Sergey F. Tikhov** - *“Physico-Chemical Principles of Porous Composite Alumina Ceramometal Based Supports and Catalysts Preparation”*

**Aleksandr A. Khassin** - *“Catalysts Based on the Layered Structures for the Processes of the Natural Gas Conversion to the Synthetic Liquid Fuels”*

**Elena G. Zhizhina** - *“Catalytic Wet Oxidation of Organic Substrates in the Presence of Mo-V-Phosphoric Heteropoly Acids”*

**Andrey N. Zagoruiko** - *“Simulation and Development of Catalytic Processes in Fixed Adiabatic Beds under Artificially Created Unsteady State of the Catalyst”*

**Oxana A. Kholdeeva** - *“Liquid Phase Selective Oxidation with Molecular Oxygen and Hydrogen Peroxide in the Presence of Single Site Catalysts”*

**Elena R. Savinova** - *“Particle Size and Structural Effects in Electrocatalysis”*

Ph.D. theses:

**Ivan S. Glaznev** - *“Kinetics of Water Adsorption on the Grains and in the Layer of CaCl<sub>2</sub>/Silicagel and CaCl<sub>2</sub>/Alumina Sorbents”*

**Sergey S. Arzumanov** - *“Mechanism Studies of the Conversion of Alkanes and Olefins over Solid Acid Catalysts Studied by <sup>13</sup>C NMR Spectroscopy”*

**Aleksandr I. Titkov** - *“Mechanisms of Palladium Surface Reconstruction and Oxidation Induced by O<sub>2</sub> Chemisorption and CO+O<sub>2</sub> Reaction”*

**Larisa V. Perminova** - *“Research and Development (R&D) of the Heterogeneous Biocatalytical Process of Dextrin Hydrolysis”*

**Natalia V. Maksimchuk** - *“Development of Methods for Fragrance Compounds Obtaining from  $\alpha$ -Pinene”*



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

### *Joint Educational Scientific Laboratories*

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

Joint **Laboratory for Catalytic Processing of Light Hydrocarbons** of the *Boreskov Institute of Catalysis* (Novosibirsk) and *Institute of Petroleum Chemistry* (Tomsk), created in 2000. Scientific Coordinators are **Prof. Aleksandr S. Noskov** (Boreskov Institute of Catalysis) and **Dr. Aleksandr V. Vosmerikov** (Institute of Petroleum Chemistry).

Main areas of scientific research of the Laboratory are:

- ◆ Development of the Scientific Basis for the Technology for Light Hydrocarbons Catalytic Processing
- ◆ Engineering Elaboration of Catalytic Processes and Devices for Light Hydrocarbons Processing
- ◆ Study of Combined Catalytic Processes for Oil and Natural Gas Processing.

Laboratory acts in close contact with Institution of Higher Education of Tomsk.

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

Main areas of scientific research of the Laboratory are:

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

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

Main areas of scientific research of the Laboratory are:

- ◆ Design of the Catalysts and Sorbents for Petrochemistry and Oil Refinery in Russia

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

## SCIENTIFIC SOCIAL LIFE

### NIO SIBUR-TOMSKNEFTEKHIM LLC BECAME THE FIRST RESIDENT OF THE SPECIAL ECONOMIC ZONE IN TOMSK

On April 26 Tomsk saw the solemn opening of the first special economic zone of technical promotion type (SEZ).

While attending the opening ceremony, President of the Russian Federation Vladimir V. Putin awarded Diploma No. 1 to NIO SIBUR-Tomskneftekhim LLC. This company was established by SIBUR Holding JSC to develop titanium-magnesium catalysts and manufacture supermolecular polyethylene of unique properties on the basis thereof.

President of SIBUR Holding JSC A.V. Dyukov and General Director of Tomskneftekhim LLC L.M. Reznikov familiarized V.V. Putin and heads of the federal ministries and departments attending the SEZ opening ceremony not only with the new production facilities located in the area of the Tomsk special economic zone, but also with the plans of SIBUR Holding JSC to increase the chemical output in the territory of the Tomsk Region.

Director of the Boreskov Institute of Catalysis **Academician Valentin N. Parmon** informed Vladimir Putin about long collaboration of headed by him Institute and Tomskneftekhim.

The technology for production of supported titanium-magnesium catalyst TMC and ultra-high molecular weight polyethylene (UHMWPE) designed by Novosibirsk scientists was approbated on pilot scale at Tomskneftekhim. The results of pilot tests became a visible evidence of availability of given developments. Joint work of the scientists from the research institute and specialists from Tomskneftekhim on design of new materials gained the status of Innovative Project of state significance.



## COMPREHENDING THE MYSTERY OF THE ORIGIN OF LIFE

November, 16 a regularly scheduled meeting devoted to the report under the Program of Russian Academy of Sciences «Origin and Evolution of Biosphere» took place at the Boreskov Institute of Catalysis of the SB RAS.

This Program of RAS was initiated several years ago. Now it is executed by the institutions of the Russian Academy of Sciences and scientific teams from the universities of Russian Federation, working in the fields of Life Sciences, Earth Sciences, chemistry, mathematics, informatics, biology, geology, who gather regularly to discuss the already done work and to share new ideas. Due to such community of interests the scientists are able to demonstrate interdisciplinary approach to decision of the problem and to come up to searching for an answer how life emerged on Earth.

In their presentation the lecturers regarded various problems related to evolution of biosphere. Problems of abiogenic synthesis and evolution of the matter under conditions of pregeological stages of the Earth evolution were considered. One of the reports was presented by **Dr. V. Snytnikov**.



Collage form yhe Journal “Science from the First Hands”

## FOR SOLVING GLOBAL PROBLEMS

Global Energy International Prize is a unique award intended to assist international cooperation in solving the most important nowadays problems in the field of power generation. On December 18, in the Central House of Scientists, Russian Academy of Science (Moscow), the final results of the Russian Contests of the Youth Energy Research Projects conducted by the “Global Energy” Award were announced. «Global Energy» Prizes were delivered to six teams of scientists to conduct research on hydrogen, nuclear power engineering, and derivation of synthetic fuel and ecology of unrenewed energy sources. In the current year the young scientists received, apart from Diploma of Honor, medals of the Youth Contests Winners which are the exact replica of the gold medal invested to “Global Energy” Award laureates.

There are two groups of young scientists of the Boreskov Institute of Catalysis among the winners. **Dr. P. Snytnikov** and **O. Netskina** represented these teams on the ceremony. Group of four researchers – **P. Snytnikov, A. Stadnichenko, S. Badmaev, M. Sidyakin**, Laboratory of Catalytic Processes in Fuel Cells, works on the Project “*Hydrogen Production from Methanol, Dimethyl Ether and Ethanol for Fuel Cells*”. The second group – **O. Netskina, O. Komova, A. Gentsler, E. Graifer**, Laboratory of Hydride Compounds Studying, works on the Project “*Development of Active and Stable Catalysts for Portable Hydrogen Gas Generators*”



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:

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

The Foundation is supported by IUPAC and some Russian sponsors.

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

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

Major part of Foundation means is spent on Zamaraev post-graduate scholarships, prizes and grants. Foundation plans to support the international cooperation of scientific youth in the field of chemical catalysis and chemical physics, i.e., their participation in international scientific conferences and seminars. In 2006 **T. Trubitsyna, A. Nuzhdin, I. Pakharukov, I. Simonova** have got the post-graduate scholarship; **V. Kolko, A. Sametova** - incentive post-graduate scholarships.

13 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 80<sup>th</sup> 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 Chemcoradiological Institute (Odessa) in 1932 through 1937 (the laboratory registry dated 1931 with records by Georgii Konstantinovich concerning the preparation and characterization of vanadium catalysts was kept); the Laboratory of Catalysis at the Research Institute for Fertilizers and Insecto-Fungicides (Moscow) in 1937 through 1946, the Laboratory of Technological Catalysis at the Karpov Institute of Physical Chemistry (Moscow), and in 1958 became the Director of the Institute of Catalysis (Novosibirsk).

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

Boreskov's activity in the area of catalysis was recognized worldwide. He was a foreign member of the National Academy of Sciences of German Democratic Republic, honorary member of the New York Academy of Sciences, Doctor HONORIS CAUSA of the Wroclaw Polytechnic Institute (Poland) and of the Poitiers University (France). Government of Bulgarian Republic awarded the Order of Kirill and Mepodium 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.



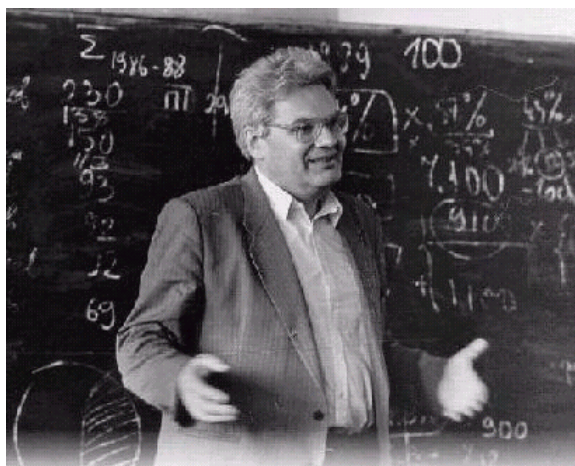


There is his writing table, case, bureau and an old push-button typewriter.

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 20<sup>th</sup> of May 1999, the day of 60<sup>th</sup> anniversary of K. Zamaraev. Establishment of the Memorial Room was promoted by the International Charitable Zamaraev Foundation and directly participated by Kirill Ilyich’s widow, Lyudmila Aleksandrovna Zamaraeva. This small museum exposition relates to the life and activities of Academician Kirill Ilyich Zamaraev, who was a hereditary scientist.



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

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



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

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

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

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



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

Everyone, who knew personally Kirill Ilyich, remember his exceptional ability not to lose 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.

# **RESEARCH ACTIVITY**

## Quantum-Chemical Investigations

### C-O BOND SCISSION IN METHOXIDE ON Pd NANOPARTICLES: A DENSITY FUNCTIONAL STUDY

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*Phys. Chem. Chem. Phys.*,  
8 (2006) pp. 2396-2401.

C-O bond scission of methoxide species adsorbed at the surface of Pd nanoparticle was studied by DF calculations for the example of cuboctahedral Pd<sub>79</sub>. To investigate different locations of adsorbed intermediates as well as the transition state of C-O bond scission, a substrate model was used, which allows one to consider adsorbates without any local geometry restrictions. In contrast to reaction sites on the flat Pd(111) surface and on extended facets, scission of the C-O bond of methoxide at cluster edges is exothermic by ~40 kJ/mol and the decomposition product CH<sub>3</sub> is found to be stabilized there. However, the high calculated activation barrier, ~140 kJ/mol, implies only a very slow reaction compared to dehydrogenation of CH<sub>3</sub>O.

### ADSORPTION OF Cu<sub>4</sub>, Ag<sub>4</sub> AND Au<sub>4</sub> PARTICLES ON THE REGULAR MgO(0 0 1) SURFACE: A DENSITY FUNCTIONAL STUDY USING EMBEDDED CLUSTER MODELS

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*Chem. Phys. Lett.*,  
417(4-6) (2006) pp. 515-520.

Cu<sub>4</sub>, Ag<sub>4</sub>, and Au<sub>4</sub> species adsorbed on the regular MgO(0 0 1) 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<sub>4</sub> moiety orthogonal to the surface and two metal atoms attached to surface oxygen anions. Au<sub>4</sub> and Cu<sub>4</sub> exhibit substantially stronger binding to the surface than Ag<sub>4</sub>.

### A DFT STUDY OF HYDROGEN-DEUTERIUM EXCHANGE OVER OXIDIZED AND REDUCED GALLIUM SPECIES IN Ga/HZSM-5 ZEOLITE

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(\*Zelinsky Institute of Organic Chemistry, Moscow, Russia; \*\*Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands)

*Catal. Lett.*, 108(3-4) (2006) pp. 187-191.

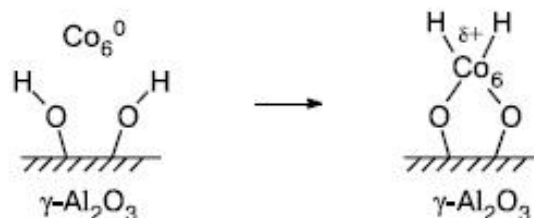
Quantum-chemical calculations give insight in the experimentally observed higher rate of hydrogen-deuterium exchange for oxidized Ga/HZSM-5 over reduced Ga/HZSM-5. The reaction is computed to be more facile over reduced (Ga<sup>+</sup>) than over oxidized (GaO<sup>+</sup>) cations. The difference lies in the difficult formation of active GaH<sub>2</sub><sup>+</sup> cations from Ga<sup>+</sup> compared to facile hydrogen dissociation over GaO<sup>+</sup> to give active GaHOH<sup>+</sup> cations. Neutral gallium oxide clusters are shown to have a lower intrinsic activity than GaO<sup>+</sup> cations.

### INTERACTION OF Co<sub>6</sub> CLUSTER WITH γ-ALUMINA SURFACE: A QUANTUM CHEMICAL STUDY

M.N. Mikhailov\*, G.M. Zhidomirov, A.Yu. Krylova\* (\*Zelinsky Institute of Organic Chemistry, Moscow, Russia)

*Russ. Chem. Bull.*, 10 (2005) pp. 2264-2269.

The interaction of Co<sub>6</sub> cluster with partially dehydroxylated γ-alumina surface was studied by the DFT method. Hydrogen atoms of surface hydroxyl groups can be transferred to the metal particle to form partially oxidized cobalt states. The energy characteristics of hydrogen transfer were determined and changes in the electronic structure of supported Co<sub>6</sub> particles were characterized.



**MoS<sub>2</sub> SINGLE SLAB AS A MODEL FOR ACTIVE COMPONENT OF HYDRODESULFURIZATION CATALYST: A QUANTUM CHEMICAL STUDY.**

**1. MOLECULAR AND ELECTRONIC STRUCTURE OF Mo<sub>12</sub>S<sub>24</sub> MACROMOLECULE AND ITS ADSORPTION COMPLEX WITH H<sub>2</sub>S**

**I.I. Zakharov, A.N. Startsev**

*Russ. Chem. Bull.*, 10 (2005) pp. 2259-2263.

The molecular and electronic structure of Mo<sub>12</sub>S<sub>24</sub> macromolecule as the MoS<sub>2</sub> single slab structure was calculated by the density functional theory (DFT) method with the B3P86 hybrid exchange-correlation functional. The results of calculations point to slight relaxation of coordinatively unsaturated Mo and S atoms, which is consistent with the published data. The calculated width of the forbidden band (0.85-0.98 eV) is comparable with the experimental value (1.30 eV) and similar to that obtained from DFT calculations with periodic boundary conditions (0.89 eV). The surface Mo centers in the Mo<sub>12</sub>S<sub>24</sub> macromolecule are more reduced than the internal Mo(IV) atoms. In order to characterize the adsorption capacity of coordinatively unsaturated Mo centers, a Mo<sub>12</sub>S<sub>24</sub>•6H<sub>2</sub>S adsorption complex was calculated. The structure and energy characteristics of the adsorption complex point to a weak donor-acceptor interaction of the  $\pi$ -lone pair of H<sub>2</sub>S molecule with the surface (reduced) Mo centers. The active center of thiophene hydrodesulfurization catalysts is formed as a result of the oxidative addition of hydrogen followed by occlusion of hydrogen into the MoS<sub>2</sub> matrix.

**THE MOLECULAR AND ELECTRONIC STRUCTURE OF THE Mo<sub>12</sub>S<sub>24</sub> MACROMOLECULE AS A MODEL OF THE ACTIVE COMPONENT OF A HYDRODESULFURIZATION CATALYST**

**I.I. Zakharov, O.V. Voroshina, A.N. Startsev**

*Russ. J. Phys. Chem.*,  
80(7) (2006) pp. 1083-1087.

The density functional theory (DFT) with the B3P86 hybrid exchange-correlation functional was used to calculate the molecular and electronic structure of the Mo<sub>12</sub>S<sub>24</sub> macromolecule as a single MoS<sub>2</sub> layered structure slab. Calculations with geometry optimization are indicative of insignificant relaxation of the coordinatively unsaturated Mo and S atoms, which corresponds with the literature DFT data on the MoS<sub>2</sub> single slab obtained with periodic boundary conditions. The calculated forbidden band

width (0.85–0.98 eV) is comparable with its experimental value (1.30 eV) and the results of DFT calculations of MoS<sub>2</sub> with periodic boundary conditions (0.89 eV). An analysis of the electronic state of the surface Mo centers in the Mo<sub>12</sub>S<sub>24</sub> macromolecule showed that these centers were reduced to a greater degree than the Mo(IV) atoms in the bulk. The adsorption complex between the Mo<sub>12</sub>S<sub>24</sub> macromolecule and six H<sub>2</sub>S molecules was calculated to characterize the adsorption ability of the coordinatively unsaturated Mo centers. The structure and energy characteristics of the adsorption complex corresponded to weak donor-acceptor interaction between the  $\pi$ -lone pair of H<sub>2</sub>S and the surface (reduced) Mo centers. The suggestion was made that the active center of the catalytic cycle of thiophene hydrodesulfurization should induce the oxidative addition of H<sub>2</sub> followed by the occlusion of hydrogen into the MoS<sub>2</sub> matrix.

**QUANTUM-CHEMICAL ANALYSIS OF THE CuCl<sub>2</sub> MOLECULE**

**S.F. Ruzankin, V.F. Anufrienko, S.A. Yashnik, Z.R. Ismagilov**

*J. Struct. Chem.*,  
47(3) (2006) pp. 404-412.

This paper reports on quantum-chemical analysis of the linear structure of CuCl<sub>2</sub> by Hartree-Fock (HF) and density functional theory (DFT) methods and also by time-dependent HF (TD HF) and DFT (TD DFT) techniques. Using pure DFT exchange correlation functional (B3LYP) yields the best agreement with the experimental electronic spectra of CuCl<sub>2</sub>. In this case, the odd electron is delocalized over the molecule, spin density on copper being 0.27. The ground state of the CuCl<sub>2</sub> molecule is <sup>2</sup> $\Pi_g$  with linear geometry.

**ASFMS: A PROGRAM PACKAGE FOR AB INITIO CALCULATION OF ABSORPTION SPECTRA BY FULL MULTIPLE SCATTERING**

**S.Ph. Ruzankin**

*Comp. Mater. Sci.*, 36(1-2) (2006) pp. 184-188.

The program package ASFMS for *ab initio* self-consistent field (SCF) all-electron full multiple scattering (MS) computations of electron structure and absorption spectra of large systems was developed. ASFMS can compute the X-ray absorption fine structure (XAFS) and near-edge structure (XANES) spectra. Unlike other programs ASFMS can be applied to calculations of pre-edge structure and transition intensity in ultraviolet region. Another advantage of

ASFMS consists in using additional cluster boundary conditions for modeling of ionic and covalent solids. Effective algorithms are implemented to reduce the time of the computation and storage.

#### **NATURE OF THE CHEMICAL BOND OF HYDROGEN AND OXYGEN ATOMS WITH Pt(100) SURFACE: QUANTUM CHEMICAL CALCULATION AND DISAPPEARANCE POTENTIAL SPECTRA**

**V.M. Tapilin, V.D. Tsybiktarov, A.R. Cholach**

*Russ. J. Struct. Chem.*,  
47(5) (2006) pp. 808-812.

Electronic structures of clean, hydrogen covered, and oxygen covered Pt(100)-(1×1) surface have been calculated. Both adsorbates form surface subzones localized below the metal conduction band and overlapping partially with it. Furthermore, the local density of states (LDOS) reveals the peaks of the resonant state on the adsorbed atoms which are narrower for hydrogen than for oxygen. The comparison of LDOS on adsorbed and Pt atoms shows that subzone surface states are responsible for the covalent component of the chemical bond between adsorbed and platinum atoms, while resonant states make the ionic contribution. The obtained LDOS were used to calculate disappearance potential spectra. Theoretical spectra are well consistent with experimental ones.

#### **ELECTRONIC STRUCTURE OF ZrO<sub>2</sub> AND HfO<sub>2</sub>**

**T.E. Perevalov\*, A.V. Shaposhnikov\*,  
K.A. Nasyrov\*, D.V. Gritsenko\*, V.A. Gritsenko\*,  
V.M. Tapilin** (\*Institute of Semiconductor Physics,  
Novosibirsk, Russia)

In “*Defects in High-k Gate Dielectric Stacks: Nano-Electronic Semiconductor Devices*”,  
NATO Science Series II: Mathematics,  
Physics and Chemistry,  
Ed. E. Gusev, Springer, 2006, pp. 423-434.

Band structures, density of states and effective masses of electrons and holes of cubic, tetragonal and monoclinic phases of ZrO<sub>2</sub> and HfO<sub>2</sub> have been calculated. Oxygen vacancy has been modeled by removing off one oxygen atom from 12-atom monoclinic cell. Incorporation of oxygen vacancy leads to formation of new filled subband formed mostly by d-electrons of the metals. Enormously high leakage current, observed in ZrO<sub>2</sub> and HfO<sub>2</sub> is explained by multi-phonon trap ionization model.

#### **TIME SAVING TECHNIQUES FOR ELECTRONIC STRUCTURE CALCULATIONS OF INFINITE AND SEMI-INFINITE CRYSTALS, INTERFACES, AND SLABS OF ARBITRARY THICKNESS**

**V.M. Tapilin**

*Comp. Mater. Sci.*, 36(1-2) (2006) pp. 106-111.

Hard confined functions (HCF) are proposed as a basis set for electronic structure calculations. The basis functions have enough number of continuous derivatives to perform space integrations numerically with desired accuracy. Replacing unconfined basis functions in ADF-AND package by HCF with cut-off radiuses of the order of the nearest neighbor distance leads to the reduction of the time of computations without losing the accuracy. For the crystals with surfaces, special techniques based on representation of the wave function as a linear combination of a finite number of HCF and Bloch waves, were elaborated. Exact finite sets of equations for coefficients of HCF and Bloch waves have been developed. The order of the sets depends only on the thickness of a perturbed region, but not on the size of the whole system. For integration of the density of states over perpendicular to the surface wave vector component and energy the residue theorem and a shift of the energy path into the complex plane are used.

#### **THE VARIATIONS OF g-TENSOR PRINCIPAL VALUES IN REDUCED [2Fe-2S] CLUSTER OF IRON-SULFUR PROTEINS**

**A.A. Shubin, S.A. Dikanov\*** (\*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia)

*Appl. Magn. Reson.*, 30(3-4) (2006) pp. 399-416.

This article discusses the present status of the theoretical and experimental studies of the electronic structure of the reduced [2Fe-2S] cluster with special emphasis on the g-tensor variations in the Rieske-type proteins. The necessity of this analysis is dictated by the fact that the changes in the EPR lineshape of the reduced cluster are broadly exploited as the basis for different mechanistic conclusions in the structure-function studies of the *bc<sub>1</sub>/bf* families.

### ANALYSIS OF THE STRUCTURAL SPECIFICITY OF ZrO<sub>2</sub> NANOPARTICLES IN PILLARED CLAYS BY MODELING OF THE CONDENSATION PROCESS IN ZrOCl<sub>2</sub>·8H<sub>2</sub>O SOLUTIONS

N.V. Mezentseva, V.A. Sadykov, V.I. Avdeev, V.L. Kuznetsov

*Mater. Res. Soc. Symp. Proc.*,  
894 (2006) LL06-05.1-05.6.

A combination of quantum-chemical approaches including DFT, semiempirical PM3 and molecular mechanics (force field MM+) methods has been applied for analysis of the structure of polynuclear hydroxocomplexes of Zr in diluted solutions of its oxochloride as precursors of zirconia nanoparticles in zirconia-pillared clays. Relative stability of complexes differing by their size and shape has been estimated.

### SURFACE CHARACTERIZATION OF NANOSTRUCTURED ZIRCONIA CATALYSTS BY ESR SPECTROSCOPY USING O<sub>2</sub><sup>-</sup> RADICAL ANIONS AS SPIN PROBES

N.V. Mezentseva, A.F. Bedilo, A.M. Volodin, V.A. Sadykov

*Mater. Res. Soc. Symp. Proc.*,  
900E (2006) O06-11.1-11.6.

O<sub>2</sub><sup>-</sup> radical anions generated by adsorption of hydrogen peroxide or NO + O<sub>2</sub> mixture were used as spin probes for EPR characterization of nanostructured zirconia catalysts, including pillared clays. Similarities and significant discrepancies observed in the formation of oxygen radical anions over catalysts with different composition and surface structure by the two methods are discussed.

### KOOPMANS' THEOREM IN THE ROHF METHOD: CANONICAL FORM FOR THE HARTREE-FOCK HAMILTONIAN

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(\*Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia)

*J. Chem. Phys.*,  
125(21)(2006) pp. 204110 (10 pages)

Since the classic work of Roothaan [Rev. Mod. Phys. 32, 179 (1960)], the one-electron energies of a ROHF method are known as ambiguous quantities having no physical meaning. Together with this, it is often assumed in present-day computational studies that Koopmans' theorem is valid in a ROHF method. In this work the specific dependence of orbital energies on the choice of the basic equations in a ROHF method which are the Euler equations and different forms of the generalized Hartree-Fock equation are analyzed. The authors first prove that the one-electron *open-shell* energies  $\epsilon_m$  derived by the *Euler equations* can be related to the respective ionization potentials  $I_m$  via the modified Koopmans' formula  $I_m = -\epsilon_m/f_m$  where  $f_m$  is an occupation number. As compared to this, neither the closed-shell orbital energies nor the virtual ones derived by the Euler equations can be related to the respective ionization potentials and electron affinities via Koopmans' theorem. Based on this analysis, the new (*canonical*) form for the Hamiltonian of the Hartree-Fock equation is derived, the eigenvalues of which obey Koopmans' theorem for the whole energy spectrum. A discussion of new orbital energies is presented on the examples of a free N atom and an endohedral N@C<sub>60</sub> ( $I_h$ ). The vertical ionization potentials and electron affinities estimated via Koopmans' theorem are compared with the respective observed data and, for completeness, with the respective estimates derived via a  $\Delta$ SCF method. The agreement between observed data and their estimates via Koopmans' theorem is qualitative and, in general, appears to possess the same accuracy level as in the closed-shell SCF.

## Monte-Carlo Simulation to Study Physico-Chemical Processes

### GRAZERS AND GRASS: MONTE CARLO SIMULATIONS

V.P. Zhdanov

*BioSystems*, 85(3) (2006) pp. 219-224.

To illustrate the interplay between grazers and grass, a novel Monte Carlo model is presented including grass-island growth, consumption of grass

by grazers, and birth, migration and death of grazers. The rates of the former and three latter processes are assumed to depend on the environment so that the conventional mean-field approximation does not hold (in particular, the model takes into account that grass grows on the grass-island boundaries, and grazers are mobile and prefer to stay on the areas covered by grass). Due to the feedback between various

processes, as expected, the model predicts stable regimes and irregular oscillations of the area of the grass islands and grazer population. The patterns observed are however different compared to those predicted by conventional Monte Carlo prey–predator models. Specifically, there is no tendency for grazers and grass to segregate. The mean-field version of the model is briefly discussed as well.

#### **TRANSIENT STOCHASTIC BISTABLE KINETICS OF GENE TRANSCRIPTION DURING THE CELLULAR GROWTH**

**V.P. Zhdanov**

*Chem. Phys. Lett.*, 424(4-6) (2006) pp. 394-398.

The feedback between mRNA and regulatory-protein production may result in bistability of gene transcription. If the mRNA and/or protein number are low, one can observe transcriptional ‘bursts’ in this case provided that the intracellular conditions are steady. Monte Carlo simulations show that for biologically reasonable kinetic parameters this effect may easily disappear if the transcription occurs during the cellular growth and division.

#### **SUPPRESSION OF BINDING EVENTS VIA EXTERNAL PERTURBATION WITH EMPHASIS ON QCM**

**V.P. Zhdanov, M. Edvardsson\*, F. Hook\*\*, B. Kasemo\*** (\*Chalmers University of Technology, Göteborg, Sweden; \*\*Lund University, Lund, Sweden)

*Chem. Phys. Lett.*, 424(1-3) (2006) pp. 214-217.

Recent experiments indicate that the external perturbations, related e.g. to high-amplitude shear oscillations of the surface of a quartz crystal microbalance sensor, may suppress binding of mesoscopic aggregates (e.g., polystyrene spheres, vesicles, large proteins, etc.) to the surface. Using a simple kinetic model, equations were derived making it possible to conceptually understand and to mathematically describe what may happen in such experiments.

#### **SIGNALING BETWEEN CELLS ATTACHED TO A SURFACE**

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

*Phys. Rev. E*,  
74 (2006) 021915 (6 pp.).

A kinetic model allowing one to classify likely scenarios of protein-mediated communication between attached cells of two distinct types is presented. Upon

treatment, messenger proteins, synthesized in type-1 cells, are considered to penetrate the external membrane of these cells, diffuse in the extracellular medium, associate with the receptors in the external membrane of cells of both types, and induce intracellular signal transduction cascades, influencing the development of cells. Protein degradation inside and outside cells is taken into account as well.

#### **IMAGING AND MANIPULATION OF ADSORBED LIPID VESICLES BY AN AFM TIP: EXPERIMENT AND MONTE CARLO SIMULATIONS**

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

*Colloids Surf. B: Biointerf.*,  
47(2) (2006) pp. 115-125.

Single lipid vesicles adsorbed on SiO<sub>2</sub> were manipulated using an atomic force microscope (AFM) operated in contact mode. For large force setpoints, single vesicles were either pushed sideways or ruptured by the tip, depending on the tip type (sharp or blunt) used, while for small force setpoints the vesicles were imaged by the tip. To extend the interpretation of and to guide the experiment, it has been developed a generic model of the vesicle–tip–substrate system and performed Monte Carlo simulations, addressing the influence of force setpoint and tip speed and shape on the type of imaging or manipulation observed. Specifically, it has been explored AFM-image height and width variations versus force setpoint, typical AFM images for small and large force setpoints, tip-induced vesicle strain versus force setpoint, typical vesicle shapes during pushing for different tip speeds, and the details of vesicle rupture induced by the tip.

#### **ADSORPTION AND SPONTANEOUS RUPTURE OF VESICLES COMPOSED OF TWO TYPES OF LIPIDS**

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

*Langmuir*, 22(8) (2006) pp. 3477-3480.

To analyze the adsorption of single vesicles composed of two types of lipids (e.g., zwitterionic and positively charged lipids or zwitterionic and negatively charged lipids), a statistical model is proposed taking into account lipid-surface interactions, lipid-lipid lateral interactions, and vesicle

bending energy. Treatment specifies how these parameters govern vesicle adsorption, shows how the radius of the vesicle-surface contact area may depend on the vesicle composition, and clarifies the conditions for vesicle rupture.

#### **SIMULATION OF THE CHARGE AND POTENTIAL DISTRIBUTION IN THE DOUBLE LAYER FORMED BY POLYMER ELECTROLYTE**

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

*Electrochem. Comm.*,  
8(4) (2006) pp. 561-564.

Monte Carlo simulations of phase separation on the nm scale in the double layer formed by wetted NAFION or NAFION-type polymer electrolyte near the charged metal surface is presented. The results obtained indicate that the phase separation may cause appreciable spatial fluctuations of the potential near the surface. If e.g. the drop of the potential in the double layer is about 1 V, the amplitude of the fluctuations of the potential may be 0.2–0.3 V. Such fluctuations may influence the rate of electrochemical reactions.

#### **KINETICS OF ELECTROCHEMICAL O<sub>2</sub> REDUCTION ON Pt**

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

*Electrochem. Comm.*, 8(7) (2006) pp. 1132-1136.

The experiments show that the kinetics of O<sub>2</sub> reduction on Pt (with NAFION as electrolyte) is first order in O<sub>2</sub> in a wide range of reaction conditions. Recent DFT calculations indicate that during this reaction the atomic-oxygen coverage may be appreciable. To adjust these two findings, the reaction kinetics corresponding to the dissociative and associative mechanisms with participation of atomic oxygen was analyzed. If the reaction steps are described by using the Langmuir equations, the kinetics is predicted to be first order only in the situations when the O coverage is low. With O–O lateral interactions, the model based on the associative mechanism is able to predict the first-order kinetics in a wide range of pressure even if the O coverage is appreciable.

#### **PROPAGATION OF A REACTION FRONT ACCOMPANIED BY ISLAND FORMATION: CO/Au/Ni(111)**

**V.P. Zhdanov, R.T. Vang, J. Knudsen, E.K. Vestergaard, F. Besenbacher** (*\*University of Aarhus, Aarhus C, Denmark*)

*Surf. Sci.*,  
600(19) (2006) L260-L264.

Recent high-pressure scanning tunneling microscopy studies, performed at room temperature, have explicitly demonstrated the specifics of the CO-mediated removal of Ni atoms from the topmost layer of an Au/Ni(111) surface alloy. After an incubation period, the reaction is found to start at step edges. On each edge, a large fraction of Ni atoms is removed from the terrace in certain areas, whereas other areas are nearly intact after a given time. With increasing time, the former areas begin to overlap and the reaction front becomes somewhat more homogeneous. The Au atoms remaining behind the front form nm-sized islands. Here, Monte Carlo simulations reproducing all these observations are presented.

#### **RELAXATION OF PLASMONS IN nm-SIZED METAL PARTICLES LOCATED ON OR EMBEDDED IN AN AMORPHOUS SEMICONDUCTOR**

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

*Surf. Sci.*,  
599(1-3) (2005) L372-L375.

Relaxation of plasmons, generated optically in nm-sized metal particles, occurs usually via excitation of electron–hole pairs inside the particles. If a metal particle is located on the surface of or embedded in a semiconductor, plasmons may also relax via local field enhanced excitation of electron–hole pairs in the semiconductor. Equations were derived describing the latter relaxation channel in the case when the semiconductor is amorphous or nanocrystalline and show that the ratio of the rates of the two channels may vary in a wide range. In particular, the latter channel may dominate under certain conditions. As an example, the Ag/TiO<sub>2</sub> system is briefly discussed.



## CHARGE DISTRIBUTION ON AND NEAR SCHOTTKY NANOCONTACTS

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*Physica E*,  
33(1) (2006) pp. 296-302.

Schottky nanocontacts are formed when nm-sized metal particles are located on the planar surface of a doped semiconductor. The charge distribution on and near such nanocontacts is analyzed in the case of disc-shaped particles. The results of calculations are presented as a function of particle size, semiconductor permittivity, dopant concentration, and Fermi level difference. In contrast to macroscopic junctions, the charging of the metal particle is demonstrated to be proportional to the Fermi level difference and accordingly to the potential difference between the metal and semiconductor, so that the junction exhibits a constant capacitance. The charging of the metal-vacuum metal surfaces may be appreciable, especially for relatively low values of the semiconductor permittivity. The tunneling barrier width at half height is shown to be close to, or less than, 3/8 of the disc diameter.

## SELF-SUSTAINED KINETIC OSCILLATIONS IN CO OXIDATION OVER SILICA-SUPPORTED Pt

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*Phys. Chem. Chem. Phys.*,  
8(23) (2006) pp. 2703-2706.

Isothermal self-sustained kinetic oscillations in CO oxidation over silica-supported Pt at near-atmospheric pressure were studied by combined *in situ* Fourier transform infrared spectroscopy and mass spectrometry. The use of a specially designed reactor and careful choice of the physical properties of the catalyst and reaction conditions made it possible to eliminate diffusion limitations, to determine the maximum CO oxidation rate per Pt site in the purely kinetic regime and to clarify the mechanism of the oscillations. Specifically, the results obtained indicate that during the high reactive periods the reaction mainly occurs on the oxide surface.

## NONADIABATIC RATE PROCESSES ON METAL SURFACE: LIMITATION BY SPIN CONVERSION

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*J. Exp. Theor. Phys.*,  
102(5) (2006) pp. 737-740.

Rate processes occurring on a metal surface may sometimes be limited by spin conversion. A generic model is presented describing this case. The results obtained are compared with the conventional two-state Landau-Zener model and with a multistate model implying one-electron transfer between the reactant and the metal. In this context, the specifics of the dissociative adsorption of O<sub>2</sub> on Ag(111) are briefly discussed.

## STATISTICAL LATTICE MODEL FOR THE BIMOLECULAR REACTION ON THE DYNAMICALLY CHANGING SURFACE OF A BODY-CENTERED METAL CRYSTAL

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*Kinet. Catal.*,  
47(4) (2006) pp. 469-480.

A statistical lattice model has been constructed for the surface of a body-centered cubic (bcc) crystal whose morphology varies under the action of external factors (temperature and adsorbate coverage). Monomolecular and dissociative bimolecular adsorption on the bcc crystal surface has been investigated. In this model, adsorption smoothens the originally rough surface owing to adsorbate molecules stabilizing their flat adsorption areas, as distinct from adsorption on the primitive cubic lattice. The model differs from the models with invariable surface morphology in that the number of its accessible adsorption sites is variable and depends on external conditions. The kinetics of a catalytic reaction proceeding by the Langmuir–Hinshelwood mechanism have been studied for the (100) face of a bcc crystal whose morphology varies under the action of the reaction medium.

## ON THE PORE SIZE DISTRIBUTIONS OF CARBONACEOUS CATALYSTS AND ADSORBENTS

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*Chem. Sustain. Devel.*, 14(6) (2006) pp. 565-569.

The modeling of a low temperature nitrogen adsorption in graphite mesopores with rectangular sections having the aspect ratio of the side lengths more than 7:1 has been executed by using the grand canonical Monte Carlo (GCMC) method. The adsorption branches of obtained GCMC isotherms were processed with the purpose of calculation of the formal pore size distributions (PSDs) by the nonlocal

density functional theory (NLDFT) and Derjaguin-Broekhoff-de Boer (D-BdB) method. It is shown that NLDFT underestimates the sizes of the model rectangular mesopores though gives good estimations of specific surface area and volume of the pores. Also, it is shown that D-BdB method very strongly underestimates specific surface area and overestimates total volume of pores. PSDs obtained from D-BdB method have a very wide distributive interval of apparent sizes and brightly expressed bimodal forms. Such completely wrong information about the size of the investigated model pores is a consequence of the macroscopic assumption of the D-BdB theory about the constancy of the capillary condensate density in pores at various pressures.

## Studying of Active Sites, Mechanism and Reaction Kinetics

### COMBINED *IN SITU* XPS AND PTRMS STUDY OF ETHYLENE EPOXIDATION OVER SILVER

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*J. Catal.*,  
238(2) (2006) pp. 260-269.

Ethylene epoxidation over silver was investigated by combined *in situ* X-ray photoelectron spectroscopy (XPS) and proton-transfer reaction mass spectrometry (PTRMS) at 300–520 K and 0.07–1 mbar. Ethylene oxide was present among the reaction products at  $T \geq 420$  K and  $p \geq 0.3$  mbar. The catalytically active surface contains two oxygen species – nucleophilic and electrophilic oxygen. The observed correlation between the abundance of electrophilic oxygen and the yield of ethylene oxide expressed as  $C_2H_4O$  partial pressure indicates that namely this oxygen species oxidizes ethylene to ethylene oxide. Opposite trend is observed for nucleophilic oxygen: the higher is the abundance of this species, the lower is the yield of ethylene oxide. This result is in line with the known fact that because of its oxidic nature, nucleophilic oxygen is active in total oxidation of ethylene to  $CO_2$  and  $H_2O$ . The low activity of silver at  $T < 420$  K is caused by the presence of carbonates and carbonaceous residues at the silver surface that reduce the available silver surface area for the catalytic reaction. Reduction of the surface area available for the formation of active species due to accumulation of the embedded oxygen species also explains the decreased rate of ethylene oxide formation with time observed for  $T \geq 470$  K.

### STRUCTURE OF THE ACTIVE COMPONENT AND CATALYTIC PROPERTIES OF CATALYSTS PREPARED BY THE REDUCTION OF LAYERED NICKEL ALUMINOSILICATES

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*Kinet. Catal.*,  
47(3) (2006) pp. 412-422.

The reduction of Ni–Mg aluminosilicates with the amesite structure was studied using thermogravimetry, high-resolution electron microscopy, XPS, and XRD. It was found that the reduction with hydrogen at 920 K resulted in the formation of nickel particles coated with a difficult-to-reduce amorphous oxide shell. The reduced samples were incapable of chemisorbing oxygen; however, they exhibited a high adsorption capacity for hydrogen. The  $Ni^0$  core–oxide shell decorated particles were highly active in steam methane reforming and CO hydrogenation reactions. At the same time, they were inactive in the formation of graphite-like carbon in both methane decomposition and CO disproportionation.

### THE NATURE OF ACTIVE SITES IN Pt PROMOTED GaZSM-5 CATALYSTS

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*React. Kinet. Catal. Lett.*,  
87(2) (2006) pp. 249-254.

Activity and selectivity of Pt-promoted GaZSM-5 catalysts in the aromatization of ethane were studied. XRD indicated that high temperature treatment of the Pt promoted GaZSM-5 zeolites results

in the formation of bimetallic GaPt clusters located on the inner surface of zeolites. Both experimental results and calculations suggest that the clusters containing Ga and Pt atoms stabilized in cationic positions are characterized by an increased activity and selectivity in the dehydrogenation of ethane.

**MECHANISM STUDIES OF THE CONVERSION OF  $^{13}\text{C}$ -LABELED *n*-BUTANE ON ZEOLITE H-ZSM-5 STUDIED BY  $^{13}\text{C}$  MAGIC ANGLE SPINNING NMR SPECTROSCOPY AND GC-MS ANALYSIS**

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*Chem. Eur. J.*, 12(2) (2006) pp. 457-465.

$^{13}\text{C}$  MAS NMR spectroscopy shows that the conversion of the selectively  $^{13}\text{C}$ -labeled *n*-butane on zeolite H-ZSM-5 proceeds at 430–470 K via two pathways: (i) a scrambling of the selective  $^{13}\text{C}$ -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*  $^{13}\text{C}$  MAS NMR and complementary *ex situ* GC-MS data provide evidence for a monomolecular mechanism of the  $^{13}\text{C}$ -label scrambling, whereas both isobutane and propane are formed via an intermolecular pathways of oligomerization-cracking and a conjunct polymerization. According to  $^{13}\text{C}$  MAS NMR kinetic measurements, the  $^{13}\text{C}$ -label scrambling as well as the formation of isobutane and propane proceed with nearly the same activation energies ( $E_a = 75 \text{ kJ mol}^{-1}$  for the scrambling and  $71 \text{ kJ mol}^{-1}$  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.

**$^1\text{H}$  MAS NMR MONITORING OF THE  $^{13}\text{C}$ -LABELED CARBON SCRAMBLING FOR PROPANE IN ZEOLITE H-ZSM-5**

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*Chem. Phys. Lett.*, 420(4-6) (2006) pp. 574-576.

It has been demonstrated that  $^1\text{H}$  MAS NMR spectroscopy can be used as a tool for *in situ* monitoring the reaction kinetics of  $^{13}\text{C}$ -labeled carbon scrambling in alkane molecules adsorbed on zeolite catalysts at the reaction temperature of 540–570 K. The accuracy of the results and the time resolution are improved compared to  $^{13}\text{C}$  MAS NMR spectroscopy.

**ASYMMETRIC OXIDATION OF SULFIDES WITH  $\text{H}_2\text{O}_2$  CATALYZED BY TITANIUM COMPLEXES WITH AMINOALCOHOL DERIVED SCHIFF BASES**

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

*J. Mol. Catal.*, 264(1-2) (2007) pp. 280-287.

Sulfoxidation catalysts generated *in situ* from titanium(IV) isopropoxide and enantiopure Schiff bases promote the enantioselective oxidation of alkyl aryl sulfides to the corresponding sulfoxides at low catalyst loadings ( $< 1 \text{ mol}\%$ ), 30% aqueous hydrogen peroxide being the terminal oxidant. Upon screening of several ligands derived from  $\beta$ -aminoalcohols and salicylaldehydes, a catalyst affording sulfoxides with over 90% chemoselectivity and up to 60% *ee* was found, and the kinetics of the catalytic reaction was analyzed by  $^1\text{H}$  NMR.

**ACTIVE OXYGEN IN SELECTIVE OXIDATION CATALYSIS**

**G.I. Panov, K.A. Dubkov, E.V. Starokon**

*Catal. Today*, 117(1-3) (2006) pp. 148-155.

The paper reviews literature data related to oxygen species available on the surface of metal oxides and their possible role in selective oxidation. With some reservations, one may conclude that the main concept accepted presently in oxidation catalysis assumes that selective oxidation is provided by strongly bonded lattice oxygen, while the full oxidation is provided by weakly bonded reactive oxygen.

Recent studies on the oxidation mechanism over FeZSM-5 zeolites with  $\text{N}_2\text{O}$  give ground to reconsider this concept in order to integrate the earlier suggested radical oxygen idea, which supposes an important role

of  $O^-$  radicals in selective oxidation. This highly reactive oxygen species can be considered as a powerful tool for activation of organic molecules.

#### PLANAR DEFECT OF THE NANO-STRUCTURED ZINC OXIDE AS THE SITE FOR STABILIZATION OF THE COPPER ACTIVE SPECIES IN Cu/ZnO CATALYSTS

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*Catal. Today*, 112(1-4) pp. 143-147.

The catalytic activity of CuZn catalysts in the synthesis of methanol is related to those reduced Cu species, which originate from the  $Cu_xZn_{1-x}O$  solid solution of wurtzite-like structure. Copper cations in the  $Cu_xZn_{1-x}O$  solid solution are localized in the extended stacking faults of the ZnO lattice. Copper sites could be supposedly described as the product of introducing  $(OH)\dots Cu\dots(OH)$  to the planar defects of zinc oxide structure. Hydroxyl groups stabilize the planar defects of ZnO. The process of the samples reduction leads to the formation of flat  $Cu^0$  particles over the surface of zinc oxide. The planar defects of ZnO structure are preserved in the reduced state. During the reoxidation, copper atoms return back to the extended stacking faults of ZnO as the tape-like clusters of flat-square coordinated copper cations.

#### AMMOXIDATION OF ETHANE ON V-Mo-Nb OXIDE CATALYSTS

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*React. Kinet. Catal. Lett.*, 87(2) (2006) pp. 377-386.

Catalytic and physicochemical properties of V-Mo-Nb oxide catalysts ( $V_{0.3}Mo_1Nb_x$ , where  $x = 0.05, 0.15, 0.22, 0.27$ ) have been studied in the reaction of ethane ammoxidation. An increase in the Nb content in the samples is accompanied by an increase in the catalytic activity and selectivity to acetonitrile. It was established that a triple  $Mo_5O_{14}$ -like phase with a variable composition ( $V_{0.23\pm 0.3}Mo_1Nb_x$ , where  $x = 0.2\div 0.37$ ) acts as an active component in the catalyst.

#### THE FORMATION OF AN ACTIVE COMPONENT IN V-Mo-Nb-O CATALYSTS OF ETHANE OXIDATION AND AMMOXIDATION

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*React. Kinet. Catal. Lett.*, 88(1) (2006) pp. 183-192.

A genesis of an active component in V-Mo-Nb oxide catalysts for the oxidation and ammoxidation of ethane was studied. It was shown that the mixing of the aqueous solutions of initial reactants leads to the formation of MoV complexes in solution and is accompanied with the formation of a sediment of a binary Nb-Mo compound. The latter is the base for formation of the active component phase (a triple V-Mo-Nb compound with a variable composition with  $Mo_5O_{14}$ -like structure) during the subsequent treatment in air flow at  $400^\circ C$ .

#### PROPERTIES AND DEACTIVATION OF THE ACTIVE SITES OF AN MoZSM-5 CATALYST FOR METHANE DEHYDROAROMATIZATION: ELECTRON MICROSCOPIC AND EPR STUDIES

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*Kinet. Catal.*, 47(3) (2006) pp. 389-394.

The MoZSM-5 (4.0 wt % Mo) catalyst has been characterized by high-resolution transmission electron microscopy, EDXA, and EPR. Two types of molybdenum-containing particles are stabilized in the catalyst in the course of nonoxidative methane conversion at  $750^\circ C$ . These are 2- to 10-nm molybdenum carbide particles on the zeolite surface and clusters smaller than 1 nm in zeolite channels. According to EPR data, these clusters contain the oxidized molybdenum form  $Mo^{5+}$ . The surface  $Mo_2C$  particles are deactivated at the early stages of the reaction because of graphite condensation on their surface. Methane is mainly activated on oxidized molybdenum clusters located in the open molecular pores of the zeolite. The catalyst is deactivated after the 420-min-long operation because of coke buildup on the zeolite surface and in the zeolite pores.

## CATALYTIC PROPERTIES AND ELECTRONIC STRUCTURE OF COPPER IONS IN Cu-ZSM-5

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*Catal. Today*,  
110(3-4) (2005) pp. 310-322.

The effect of ion exchange conditions, such as Si/Al ratio, precursor copper salt, pH and concentration of the solution, on the catalytic activity in SCR of NO by propane and on the electronic state of copper ions in Cu-ZSM-5 has been studied. The NO conversion in NO SCR by C<sub>3</sub>H<sub>8</sub> has been found to reach a maximum value at Cu/Al ratio about 0.37-0.4 and remain constant at higher Cu/Al. ESR and UV-vis DR spectroscopy have been used to elucidate stabilization conditions of copper ions in Cu-ZSM-5 zeolites as isolated Cu<sup>2+</sup> ions, chain copper oxide structures and square-plan oxide clusters. The ability of copper ions for reduction and reoxidation in the chain structures may be responsible for the catalytic activity of Cu-ZSM-5. These transformations of copper ions are accompanied by the observation of intervalence transitions Cu<sup>2+</sup>-Cu<sup>+</sup> and CTLM of the chain structures in the UV-vis spectra.

## MECHANISM OF β-PICOLINE OXIDATION TO NICOTINIC ACID ON V-Ti-O CATALYST AS STUDIED BY *IN SITU* FTIR

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*React. Kinet. Catal. Lett.*,  
87(2) (2006) pp. 387-394.

*In situ* FTIR spectroscopy was used to study the interaction of β-picoline with the surface of a V-Ti-O catalyst in the temperature range of 120–300°C. β-Picoline was found to react with the Lewis acid sites of the catalyst to form a nitrogen coordinated complex. This complex turns into an aldehyde-like complex at 150–250°C and then into a nicotinate, which is a direct precursor of nicotinic acid.

## COMPOSITE MECHANISM OF THE CATALYTIC HYDROGENATION OF UNSATURATED HYDROCARBONS ON HYDRIDED MAGNESIUM INTERMETALLIDES

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*Kinet. Catal.*, 47(5) (2006) pp. 744-746.

Two temperature ranges are distinguished in the catalytic hydrogenation of unsaturated hydrocarbons on magnesium intermetallide hydrides. In the lower

temperature range, the reaction proceeds by a composite mechanism, as is indicated by the fact that the rate of the catalytic hydrogenation of ethylene, *n*-butenes, and butadiene is equal to the rate of the reduction of these hydrocarbons with hydride hydrogen. It is assumed that, at higher temperatures, the reaction proceeds by a heterogeneous–homogeneous mechanism.

## NO<sub>x</sub> SCR BY DECANE AND PROPYLENE ON Pt + Cu/Zr-PILLARED CLAYS IN REALISTIC FEEDS: PERFORMANCE AND MECHANISTIC FEATURES VERSUS STRUCTURAL SPECIFICITY OF NANOSIZED ZIRCONIA PILLARS

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*Catal. Today*, 114(1) (2006) pp. 13-22.

Pt + Cu-loaded ZrPILC tested in the reactions of NO<sub>x</sub> selective catalytic reduction by propylene and decane in realistic feeds with a high content of water, oxygen and an admixture of SO<sub>2</sub> demonstrated promising performance at high space velocities (up to 100 000 h<sup>-1</sup>) in the temperature range of 150–400°C. A strong promoting effect of water, oxygen and the catalyst presulfation on the degree of NO<sub>x</sub> conversion into N<sub>2</sub> was revealed. The specificity of these catalysts action in realistic feeds was explained by taking into account the textural, structural and surface features of zirconia-pillared clays as well as the mechanism of NO<sub>x</sub> HC SCR reaction including participation of strongly bound species in key stages.

**REACTION PATHS OF THE FORMATION AND CONSUMPTION OF NITROORGANIC COMPLEX INTERMEDIATES IN THE SELECTIVE CATALYTIC REDUCTION OF NITROGEN OXIDES WITH PROPYLENE ON ZIRCONIA-PILLARED CLAYS ACCORDING TO *IN SITU* SPECTROSCOPIC DATA**

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*Kinet. Catal.*, 47(5) (2006) pp. 747-755.

It was found that the adsorption and catalytic properties of nanosized ZrO<sub>2</sub> particles as the pillar constituents of ZrO<sub>2</sub>-pillared clay and bulk ZrO<sub>2</sub> are essentially different. The interaction of NO with the surface of bulk ZrO<sub>2</sub> resulted in the formation of three types of nitrate complexes. Only two nitrate species were formed on ZrO<sub>2</sub>-pillared clay (the monodentate species was absent). Only an acetate complex was formed in the interaction of a mixture of propylene and oxygen with the surface of bulk ZrO<sub>2</sub>, whereas an isopropoxide complex was the main propylene activation species on ZrO<sub>2</sub>-pillared clay. On the surface of ZrO<sub>2</sub>-pillared clay, isopropoxide and nitrate intermediates formed a complex structurally similar to adsorbed dinitropropane. On the surface of bulk ZrO<sub>2</sub>, acetate and monodentate nitrate complexes formed a complex structurally similar to adsorbed nitromethane. The dinitropropane complex on ZrO<sub>2</sub>-pillared clay was consumed in reactions with surface nitrates. The decomposition reaction of a dinitropropane compound with the formation of acetate complexes and ammonia predominated on the surface containing no nitrate complexes in the absence of NO + O<sub>2</sub> from a gas phase. The found differences in reactant activation species and their thermal stabilities explained differences in the activities of bulk ZrO<sub>2</sub> and nanosized ZrO<sub>2</sub> particles as pillars in pillared clay in the course of the selective catalytic reduction of nitrogen oxides with propylene in an excess of oxygen.

**ROLE OF NITROGEN DIOXIDE IN THE OXIDATION OF DIESEL SOOT ON PROMOTED MIXED CATALYSTS WITH FLUORITE AND PEROVSKITE STRUCTURES**

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*Kinet. Catal.*, 47(3) (2006) pp. 400-411.

The oxidation of soot on catalysts with the perovskite and fluorite structures (including platinum-promoted catalysts) in the presence and in the absence of NO<sub>2</sub> was studied using *in situ* IR spectroscopy and temperature-programmed techniques (TPR, TPD, and TPO). It was found that, as a rule, the temperature of the onset of soot oxidation considerably decreased upon the addition of NO<sub>2</sub> to a flow of O<sub>2</sub>/N<sub>2</sub>, whereas the amount of oxygen consumed in soot oxidation considerably increased. To explain these facts, it was hypothesized that the initiation of soot combustion in the presence of NO<sub>2</sub> was related to the activation of the NO<sub>2</sub> molecule through the formation (at a low temperature) and decomposition (at a high temperature) of nitrate structures on the catalyst. Superequilibrium amounts of NO<sub>2</sub> resulted from the decomposition of nitrate complexes immediately on the catalyst for soot combustion. Based on a comparison between catalyst activities and data obtained by TPR and the TPD of oxygen, a conclusion was drawn that the presence of labile oxygen in the catalyst is a necessary but insufficient condition for the efficient occurrence of a soot oxidation reaction in the presence of NO<sub>2</sub>. The introduction of platinum as a constituent of the catalyst increased the amount of labile oxygen and, as a consequence, increased the amount of highly reactive nitrate complexes. As a result, this caused a decrease in the temperature of the onset of soot combustion.

**REACTION PATHS OF THE FORMATION AND CONSUMPTION OF NITROORGANIC COMPLEX INTERMEDIATES IN THE SELECTIVE CATALYTIC REDUCTION OF NITROGEN OXIDES WITH PROPYLENE ON ZIRCONIUM DIOXIDE ACCORDING TO *IN SITU* FOURIER TRANSFORM IR SPECTROSCOPIC DATA**

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*Kinet. Catal.*,  
47(4) (2006) pp. 593-602.

Nitrate, acetate, and nitroorganic complexes were detected on the surface of ZrO<sub>2</sub> under the reaction conditions of nitrogen oxide reduction with propylene using Fourier transform IR spectroscopy. The nitroorganic complex was formed in the reaction between acetate and nitrate complexes by the replacement of the carboxyl group in the acetate complex by the nitro group. Monodentate nitrate was the most reactive species in this process. The adsorption of various nitroorganic substances was studied. It was found that the nitroorganic complex was structurally analogous to the nitromethane molecule bound to the surface through the nitro group. The experimental data led to a conclusion that nitroorganic compounds were subsequently consumed in reactions with nitrate complexes. In this surface reaction, monodentate nitrate was also the most reactive species. The presence of oxygen had no effect on the consumption of the nitroorganic complex.

**AMMONIA OXIDATION ON Pt(410)**

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*J. Catal.*, 242(1) (2006) pp. 184-194.

The adsorption of both O<sub>2</sub> and NH<sub>3</sub> on Pt(410) was studied using temperature-programmed desorption (TPD) and X-ray photoelectron spectroscopy (XPS). Molecular NH<sub>3</sub> desorbed from Pt(410) between 100 and 450 K, and dissociation was not observed. Radiation (X-Rays, electrons) induced NH<sub>3ad</sub> dissociation, and as a result several dissociation products (NH<sub>2ad</sub>, NH<sub>ad</sub>, and N<sub>ad</sub>) were observed in the N 1s core-level spectrum. NH<sub>ad</sub> is a rather stable dissociation product that starts to dehydrogenate

above 350 K. The N<sub>ad</sub> and H<sub>ad</sub> formed in this process desorbed on formation (as N<sub>2</sub> and H<sub>2</sub>). Both molecular and dissociative O<sub>2</sub> adsorption were observed after the surface was exposed to O<sub>2</sub>(g) at 100 K. Molecularly adsorbed O<sub>2</sub> desorbed below 200 K, whereas atomic oxygen desorbed (as O<sub>2</sub>) between 600 and 900 K, in two distinct desorption peaks. In the O 1s core-level spectrum, both molecular O<sub>2</sub> and two different types of O<sub>ad</sub> were distinguished. NH<sub>3ad</sub> dissociation was observed on an oxygen-presaturated surface. The NH<sub>3ad</sub> oxy-dehydrogenation started at 150 K. NO<sub>ad</sub> and NO(g) were also observed, but only during experiments in which an excess of O<sub>ad</sub> was available. NO<sub>ad</sub> desorbed/decomposed between 400 and 500 K. For the steady-state ammonia oxidation reaction, N<sub>2</sub> and H<sub>2</sub>O were the major products at low temperatures, whereas the selectivity toward NO and H<sub>2</sub>O changed at higher temperatures. This selectivity change can be attributed to changes in surface composition.

**SELECTIVE, C,C-DOUBLE BOND REDUCTION OF  $\alpha,\beta$ -UNSATURATED CARBONYL COMPOUNDS WITH CYCLOHEXANE USING ZEOLITES**

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*J. Mol. Catal. A: Chem.*,  
245(1-2) (2006) pp. 231-234.

Selective ionic hydrogenation of  $\alpha,\beta$ -unsaturated carbonyl compounds with alkanes (cyclohexane and others) was previously known to proceed only in superacidic conditions due to the necessity of dicationic, superelectrophilic activation of the enones. In present paper it is disclosed that H-form zeolites with acidity well below superacidity, are able however to induce the reduction of  $\alpha,\beta$ -unsaturated carbonyl compounds with cyclohexane in strong analogy to the "parent", superacid mediated reactions. The probable interpretation of these results in terms of highly electrophilic (superelectrophilic) intermediates on the solid is discussed.

**SUPERACIDIC ACTIVATION OF MALEIMIDE AND PHTHALIMIDE AND THEIR REACTIONS WITH CYCLOHEXANE AND AROMATIC COMPOUNDS**

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*Eur. J. Org. Chem.*, 21 (2006) pp. 4861-4866.

When activated in the CF<sub>3</sub>SO<sub>3</sub>H/SbF<sub>5</sub> acid system maleimide (1) and phthalimide (2) undergo selective ionic hydrogenation with cyclohexane to give

1,5-dihydropyrrol-2-one (3) and phthalimidine (11), respectively. When treated with aluminum halides, *N*-phenylmaleimide (4) reacts with cyclohexane to give *N*-phenylsuccinimide (5), whereas 2 still gives 11. Imide 1 also condenses with benzene in trifluoromethanesulfonic acid (CF<sub>3</sub>SO<sub>3</sub>H) to give 1,5-dihydro-5,5-diphenylpyrrol-2-one (7) as the major product. However, in the presence of aluminum halides 1 reacts with benzene, toluene, and *o*-dichlorobenzene to give 3-arylsuccinimides 8-10, respectively. Imide 2 reacts with benzene under the influence of trifluoromethanesulfonic acid as well as aluminum halides to yield 3,3-diphenylphthalimidine (12). The mechanism of these reactions, with potential involvement of superelectrophilic dicationic intermediates, is discussed.

#### ISOTOPE EXCHANGE BETWEEN NO AND H<sub>2</sub>O ON A PLATINUM-CONTAINING CATALYST BASED ON FIBERGLASS

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L.G. Simonova, E.A. Paukshtis, B.S. Bal'zhinimaev

*Kinet. Catal.*,  
47(1) (2006) pp. 131-138.

The dynamics of <sup>18</sup>O isotope exchange between NO or H<sub>2</sub>O and a catalyst and the dynamics of <sup>18</sup>O label transfer from NO to H<sub>2</sub>O have been studied under conditions of sorption-desorption equilibrium. The occurrence of a reaction of oxygen exchange between NO and water sorbed in the bulk of the catalyst was detected. This reaction occurs at platinum sites with the participation of acid sites of the glass matrix. The rate constants of the reaction of NO with platinum sites and the diffusion coefficients of water in the bulk of the glass matrix are evaluated.

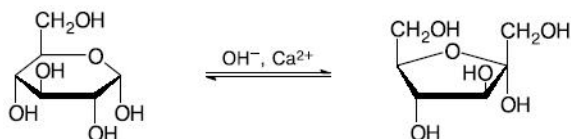
### Application of Physicochemical Methods for Characterization of Catalysts, Supports, Synthesized Substances and Materials

#### <sup>13</sup>C NMR STUDIES OF ISOMERIZATION OF D-GLUCOSE IN AN AQUEOUS SOLUTION OF Ca(OH)<sub>2</sub>. THE EFFECT OF MOLECULAR OXYGEN

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V.N. Parmon

*Russ. Chem. Bull.*,  
8 (2005) pp. 1967-1972.

Isomerization of D-glucose to fructose and mannose in aqueous solutions of Ca(OH)<sub>2</sub> with the initial pH 11.4 in a temperature interval of 20-90°C was studied by <sup>13</sup>C NMR spectroscopy in the presence and absence of dissolved oxygen. In the presence of oxygen, the apparent equilibrium isomerization constant is much lower than that in the absence of oxygen. This is related to the oxidation of monosaccharides to formic and aldonic acids, a decrease in the pH of solutions, and cessation of isomerization at pH < 9.



#### NMR STUDIES OF MOLECULAR MOTION OF ULTRADISPERSED POLYTETRAFLUOROETHYLENE

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*J. Struct. Chem.*, 47(4) (2006) pp. 668-673.

Molecular motion in ultradispersed polytetrafluoroethylene obtained by special gas-phase technology has been studied experimentally and theoretically based on a temperature dependence of the second moment of <sup>19</sup>F NMR spectra and the time of spin-lattice relaxation. The results of observations are interpreted as the consequence of reorientation motion of CF<sub>2</sub> groups around the axis of macromolecules at low temperature and of translational motion of macromolecules in the high temperature region. Qualitative differences from the molecular motion in industrial polytetrafluoroethylene (teflon-4) were detected and parameters of dynamic processes determined.



## SOLID STATE MULTINUCLEAR NMR STUDIES OF NANOSTRUCTURED THIN OXIDE FILMS

O.B. Lapina

*Chinese J. Light Scatt.*, 17(10) (2005) pp. 287-288.

Detailed knowledge of the molecular structure and electronic structures of surface thin oxide films, their active sites and their corresponding reactivity/selectivity relationships are the critical fundamental information that is necessary for the molecular engineering of active surface oxide species for specific catalytic applications. Modern solid state NMR techniques became a keystone technique for characterization of local structure of quadrupolar nuclei ( $^{51}\text{V}$ ,  $^{93}\text{Nb}$ ,  $^{27}\text{Al}$ ,  $^{45}\text{Sc}$ ,  $^{17}\text{O}$ ) in different oxide systems. Herein the current state of solid state NMR techniques in their applications to thin oxide films is discussed.

## $^{129}\text{Xe}$ NMR STUDY OF PITCH-BASED ACTIVATED CARBON MODIFIED BY AIR OXIDATION/PYROLYSIS CYCLES: A NEW APPROACH TO PROBE THE MICROPORE SIZE

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*J. Phys. Chem. B.*, 110(7) (2006) pp. 3055-3060.

$^{129}\text{Xe}$  NMR has been used to study a series of homologous activated carbons obtained from a KOH activated pitch-based carbon molecular sieve modified by air oxidation/pyrolysis cycles. A clear correlation between the pore size of microporous carbons and  $^{129}\text{Xe}$  NMR of adsorbed xenon is proposed for the first time. The virial coefficient  $\delta_{\text{Xe-Xe}}$  arising from binary xenon collisions varied linearly with the micropore size and appeared a better probe of the microporosity than the chemical shift extrapolated to zero pressure. This correlation related to SFD (single file diffusion) phenomenon indicated that the xenon collision frequency increases with increasing micropore size. The chemical shift has been shown to vary very weakly with temperature (less than 9 ppm) for xenon trapped inside narrow and wide micropores. This is indicative of smooth xenon – surface interaction potential.

## ACTIVATION OF *rac*- $\text{Me}_2\text{Si}(\text{ind})_2\text{ZrCl}_2$ BY METHYLALUMOXANE MODIFIED BY ALUMINUM ALKYL: AN EPR SPIN-PROBE, $^1\text{H}$ NMR, AND POLYMERIZATION STUDY

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*Macromol. Chem. Phys.*, 207(3) (2006) pp. 327-335.

Solutions containing mixtures of methylalumoxane (MAO) and  $^i\text{Bu}_3\text{Al}$  give rise to  $^1\text{H}$  NMR signals indicative of the presence of the mixed alkyl aluminum dimers  $^i\text{Bu}_2\text{Al}(\mu\text{-Me})_2\text{Al}^i\text{Bu}_2$  and of mixed clusters of the type  $(\text{AlMe}_{(1+2x-y)}^i\text{Bu}_y\text{O}_{(1-x)})_n$ . These mixed clusters, as well as related species present in solutions containing either MAO- $\text{Et}_3\text{Al}$  or commercially available modified MAO (MMAO), appear to have stronger Lewis acidic sites and greater hydrodynamic radii than comparable clusters present in solutions of MAO alone, as judged from EPR signals observed in these solutions upon addition of TEMPO. When (SBI)ZrCl<sub>2</sub> (SBI = *rac*- $\text{Me}_2\text{Si}(\text{ind})_2$ ) is reacted with one of these mixed activator reagents, the mixed heterobinuclear cation  $[(\text{SBI})\text{Zr}(\mu\text{-Me})_2\text{AlMe}^i\text{Bu}]^+$  appears to be formed, together with its methyl counterpart  $[(\text{SBI})\text{Zr}(\mu\text{-Me})_2\text{AlMe}_2]^+$ , which is normally predominant in the (SBI)ZrCl<sub>2</sub>/MAO system at  $[\text{Al}]_{\text{MAO}}/[\text{Zr}]$  ratios above 100. In the presence of  $^i\text{Bu}_3\text{Al}$ , the formation of heterobinuclear cations is suppressed in favor of ion pairs containing the cation  $[(\text{SBI})\text{ZrMe}]^+$  in contact with a (MAO-TIBA)-derived counter anion. The greater reactivity of these contact ion pairs, as compared to the normally prevalent  $\text{AlMe}_3$  adducts, as well as an increased Lewis acidity of MMAO, and the ensuing decreased coordination ability of the  $[\text{Me}(\text{MAO-TIBA})]^-$  counter ion as compared to  $[\text{Me-MAO}]^-$ , are likely to contribute to the positive effects of TIBA additions on the co-catalytic activity of MAO.

## NMR IMAGING AS A TOOL FOR STUDYING MASS TRANSPORT IN POROUS MATERIALS

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In "Fluid Transport in Nanoporous Materials",  
NATO Science Series II: Mathematics, Physics and  
Chemistry, vol. 219, Eds. W.C. Conner, J. Fraissard,  
Springer, 2006, pp. 353-374.

Modern magnetic resonance is an extremely broad field of scientific research, which embraces a vast variety of experiments and techniques. To better

define the place of NMR imaging in magnetic resonance, it might be advantageous to consider the majority of the magnetic resonance (MR) experiments as being performed in a multidimensional space of frequencies, spatial coordinates and time. Each particular MR experiment then addresses a certain subset of the parameter space. For instance, 2D (two-dimensional) NMR spectroscopy utilizes two frequency coordinates, while diffusion studies with PFG (pulsed field gradient) NMR use one spatial and one temporal coordinates, etc. NMR imaging (MRI) experiments can thus be defined as those which involve at least one spatial coordinate. Since the encoding of a spatial coordinate can be added to almost any MR experiment, this gives an infinite number of possibilities for performing MRI studies.

#### COMPLEXES OF THE PROTON AND ITS HYDRATES WITH CARBAMOYLPHOSPHINE OXIDE IN WET DICHLOROETHANE SOLUTIONS

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*J. Phys. Chem. A*, 110(30) (2006) pp. 9505-9512.

To better understand the complex equilibria involved in the UNEX process for acidic solvent extraction of radionuclides, the interaction of a carbamoylphosphine oxide ligand (L) with the proton of hydrated chlorinated cobalt(III)dicarbollide acid,  $H[Co(C_2B_9H_8Cl_3)_2]$ , has been studied in wet 1,2-dichloroethane (DCE) solution using IR and NMR ( $^{13}C$  and  $^{31}P$ ) spectroscopy. The formation of two groups of complexes has been determined. The first group contains three complexes with 1:1 composition of acid to ligand. The second group of complexes has 1:2 composition in the equilibrium. Within each group, the complexes differ in composition only by the number of incorporated water molecules. The equilibria are both very sensitive to the content of self-associated water in solution and are driven by its concentration, which is unsteady and depends on the solution preparation history. The simultaneous presence of both anhydrous and hydrated proton solvates indicates that the enthalpies of carbamoylphosphine oxide complex formation with  $H^+$ ,  $H_3O^+$ , and  $H_5O_2^+$  are very close to each other.

#### THE STRUCTURE OF THE $H_3O^+$ HYDRONIUM ION IN BENZENE

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*J. Am. Chem. Soc.*,  
127(21) (2005) pp. 7664-7665.

Infrared, X-ray structural,  $^1H$  NMR, and computational evidence for  $\pi$ -solvation of  $H_3O^+$  by benzene molecules is presented. A salt with a discrete  $[H_3O \cdot 3benzene]^+$  cation can be isolated using a very weakly interacting carborane counterion,  $CHB_{11}Cl_{11}^-$ .  $\pi$ -Arene solvation of  $H_3O^+$  explains the solubility of this salt in benzene solution. Similar results are indicated for the "Zundel-type"  $H_5O_2^+$  ion. These findings suggest structures for the active protonating species when strong acids are used as catalysts in arene solvents containing trace water. They are also relevant to structures that may be present in biological proton transport.

#### NMR STRUCTURAL ASPECTS OF THE CHEMISTRY OF V, Mo, W POLYOXOMETALATES

**M.A. Fedotov, R.I. Maksimovskaya**

*Russ. J. Struct. Chem.*, 47(5) 2006) pp. 952-978.

The results of structural investigations of vanadium, molybdenum, and tungsten polyoxoanions (PA) by  $^{17}O$ ,  $^{51}V$ ,  $^{95}Mo$ ,  $^{183}W$ , and heteroatom NMR are generalized in this review. NMR spectroscopy possibilities to determine the structure of PA are discussed. NMR data on PA of different structures compositions nuclei are demonstrated.

#### TOMOGRAPHY RECONSTRUCTION OF HABITUS OF METAL NANOCRYSTALLS ACCORDING TO PEM DATA

**O.G. Abrosimov, A.L. Chuvilin\*, E.M. Moroz**  
(\**University of Ulm, Ulm, Germany*)

*Bull. Russ. Acad. Sci.: Physics*,  
70(4) (2006) pp. 549-552.

The High Angle Centered Dark Field (HACDF) registration mode has been developed at the Boreskov Institute of Catalysis and used for the first time to acquire angle series of strongly dissipating objects for the further tomographic reconstruction of their spatial structure. Special tomographic holder and gauzes have been developed, the algorithm for equalization of the angle series suggested and applied.

The developed method provides unique potentialities for studying morphological features of nanosized objects.

## ELECTRON MICROTOMOGRAPHY: A NEW METHOD FOR STUDYING THE SPATIAL STRUCTURE OF CATALYSTS

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*Kinet. Catal.*,  
47(3) (2006) pp. 464-466.

The spatial arrangement of active component (Pt) particles on the surface of a support (Sibunit globule) has been studied by bright-field electron tomography. A tomographic attachment for a standard specimen holder and tomographic grids have been designed. The tomographic procedure has been refined, and adequate tilt series alignment and tomographic reconstruction algorithms have been chosen. The 3D distribution of the active component in the catalyst grain has been studied: particles hidden in micropores have been directly observed, and the size of the pores connecting internal cavities with the exterior has been estimated.

## NEW DATA ON THE STRUCTURE OF FINE ALUMINIUM HYDROXIDE

K.I. Sheffer, D.A. Zyuzin, E.M. Moroz

*Bull. Russ. Acad. Sci.: Physics*,  
70(4) (2006) pp. 1068-1070.

The structure of aluminium hydroxides – pseudoboehmites with various characteristics produced by different methods was studied by method of wide-angle X-ray scattering. In contrast to reference data, it was found that modifications in the structure of pseudoboehmite layers occur *via* the insertion of additional water molecules.

## LOCAL STRUCTURE OF PSEUDOBOEHMITES

E.M. Moroz, K.I. Sheffer, D.A. Zyuzin,  
A.S. Ivanova, E.V. Kulko, V.V. Goidin,  
V.V. Molchanov

*React. Kinet. Catal. Lett.*,  
87(2) (2006) pp. 367-375.

The structure of pseudoboehmite was studied by the method of wide-angle X-ray scattering (WAXS). The samples of pseudoboehmite with various characteristics produced by different methods were examined in order to obtain the most complete information about their structure. In contrast to reference data, it was found that modifications in the structure of pseudoboehmite layers occur *via* the insertion of additional water molecules.

## X-RAY, RAMAN AND FTIRS STUDIES OF THE MICROSTRUCTURAL EVOLUTION OF ZIRCONIA PARTICLES CAUSED BY THE THERMAL TREATMENT

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E.B. Burgina, V.A. Sadykov, V.G. Kostrovskii\*,  
V.A. Matyshak\*\* (\*Institute of Solid State Chemistry  
and Mechanochemistry, Novosibirsk, Russia;  
\*\*Semenov Institute of Chemical Physics, Moscow,  
Russia)

*J. Solid State Chem.*, 179(10) (2006) pp. 2965-2971.

Genesis of the structure of zirconia particles prepared by precipitation of amorphous hydrated zirconia by ammonia from the  $ZrO(NO_3)_2$  solution followed by a mild hydrothermal treatment (HTT) of precipitate, washing and calcination under air up to 1000°C has been studied by X-ray diffraction (XRD), Raman and FTIRS. As revealed by FTIRS of lattice modes, the local structure of amorphous zirconia subjected to HTT is close to that in  $\mu$ -ZrO<sub>2</sub>. This helps to obtain nearly single-phase monoclinic nanozirconia (particle size 5–15 nm) already after a mild calcination at 500°C. Stability of this phase with nanoparticles sizes below the critical value determined by thermodynamic constraints is due to its excessive hydroxylation demonstrated by FTIRS. Dehydroxylation and sintering of these nanoparticles at higher (600–650°C) temperatures of calcination leads to reappearance of the (111) “cubic” reflection in XRD patterns. Modeling of XRD patterns revealed that this phenomenon could be explained by polysynthetic (001) twinning earlier observed by HRTEM.

## PROBING THE BRØNSTED AND LEWIS ACIDITY OF Fe-SILICALITE BY FTIR SPECTROSCOPY OF H<sub>2</sub> ADSORBED AT 20 K: EVIDENCES FOR THE FORMATION OF Fe<sup>3+</sup>/H<sub>2</sub> AND Fe<sup>2+</sup>/H<sub>2</sub> MOLECULAR ADDUCTS

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*J. Catal.*, 238(2) (2006) pp. 243-249.

The spectroscopic characterisation of a Fe-silicalite sample in terms of Brønsted and Lewis acidity using H<sub>2</sub> as a probe molecule at low temperature (20 K) is reported. At 20 K, H<sub>2</sub> is able to form adducts with surface sites present in the internal (and external) surface of zeolites: Brønsted, silanols, and metal ions. The spectroscopic manifestations of the different H<sub>2</sub> adducts are found in distinct spectral regions depending on the nature and strength of the adducts:  $\nu_{HH}$  modes of OH-H<sub>2</sub> adducts are found in the 4170-4100 cm<sup>-1</sup> region, and those of Fe<sup>x+</sup>...H<sub>2</sub> adducts are found in the 4100–3900 cm<sup>-1</sup> region. Four

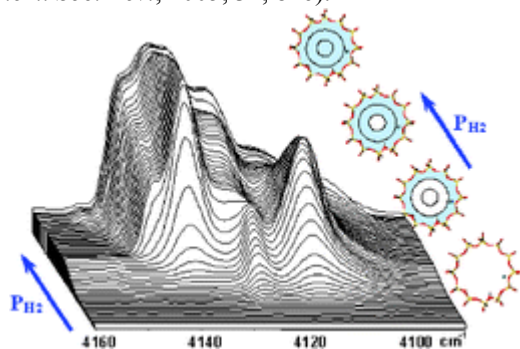
distinct  $\text{Fe}^{x+} \dots \text{H}_2$  adducts (at 4050, 4028, 3990, and  $3960 \text{ cm}^{-1}$ ) were formed on extra-framework Fe sites, created by controlled migration of Fe from the framework as a consequence of thermal treatments. The dependence on red-ox treatments of the relative concentration of these sites allowed identification of two  $\text{Fe}^{2+}$  and two  $\text{Fe}^{3+}$  distinct sites, interacting with  $\text{H}_2$  mainly by electrostatic forces. The importance of these sites as active species for the selective oxidation of hydrocarbons with  $\text{N}_2\text{O}$  is discussed.

**VIBRATIONAL AND THERMODYNAMIC PROPERTIES OF Ar, N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub> AND Co ADSORBED AND CONDENSED INTO (H, Na)-Y ZEOLITE CAGES AS STUDIED BY VARIABLE TEMPERATURE IR SPECTROSCOPY**

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*Phys. Chem. Chem. Phys.*, 8(10) (2006) pp. 1186-1196.

The adsorption of Ar, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub> and CO on (H,Na)-Y zeolite (Si/Al = 2.9, H<sup>+</sup>/Na<sup>+</sup> ≈ 5) has been studied at variable-temperature (90–20 K) and sub-atmospheric pressure (0–40 mbar) by FTIR spectroscopy. Unprecedented filling conditions of the zeolite cavities were attained, which allowed the investigation of very weakly adsorbed species and of condensed, liquid-like or solid-like, phases. Two pressure regimes were singled out, characterized by: (i) specific interaction at low pressure of the probe molecules (P) with the internal Brønsted and Lewis sites, and (ii) multilayer adsorption at higher pressure. In the case of CO the perturbation of the protonic sites located inside the sodalite cages was also observed. As the molecule is too large to penetrate the sodalite cage, the perturbation is thought to involve a proton jump tunneling mechanism. The adsorption energy for the (HF)OH<sup>+++</sup>P (P = Ar, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub> and CO) specific interaction involving the high frequency Brønsted acid sites exposed in the supercages was derived following the VTIR (variable temperature infrared spectroscopy) method described by E. Garrone and C. Otero Arean (*Chem. Soc. Rev.*, 2005, 34, 846).



**NEW FRONTIER IN TRANSMISSION IR SPECTROSCOPY OF MOLECULES ADSORBED ON HIGH SURFACE AREA SOLIDS: EXPERIMENTS BELOW LIQUID NITROGEN TEMPERATURE**

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*Catal. Today*, 113(1-2) (2006) pp. 65-80.

IR spectroscopy of adsorbed probe molecules is one of the most powerful characterization techniques for the investigation of surface active sites on high surface area materials like oxides and zeolites. In the last 20 years the use of specific IR cells allowing the *in situ* sample activation, gas dosage and sample cooling down to liquid nitrogen temperature has remarkably improved the number and the quality of the information on the surface structure with respect to the first experiments carried out at room temperature. Commercial cryostats able to reach liquid helium temperatures are available since decades, but the incompatibility of the materials used to reach and confine very low temperatures with the high temperatures usually needed to activate the surfaces of catalysts has prevented for long time the breaking down of the 77 K frontier in IR experiments of species adsorbed on active surface sites. It was recently designed, realized and tested a new experimental set-up able to perform IR experiments in the 15–300 K interval on samples previously activated under vacuum conditions ( $P < 10^{-4}$  Torr, 1 Torr ~ 133.3 Pa), or in the desired atmosphere, up to 1073 K [G. Spoto, E.N. Gribov, G. Ricchiardi, A. Damin, D. Scarano, S. Bordiga, C. Lamberti, A. Zecchina, *Prog. Surf. Sci.*, 76 (2004) 71]. The first results obtained with this innovative instrument will be reviewed and summarized in this work and compared with previous literature results on similar experiments performed at liquid nitrogen temperature. In particular, it will be discussed the adsorption of CO and H<sub>2</sub> on MgO and H-SSZ-13 zeolite, and of H<sub>2</sub> on Cu<sup>+</sup>-ZSM-5 zeolite.

**INFLUENCE OF COHERENT CONNECTION OF CRYSTALLINE BLOCKS ON THE DIFFRACTION PATTERN OF NANOSTRUCTURED MATERIALS**

**S.V. Cherepanova, S.V. Tsybulya**

*Z. Kristallogr.*, suppl\_23 (2006) pp. 155-160.

The diffraction effects such as anisotropic broadening of diffraction peaks, their splitting to the

relatively broad and narrow components, their shifts and/or the appearance of new ones can result from a coherent connection of nanoblocks. These effects can be mistakenly ascribed to size or strain anisotropy, bimodal size distribution, change in lattice constants and/or the presence of additional phases correspondingly. Developed software provides correct interpretation of the peculiarities of the X-ray diffraction patterns of materials containing planar defects arising from coherent connection of nanoblocks, that is illustrated by several examples. For 1D nanostructured materials, the type and the concentration of the planar defects can be determined on the basis of fitting of the whole pattern. If the microstructure is modulated in more than one direction, only single diffraction peaks can be analysed using the model of 1D disordered crystal.

#### **INTERACTION OF COPPER-BASED SOLID SOLUTIONS WITH LIQUID GALLIUM EUTECTICS**

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*Russ. Metallurgy,*  
2 (2006) pp. 143-146.

The interaction of binary solid solutions with binary gallium eutectics is studied *in situ* by X-ray diffraction using synchrotron radiation to reveal the sequence of phase formation for the elements that leave a solid solution and a eutectic during the formation of the first intermetallic phase. A comparison of the chemical interactions of the solid solution of tin in copper with the gallium-indium eutectic, the solid solution of indium in copper with the gallium-tin eutectic, and the solid solution of bismuth in copper with these eutectics shows that phase formation during interaction depends on the state of the element (liquid or solid).

#### **MECHANISMS OF Pd(110) SURFACE RECONSTRUCTION AND OXIDATION: XPS, LEED AND TDS STUDY**

**A.I. Titkov, A.N. Salanov, S.V. Koscheev, A.I. Boronin**

*Surf. Sci.*, 600(18) (2006) pp. 4119-4125.

Oxygen interaction with Pd(110) has been studied in a wide range of pressures ( $P_{O_2}=10^{-6}$ –100 Pa) and temperatures ( $T = 400$ –600 K) by X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and thermal desorption

spectroscopy (TDS). The amount of oxygen absorbed by Pd(110) single crystal grows to more than 100 ML when the reaction temperature and the  $O_2$  exposure are increased. Several reconstructed and oxide structures are sequentially formed on Pd(110) as the amount of adsorbed and absorbed oxygen increases. During oxygen adsorption ( $1 \times 2$ ) reconstruction occurs and a  $c(2 \times 4)$  structure is formed on Pd(110) at  $\theta = 0.5$  ML. When the amount of absorbed oxygen increases from 0.5 to 2.0 ML, oxygen penetrates into subsurface Pd layers to the depth exceeding 15–20 Å while retaining the  $c(2 \times 4)$  structure. When the amount of absorbed oxygen is between 2 and 5 ML, the surface is subjected to reconstruction with the formation of a surface oxide with  $\theta \sim 0.8$  that has a complex LEED diffraction pattern. Further increase of the amount of absorbed oxygen beyond 5 ML leads to oxygen location in the subsurface region forming PdO clusters. They gradually grow to form an almost continuous layer composed of PdO clusters.

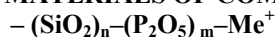
#### **OXYGEN INTERACTION WITH Pd(110): SURFACE OXIDE FORMATION**

**A.I. Titkov, A.N. Salanov, S.V. Koscheev, A.I. Boronin**

*Phys. Low-Dimensional Struct.*,  
2 (2006) pp. 107-118.

Oxygen interaction with Pd(110) has been studied in a wide range of pressures ( $P_{O_2}=5 \times 10^{-7}$  – 10 Pa) at  $T = 400$  K by X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). When the  $O_2$  exposure grows by increasing the treatment time and oxygen pressure from  $5 \times 10^{-7}$  to 10 Pa, the amount of oxygen absorbed by Pd(110) monocrystal increases up to 4.5 ML. The oxygen coverage increasing to 0.5 ML leads to the formation of the  $c(2 \times 4)$  structure on Pd(110). When the amount of absorbed oxygen increases from 0.5 to 2 ML, oxygen penetrates into subsurface Pd layers to the depth more than 15-20 Å whereas the  $c(2 \times 4)$  structure is preserved. When the amount of oxygen increases from 2 ML to 4.5 ML a new surface phase is formed on Pd(110) surface. XPS characteristics of this phase were attributed to a surface oxide.

## SYNTHESIS OF SILICA POLYPHOSPHATE MATERIALS OF COMPOSITION:



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*Academy Proceed., Physics,*  
49(3) (2006) pp. 6-9.

X-ray photoelectron spectroscopy (XPS) was used to study catalysts obtained by sol-gel technique for synthesis of Ag catalysts. Peculiarity of these catalysts is formation of active component as Ag nanoparticles directly on the stages of synthesis and subsequent drying and calcination.

## STUDYING OF THE POWDERS FOR NONLEADED PASTE FOR HIGH-TEMPERATURE SOLDERING OF COPPER ALLOYS

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*Chem. Sustain. Devel.*, 14(2) (2006) pp. 141-146.

X-ray photoelectron spectroscopy is used to study a series of fine powders of copper alloy with adding of 15 mass % of Sn, 4 mass % of Ni and 5 mass % of P. It is shown that chemical composition of near-surface layer of powder particles of solder depends on the method of preparation and significantly influences on the quality of soldering.

## PLASMA DEPOSITION AND PROPERTIES OF SILICON CARBONITRIDE FILMS

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*Inorg. Mater.*,  
41(7) (2005) pp. 706-712.

A variety of advanced analytical techniques were used to characterize silicon carbonitride films grown from new volatile nitrogen-rich silyl derivatives of asymmetrical dimethylhydrazine:  $(\text{CH}_3)_2\text{HSiHN}(\text{CH}_3)_2$  (DMDMSH) and  $\text{Me}_2\text{Si}(\text{NHNMe}_2)_2$  (bisDMHDMS). The results demonstrate that the films contain only Si-C, Si-N, and  $\text{C}(\text{sp}^3)\text{-N}$  bonds, in relative amounts that depend on the molecular structure of the precursor and deposition conditions. The  $\text{Si-C}/[\text{Si-N} + \text{C}(\text{sp}^3)\text{-N}]$  ratio is considerably larger in the films grown from DMDMSH. The data obtained by a variety of

spectroscopic techniques provide solid evidence that some of the films contain  $\text{C}(\text{sp}^3)\text{-N}$  bonds, characteristic of superhard materials, and that the films have a complex, framework structure, rather than being a mixture of  $\text{Si}_3\text{N}_4$ , SiC, and  $\text{C}_3\text{N}_4$ . The structure of the films depends on the N : Si ratio in the precursor: at N : Si = 2, the films are amorphous and contain nanocrystalline inclusions with a tetragonal structure; at N : Si = 4, the films are purely amorphous. The ability to control the chemical composition and structure of deposits allowed to produce films with various physicochemical and electrical properties.

## CHEMICAL VAPOR INFILTRATION METHOD FOR DEPOSITION OF GOLD NANOPARTICLES ON POROUS ALUMINA SUPPORTS

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*J. Struct. Chem.*,  
47(3) (2006) pp. 458-464.

Knudsen's effusion method with mass spectral analysis of the composition of the gas phase was used to measure the temperature dependence of the saturated vapor of several  $(\text{CH}_3)_2\text{AuL}$  chelate complexes and to determine the thermodynamic parameters of their sublimation. Based on the results of this study, conditions for chemical vapor deposition of gold using dimethylgold(III) chelates were chosen. Gold nanoparticles were synthesized by chemical vapor deposition (infiltration) of  $(\text{CH}_3)_2\text{Au}(\text{acac})$  on porous granules of  $\gamma\text{-Al}_2\text{O}_3$  with subsequent calcination in air at 325°C. Particle size and the chemical state of gold in  $\text{Au}/\gamma\text{-Al}_2\text{O}_3$  systems were evaluated by transmission electron microscopy (TEM) and X-Ray photoelectron spectroscopy (XPS). A vapor infiltration procedure is suggested to prepare metallic gold particles  $\leq 5$  nm in diameter from  $\text{Au}/\gamma\text{-Al}_2\text{O}_3$ . It is shown that  $\text{Au}/\gamma\text{-Al}_2\text{O}_3$  systems obtained by chemical vapor infiltration and containing small gold crystallites possess high catalytic activity in CO oxidation reactions at 40°C.

### MODEL CATALYST STUDIES OF THE STRONG METAL-SUPPORT INTERACTION: SURFACE STRUCTURE IDENTIFIED BY STM ON Pd NANOPARTICLES ON TiO<sub>2</sub>(110)

**M. Bowker\***, **P. Stone\*\***, **P. Morrall\*\***, **R. Smith\*\***, **R. Bennett\*\***, **N. Perkins\*\***, **R.I. Kvon**, **C. Pang\*\***, **E. Fourre\***, **M. Hall\*** (\**Surface Science and Catalysis Group, Cardiff University, Cardiff, UK*; \*\**Centre for Surface Science and Catalysis, University of Reading, Reading, UK*)

*J. Catal.*,  
234(1) (2005) pp. 172-181.

Model catalysts of Pd nanoparticles and films on TiO<sub>2</sub>(110) were fabricated by metal vapour deposition (MVD). Molecular beam measurements show that the particles are active for CO adsorption, with a global sticking probability of 0.25, but that they are deactivated by annealing above 600 K, an effect indicative of SMSI. The Pd nanoparticles are single crystals oriented with their (111) plane parallel to the surface plane of the titania. Analysis of the surface by atomic resolution STM shows that new structures have formed at the surface of the Pd nanoparticles and films after annealing above 800 K. There are only two structures, a zigzag arrangement and a much more complex “pinwheel” structure. The former has a unit cell containing 7 atoms, and the latter is a bigger unit cell containing 25 atoms. These new structures are due to an overlayer of titania that has appeared on the surface of the Pd nanoparticles after annealing, and it is proposed that the surface layer that causes the SMSI effect is a mixed alloy of Pd and Ti, with only two discrete ratios of atoms: Pd/Ti of 1:1 (pinwheel) and 1:2 (zigzag). It is proposed that it is these structures that cause the SMSI effect.

### THE PENETRATION OF INDIUM-GALLIUM MELT COMPONENTS INTO ALUMINUM

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*Russ. J. Phys. Chem.*,  
80(7) (2006) pp. 1110-1114.

The penetration of indium–gallium melt into aluminum alloys was studied by X-ray fluorescence spectroscopy, X-ray diffraction, and optical microscopy. The X-ray fluorescence data were used to suggest a method for estimating the bulk diffusion coefficient of liquid gallium into grains of polycrystalline aluminum alloys of various brands.

### PHYSICO-CHEMICAL INVESTIGATION INTO THE SPECIFIC FEATURES OF THE PHASE TRANSFORMATIONS IN ELECTRODEPOSITED NANOCRYSTALLINE OXOTUNGSTATE FILMS

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*Cryst. Rep.*, 51(suppl. 1) (2006) pp. 130-138.

The structure of oxotungstate films (as-deposited and subjected to heat treatment at temperatures of up to 600°C) prepared through electrodeposition on platinum and gold polycrystalline substrates is investigated using different physicochemical methods. It is shown that the oxotungstate films consist of X-ray amorphous hydrated mixtures of isopoly compounds, predominantly in the form of paratungstates with [H<sub>2</sub>W<sub>12</sub>O<sub>42</sub>]<sup>10-</sup> anions. The structural transformation with an increase in the temperature in air is accompanied by the loss of water, the transformation of paratungstate anions into more oxidized forms, their destruction, and the crystallization of nonstoichiometric hydroxylated oxide phases.

### EXAFS INVESTIGATION OF THE LOCAL ATOMIC STRUCTURE OF Fe-Ge NANOCRYSTALLINE DISORDERED ALLOYS

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*Crystallogr. Rep.*,  
51(Suppl. 1) (2006) pp. 183-191.

This paper reports on the results of EXAFS investigations (Fe K and Ge K absorption edges) of binary supersaturated nanocrystalline solid solutions Fe<sub>100-x</sub>Ge<sub>x</sub> (x = 15–40 at % Ge) prepared by mechanical alloying. The nanocrystalline disordered structure of the single-phase alloys is characterized using X-ray diffraction, Mössbauer spectroscopy, and magnetic measurements. The EXAFS spectra are analyzed by solving the inverse binary problem with the use of combined data on the Fe K and Ge K absorption edges. The parameters of the partial pair correlation functions obtained indicate that the crystal lattice is characterized by strong local static distortions and short-range chemical order increasing with an increase in the germanium content. Moreover, the formation of a hexagonal-type macrostructure in the body-centered cubic (bcc) lattice occurs through a “local” stage.



**EXAFS, X-RAY DIFFRACTION AND RAMAN STUDIES OF  $(\text{Pb}_{1-x}\text{La}_x)(\text{Zr}_{0.65}\text{Ti}_{0.35})\text{O}_3$  ( $x=0.04$  AND  $0.09$ ) CERAMICS IRRADIATED BY HIGH-CURRENT PULSED ELECTRON BEAM**

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*J. Phys. Chem. Solids*,  
67(9-10) (2006) pp. 2007-2012.

The effect of pulsed electron beam irradiation on the long-range and short-range atomic structure, as well as on the Raman phonon modes, of perovskite  $(\text{Pb}_{1-x}\text{La}_x)(\text{Zr}_{0.65}\text{Ti}_{0.35})\text{O}_3$ ,  $x=0.04$  and  $0.09$  (PLZT 4/65/35 and 9/65/35) ferroelectric ceramics is reported. X-ray powder diffraction (XRD) spectra from the single-pulse-irradiated PLZT 9/65/35 samples reveal transformation of the cubic Pm3m ( $Z=1$ ) into the orthorhombic Pmmm ( $Z=1$ ) structure. This symmetry change is however not observed for 10-pulse irradiation performed under the same conditions: here only an increase in the coherent scattering regions, lattice volume, and the Zr–O distance distribution is observed, as revealed by XRD and X-ray absorption spectroscopy at Zr  $K$ -edge. Raman scattering from PLZT 9/65/35 ceramics is in agreement with the symmetry reduction after single-pulse irradiation and reveals significant Raman signal intensity decrease after multiple-pulse irradiation. On the contrary, no significant structural changes could be detected in PLZT 4/65/35 ceramics after single- or multiple-pulse irradiation. Possible mechanisms of pulsed electron irradiation effects in PLZT 4/65/35 and 9/65/35 ceramics are discussed.

**FIRST EXPERIMENTAL AND SIMULATION STUDY ON THE SECONDARY ELECTRON AND PHOTOELECTRON YIELD OF NEG MATERIALS (Ti–Zr–V) COATING UNDER INTENSE PHOTON IRRADIATION**

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*Nucl. Instrum. Methods Phys. Res., Sect. A*,  
554 (2005) pp. 92-113.

A beam duct coated with NEG materials (Ti, Zr, V), which had been known to have a low secondary electron yield (SEY), was studied for the first time under intense photon irradiation using a positron beam at the KEK B-Factory (KEKB) to investigate a way to suppress the electron cloud instability (ECI). A 2.56 m test copper chamber was coated with the NEG materials (it is called NEG coating here) by magnetron sputtering. It was installed at an arc section of the KEKB positron ring, where the chamber was irradiated by direct photons with a line density of  $6.5 \times 10^{14}$  photons  $\text{m}^{-1} \text{s}^{-1} \text{mA}^{-1}$ . The vacuum pressure around the test chamber during a usual beam operation was lower than the case of non-coated copper chambers by a factor of 4–5. The number of electrons around positron bunches was measured by a special electron monitor up to a stored beam current of 1600 mA. The measured electron current, however, was almost the same as a non-coated copper chamber, especially at low-beam currents, and the effect of the NEG coating was smaller than expected. A simulation explained the result that abundant photoelectrons in the positron ring reduce the effect of the low SEY. The maximum SEYs of the NEG coating and non-coated copper were evaluated using a simulation as about 0.9–1.0 and 1.1–1.3, respectively, which were consistent with the values after a sufficient electron bombardment. Their photoelectron yields were also estimated as 0.22–0.28 and 0.26–0.34, respectively, and were in good agreement with the previous experimental results. The study indicates that the suppression of photoelectrons, by a beam duct with an antechamber, for example, is indispensable to make effective use of a surface with a low SEY, such as the NEG coating.

### EFFECT OF HIGH-CURRENT PULSED ELECTRON BEAM IRRADIATION ON THE STRUCTURE OF $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$ POWDER

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*J. Phys. Chem. Solids*,  
67(9-10) (2006) pp. 2001-2006.

The effect of pulsed electron irradiation on the long- and short-range order in the  $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$  ceramics is reported. Neutron and X-ray powder diffraction reveal that the unit cell symmetry and single-phase state of single and multiple irradiated  $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$  are preserved, while the oxygen atoms coordination changes towards the  $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3$  structure. X-ray absorption data confirm this observation and further reveal the details of the shift and splitting of the  $\text{Co}^{3+} t_{2g}$  and  $e_g$  atomic orbitals. Possible mechanisms of pulsed electron irradiation effect in  $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$  are discussed.

### PHASE SEPARATION IN $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ SOLID SOLUTIONS WITH A PEROVSKITE STRUCTURE

V.V. Sikolenko\*\*\*, A.P. Sazonov\*\*\*\*\*, V.V. Efimov\*\*, E.A. Efimova\*\*, V.V. Kriventsov, D.I. Kochubey, U. Zimmermann\*\*\*\*\* (\*Hahn Meitner Institut, Berlin, Germany; \*\*Joint Institute for Nuclear Research, Dubna, Russia; \*\*\*Institute of Solid-State and Semiconductor Physics, Minsk, Belarus; \*\*\*\*Institut für Kristallographie, Technische Hochschule Aachen, Aachen, Germany; \*\*\*\*\*Paul Scherrer Institute, Villigen, Switzerland)

*Crystallogr. Rep.*,  
51(Suppl. 1) (2006) pp. 67-75.

The properties of  $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$  ( $x = 0, 0.15, 0.20, 0.30$ ) solid solutions are investigated using neutron diffraction, positive-muon spin relaxation (precession) measurements, and extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structure (XANES) spectroscopy. The results obtained are interpreted within the model of phase separation into ferromagnetic regions enriched with  $\text{Sr}^{2+}$  ions and nonmagnetic regions similar in composition to the  $\text{LaCoO}_3$  compound.

### STRUCTURE OF ZIRCONIUM BUTOXIDE COMPLEXES IN *N*-BUTANOL SOLUTIONS

V.V. Kanazhevskii, V.P. Shmachkova, N.S. Kotsarenko, V.N. Kolomiichuk, D.I. Kochubey

*J. Struct. Chem.*,  
47(3) (2006) pp. 453-457.

EXAFS and SAXS were used for structure elucidation of zirconium butoxide complexes in *n*-butanol at concentrations from 0.3 g to 0.015 g  $\text{ZrO}_2$  in 1 ml. The basic structural unit of the complex is a tetramer. It has two equal sides with zirconium atoms linked by double oxygen bridges and with zirconium-zirconium distances of 3.5 Å. The other sides in the tetramer are 3.3 Å and 3.9 Å. This difference in bond lengths is explained by the different numbers of double or single ligand bridges between zirconium atoms. The tetramers are apt to undergo oligomerization to form particles with a diameter of 80 Å in solution.

### CHANGES IN THE ZIRCONIUM LOCAL SURROUNDING ON LIGAND SUBSTITUTION IN SOLUTIONS

V.V. Kanazhevskii, V.P. Shmachkova, N.S. Kotsarenko, V.N. Kolomiichuk, D.I. Kochubey

*J. Struct. Chem.*,  
47(5) (2006) pp. 860-868.

EXAFS and SAXS methods have been used to examine zirconium hydroxide and oxychloride aqueous solutions in the presence of sulfuric acid in a wide range of concentrations, as well as a zirconium sulfate aqueous solution. The structure of the complexes and their transformation regularities were determined. Structures of the given complexes and structures of zirconium hydroxide and zirconium oxychloride and hydroxide complexes in aqueous solutions were compared. Complexes in zirconium hydroxide and oxychloride aqueous solutions have identical structures in the presence of sulfuric acid. When the concentration ratio of sulfuric acid and the initial compound is low (20–30), the complex is an open trimer with zirconium atoms bonded by sulfate groups. Bridge sulfate groups form Zr-O-S-O-Zr bonds. Apart from the bridge sulfate groups, there are three terminal sulfate groups and three terminal hydroxyl groups for each zirconium atom. When the concentration of sulfuric acid is increased (up to a ratio of 40–100), closed trimers are observed in the solution.

**CHANGE IN THE COORDINATION MODE OF NITROSYL GROUPS: TRANSFORMATION OF Pd<sub>4</sub>(μ-NO)<sub>4</sub>(μ-OCOCF<sub>3</sub>)<sub>4</sub> INTO Pd<sub>3</sub>(NO)<sub>2</sub>(μ-OCOCF<sub>3</sub>)<sub>4</sub>(C<sub>6</sub>H<sub>5</sub>Me)<sub>2</sub>**

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**L.S. Alekseev\*\***, **R.S. Shamsiev\***, **A.P. Belov\***,  
**D.I. Kochubey**, **B.N. Novgorodov** (\**Lomonosov Moscow State Academy of Fine Chemical Technology, Moscow, Russia*; \*\**Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia*)

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

The reaction of the tetranuclear complex of composition Pd<sub>4</sub>(CO)<sub>4</sub>(CF<sub>3</sub>COO)<sub>4</sub> (**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<sub>4</sub>(NO)<sub>4</sub>(CF<sub>3</sub>COO)<sub>4</sub> (**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<sub>3</sub>(NO)<sub>2</sub>(CF<sub>3</sub>COO)<sub>4</sub>(TolH)<sub>2</sub> (**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.

**ANALYSIS OF THE NATURE OF ADSORBED LAYERS OF ATMOSPHERIC AEROSOLS**

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**K.P. Kutsenogii\***, **V.I. Makarov\*** (\**Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*)

*Chem. Sustain. Devel.*,  
14(5) (2006) pp. 449-452.

Secondary Ion Mass Spectrometry technique was used for comparison testing of the nature of adsorbed compounds on the surface of continental atmospheric aerosols, taken in industrial and background regions of Novosibirsk and Yamalo-Nenetsk, and also sea atmospheric aerosols, taken in the White Sea region.

**FMR FINE STRUCTURE – A TOOL TO INVESTIGATE THE SPATIAL MAGNETIC PHASE SEPARATION PHENOMENA IN MANGANITES**

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**N.V. Volkov\*\***, **K.A. Sablina\*\*** (\**Budker Institute of Nuclear Physics, Novosibirsk, Russia*; \*\**Kirensky Institute of Physics, Krasnoyarsk, Russia*)

*Phys. Status Solidi (Rapid Research Lett.)*,  
1(1) (2007) pp. R22-R24.

An original approach is proposed to study the magnetic phase separation phenomenon. It is based on the registration of the noise-like FMR Fine Structure (FMR FS) caused by the magnetic interparticle dipole-dipole interaction between spatially separated ferromagnetic regions. Data obtained for a La<sub>0.7</sub>Pb<sub>0.3</sub>MnO<sub>3</sub> single crystal point to the existence of spatially separated ferromagnetic regions. It is shown that FMR FS of the La<sub>0.7</sub>Pb<sub>0.3</sub>MnO<sub>3</sub> single crystal is temperature reversible and disappears at the maximum of magnetoresistance.

**LIFTED RECONSTRUCTION AS A FEEDBACK MECHANISM IN THE OSCILLATING CO OXIDATION ON Pt NANOFACETS: MICROSCOPIC EVIDENCE**

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**V.K. Medvedev\*\***, **H. Weiss\*** (\**Chemisches Institut, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany*; \*\**Department of Chemical Engineering, University of Washington, USA*)

*Surf. Sci.*,  
600(8) (2006) pp. 1579-1585.

Global and local oscillations in the CO oxidation reaction have been visualized *in situ* on the apex of a [1 0 0]-oriented Pt field emitter tip used as a well-defined model for catalytically active, nm-sized particles by Field Emission (FEM) and Lithium Field Desorption (Li-FDM) Microscopes. For the first time experimental evidence is provided that the reconstruction feedback mechanism of the self-maintained oscillations for the [1 0 0] and [1 1 0] orientations, which is well established on macroscopic single crystals, is also valid in the heterogeneous, nm-sized system with its different crystallographic orientations which are coupled by surface diffusion.

## THE USE OF $O_2^-$ RADICAL ANIONS AS SPIN PROBES FOR TESTING NANOSTRUCTURED MATERIALS BASED ON ZIRCONIUM OXIDE

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V.A. Sadykov, V.V. Lunin\* (\*Moscow Lomonosov  
State University, Moscow, Russia)

*Russ. J. Phys. Chem.*,  
80(7) (2006) pp. 1088-1092.

The conditions of formation of  $O_2^-$  radical anions on the surface of zirconium oxide systems, including nanostructured pillared clays, in interaction with hydrogen peroxide and an  $NO + O_2$  mixture of gases were studied by the EPR method. The special features of the formation of these radicals depending on the phase composition, structure, and degree of hydroxylation of the surface are discussed.

## FORMATION OF MIXED Fe-Mo OXO CLUSTERS IN THE GAS PHASE

V.B. Goncharov

*Russ. J. Phys. Chem.*, 80(2) (2006) pp. 288-290.

Reactions of oxygen-containing molybdenum clusters  $Mo_xO_y$  ( $x = 1-3$ ,  $y = 1-9$ ) with iron carbonyl ions  $Fe(CO)_n^+$  ( $n = 1-3$ ) were studied by the ion cyclotron resonance technique. The reactions were found to yield mixed Fe-Mo oxo clusters  $Mo_xO_yFe^+$  ( $x = 2, 3$ ;  $y = 5, 6, 8, 9$ ).

## REACTIVITY AND HYDROGEN AFFINITY OF CHARGED MOLYBDENUM OXOCLUSTERS IN THE GAS PHASE

V.B. Goncharov

*Russ. J. Phys. Chem.*,  
80(3) (2006) pp. 486-488.

The available experimental data on proton affinity were used to calculate the hydrogen affinity ( $HA$ ) of oxygen-containing molybdenum clusters. As the  $HA$  increases, the direct incorporation of the ion into a C-H bond of a hydrocarbon molecule gives way to the direct abstraction of the hydrogen atom accompanied by charge transfer to the organic fragment.

## STRUCTURAL FEATURES OF MAGNESIUM OXIDES DERIVED FROM VARIOUS PRECURSORS

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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.

## DETECTION OF HYDROGEN-COPPER CLUSTERING IN $Zn_{1-x}Cu_xO$ COMPOUNDS USING NEUTRON SCATTERING METHODS

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*Phys. Solid. State*, 48(7) (2006) pp. 1291-1297.

The atomic and cluster structure of hydrogen-treated Cu/ZnO (the major component of methanol synthesis catalysts) was studied using Bragg powder and small-angle neutron diffraction. Isotopic substitution of Cu and H was used to obtain reliable results indicating Cu and H clustering. The clusters form on the boundaries of ZnO particles and have a complex structure: a copper cluster surrounded by an adsorbed hydrogen shell has a hydrogen core. It can be assumed that this cluster configuration has a strong effect on the catalytic activity of these compounds.

## PECULIARITIES OF THE ELECTRONIC SPECTRA OF MODEL Cu-Zn CATALYSTS OF METHANOL SYNTHESIS IN THE OXIDIZED AND REDUCED STATES

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A.A. Altynnikov, T.V. Larina,  
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*Doklady Phys. Chem.*,  
409(2) (2006) pp. 193-197.

The anion-modified oxide  $Cu_{0.08}Zn_{0.92}O$  was studied to reveal the uniform light absorption over the whole visible and UV ranges. The observed

phenomenon is accounted for by shifting the edge of background absorption by the high-defect structure of zinc oxide due to the appearance of impurity levels in the ZnO band gap. The oxide reduction in hydrogen at above 210°C gives rise to an absorption band at 14500–16700 cm<sup>-1</sup> which can relate to resonance absorption of electromagnetic energy (RAEE) by copper metal nanoparticles. The observed difference of the absorption maximum from the known RAEE of copper nanoparticles (17800 cm<sup>-1</sup>) is due to decoration of the copper metal nanoparticles with zinc oxide to change dielectric permeability in the surroundings of the metal nanoparticles.

#### **INTERACTION BETWEEN 193-nm PULSED LASER RADIATION AND $\alpha$ -ALUMINA**

**V.O. Stoyanovsky, V.N. Snytnikov, N.A. Rudina, V.N. Parmon**

*Techn. Phys.*,  
51(4) (2006) pp. 514-518.

The threshold power density of 15-ns laser pulses with a wavelength 193 nm is determined for basic modes of interaction between the radiation and  $\alpha$ -alumina. As power density  $Q$  on the target varying in the range 0.001–100 MW/cm<sup>2</sup> increases, first the interaction mechanism changes from single-photon interaction to two-photon interaction at  $Q \approx 0.1$  MW/cm<sup>2</sup>. At  $Q \approx 5$  MW/cm<sup>2</sup>, the material sublimates and then the sublimation products ionize at  $Q \approx 15$  MW/cm<sup>2</sup>. At  $Q \approx 100$  MW/cm<sup>2</sup>, the material is removed from the surface at a rate of  $\approx 10$  nm per pulse.

#### **MECHANISMS OF OXYGEN ADSORPTION AND DESORPTION ON POLYCRYSTALLINE PALLADIUM**

**A.N. Salanov, A.I. Titkov, V.N. Bibin**

*Kinet. Catal.*,  
47(3) (2006) pp. 430-436.

The adsorption and desorption of oxygen on a polycrystalline palladium (Pd(poly)) surface (10- to 100- $\mu$ m crystallites;  $\sim 32\%$  (100),  $\sim 18\%$  (111),  $\sim 34\%$  (311), and  $\sim 15\%$  (331)) at  $P_{O_2} \leq 1.3 \times 10^{-5}$  Pa and  $T = 500$ – $1300$  K have been studied by TPD and mathematical modeling. The kinetics of O<sub>2</sub> adsorption and desorption on Pd(poly) are primarily governed by the formation and decomposition of oxygen adsorption structures on the (100) and (111) crystallite faces. The O<sub>2</sub> adsorption rate is constant at  $\theta \leq 0.15$ – $0.25$  owing to the formation of the  $p(2 \times 2)$  structure with an O<sub>ads</sub>–surface bonding energy of

$D(\text{Pd-O}) = 364$  kJ/mol on the (100) and (111) faces. The adsorption rate decreases with increasing coverage at  $\theta \leq 0.15$ – $0.25$  because of the growth, on the (100) face, of the  $c(2 \times 2)$  structure, in which  $D(\text{Pd-O})$  is reduced to 324 kJ/mol by lateral interactions in the adsorption layer. A high-temperature ( $\sim 800$  K) O<sub>2</sub> desorption peak is observed for  $\theta \leq 0.25$ , which is due to O<sub>2</sub> desorption from a disordered adsorption layer according to a second-order rate law with an activation energy of  $E_{\text{des}} = 230$  kJ/mol. A lower temperature ( $\sim 700$  K) O<sub>2</sub> desorption peak is observed for  $\theta \leq 0.25$ , which is due to O<sub>2</sub> released by the  $c(2 \times 2)$  structure according to a first-order rate law with  $E_{\text{des}} = 150$  kJ/mol. At  $\theta \leq 0.25$ , there are repulsive interactions between O<sub>ads</sub> atoms on Pd(poly) ( $C_{\text{aa}} = 5$ – $10$  kJ/mol).

#### **STATE OF DISPERSE ALLOY PARTICLES CATALYZING HYDROCARBON DECOMPOSITION BY THE CARBIDE CYCLE MECHANISM: TEM AND EDX STUDIES OF THE Cu-Ni/Al<sub>2</sub>O<sub>3</sub> AND Cu-Co/Al<sub>2</sub>O<sub>3</sub> CATALYSTS**

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

*Kinet. Catal.*,  
47(4) (2006) pp. 603-609.

The state of disperse bimetallic alloy particles in the Cu-Ni/Al<sub>2</sub>O<sub>3</sub> and Cu-Co/Al<sub>2</sub>O<sub>3</sub> catalysts during their carbonization in butadiene-1,3 is studied by high-resolution electron microscopy and energy-dispersive X-ray analysis. During the formation of carbon nanofilaments by the carbide cycle mechanism, the catalyst is in a dissipative state such that the bimetallic particles vary in composition and have an anomalous component distribution in their bulk. The extrapolation of this state provides insight into the processes occurring in the dissipative system.

#### **MANGANESE FERRITE NANOPARTICLES IN BORATE GLASS AND THEIR INFLUENCE ON THE MAGNETO-OPTICAL PROPERTIES**

**I.S. Edel'man\*, S.A. Stepanov\*\*, G.T. Petrovskii\*\*, V.I. Zaikovskii, R.D. Ivantsov\*, O.S. Ivanova\*, D.E. Prokof'ev\*, T.V. Zarubina\*\*, E.E. Kornilova\*\*** (\*Kirensky Institute of Physics, Krasnoyarsk, Russia; \*\*Vavilov State Optical Institute, All-Russia Research Center, St. Petersburg, Russia)

*Glass Phys. Chem.*,  
31(2) (2005) pp. 177-186.

Nanoparticles that are formed in the course of additional heat treatment in borate glasses containing

iron and manganese oxide additives at low concentrations are directly observed for the first time using electron microscopy. The size, the shape, and the structure of nanoparticles and their volume distribution in the glass matrix are determined. Correlations between the nanoparticle parameters and the magnetic and magneto-optical properties of the glasses containing these particles are revealed.

#### **GAS CHROMATOGRAPHIC ANALYSIS OF GAS EMISSIONS CONTAINING IMPURITIES OF HYDROCYANIC ACID AND CARBON OXYSULFIDE**

**V.I. Zheivot, S.I. Afanasieva, A.V. Simakov**

*J. Analyt. Chem.*, 61(3) (2006) pp. 253-258.

Gas chromatography was used for studying the retention of HCN, COS, H<sub>2</sub>S, H<sub>2</sub>O, CO<sub>2</sub>, CO, and H<sub>2</sub> on organic porous polymer sorbents Chromosorb-104 and Hayesep C either unmodified or modified with different amounts of H<sub>3</sub>PO<sub>4</sub>. The effect of water on the signal of the thermionic detector was studied, and the conditions of the determination of 6–23 ppm HCN in aqueous solutions were found: column (3 m × 2 mm) with Hayesep C containing 15 wt % H<sub>3</sub>PO<sub>4</sub>. A procedure was developed for the determination of 15-1000 ppm COS in the presence of high concentrations (up to 1 vol %) of H<sub>2</sub>S on a column (3 m × 2 mm) packed with Chromosorb-104 modified with 0.5 wt % H<sub>3</sub>PO<sub>4</sub> with a flame photometric detector (396 nm). A basic scheme was proposed for the gas chromatographic analysis of the products of the catalytic detoxication of gas emissions in the process of coal gasification.

#### **SPECIFIC FEATURES OF THE GAS-CHROMATOGRAPHIC DETERMINATION OF THE REACTION PRODUCTS IN THE CATALYTIC DECOMPOSITION OF HYDROGEN SULFIDE**

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*J. Analyt. Chem.*, 61(4) (2006) pp. 334-337.

Specific features of the determination of hydrogen sulfide in the presence of hydrogen were studied by gas chromatography with the use of a thermal conductivity detector and argon as the carrier gas. A chromatographic column with HayeSep A modified with 10 wt % H<sub>3</sub>PO<sub>4</sub> was proposed for the simultaneous determination of both components. It was demonstrated that the elution curve of hydrogen

sulfide in an argon atmosphere has a non-Gaussian shape because of the interaction of hydrogen sulfide with the tungsten filament of the sensing element of the catarometer. To eliminate this interaction, it was recommended that a gold-plated tungsten filament be used in the detector.

#### **GAS CHROMATOGRAPHY ON CARBON ADSORBENTS: CHARACTERIZATION, SYSTEMATIZATION, AND PRACTICAL APPLICATIONS TO CATALYTIC STUDIES**

**V.I. Zheivot**

*J. Analyt. Chem.*, 61(9) (2006) pp. 832-852.

The results of the characterization of graphite-like carbon materials by X-ray diffraction, electron microscopy, and adsorption and gas chromatography are discussed. All carbon-containing adsorbents are systematized in accordance with their structure and adsorption characteristics, chemical nature, and chromatographic surface properties. The adsorption and gas-chromatographic properties of carbons and other adsorbents are compared. The purposeful regulation of the chemical nature of carbon adsorbent surfaces is considered; it significantly extended the gas-chromatographic capabilities of carbon-containing materials, in particular, in studies of the product composition of catalytic reactions.

#### **DISSOLUTION KINETICS OF CsHSO<sub>4</sub> AND CsHSO<sub>4</sub>/SiO<sub>2</sub> COMPOSITES IN AQUEOUS SOLUTIONS**

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*Inorg. Mater.*, 42(10) (2006) pp. 1115-1120.

Using a differential dissolution method, the dissolution kinetics of CsHSO<sub>4</sub> and CsHSO<sub>4</sub>/SiO<sub>2</sub> composites (40, 60, and 70 mol % SiO<sub>2</sub>) in aqueous solutions have been studied. The results demonstrate that the composites and bulk CsHSO<sub>4</sub> differ markedly in dissolution rate. In addition, the dissolution rate depends on the composition of the composite and decreases significantly as the SiO<sub>2</sub> content is raised from 0 to 70 mol %, even though the particle size of the salt is notably smaller in the composites. The composites of the same composition may contain cesium hydrogen sulfate in several states, differing in dissolution rate.

## TEXTILES FROM FROZEN TOMBS OF IV–III CENTURIES B.C. IN THE ALTAI MOUNTAINS

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Novosibirsk, Publishing House SB RAS, 2006, 265 pp.

Results of studying inorganic components of ancient textile samples are reported. Inductively coupled plasma–atomic emission spectrometry (ICP-AES) and X-ray fluorescent spectroscopy (XRFS) techniques were used to determine the textile elemental composition. In general, more than 100 fragments of ancient textiles were characterized. A new reference-free high-sensitive method of differential dissolution (DD) was used for the first time for identification and quantitative determination of the phase (mineral) composition of inorganic constituents of the ancient textiles.

## PHYSICO-CHEMICAL STUDIES OF CERAMICS (WITH WARES OF THE TRANSITION PERIOD FROM BRONZE TO THE IRON AGE AS AN EXAMPLE)

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Eds. V.V. Boldyrev, V.I. Molodin, Novosibirsk, Publishing House SB RAS, 2006, 98 pp.

An economically and informatively optimal set of analytic physicochemical tools was chosen for studying specimens of ancient ceramics. The authors found it most appropriate to combine thermogravimetric (TG), powder X-ray diffraction (XRD) and petrographic techniques. TG and XRD are most effective for characterization of clay minerals including their thermal treatment products and of well crystalline nonplastic minerals, while petrography provides quantitative data on the ratio of clay components and nonplastic debris. Algorithms of analytic procedures were developed for each of these methods.

## Fundamental and Practical Approach to Catalyst Preparation

### COPPER-PROMOTED COBALT CATALYSTS FOR 2,3-DIHYDROFURAN SYNTHESIS

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*Appl. Catal.*, A, 311 (2006) pp. 86-93.

The conversion of 1,4-butanediol to 2,3-dihydrofuran in the liquid phase has been studied over novel kaolin-supported Co–Cu catalysts, prepared by means of a simple mechanochemical method. The improvement of the catalytic properties and decrease in the optimum reduction temperature of Co–kaolin catalysts, promoted by copper, has been observed. It was established that a Co:Cu ratio 5:1 is optimum for the specific activity and for the yield in the conversion of 1,4-butanediol to 2,3-dihydrofuran. In the present study, the highest 2,3-dihydrofuran yield (81%) was obtained with the ultrasonically treated catalyst and after reduction pretreatment at 320–350°C. The existence of an optimum reduction

temperature for the catalyst pretreatment was established. In agreement with the results, obtained in previous studies, the high 2,3-dihydrofuran yield is favoured by the coexistence of cobalt both in the metallic and oxidic state. The increased specific activity of copper-containing catalysts could be related to the lowering of the reduction temperature, which leads to a hexagonal metallic cobalt phase formation. The latter is favourable for 2,3-dihydrofuran synthesis. The advantage of mechanochemical preparation of Co–Cu (5:1) catalyst is that the method prevents penetrating of cobalt ions into the support, thus the whole amount of cobalt loaded is available for the catalyst performance. This is one of the probable reasons for higher specific activity of the 2,3-DHF formation over these catalysts.



#### CATALYST FOR DEHYDROGENATION OF LOWER C<sub>3</sub>-C<sub>5</sub> PARAFFINS IN FIXED BED OVER NOVEL ALUMINA CERAMOMETAL SUPPORT

N.A. Pakhomov, S.F. Tikhov, Yu.N. Bespalko, V.S. Babenko, A.I. Titkov, A.N. Salanov, V.A. Sadykov, R.A. Buyanov

*Crit. Technol. Membranes*,  
29(1) (2006) pp 38-42.

The effect of a ratio of powder metallic aluminum and the product of thermochemical activation gibbsite in the initial charge on the textural and strength properties of the ceramic-metal Al<sub>2</sub>O<sub>3</sub>-Al catalysts has been studied. The optimal composition of the initial charge, providing preparation of a support with the best texture-mechanical properties, was determined. The chromium oxide catalyst supported on a new ceramic-metal support cermet exhibits in the reaction of lower C<sub>3</sub>-C<sub>4</sub> paraffin dehydrogenation the activity and selectivity which comply with the best world analogs.

#### THE HEAT OF WETTING OF ALUMINUM HYDROXYOXIDE OBTAINED BY THE THERMAL ACTIVATION OF HYDRARGILLITE

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*Russ. J. Phys. Chem.*,  
80(7) (2006) pp. 1037-1043.

Changes in the volume and surface properties of thermally activated hydrargillite, so-called centrifugal thermal activation (CTA) product (empirical formula Al<sub>2</sub>O<sub>3</sub> · 0.85H<sub>2</sub>O), during its calcining in air with gradually increasing temperature from 90 to 1100°C were studied. At each stage of calcining, weight loss, phase composition, texture characteristics, and the heat of wetting with water at 25°C were determined. Measurements of the heat of wetting showed that the energy and, therefore, chemical state of the surface changed during thermal treatment. The data obtained were used to calculate the heats of adsorption  $q_{ads}$  of water vapor by CTA samples with different water contents; the range of  $q_{ads}$  variations was 50-250 kJ/mol. The values obtained are compared with literature data.

#### ACID-BASE PROPERTIES OF ALUMINA PREPARED FROM A HYDRATED PRODUCT OF CENTRIFUGAL THERMAL ACTIVATION OF HYDRARGILLITE (CTA-PRODUCT)

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

*React. Kinet. Catal. Lett.*,  
88(2) (2006) pp. 381-390.

Acid-base properties of aluminas prepared by thermal treatment of a hydrated CTA-product at 600°C were studied. The CTA-oxides, representing  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, were shown to contain terminal and bridged OH-groups. The concentration of the terminal OH-groups in the CTA-oxides was found to exceed their concentration in  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> prepared by dehydration of the "precipitated" pseudoboehmite, whereas the concentration of the bridged OH-groups in the CTA-oxides was lower than that in  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> prepared from pseudoboehmite. The total concentration of the surface Lewis acid sites in CTA-oxides varies within the limits of 2.80–4.14  $\mu\text{mol}/\text{m}^2$  and is essentially above that in  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> (2.25  $\mu\text{mol}/\text{m}^2$ ). The distinctive feature of the CTA-oxides is that their surface contains strong Lewis acid sites with  $\nu_{CO} = 2220$  and  $2238 \text{ cm}^{-1}$ . The total concentration of basic sites in the CTA oxides is lower than that in  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, however, in contrast to  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, they contain strong basic sites with  $\nu_{CDCl_3} = 2200 \text{ cm}^{-1}$ .

#### PREPARATION FACTORS INFLUENCING THE EFFECTIVENESS OF SAPO CATALYSTS IN N-PARAFFINS HYDROISOMERIZATION

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*Stud. Surf. Sci. Catal.*,  
162 (2006) pp. 897-904.

The present work deals with a comparison of synthesis procedures of silicoaluminophosphates of AEL and ATO structural types starting with the same Al, P and Si sources but differing in template origin. On the base of performed experiments on preparation of these materials by means of hydrothermal synthesis of initial silicoaluminophosphate gel general factors which determine a quality of final product have been specified. It is shown that within both crystalline systems a treatment of starting reaction mixture with a wide range of Si/Al ratios is possible to result in high crystalline goal material with no admixture of impurity phases. It is found that AEL phase allows much broader variations in its preparation conditions comparatively with ATO phase synthesis. The next parameters are determined to have more expressed importance for preparation of good

quality SAPO-31 samples: order of reagent mixing, intensity and duration of stirring, pH control for each stage of preparation. Disturbance of the reaction boundary conditions leads to incomplete crystallization of initial gel or else to appearance of competing phase. Both cases may be a matter for insufficient quality of goal hydroisomerization catalyst in respect to its activity and selectivity.

In the present work influence of parameters of preparation of SAPO-11 and SAPO-31 materials is demonstrated in terms of their catalytic performance in hydroconversion of n-octane.

The effect of pore structure differences between AEL and ATO on group distribution of C<sub>8</sub> isomers as well as on isomer distribution within methylheptanes and dimethylhexanes is shown for high quality samples.

Taking into account obtained experimental data a conclusion is made on possibility of use of substituted aluminophosphate with ATO structure with regard to hydroisomerization of long-chain paraffin molecules. Catalytic properties of these materials are totally determined by a possibility of synthesis of high crystalline pure ATO phase with high degree of substitution of Al and P atoms of crystalline lattice with isomorphous element.

#### **NANOSTRUCTURED V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub> (ANATASE) CATALYSTS: SYNTHESIS, CHARACTERIZATION, CATALYTIC PROPERTIES**

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

In "New Challenges in Catalysts 4",  
Eds. P. Putanov, Belgrade,  
The Serbian Academy of Science and Arts,  
Branch in Novi Sad., 2005, pp. 239-254.

This paper describes a synthesis of the nanostructured vanadia-based catalysts possessing interfacial boundaries between V<sub>2</sub>O<sub>5</sub> and TiO<sub>2</sub> (anatase) particles. The process of structural formation of the interface at the different stages of the synthesis of catalysts with V<sub>2</sub>O<sub>5</sub> loading lying between 5 and 50 % wt has been studied. XRD, TEM, ESR, <sup>51</sup>V NMR and Raman spectroscopies provide detailed characterization of the materials, particularly, the atomic arrangement of the interface and state of oxidation the vanadium ions. Data on the determination of catalysts texture in a wide temperature region are given. These catalysts appear to be effective for some selective oxidation reactions.

#### **THE STATE OF THE ART AND PROSPECTS FOR DEVELOPMENT IN THE FIELD OF SUPPORTED PALLADIUM CATALYSTS**

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*Russ. Chem. J.*,  
50(4) (2006) pp. 140-153.

The present-day status of researches in the field of supported catalysts with metallic palladium as the active phase is briefly reviewed. Most attention is given to peculiarities of catalyst synthesis from different metal precursors on oxide and carbon supports, to interaction of the active phase with the support, and to comparison of Pd and Pt catalysts. Multiplicity of the factors acting during the catalyst genesis, and a close and intricate relationship between these factors have been pointed out. The nature of the metal precursor, texture and functional coverage of the support, as well as various treatments prove capable of affecting strongly the catalytic properties but none of the factors can be considered principal one, and any can play both positive and negative role, depending on other conditions. Possibilities for further improving and new ways for industrial application of Pd catalysts are also noted.

#### **EFFECTS OF CARBON SURFACE OXIDES ON THE DISPERSION OF Pt/C CATALYSTS PREPARED VIA ADSORPTION OF HEXACHLOROPLATINIC ACID: A NEW INSIGHT**

**A.N. Kholodovich, P.A. Simonov**

*React. Kinet. Catal. Lett.*,  
89(1) (2006) pp. 167-175.

A new concept is advanced to explain some effects of oxygen-containing groups of the carbon surfaces on the dispersion of Pt/C catalysts prepared through the adsorption of H<sub>2</sub>PtCl<sub>6</sub> onto porous carbon powders followed by the reduction with H<sub>2</sub>. These groups alter the electrochemical properties of the support and, therefore, influence the nature and amount of the adsorbed catalyst precursors formed during a redox reaction between the carbon surface and H<sub>2</sub>PtCl<sub>6</sub>, that reflects on the dispersion of Pt/C. A way to account for their impact on platinum dispersion is offered. It allows revising and uniting many literature data related to this problem.

## INVESTIGATIONS OF THE ACTIVATION OF ALUMINIUM METAL AS THE INITIAL STAGE OF PREPARATION OF ALUMINA-BASED CATALYSTS AND SUPPORTS

**M.V. Trenikhin\***, **V.K. Duplyakin**, **A.I. Nizovskii**, **A.G. Kozlov\*\*** (\**Institute of Hydrocarbons Processing, Omsk, Russia*; \*\**Omsk Department of the Institute of Semiconductor Physics, Omsk, Russia*)

*Chem. Sustain. Devel.*, 14(1) (2006) pp. 63-71.

The initial stage of synthesis of 'metal of alumina' catalysts is studied. The proposed procedure allows the amount of harmful waste to be decreased considerably. The method is based on the direct interaction of pre-treated aluminium metal and water. It is shown that diffusion phenomena underlie the process of aluminium activation with a fluid In-Ga metal fusion. A method is proposed for estimation of the coefficient of gallium bulk diffusion into grains of polycrystalline aluminium.

## CHEMICAL INTERACTION OF THE In-Ga EUTECTIC WITH Al AND Al-BASE ALLOYS

**M.V. Trenikhin\***, **A.V. Bubnov\***, **A.I. Nizovskii**, **V.K. Duplyakin\*** (\**Institute of Hydrocarbons Processing, Omsk, Russia*)

*Inorg. Mater.*, 42(3) (2006) pp. 256-260.

The chemical interaction of the indium-gallium eutectic with Al and Al-base alloys is studied by X-ray diffraction, optical microscopy, and electron microscopy. Experimental data are presented that shed light on the reaction mechanism and the diffusion processes responsible for the subsequent disintegration of the material and its dissolution in water. Mechanical tests show that the activation of aluminum leads to a transition from plastic to brittle fracture.

## HIGH-TEMPERATURE CATALYSTS WITH A SYNERGETIC EFFECT OF Pd AND MANGANESE OXIDES

**S.A. Yashnik**, **Z.R. Ismagilov**, **V.V. Kuznetsov**, **V.V. Ushakov**, **V.A. Rogov**, **I.A. Ovsyannikova**

*Catal. Today*, 117(4) (2006) pp. 525-535.

A synergetic effect in the catalytic activity has been found after palladium introduction in Mn-Al-O systems. The magnitude of the synergetic effect depends on the types of the oxidic manganese species: oxide  $Mn_3O_4$ , spinel  $(Mn, Mg)[Mn, Al]_2O_4$  or hexaaluminate  $(Mn, Mg)LaAl_{11}O_{19}$ . The synergetic effect of Pd and manganese-containing compounds is observed only if palladium is introduced to the low-temperature precursor of the manganese alumina spinel or manganese hexaaluminate. The synergetic

effect is not observed when high-temperature samples with formed spinel or hexaaluminate phases are modified with Pd.

## CARBONIZATION AND REGENERATION OF Mo/ZSM-5 CATALYSTS FOR METHANE DEHYDROAROMATIZATION

**Z.R. Ismagilov**, **L.T. Tsykoza**, **E.V. Matus**, **G.S. Litvak**, **I.Z. Ismagilov**, **O.B. Sukhova**

*Eurasian Chem.-Tech. J.*, 7(2) (2005) pp. 115-121.

The character of carbonaceous deposits formed during methane dehydroaromatization reaction in the presence of Mo/ZSM-5 catalyst was studied by differential thermal analysis. The dependence of the concentration and condensation degree (C/H ratio) of the carbonaceous deposits on the catalyst synthesis conditions (Mo content = 1-10%, Si/Al ratio in the initial H-ZSM-5 = 17-45) and reaction conditions (feed flow rate = 405-1620 h<sup>-1</sup>, methane concentration = 90-98%, reaction temperature = 720-780°C) was investigated. The oxidative treatment conditions of carbonized Mo/ZSM-5 catalysts providing stable operation of the catalysts under multiple reaction-oxidative treatment cycles were selected.

## ON THE H-FORM OF NATROLITE

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*Eur. J. Mineral.*, 18(3) (2006) pp. 345-350.

To resolve the problem of existence of the H-form of natrolite, the thermal decomposition of NH<sub>4</sub>-exchanged natrolite (as a precursor of the H-form) was studied by gas chromatography, IR spectroscopy and X-ray diffraction. Throughout the decomposition, the de-ammoniation is immediately followed by dehydroxylation, which is evidence for the instability of the H-natrolite formed after the removal of NH<sub>3</sub>, and leads to a negligibly small concentration of the OH-groups. The natrolite structure can not persist after the removal of NH<sub>3</sub>.

In the final step of decomposition, the adsorption of NH<sub>3</sub> onto Lewis centres accumulated in the amorphosed framework hinders the de-ammoniation. This seems to be one of the major factors which influence the observed increase in the activation energy for NH<sub>3</sub> desorption from 117(±13) kJ/mol in the initial step to 270(±20) kJ/mol.

Smooth vacuum degassing of NH<sub>4</sub>-natrolite at 550 K leads to partial de-ammoniation, rather than formation of H-natrolite.

**A HOMOCHIRAL METAL-ORGANIC MATERIAL WITH PERMANENT POROSITY, ENANTIOSELECTIVE SORPTION PROPERTIES, AND CATALYTIC ACTIVITY**

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*Angew. Chem. Int. Ed.*,  
45(6) (2006) pp. 916-920.

A new approach to the synthesis of homochiral metal-organic porous materials starting from readily available chemicals is described. A 3D homochiral microporous framework that has permanent porosity, size- and enantioselective guest-sorption properties, as well as remarkable catalytic activity with size and chemoselectivity, and high conversion in the oxidation of thioethers to sulfoxides was successfully produced.

**SYNTHESIS OF METHYLFORMATE THROUGH CATALYTIC DEHYDROGENATION OF METHANOL OVER COPPER-CONTAINING CATALYSTS**

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*Ind. Chem.*,  
10 (2005) pp. 492-497.

The work is devoted to optimization of the composition and preparation conditions of copper-containing catalysts for dehydrogenation of methanol into methylformate. It is shown that the effective catalysts can be prepared using copper nitrate as the active component precursor. The optimal copper loading in the catalyst is established at the level of 5%.

**DETONATIVE SPUTTERING FOR DECISION OF PROBLEMS OF HYDROGEN ENERGY**

**V.Yu. Ulyanitskii\***, **A.A. Shtertser\***, **S.B. Zlobin\***, **V.I. Matrenin\***, **I.V. Schipanov\***, **S.Yu. Serykh\***, **A.S. Stikhin\***, **L.M. Tretiakova\***, **V.A. Sadykov**, **S.N. Pavlova**, **S.F. Tikhov**, **V.A. Kuzmin** (\*Institute of Hydrodynamics, Novosibirsk, Russia)

*Int. Sci. J. Alternative Energy Ecol.*,  
9 (2006) pp. 137-144.

Regularities for preparation of supports and catalysts based on layered metal-oxide composites, obtained by detonative sputtering of powder oxides on metal foil, and its application for catalysis, is studied.

**THE YTTRIA-STABILIZED ZIRCONIA INTERFACIAL COATINGS ON NICALON FIBER**

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*J. Eur. Ceramic Soc.*,  
26(9) (2006) pp. 1725-1736.

Sols of yttria-stabilized zirconia may be used as simple, readily processable and accurate controllable precursors for the ZrO<sub>2</sub> interfacial coatings on SiC-based Nicalon<sup>TM</sup> fibers. The ZrO<sub>2</sub> interfacial coatings of predictable crystal phase compositions were obtained in dependence of yttria dopant level. The morphology, composition and oxidation resistance of coated fibers were evaluated by SEM, EDS, XPS, XRD, and Raman analysis. All coatings obtained are uniform, continuous and adherent to substrates. The delamination within the ZrO<sub>2</sub> interfacial coating was found. Possible reasons of this phenomenon are discussed. The peculiarities of the behavior of Y-stabilized ZrO<sub>2</sub>-coated fibers in air at elevated temperature are considered.

**FORMATION OF Pt(O)/Si(Ca)O<sub>2</sub> NANOFIBERS UPON THE REACTION OF PLATINUM AEROSOL PARTICLES WITH A CALCIUM- AND SILICON-CONTAINING MATERIAL**

**A.S. Ivanova**, **E.M. Slavinskaya**, **V.I. Zaikovskii**, **I.N. Polukhina**, **O.V. Chub**, **A.S. Noskov**

*Doklady Phys. Chem.*,  
407(1) (2006) pp. 80-83.

It was found that crystalline nanofibers (up to 1000 nm high and about 50 nm in diameter) are formed on the surface of the calcium- and-silicon-containing high-temperature material upon its interaction with platinum aerosol particles at 900°C. The nascent nanofibers represented quartz containing dissolved calcium, Si(Ca)O<sub>2</sub>, the calcium concentration being higher on the top of the fibers. Platinum is also present on the top of the nanofibers, in particular, oxidized platinum occurs on the surface and metal particles (~5 nm) are located under the Si(Ca)O<sub>2</sub> layer.

## TEXTUROLOGY

V.B. Fenelonov, M.S. Melgunov

In "Surface and Nanomolecular Catalysis",  
Ed. R. Richards, CRC Press, 2006, pp. 257-336.

Review of modern state-of-art in the field of texturology of catalyts and other porous materials.

## IS IT POSSIBLE TO GENERALIZE THE PROBLEMS OF POROUS MATERIALS FORMATION, STUDY AND EXPLOITATION?

M.S. Melgunov, V.B. Fenelonov

In "Surface Chemistry in Biomedical and Environmental Science",  
Eds. J.P. Blitz, V.M. Gun'ko, Springer,  
The Netherlands, 2006, pp. 69-78.

The transition from the variety of "scientific bases of preparation" of porous materials (adsorbents, catalyts, etc.) to a uniform fundamental knowledge is discussed. This transition is based on allocation of two different but general levels of porous materials science: molecular (atomic) and supramolecular (textural). Fundamental relationships and laws are discussed in the application of porous materials for catalysis and adsorbents with respect to texture and structure.

## CrAl ALLOY-BASED MONOLITH WITH POLYMODAL PORE STRUCTURE FOR PARTIAL OXIDATION OF METHANE TO SYNTHESIS-GAS

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S.N. Pavlova, O.I. Snegurenko, L.L. Gogin,  
Z.Yu. Vostrikov, A.N. Salanov, S.V. Tsybulya,  
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*Stud. Surf. Sci. Catal.*,  
162 (2006) pp. 641-648.

The main stages of the CrAl alloy-based monoliths preparation from the Al and Cr powders through mechanical alloying, hydrothermal treatment and calcination have been described. The textural, mechanical and catalytic properties in the partial oxidation of methane on the monolithic cermets are presented.

## DEFECT MAGNESIUM OXIDES CONTAINING ACETATE AND NITRATE ION FRAGMENTS INCORPORATED IN THE OXIDE STRUCTURE

N.A. Vasilieva, L.M. Plyasova, G.V. Odegova

*Kinet. Catal.*,  
47(3) (2006) pp. 437-444.

The results of studies on the synthesis of defect magnesium oxides by MgO hydration in salt solutions are summarized. The incorporation of oxygen-containing salt anions into the anionic hydroxide/oxide framework is described. In this case, the anion residue whose oxygen atoms belong to the oxygen framework of the oxide is incorporated in the octahedral oxygen cell of the oxide to occupy the place of a virtual magnesium cation. A portion of cationic vacancies remains free, whereas a portion is occupied by the transformed anion residue with a positive charge other than 2+. As a result, defect magnesium oxides are formed as substitutional solid solutions. The structure and charge heterogeneity of defect oxides is responsible for their high catalytic activity.

## WO<sub>3</sub>/MO<sub>2</sub> (M = Zr, Sn, Ti) HETEROGENEOUS ACID CATALYSTS: SYNTHESIS, STUDY, AND USE IN CUMENE HYDROPEROXIDE DECOMPOSITION

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*Kinet. Catal.*,  
47(4) (2006) pp. 564-571.

Thirty (5–40)% WO<sub>3</sub> /MO<sub>2</sub> (M = Zr, Ti, Sn), heterogeneous acidic catalysts have been synthesized by two methods, specifically, via homogeneous acid solutions and from solutions brought to pH 9 with ammonia, both followed by calcination at 600-900°C. The catalysts have been characterized by IR spectroscopy and scanning electron microscopy, and their aqueous washings have been analyzed. Their acidity has been determined by the thermal analysis of samples containing adsorbed pyridine, and in terms of the proton affinity scale. Catalytic activities have been compared for cumene hydroperoxide (CHP) decomposition at 40°C in cumene and acetone. For all M, the catalysts are one type and contain W in strongly and weakly bound states, the latter being a polyoxometalate that can be washed off. Both tungstate phases are active in acid catalysis. Brønsted acid sites with a broad strength distribution have been

found. The strongest of them are heteropolyacid protons. The catalysts 30% WO<sub>3</sub>/SnO<sub>2</sub> and 20% WO<sub>3</sub>/ZrO<sub>2</sub> (in acetone) and 10–20% WO<sub>3</sub>/TiO<sub>2</sub> (in cumene) are the most active in CHP decomposition, and their activity is not related to their total acidity. Phases containing W<sup>6+</sup> that form during the high-temperature synthesis are responsible for the high acidity, and additional protons that may appear owing to W<sup>6+</sup> reduction can play only a minor role.

#### **NANOSCALE OXIDES AS DESTRUCTIVE SORBENTS FOR HALOGENATED HYDROCARBONS**

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*Surf. Chem. Biomed. Environ. Sci., NATO Science Series II: Mathematics, Physics & Chemistry, Springer-Verlag GmbH, Eds. J. Blitz, V. Gun'ko, 2006, pp. 403–412.*

Destructive adsorption of halocarbons on nanocrystalline oxides has been studied. The effect of the nanoparticle size and phase composition on the reaction kinetics is discussed. The reactivity of nanocrystalline oxides has been found to increase after deposition of a permeable carbon coating. The possibility of synthesis of new nanocrystalline halogenated materials using nanoscale oxides as precursors has been demonstrated.

#### **MESOPOROUS TITANIUM SILICATES AS CATALYSTS FOR THE LIQUID-PHASE SELECTIVE OXIDATION OF ORGANIC COMPOUNDS**

**O.A. Kholdeeva, N.N. Trukhan**

*Russ. Chem. Rev., 75(5) (2006) pp. 411–432.*

The data on the synthesis, physicochemical and catalytic properties of mesoporous titanium silicate materials published to date are surveyed. The relationship between the structure of these materials and their catalytic properties in the liquid-phase selective oxidation of organic compounds with peroxides is considered. The emphasis is placed on the problems of stability of mesoporous titanium silicate catalysts and the possibility of their recycling. The bibliography includes 264 references.

#### **RELATION BETWEEN THE SUPERMOLECULAR STRUCTURE AND OPTICAL PROPERTIES OF LIQUID CRYSTAL – PHOTOPOLYMER COMPOSITE FILMS**

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*Mol. Cryst. Liq. Cryst., 449 (2006) pp. 57–70.*

Composite materials with spatially alternating polymer and nematic liquid crystal layers have been obtained. The tetraacrylate pentaerythritol monomer, methylene blue and nematic liquid crystals were used as the pre-polymer composition. Scanning electron microscopy results show that the supermolecular structure holographically formed in the film depends on the relation between the nematic liquid crystal and dye concentrations in the pre-polymer composition and the curing energy. This system allows preparation of electrically switchable transmission gratings with first-order diffraction efficiencies up to 30–55%. The formed gratings could be switched from diffracting to transparent state at 4.5–7.5 V/μm. The turn-on and turn-off times were 200–300 μs and 1.2–3 ms, depending on the particular composition of the initial composition. Stability of grating characteristics was examined over a 1.5-year period of grating storage.

#### **FORMATION OF NANOPARTICLES OF TiO<sub>2</sub> AND Al<sub>2</sub>O<sub>3</sub> AT COMBUSTION OF METAL DROPLETS**

**S.A. Khromova, V.V. Karasev\*, A.A. Onischuk\*, O.G. Glotov\*, V.E. Zarko\*** (*\*Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia*)

*In "Nonequilibrium Processes", vol. 2: Plasma, Aerosols, and Atmospheric Phenomena,*

*Eds. G. Roy, S. Frolov, A. Starik, TORUSPRESS, Moscow, 2005, pp. 225–234.*

The investigations of metal droplets combustion are inspired by both fundamental interest and possible applications. In particular the combustion of metal powder can be an effective way of synthesis semiconductor and ceramic oxide nanoparticles. Aluminum powder serves as an energetic additive to the rocket propellants. In respect to this application a single metal particle burning in air at 1 atm was selected by many researches as a simple model for theoretical and experimental study. Even though in most practical propellants metal particles burn at high pressures, with CO<sub>2</sub>, CO, and H<sub>2</sub>O oxidizers, the

knowledge of more simple mechanism details will give an insight to the processes occurring in the real systems. Combustion of Ti droplets results in formation of TiO<sub>2</sub> nanoparticle predominantly in anatase crystal modification. The anatase modification is active in various photocatalytic redox reactions. That is why the combustion route of synthesis of TiO<sub>2</sub> nanoparticles has attracted a great interest in the literature. However at present there is lack of experimental data on metal oxide nanoparticle formation which prevents elaboration of appropriate model of the metal particle combustion which can predict the characteristics of oxide nanoaerosol. In this work TiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> nanoparticle formation was studied during combustion of Ti and Al droplets in air at atmospheric pressure.

#### **IMMOBILIZED GLUCOAMYLASE: A BIOCATALYST OF DEXTRIN HYDROLYSIS**

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Russia)

*Appl. Biochem. Microbiol.*,  
42(2) (2006) pp. 145-149.

Heterogeneous biocatalysts of starch saccharification based on glucoamylase and carbon-containing carriers were obtained, and their biocatalytic properties in the enzymatic hydrolysis of corn dextrans were studied. It was shown that the morphology of the surface carbon layer of carriers markedly affected the properties of biocatalysts. Glucoamylase immobilized by adsorption on the surface of carriers covered with a layer of catalytic filamentous or pyrolytic carbon had the maximum enzymatic activity and stability, whereas biocatalysts prepared on the basis of carriers that had no carbon layer or were covered with graphite-like surface carbon had a low activity and stability.

### **Ceria Based Composites:**

#### **Synthesis, Structural Features and Catalytic Properties**

##### **MODIFIED CERIA-ZIRCONIA FLUORITE-LIKE CATALYSTS FOR THE COMBUSTION OF METHANE**

**T.G. Kuznetsova, V.A. Sadykov, L.Ch. Batuev,  
E.M. Moroz, E.B. Burgina, V.A. Rogov,  
V.V. Kriventsov, D.I. Kochubey**

*J. Natural Gas Chem.*,  
15(3) (2006) pp. 149-163.

For dispersed ceria-zirconia-based solid solutions prepared via the polymerized complex method and annealed at 700°C, effects of bulk doping by Ca, Mn, Co, Bi or Nb cations and surface modification by Mn and Pt on their structural features, surface/bulk oxygen reactivity and catalytic activity in methane combustion are considered. With up to 20 mol% doping, a structural type of homogeneous solid solutions of anion-deficient fluorite with disordered anion vacancies is formed. Doping by transition metal cations or Pt increases the mobility and reactivity of the surface/bulk oxygen. A broad variation in specific rates of methane combustion for the studied systems was observed, suggesting structural sensitivity of this reaction. In general, there is no universal relationship between the oxygen mobility, the reactivity and the catalytic activity in methane combustion, which is explained by the factor of specific methane activation on surface active sites. For the Pt-

promoted samples, Pt efficiency in methane activation depends on the Pt-support interaction, and the most favorable ones being mixed Pt/MnO<sub>x</sub> and Pt/NbO<sub>x</sub> clusters on the surface of the supports that exhibit high lattice oxygen mobilities.

##### **FUEL-RICH METHANE COMBUSTION: ROLE OF THE Pt DISPERSION AND OXYGEN MOBILITY IN A FLUORITE-LIKE COMPLEX OXIDE SUPPORT**

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Yu.V. Frolova-Borchert, 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, L.Ch. Batuev,  
V.N. Parmon, S. Neophytides\*, E. Kemnitz\*\*,  
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Patras, Greece; \*\*Institute for Chemistry, Humboldt  
University, Berlin, Germany; \*\*\*Institut de  
Recherches sur la Catalyse, Villeurbanne, France)

*Catal. Today*, 117(4) (2006) pp. 475-483.

For catalysts comprised of Pt supported onto dispersed complex fluorite-like oxides (ceria doped by Pr, Gd, Sm, or CeO<sub>2</sub>-ZrO<sub>2</sub> doped by La, Gd or Pr), the effects of the oxygen mobility in supports and Pt



dispersion on the performance in methane selective oxidation into syngas at short contact times were elucidated using combination of kinetic and spectroscopic methods. While in general any simple universal relation between the oxygen mobility, Pt dispersion and the rate of methane transformation into syngas was not found, for some series, a good correlation was observed agreeing with the bifunctional scheme of the methane selective oxidation into syngas.

#### **PROPERTIES OF Ce–Zr–La–O NANO-SYSTEM WITH RUTHENIUM MODIFIED SURFACE**

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*Prog. Solid State Chem.*,  
33(2-4) (2005) pp. 317-325.

Structural peculiarities of Ce–Zr–La–O and Ce–Zr–La–O/Ru samples in mean of catalytic properties are compared. The samples (Ce:Zr = 1:1, La = 10÷30 mol.%, Ru = 1.5 wt.%) were obtained by sol–gel method (X-samples) and co-precipitation (P-samples). It is shown that Ce<sub>0.45</sub>Zr<sub>0.45</sub>La<sub>0.1</sub>O<sub>2-δ</sub>/Ru X-samples are characterized by high thermal stability and the highest catalytic activity in partial methane oxidation reaction. According to XRD, BET, FTIR, EPR and XPS data it is concluded that the difference in the samples catalytic activity is caused by various disposition of Ru-containing phase on the support surface. The distinction in the dimension of Ru-containing particles (3D or 2D) is conditioned by structural peculiarities of Ce<sub>0.45</sub>Zr<sub>0.45</sub>La<sub>0.1</sub>O<sub>2-δ</sub> and Ce<sub>0.35</sub>Zr<sub>0.35</sub>La<sub>0.3</sub>O<sub>2-δ</sub> P- and X-samples.

#### **SYNTHESIS AND SINTERING OF CERAMIC NANOCOMPOSITES WITH HIGH MIXED CONDUCTIVITY**

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S. Neophytides\*\*\*\*** (\*Institute of Solid State  
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Russia; \*\*Belarusian State University, Minsk,  
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*Sci. Sintering*,  
37(1) (2005) pp. 45-54.

Metastable solid solutions of complex oxides with fluorite and perovskite structures are obtained by

mechanosynthesis. Dense ceramics on the base of these metastable phases was obtained by thermal sintering of nanopowders due to kinetic stabilization. Different degrees of a chemical interaction (interdiffusion) are observed during sintering of “perovskite+fluorite” and “perovskite+perovskite” composites. It is shown, that optimization of the composition, mixing conditions of individual phases and their sintering, preparation of ceramic composites with mixed conductivity for use in catalytic membrane reactors is possible. Unusual behavior of complex perovskites and fluorites is discovered during sintering, enabling determination of an optimum sintering temperature and time for which a qualitative explanation is given. It is established that rearrangement of fine crystalline particles as a whole plays a key role in shrinkage.

#### **NANOCRYSTALLINE CATALYSTS BASED ON CeO<sub>2</sub>-ZrO<sub>2</sub> DOPED BY PRASEODYMIUM OR GADOLINIUM: SYNTHESIS AND PROPERTIES**

**V.A. Sadykov, Yu.V. Frolova-Borchert,  
N.V. Mezentseva, G.M. Alikina,  
A.I. Lukashovich, E.A. Paukshtis,  
V.S. Muzykantov, L.Ch. Batuev,  
T.G. Kuznetsova, E.M. Moroz, D.A. Zyuzin,  
V.P. Kolko, E.B. Burgina, V.V. Kriventsov,  
D.I. Kochubey, E. Kemnitz\*, K. Scheurell\***  
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*Mater. Res. Soc. Symp. Proc.*,  
900E (2006) 0900-O10-04.1-04.6.

The structural features of nanocrystalline samples of Pr- or Gd-doped ceria-zirconia solid solutions prepared by polymerized precursor (Pechini) route and calcined at 500°C were studied using XRD, EXAFS, Raman, while their surface features before and after Pt supporting were characterized by IR spectroscopy of adsorbed CO test molecules. Effect of the nature and content of a dopant on the structural and surface features of studied systems as related to the oxygen mobility and catalytic activity in the reaction of methane selective oxidation into syngas at short contact times was considered.

## ONE-POT SYNTHESIS OF MIXED IONIC-ELECTRONIC CONDUCTING NANOCOMPOSITES COMPRISED OF FLUORITE-LIKE AND PEROVSKITE-LIKE PHASES AS CATALYTIC MATERIALS FOR SOFC

V.A. Sadykov, Yu.V. Frolova-Borchert, G.M. Alikina, A.I. Lukashovich, R.V. Bunina, G.V. Zaboltnaya, N.V. Mezentseva E.M. Moroz, V.I. Zaikovskii, D.Yu. Zyuzin, N.F. Uvarov\*, V.V. Zyryanov\*, N.A. Orlovskaya\*\* (*\*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

*Mater. Res. Soc. Symp. Proc.*,  
900E (2006) O10.08.1-08.6.

Nanocomposites comprised of fluorite-like (doped ceria) and perovskite-like (doped manganite) phases were prepared using a polymerized precursor (Pechini) route and two sources of lanthanides (Ln) - either pure Gd and Ce salts or an industrial ceria-rich mixture of Ln carbonates. Genesis of the structure of composites with annealing temperature has been studied by X-ray diffraction, Transmission Electron Microscopy and Raman. Up to 1300°C, particle sizes of both fluorite and perovskite phases remain in the nano-range. Nanocomposites possess a high conductivity, lattice oxygen mobility and reactivity with respect to methane exceeding that of individual phases. They are also good catalysts for oxidation of decane by O<sub>2</sub> without coking. Nanocomposite prepared from the industrial Ln source demonstrates better performance than that prepared from pure salts.

## NANOCOMPOSITES COMPRISED OF DOPED CERIUM DIOXIDE AND LANTHANUM MANGANITE FOR SYNGAS PRODUCTION

Yu.V. Frolova-Borchert, V.A. Sadykov, G.M. Alikina, A.I. Lukashovich, E.M. Moroz, D.I. Kochubey, V.V. Kriventsov, V.I. Zaikovskii, V.V. Zyryanov\*, N.F. Uvarov\* (*\*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia*)

*Solid State Ionics*,  
177(26-32) (2006) pp. 2533-2538.

Nanocomposites comprised of fluorite-like (Gd- or Pr-doped ceria) and perovskite-like (LaMnO<sub>3+δ</sub>) phases were prepared using a polymerized precursor (Pechini) route. Genesis of the structure of composites with annealing temperature has been studied by X-ray diffraction, Transmission Electron Microscopy and EXAFS. Up to 1300°C, particle sizes of both fluorite and perovskite phases remain in the nano-range. Interaction between components is reflected in the increase of doped ceria lattice parameter and disordering of Mn coordination

sphere. Despite this interaction, nanocomposites possess a high conductivity along with a high lattice oxygen mobility and reactivity. The addition of CoO improves sintering of nanocomposites.

## DOPED CERIA - LaMeO<sub>3</sub> (Me=Mn, Fe, Co) NANOCOMPOSITES: SYNTHESIS VIA MECHANOCHEMICAL ACTIVATION ROUTE AND PROPERTIES

L.A. Isupova, E.A. Obyskalova, V.A. Rogov, S.V. Tsybulya, L.S. Dovlitova, E.B. Burgina, A.V. Ischenko, V.I. Zaikovskii, V.A. Sadykov, N.A. Orlovskaya\*

*Mater. Res. Soc. Symp. Proc.*,  
885E (2006) A03-04 83-04 88.

Nanocomposite materials composed of fluorite and perovskite phases were prepared by mechanical treatment of the mixture of industrial raw material – mixed lanthanide oxide and 3d oxide followed by calcinations in the range of 900-1100°C. Samples were investigated with XRD, TEM, BET, IR, Raman and H<sub>2</sub> TPR. Composites demonstrate a high lattice oxygen mobility and reactivity exceeding that of individual phases, being rather insensitive to calcination temperature.

## DESIGN OF MULTILAYERED CERAMIC MIEC MEMBRANES

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*Desalination*, 199(1-3) (2006) pp. 299-301.

Nanopowders of LaGaO<sub>3</sub>- and LaMnO<sub>3</sub>-based complex perovskites P and ceria based fluorites F are derived by mechanochemical synthesis. Compatible nanocomposites F+P and P+P with MIEC properties were prepared and sintered at moderate temperatures up to dense ceramics. Obtained materials were studied by means of XRD, electrical conductivity measurements, TP reduction by methane and TP oxidation. New strategy based on facilities of mechanochemical ceramic approach is proposed to design multilayer ceramic membranes for CMR. Casting technology and one step sintering were used for production a thin film membrane with MIEC properties on porous substrate. Large fraction of as-milled powders from agglomerates with density ~70% was used for porous substrate and fine fractions of aggregates with sizes <1 μm were used in preparation of composites for thin dense films. Ceria based composites derived by Pechini route and/or mechanochemical approach are proposed as materials for protected thin films.

## **Ce-SILICA MESOPOROUS SBA-15 TYPE MATERIALS FOR OXIDATIVE CATALYSIS: SYNTHESIS, CHARACTERIZATION AND CATALYTIC APPLICATION**

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*Appl. Catal., A*,  
317(1) (2007) pp. 1-10.

Cerium-containing mesoporous materials have been synthesized by hydrothermal method and characterized by IR, DR-UV-vis and DRIFT

spectroscopy, XRD and N<sub>2</sub> adsorption methods. It was established that the  $d_{100}$  and unit-cell ( $a_0$ ) parameter increase with the increase of cerium content up to 2% in SBA-15 and then tend to remain the same. According to DR-UV-vis spectroscopic data, an agglomeration of cerium atoms was observed in the form of fine CeO<sub>2</sub> crystallites. Important factors affecting the catalytic activity of Ce-SBA-15, namely the effect of cerium content, the state of cerium ions, the state of silanol groups on the surface of Ce-SBA-15, and stability of the catalyst have been studied in the cyclohexanol and cyclohexene oxidation with hydrogen peroxide.

## **Carbon and Carbon Related Materials**

### **PECULIARITIES OF FORMATION OF CARBON NANOFILAMENTS WITH VARIOUS CRYSTALLOGRAPHIC STRUCTURE FROM HYDROCARBONS OVER THE CATALYSTS CONTAINING IRON SUBGROUP METALS**

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

*Crit. Technol. Membranes*,  
28(4) (2005) pp. 75-79.

Electron microscopy and XRD were used to study the mechanism of formation of carbon filaments from hydrocarbons in the presence of iron subgroup metal catalysts.

Carbon nanofilaments with a coaxial-conical structures form from hydrocarbons on the NiAl<sub>2</sub>O<sub>3</sub>, Ni/MgO catalysts in a temperature range of 400-600°C. The kinetic curves of growth of filamentous carbon exhibit four periods such as induction, acceleration, stationary and deactivation. The reasons and processes providing transformation of catalytic particles and morphology itself of the filamentous carbon in each period of growth of the filamentous carbon has been established.

It is possible to synthesize three “basic” structure types of graphite filaments depending on the properties of a catalyzing metal particle and conditions of the process performance. The work gives an explanation of the reasons and features of formation of three main types of carbon filaments. It is shown that the properties of metal particles are significantly controlled by methods of their preparation and additives of other metals. Note that the lattice parameters and some other characteristics of the alloyed particles, affecting both crystallographic and morphological properties of graphite filaments, change. The models of growth of carbon filaments with different crystallographic structures are presented.

### **ON THE MECHANISM OF FORMATION OF CARBON NANOFILAMENTS DURING CATALYTIC DECOMPOSITION OF HYDROCARBONS OVER IRON SUBGROUP METALS**

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

*Catal. Ind.*, 2 (2006) pp. 3-15.

The progress in the science and technology is related to design of new composite materials, in particular, carbon filaments and fibers based products. In recent 20 years, the scientists paid special attention to a possibility of producing a new generation of such products as carbon nanosized filaments by various methods. The achievement of the optimal conditions requires the knowledge of the process mechanism to choose a catalyst, starting hydrocarbon raw material, and the process conditions. The review proposed generalizes the results of the complex investigations of regularities of carbon nanofilament formation during catalytic decomposition of hydrocarbons over iron-subgroup metals according to the «carbide cycle» mechanism. The process of production of these materials is shown to consist of two stages: chemical (catalytic) and physical ones. Four periods: induction, acceleration, stationary, and inactivation were defined in the course of generation and growth of carbon nanofilaments. The nature, mechanisms, and regularities of the stages and periods are explained. The scientific principles of carbon nanofilaments of various crystallographic characteristics were formulated.

### EFFECT OF ZINC ADDED TO THE Co/Al<sub>2</sub>O<sub>3</sub> CATALYST ON THE FORMATION OF CARBON NANOFILAMENTS FROM METHANE AND BUTADIENE-1,3

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

*Kinet. Catal.*,  
47(3) (2006) pp. 445-450.

The dynamics of carbon nanofilament growth from methane and butadiene-1,3 on Co-Zn/Al<sub>2</sub>O<sub>3</sub> catalysts have been studied in the temperature range 500–750°C. The rate-limiting step in the growth of nanofilaments from butadiene is carbon atom diffusion through the bulk of the metal particle. In the case of methane, the process is controlled by one of the stages of hydrocarbon decomposition on the metal particle. The structure and morphology of the nanofilaments (composites) forming by the carbide cycle mechanism on fine zinc-promoted cobalt particles have been studied by electron microscopy and X-ray diffraction. The morphology and crystallographic properties of the nanofilaments depend on the ratio of the hydrocarbon decomposition rate (which is determined by the nature of the hydrocarbon) to the rate at which carbon atoms diffuse from their formation sites to the nanofilament formation sites (which is determined by the nature of the metal particle and by the carbon diffusion coefficient in the particle bulk). The properties of the resulting carbon nanofilaments can be controlled by varying the nature of the hydrocarbon to be decomposed and the reaction temperature and by introducing another metal into the cobalt particles.

### PROPERTIES OF INDIVIDUAL FRACTIONS OF DETONATION NANODIAMOND

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*Diamond Relat. Mater.*,  
15 (2006) pp. 1804-1808.

Detonation nanodiamonds synthesized and purified on an industrial scale were additionally purified and separated into narrow size fractions by centrifugation. The average particle size for the smallest fraction was lower than 30 nm and the yield was about 20 wt.%. Using FTIR spectra analysis, it was demonstrated that ND aggregates of different sizes, separated from the same pristine ND, have different surface compositions of active surface groups, particularly oxygen-containing groups, which

finally influence their zeta potential values and hydrosol stability. Using DTA analysis, the higher reactivity of the smallest fractions during heat treatment in air was also demonstrated.

### THE THERMAL STABILITY OF NANODIAMOND SURFACE GROUPS AND ONSET OF NANODIAMOND GRAPHITIZATION

Yu.V. Butenko, V.L. Kuznetsov, E.A. Paukshtis, A.I. Stadnichenko, I.N. Mazov, S.I. Moseenkov, A.I. Boronin, S.V. Koscheev

*Fullerenes, Nanotubes, Carbon Nanostruct.*,  
14(2-3) (2006) pp. 557-564.

The results of study of the surface chemistry of nanodiamonds treated by a mixture of HClO<sub>4</sub> and H<sub>2</sub>SO<sub>2</sub> acids are presented. Changes of the composition of surface diamond groups brought up by thermal annealing were monitored by Fourier transformed infrared spectroscopy and temperature-programmed desorption. The decomposition of oxygen-containing groups is observed at 300–900°C; CH<sub>x</sub> groups decompose at 700–1150°C. The process of the annealing of ND was investigated by the X-ray photoelectron spectroscopy. The clear onset of ND graphitization was observed at temperature of 950°C that is supported by the appearance of *sp*<sup>2</sup> component in the C1s spectrum. The presence of the N1s peak in spectra of ND is observed in initial and partially graphitized ND annealed up to 1100°C.

### WHO SHOULD BE GIVEN THE CREDIT FOR THE DISCOVERY OF CARBON NANOTUBES?

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*Carbon*,  
44(9) (2006) pp. 1621-1623.

Due to a unique combination of physical properties and potential applications, carbon nanotubes have evolved into one of the hottest research topics today. Most publications on nanotubes refer back to the article by Sumio Iijima, published in *Nature* 354 (1991) 56, which started the present "nanotube boom". This article reviews some of the earlier publications, which reported likely synthesis and observation of nanotubes and related filamentous structures. The finite list of references will probably inspire further discussion. In spite of several inaccurate technical statements, this intriguing review makes a point by illustrating that a discovery often needs to await its time to cause a large societal impact.

## ELECTRON-ELECTRON INTERACTION IN CARBON NANOSTRUCTURES

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*Cond. Mat.*,  
(2006) 0608437.

The electron-electron interaction in carbon nanostructures was studied. A new method which allows to determine the electron-electron interaction constant  $\lambda$  from the analysis of quantum correction to the magnetic susceptibility and the magnetoresistance was developed. Three types of carbon materials: arc-produced multiwalled carbon nanotubes (arc-MWNTs), CVD-produced catalytic multiwalled carbon nanotubes (c-MWNTs) and pyrolytic carbon were used for investigation. It was found that  $\lambda=0.2$  for arc-MWNTs (before and after bromination treatment);  $\lambda=0.1$  for pyrolytic graphite;  $\lambda > 0$  for c-MWNTs. It was concluded that the curvature of graphene layers in carbon nanostructures leads to the increase of the electron-electron interaction constant  $\lambda$ .

## QUASI-TWO-DIMENSIONAL CONDUCTIVITY AND MAGNETOCONDUCTIVITY OF GRAPHITE-LIKE NANOSIZE CRYSTALLITES

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*Solid State Commun.*,  
137(11) (2006) pp. 625–629.

The temperature dependence of electrical conductivity and magnetoconductivity of new type of carbon films composed of nanosize thin graphite-like crystallites were investigated at temperature interval of 4.2–300 K and in the magnetic field range of 0–12 kG at 4.2 K, respectively. The crystallites consist of several (5–50) graphene layers which have predominant orientation perpendicularly to a film surface. At temperature  $\leq 30$  K the logarithmic conductivity decreases linearly with temperature. The positive magnetoconductivity of the films was observed in a magnetic field directed perpendicularly to the film surface in all intervals of field values. In magnetic field  $B \geq 4$  kG the logarithmic asymptotic of conductivity from magnetic field was observed. That

is characteristic of the systems with two-dimensional quantum corrections to magnetoconductivity. In a magnetic field directed along a film surface, the crossover from negative to positive magnetoresistivity is observed at  $B \geq 8$  kG.

## THERMAL BEHAVIOR OF FLUORINATED DOUBLE-WALLED CARBON NANOTUBES

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**Yu.V. Lavskaya\***, **N.F. Yudanov**, **L.I. Yudanova\***,  
**O.G. Abrosimov**, **E.M. Pazhetnov**, **A.I. Boronin**,  
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Materiaux, Université Paul-Sabatiér, Toulouse cedex,  
France)

*Chem. Mater.*,  
18(20) (2006) pp. 4967–4971.

Double-walled carbon nanotubes (DWNTs), produced by a catalytic chemical vapor deposition method, have been fluorinated using a volatile mixture of  $\text{BrF}_3$  and  $\text{Br}_2$ . Optical absorption spectroscopic study on the product detected nonfluorinated nanotubes, which could correspond to the inner walls of DWNTs. The fluorinated DWNTs have been annealed in vacuum at fixed temperatures, and X-ray photoelectron spectroscopy showed almost no fluorine in the sample heated to 300°C. Comparison between X-ray fluorescent C K $\alpha$  spectra of the pristine DWNT sample and the annealed fluorinated sample revealed change of the atomic structure of graphitic shells in the process of thermal defluorination.

## CARBON FILMS GROWN ON Pt(1 1 1) AS SUPPORTS FOR MODEL GOLD CATALYSTS

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**A.I. Stadnichenko**, **A.I. Boronin**,  
**S.K. Shaikhutdinov\*** (\*Department of Chemical  
Physics, Fritz-Haber Institute, Berlin, Germany)

*Surf. Sci.*, 600(13) (2006) pp. 2688–2695.

Carbon films were grown on a Pt(1 1 1) single crystal by ethylene decomposition at elevated temperatures (1000–1300 K). Depending on the preparation conditions, different carbon structures formed on the metal surface such as flat and curved graphitic layers, carbon particles and carbon nanowires. Although these carbon films exhibited a high density of surface defects, gold interacted only weakly with the carbon surface. CO adsorption on the Au/carbon systems was very similar to that observed for various Au/oxide systems previously studied. This finding strongly indicates that CO adsorption on gold is essentially independent of the nature of support.

**XPS STUDY OF CARBON FILMS ON THE Pt(III) SURFACE OBTAINED BY HIGH TEMPERATURE DECOMPOSITION OF METHANE AND ETHYLENE**

**E.M. Pazhetnov, A.I. Boronin**

*Chem. Sustain. Devel.*,  
14(6) (2006) pp. 599-603.

The carbon films grown on Pt(III) surface by the high temperature catalytic decomposition of methane and ethylene were investigated with aid of X-ray photoelectron spectroscopy (XPS). It was observed that photoelectron spectra of carbon films depend on the hydrocarbon used as a reagent. It was shown that in case of methane used as the reagent the flat graphite films are deposited on the Pt(III) surface while ethylene or ethylene/methane mixture stimulates the carbon films distortion resulting in curved fullerites/like structures. The formation of curved carbon films occurs through the formation of flat graphenes as the intermediate structures. It was determined that this topographic transition is reversible and has dynamic character depending on the crystal temperature and ethylene presence in the gas phase. The role of the diffusion-segregation phenomenon of carbon atoms in the formation of the curved films was established.

**CHEMICAL PROPERTIES OF THE SURFACE OF NANOFIBROUS CARBONACEOUS MATERIALS PRODUCED BY CATALYTIC METHANE DECOMPOSITION**

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*Russ. J. Phys. Chem.*,  
80(6) (2006) pp. 886-891.

The chemical behavior of nanofibrous carbonaceous materials prepared by the catalytic decomposition of methane was studied by IR spectroscopy, X-ray photoelectron spectroscopy, and titration. Initial carbon was shown to be virtually devoid of functional groups on its surface. Treatment of carbonaceous samples with alkali, ammonia, or nitric acid modified the surface of carbon and increased the number of functional groups.

**STUDYING OF THE STRUCTURE OF POROUS CARBON NANOFIBRES AND SUPPORTED Pd PARTICLES**

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*Russ. Chem. J. (Mendeleev Chem. J.)*,  
50(1) (2006) pp. 104-106.

Texture properties of porous carbon nanofibres, size of supported Pd particles and character of their distribution are studied. Texture properties of porous carbon nanofibres were studied by electron microscopy and adsorption analysis. It is established, that homogeneous Pd distribution in pores of support is achieved due to developed nanoporous structure presented by pores of practically uniform size. Supported Pd particles are 4-5 nm in size.

**SPECTROSCOPY OF SMOOTH DEUTERATED CARBON FILMS REDEPOSITED FROM PLASMA DISCHARGE IN THE TOKAMAK T-10**

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*Crystallogr. Rep.*,  
51(Suppl. 1) (2006) pp. 158-162.

Smooth deuterated carbon films redeposited from a deuterium plasma discharge in the tokamak T 10 vacuum chamber have been investigated by different spectroscopic methods and temperature measurements. The photoluminescence excitation spectra of  $sp^3$ - $sp^2$  nanostructures of tokamak films and  $sp^2$  nanostructures of fullerite C60 films are compared. The effect of defect states on the photoluminescence and its temperature quenching is discussed. It is concluded that the mechanism of thermal luminescence quenching for Smooth deuterated tokamak films is close to the corresponding mechanism for amorphous  $a$ -C:H films.

## **PORE SIZE DISTRIBUTION ANALYSIS OF ACTIVATED CARBONS: APPLICATION OF DENSITY FUNCTIONAL THEORY USING NONGRAPHITIZED CARBON BLACK AS A REFERENCE SYSTEM**

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Brisbane, Australia)

*Carbon*, 44(4) (2006) pp. 653-663.

The application of nonlocal density functional theory (NLDFT) to determine pore size distribution (PSD) of activated carbons using a nongraphitized carbon black, instead of graphitized thermal carbon black, as a reference system is explored. It was shown that in this case nitrogen and argon adsorption isotherms in activated carbons are precisely correlated by the theory, and such an excellent correlation would never be possible if the pore wall surface was assumed to be identical to that of graphitized carbon black. It suggests that pore wall surfaces of activated carbon are closer to that of amorphous solids because of defects of crystalline lattice, finite pore length, and the presence of active centers, etc. Application of the NLDFT adapted to amorphous solids resulted in quantitative description of N<sub>2</sub> and Ar adsorption isotherms on nongraphitized carbon black BP280 at their respective boiling points. In the present paper it

is determined solid-fluid potentials from experimental adsorption isotherms on nongraphitized carbon black and subsequently used those potentials to model adsorption in slit pores and generate a corresponding set of local isotherms, which were used to determine the PSD functions of different activated carbons.

## **MAGNETORESISTANCE AND RESISTANCE VERSUS TEMPERATURE DEPENDENCE OF A MESOPOROUS MESOPHASE CARBON**

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Grenoble, France)

*Physica E -  
Low-Dimensional Syst. & Nanostruct.*,  
34(1-2) (2006) pp. 655-657.

In the present work the transport properties of mesoporous mesophase carbon (MMC) powder have been investigated in wide temperature and magnetic field ranges. It has been found that in the range 1.5-42 K the temperature dependence of the resistivity of this material can be described by Efros-Shklovskii variable range hopping law. In the same temperature range the magnetoresistance is positive but does not fit the exponential dependence expected in the hopping regime.

## **Catalysis by Heteropoly Compounds and Polyoxometallates**

### **CATALYTIC OXIDATION OF 2,3,6-TRIMETHYLPHENOL AND 2-METHYLNAPHTHOL-1 INTO CORRESPONDING PARA-QUINONES BY DIOXYGEN IN THE PRESENCE OF Mo-V-PHOSPHORIC HETEROPOLY ACID SOLUTIONS AS KEY STAGES OF TOCOPHEROL AND K VITAMIN SYNTHESIS**

**E.G. Zhizhina, V.F. Odyakov, K.I. Matveev**

*Catal. Ind.*, 6 (2005) pp. 19-27.

Solutions of Mo-V-phosphoric heteropoly acids (HPA) are efficient catalysts for oxidation of alkyl phenols of benzene and naphthalene series by dioxygen into corresponding alkyl-1,4-quinones. The most important reactions are oxidation of 2,3,6-trimethylphenol (TMP) into 2,3,5-trimethyl-1,4-benzoquinone (TMQ, key intermediate product of tocopherol synthesis) and oxidation of 2-methylnaphthol-1 into 2-methyl-1,4-naphthoquinone (vitamin K<sub>3</sub>). In industry, TMP is oxidized into TMQ by dioxygen in the presence of copper chlorides. The

disadvantage of such a catalyst is its chlorinating ability. In any case, ecologically dangerous chlorinated quinones (related to dioxins) must be thoroughly separated and detoxified. In the industry, vitamin K<sub>3</sub> is produced by uncatalyzed oxidation of 2-methylnaphthalene by chromic acid. Both oxidation processes are non-ecological. They became long-outdated. In the presence of HPA, the oxidation is carried out at 50÷60°C in two-phase systems (aqueous solution of HPA + solution of substrate and product in organic solvent). The product is separated from the catalyst by phase separation. The TMQ selectivity reaches 99%, and vitamin K<sub>3</sub> selectivity - 90%. Such high characteristics allow to use TMQ without purification in following stages of tocopherol synthesis, to lower the number of operations, and to obtain more pure final product. The method proposed for TMQ synthesis may be taken as a basis of an ecological technology of tocopherol preparation. The method proposed for vitamin K<sub>3</sub> synthesis by oxidation of 2-methylnaphthol-1 in the presence of



HPA was used for development of a low-waste process "Vikasib" for synthesis of K group vitamins at the Boreskov Institute of Catalysis. In this article results of investigations of development of new ecological catalytic methods of tocopherol and vitamin K<sub>3</sub> synthesis are presented.

#### **PRODUCTION OF K<sub>3</sub> VITAMIN BY THE REACTION OF DIENE SYNTHESIS IN THE PRESENCE OF THE SOLUTIONS OF Mo-V-PHOSPHORIC HETROPOLY ACIDS AS CATALYSTS**

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*Academy Proceed., Chem. Chem. Techn.,*  
49(9) (2006) pp. 20-23.

The principal opportunity of preparation of vitamin K<sub>3</sub> (2-methyl-1,4-naphthoquinone) from such accessible substrates as 2-methylphenol (o-cresol) or 2-methylaniline (o-toluidine) is shown. These processes proceed by reaction of diene synthesis. Solutions of Mo-V-phosphoric hetropoly acids are polyfunctional catalysts of such processes. It allows to carry out oxidation and diene synthesis by one technological stage. Solutions of catalysts are regenerated at 140-160°C under O<sub>2</sub> pressure.

#### **KINETICS AND MECHANISM OF THE WET OXIDATION OF PROPENE TO ACETONE IN THE PRESENCE OF Pd<sup>2+</sup> IONS AND Mo-V-PHOSPHORIC HETEROPOLY ACIDS**

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

*React. Kinet. Catal. Lett.,*  
89(1) (2006) pp. 157-166.

Oxidation of propene to acetone in water solutions in the presence of homogeneous catalysts (Pd<sup>2+</sup> + HPA-x, where HPA-x = H<sub>3+x</sub>PV<sub>x</sub>Mo<sub>12-x</sub>O<sub>40</sub>, x = 1-4) is studied. This reaction is shown to be of 1st order with respect to C<sub>3</sub>H<sub>6</sub> and of the 0.5th order with respect to Pd. The reaction rate does not depend on the concentration of HPA-x and acidity of the catalyst solution. The apparent activation energy of the reaction is 21 kJ/mol. A reaction mechanism is proposed.

#### **H<sub>2</sub>O<sub>2</sub> AND O<sub>2</sub>/H<sub>2</sub> OXIDATION OF AROMATIC COMPOUNDS IN CATALYTIC SYSTEMS CONTAINING HETEROPOLY COMPOUNDS**

**N.I. Kuznetsova, N.V. Kirillova, L.I. Kuznetsova, M.Yu. Smirnova, V.A. Likholobov\*** (\*Institute of Hydrocarbons Processing, Omsk, Russia)

In "Environmental Applications of Advanced Oxidation Processes",  
Chania, 2006, e-Proceedings, 158 (8 pages).

Hydrogen peroxide and Pt activated mixture of gaseous O<sub>2</sub> and H<sub>2</sub> have been applied to oxidation of aromatic compounds in the presence of red-ox active heteropoly compounds in the form of acid H<sub>4</sub>PMo<sub>11</sub>VO<sub>40</sub> and tetrabutylammonium (TBA) salts TBA<sub>4</sub>PMo<sub>11</sub>VO<sub>40</sub> and TBA<sub>4</sub>HPW<sub>11</sub>Fe(OH)O<sub>39</sub>. Benzene, toluene and phenol were subjected to hydroxylation of the ring, that was accompanied by secondary oxidation in reaction with hydrogen peroxide. Oxygenation of toluene was equally directed to the ring and to methyl group. The total reactivity of substrates was increased in order of benzene < toluene < phenol in oxidation by both O<sub>2</sub>/H<sub>2</sub> and H<sub>2</sub>O<sub>2</sub>, that indicated identical nature of active intermediates for both oxidants. It was suggested HPC bonded radical species to be responsible for oxidation of hydrocarbons.

#### **INTERACTION OF PLATINUM AND MOLYBDOPHOSPHORIC HETEROPOLY ACID UNDER CONDITIONS OF CATALYST PREPARATION FOR BENZENE OXIDATION TO PHENOL WITH AN O<sub>2</sub>-H<sub>2</sub> GAS MIXTURE**

**L.I. Kuznetsova, N.I. Kuznetsova, S.V. Koscheev, V.A. Rogov, V.I. Zaikovskii, B.N. Novgorodov, L.G. Detusheva, V.A. Likholobov\*, D.I. Kochubey** (\*Institute of Hydrocarbons Processing, Omsk, Russia)

*Kinet. Catal.,* 47(5) (2006) pp. 704-714.

The transformations of platinum and a heteropoly acid (HPA) in binary systems prepared from H<sub>2</sub>PtCl<sub>6</sub> or H<sub>2</sub>PtCl<sub>4</sub> and H<sub>3</sub>PMo<sub>12</sub>O<sub>40</sub> were studied using IR and UV-VIS spectroscopy, elemental analysis, XPS, EXAFS, TPR, and HREM. The calcination of platinum chloride with the HPA to 450°C resulted in the formation of a platinum salt of the HPA along with decomposition products (mixture **I**). The reduction of calcined samples containing Pt : HPA = 1 : 1 with hydrogen at 300°C (mixture **II**) followed by exposure to air resulted in the regeneration of the HPA structure. The resulting solid samples of (Pt<sup>0</sup><sub>1-n</sub> Pt<sup>II</sup><sub>n</sub>Cl<sub>m</sub>O<sub>x</sub>H<sub>y</sub>)·(H<sub>3+p</sub>PMo<sup>VI</sup><sub>12-p</sub>Mo<sup>V</sup><sub>p</sub>O<sub>40</sub>) (**III**) contained platinum and molybdenum in both oxidized

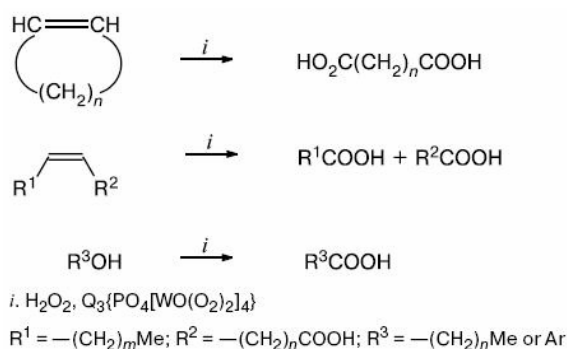
and reduced states. The following association species were isolated from mixtures **I** and **II** by dissolving in water:  $[\text{Pt}^{\text{II}}_n \cdot \text{PMo}_{12}\text{O}_{40}]$ , (**I<sub>s</sub>**) ( $n = 0.3-0.8$ ) and  $[\text{Pt}^{\text{0}}_n \cdot \text{PMo}^{\text{BOC}}_{12}\text{O}_{40}]$  (**II<sub>s</sub>**) ( $n \approx 1$ ). Under exposure to air, the solutions of **I<sub>s</sub>** were stable (pH  $\sim 2$ ), whereas  $\text{Pt}^{\text{met}}$  was released from **II<sub>s</sub>**. After the drying of **I<sub>s</sub>**, the solid association species  $(\text{Pt}^{\text{II}}_n \text{Cl}_m \text{O}_x \text{H}_y) \cdot (\text{H}_3\text{PMo}_{12}\text{O}_{40})$ , where  $n = 0.3-0.8$ ,  $m = 0.2-1$ , and  $x = 3-0$ , (**I<sub>solid</sub>**) were obtained. The **I<sub>solid</sub>**/SiO<sub>2</sub> supported samples were prepared by impregnating SiO<sub>2</sub> with a solution of **I<sub>s</sub>** and drying at 100°C. Platinum metal particles of size  $\sim 20$  Å and a mixed-valence association species of platinum with the HPA were observed after the reduction of **I<sub>solid</sub>**/SiO<sub>2</sub> with hydrogen at 100–250°C. These samples were active in the gas-phase oxidation of benzene to phenol at 180°C with the use of an O<sub>2</sub>-H<sub>2</sub>-N<sub>2</sub> mixture.

#### CATALYTIC OXIDATION OF OLEFINS AND ALCOHOLS WITH HYDROGEN PEROXIDE IN A TWO-PHASE SYSTEM GIVING MONO- AND DICARBOXYLIC ACIDS

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*Russ. Chem. Bull.*,  
54(8) (2005) pp. 1847-1854.

The present study considered the influence of various factors on the catalytic activity of systems based on a combination of tetrakis(oxodiperoxotungsto)phosphate(3-) with quaternary ammonium cations, for example, with methyltri-n-octylammonium  $[\text{Me}(\text{n-C}_8\text{H}_{17})_3\text{N}]^+$ . The catalysts were tested in oxidation of cycloolefins (cyclohexene and cyclooctene), alcohols (octan-1-ol and phenylmethanol), and unsaturated fatty acids (cis-9-octadecenoic and 12-hydroxy-9Z-octadecenoic acids) with a 30% hydrogen peroxide solution. These reactions proceed under mild conditions (atmospheric pressure, 80-90°C) to give carboxylic acids. The catalytic systems were characterized by vibrational (IR and Raman) spectroscopy. The state of the systems formed from various precursors, viz., polyoxometallates and phase-transfer catalysts, was studied. It was demonstrated for the first time that the structure formation of peroxo complexes depends on the nature of the halide anion of the quaternary ammonium salt used. The melting points of individual catalytic complexes were determined. The optimal conditions for oxidation were found.



#### PHASE-TRANSFER CATALYTIC OXIDATION OF THE ORGANIC COMPOUNDS WITH THE HYDROGEN PEROXIDE IN THE PRESENCE OF PEROXOPOLYOXOMETALLATES

Z.P. Pai, P.V. Berdnikova, A.G. Tolstikov, T.B. Khlebnikova, N.V. Selivanova

*Catal. Ind.*,  
5 (2006) pp. 12-23.

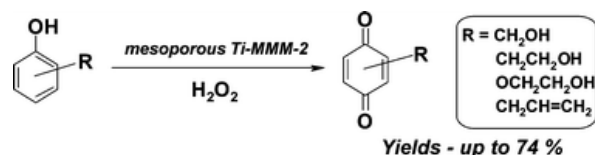
Modern approaches to the development of ecologically and economically acceptable methods of manufacturing of industrially important large-tonnage organic products or fine chemicals with the use of petrochemistry products and renewable raw materials are considered in the presented review. The prospects of the application of phase-transfer catalysis (PTC) method in organic synthesis are shown in the introduction. In the part of the review concerning catalysts the comparison of data on the synthesis of catalytic systems on the base of peroxopolyoxometallates in combination with phase-transfer catalysts applied for the catalytic oxidation of organic compounds including compounds with double bonds and asymmetric centers is carried out. In the part concerning carboxylic acids manufacturing the analysis of tradition processes of their production and the market needs is performed. With the purpose to demonstrate the advantages of the carboxylic acids one-stage producing the examples of the oxidation of cyclic olefins, alcohols and unsaturated fatty acids in two-phase solutions with the use of the PTC method are given.

**H<sub>2</sub>O<sub>2</sub>-BASED OXIDATION OF FUNCTIONALIZED PHENOLS CONTAINING SEVERAL OXIDIZABLE SITES TO *p*-QUINONES USING A MESOPOROUS TITANIUM-SILICATE CATALYST**

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*Green Chem.*,  
 8 (2006) pp. 883-886.

The oxidation of 2-allylphenol and different phenols bearing alcohol functional groups with aqueous H<sub>2</sub>O<sub>2</sub> as oxidant and heterogeneous titanium-silicate Ti-MMM-2 as catalyst exhibits an unusual selectivity affording the corresponding *p*-quinones with good to moderate yield and keeping the other oxidizable sites intact. The use of hydrogen peroxide and heterogeneous titanium-silicate catalyst is a green alternative to the stoichiometric oxidation with hypervalent iodine compounds that provides better yields of structurally complex quinones in one step.



**Zr<sup>IV</sup>-MONOSUBSTITUTED KEGGIN-TYPE DIMERIC POLYOXOMETALATES: SYNTHESIS, CHARACTERIZATION, CATALYSIS OF H<sub>2</sub>O<sub>2</sub>-BASED OXIDATIONS, AND THEORETICAL STUDY**

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*Inorg. Chem.*, 45(18) (2006) pp. 7224-7234.

The previously unknown Zr<sup>IV</sup>-monosubstituted Keggin-type polyoxometalates (Zr-POMs), (n-Bu<sub>4</sub>N)<sub>7</sub>H[ {PW<sub>11</sub>O<sub>39</sub>Zr(μ-OH)}<sub>2</sub>] (1), (n-Bu<sub>4</sub>N)<sub>8</sub>[ {PW<sub>11</sub>O<sub>39</sub>Zr(μ-OH)}<sub>2</sub>] (2), and (n-Bu<sub>4</sub>N)<sub>9</sub>[ {PW<sub>11</sub>O<sub>39</sub>Zr}<sub>2</sub>(μ-OH)(μ-O)] (3) differing in their protonation state, have been prepared starting from heteropolyacid H<sub>5</sub>PW<sub>11</sub>ZrO<sub>40</sub>·14H<sub>2</sub>O. The compounds were characterized by elemental analysis, potentiometric titration, X-ray single-crystal structure, and IR, Raman, and <sup>31</sup>P and <sup>183</sup>W NMR spectroscopy. The single-crystal X-ray analysis of 2 reveals that two Keggin structural units [PW<sub>11</sub>O<sub>39</sub>Zr]<sup>3-</sup> are linked through two hydroxo bridges Zr-(OH)-Zr with Zr<sup>IV</sup> in 7-fold coordination. The IR spectra of 1 and 2 show a

characteristic band at 772 cm<sup>-1</sup>, which moves to 767 cm<sup>-1</sup> for 3, reflecting deprotonation of the Zr-(OH)-Zr bond. Potentiometric titration with methanolic Bu<sub>4</sub>NOH indicates that 1-3 contain 2, 1, and 0 acid protons, respectively. <sup>183</sup>W NMR reveals C<sub>s</sub> symmetry of 2 and 3 in dry MeCN, while for 1, it discovers nonequivalence of its two subunits and their distortion resulting from localization of the acidic proton on one of the Zr-O-W bridging O atoms. The <sup>31</sup>P NMR spectra of 2 and 3 differ insignificantly in dry MeCN, showing only signals at δ-12.46 and -12.44 ppm, respectively, while the spectrum of 1 displays two resonances at δ-12.3 (narrow) and -13.2 (broad) ppm, indicating slow proton exchange on the <sup>31</sup>P NMR time scale. The theoretical calculations carried out at the density functional theory level on the dimeric species 1-3 propose that protonation at the Zr-O-Zr bridging site is more favorable than protonation at Zr-O-W sites. Calculations also revealed that the doubly bridged hydroxo structure is thermodynamically more stable than the singly bridged oxo structure, in marked contrast with analogous Ti- and Nb-monosubstituted polyoxometalates. The interaction of 1-3 with H<sub>2</sub>O and H<sub>2</sub>O<sub>2</sub> in MeCN has been studied by both <sup>31</sup>P and <sup>183</sup>W NMR. The stability of the [PW<sub>11</sub>O<sub>39</sub>ZrOH]<sup>4-</sup> structural unit toward at least 100-fold excess of H<sub>2</sub>O<sub>2</sub> in MeCN was confirmed by both NMR and Raman spectroscopy. The interaction of 1 and 2 with H<sub>2</sub>O in MeCN produces most likely monomeric species (n-Bu<sub>4</sub>N)<sub>3+n</sub>[PW<sub>11</sub>O<sub>39</sub>Zr(OH)<sub>n</sub>(H<sub>2</sub>O)<sub>3-n</sub>] (n = 0 and 1) showing a broad <sup>31</sup>P NMR signal at δ-13.2 ppm, while interaction with H<sub>2</sub>O<sub>2</sub> leads to the formation of an unstable peroxy species (δ-12.3 ppm), which reacts rapidly with cyclohexene, producing 2-cyclohexen-1-one and *trans*-cyclohexane-1,2-diol. Both 1 and 2 show a pronounced catalytic activity in H<sub>2</sub>O<sub>2</sub> decomposition and H<sub>2</sub>O<sub>2</sub>-based oxidation of organic substrates, including cyclohexene, α-pinene, and 2,3,6-trimethylphenol. The oxidation products are consistent with those of a homolytic oxidation mechanism. On the contrary, 3 containing no acid protons reacts with neither H<sub>2</sub>O nor H<sub>2</sub>O<sub>2</sub> and shows negligible catalytic activity. The Zr-monosubstituted polyoxometalates can be used as tractable homogeneous probes of Zr single-site heterogeneous catalysts in studying mechanisms of H<sub>2</sub>O<sub>2</sub>-based oxidations.

## TITANIUM-MONOSUBSTITUTED POLYOXOMETALATES: RELATION BETWEEN HOMOGENEOUS AND HETEROGENEOUS Ti-SINGLE-SITE-BASED CATALYSIS

O.A. Kholdeeva

*Top. Catal.*,  
40(1-2) (2006) pp. 229-243.

The similarity in the catalytic behaviour of titanium-monosubstituted Keggin type polyoxometalates  $[\text{PTi(L)W}_{11}\text{O}_{39}]^{n-}$  (Ti-POMs) and

heterogeneous titanium single-site catalysts in selective oxidations with  $\text{H}_2\text{O}_2$  is demonstrated. Recent achievements in the application of Ti-POMs as soluble molecular models for studying mechanisms of oxidation catalysis are reviewed.

## Photocatalytic and Related Processes

### EXPERIMENTAL STUDY OF DIMETHYL METHYLPHOSPHONATE DECOMPOSITION OVER ANATASE $\text{TiO}_2$

D.A. Trubitsyn, A.V. Vorontsov

*J. Phys. Chem. B*,  
109(46) (2005) pp. 21884-21892.

Removal from air and decomposition of dimethyl methylphosphonate (DMMP) over high surface area anatase  $\text{TiO}_2$  at ambient temperature have been quantitatively studied by employing Fourier transform infrared (FTIR) technique under static conditions. In the first scenario of air purification, DMMP underwent reactive adsorption that upon completion was followed by photocatalytic oxidation. DMMP was captured over the  $\text{TiO}_2$  surface at the speed of external diffusion. Hydrolysis of adsorbed DMMP led to methanol and methyl methylphosphonate (MMP). At low DMMP coverage quantity, it hydrolyzed completely with the formation of completely surface-bound methanol at 1% relative humidity (RH) and mostly gaseous methanol at 50% RH. Photocatalytic oxidation generated  $\text{CO}_2$  as the only carbonaceous gaseous product and bidentate formates as the intermediate surface product. At high DMMP coverage quantity, it was captured incompletely and hydrolyzed partially with  $\text{CH}_3\text{OH}$  in the gas phase only, 50% RH enhancing both processes. Photocatalytic oxidation generated gaseous  $\text{HCOOH}$ ,  $\text{CO}$ , and  $\text{CO}_2$  and was incomplete due to catalyst deactivation by nonvolatile products. In the second scenario of air purification, DMMP underwent adsorption, hydrolysis, and photooxidation at the same time. It resulted in the quickest removal of DMMP from the gas phase and completion of oxidation in 30 min, suggesting this process for practical air decontamination. At least  $0.8 \text{ nm}^2$  of  $\text{TiO}_2$  surface per

each DMMP molecule should be available for complete purification of air.

### PHOTOINDUCED HETEROGENEOUS PROCESSES ON PHASE CHEMICAL 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 ( $\text{In}_2\text{O}_3$ ,  $\text{Sc}_2\text{O}_3$ ,  $\text{V}_2\text{O}_5$  and  $\text{MoO}_3$ ) and insulator type ( $\text{MgO}$ ). 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.

### 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.

## STUDY OF THE PHOTOINDUCED FORMOSE REACTION BY FLASH AND STATIONARY PHOTOLYSIS

O.A. Snytnikova\*, A.N. Simonov, O.P. Pestunova, V.N. Parmon, Yu.P. Tsentalovich\* (\*International Tomography Center, Novosibirsk, Russia)

*Mendeleev Commun.*, 16(1) (2006) pp. 9-11.

The chemical condensation of formaldehyde into more complex aldehydes (glycolaldehyde and glyceraldehyde) and monosaccharides (glucose, lyxose, erythrose and erythrulose) under UV irradiation was found to proceed in acidic aqueous solutions in the absence of catalysts and initial primers.

## HETEROGENEOUS FENTON SYSTEM FOR DEEP OXIDATION OF TOXIC ORGANIC SUBSTANCES IN WATER SOLUTIONS

O.A. Makhotkina, E.V. Kuznetsova, L.G. Matvienko, V.N. Parmon

*Catal. Ind.*, 4 (2006) pp. 30-37.

The Fenton heterogeneous system FeZSM-5/H<sub>2</sub>O<sub>2</sub> was investigated in deep oxidation of toxic organic contaminants, such as 1,1-dimethylhydrazine (NDMH), N-nitrosodimethylamine (NDMA), dimethyl keton, and others, in water solutions. Adsorption characteristics of FeZSM-5 with respect to H<sub>2</sub>O<sub>2</sub>, NDMH, NDMA, dimethyl keton, and ethanol as well as the kinetic behavior of NDMH catalytic oxidation by hydrogen peroxide were studied. An analysis of intermediate and final products of NDMH oxidation by hydrogen peroxide over FeZSM-5 was carried out. The system investigated is heterogeneous and ecologically safe. It provides more effective use of the oxidizer and a possibility of full oxidation of toxic organic compounds to harmless substances and it is very promising system for deactivation of water solutions.

## CATALYTIC DETOXIFICATION OF 1,1-DIMETHYLHYDRAZINE AQUEOUS SOLUTIONS IN HETEROGENEOUS FENTON SYSTEM

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*Appl. Catal., B*, 68(2-3) (2006) pp. 85-91.

The experimental study into catalytic properties of FeZSM-5 was undertaken into oxidation of 1,1-dimethylhydrazine (UDMH) aqueous solutions using hydrogen peroxide. The performances of

heterogeneous and homogeneous Fenton systems were compared. UDMH complete mineralization was achieved. Formic and acetic acids, as well as nitromethane, were identified as oxidation by-products. Adsorption properties of FeZSM-5 with respect to hydrogen peroxide, 1,1-dimethylhydrazine and N-nitrosodimethylamine have been studied. The effects of the oxidant and the target compound concentrations, temperature and pH of aqueous solution were established

## NOBLE METAL AND SULFURIC ACID MODIFIED TiO<sub>2</sub> PHOTOCATALYSTS: MINERALIZATION OF ORGANOPHOSPHOROUS COMPOUNDS

E.A. Kozlova, A.V. Vorontsov

*Appl. Catal., B*, 63(1-2) (2006) pp. 114-123.

Photocatalytic oxidation by oxygen of air in water suspension of TiO<sub>2</sub>-based catalysts was carried out for dimethyl methylphosphonate (DMMP) and trimethyl phosphate (TMP) — simulants of warfare agents. Active photocatalysts were prepared via surface modification of standard photocatalyst Degussa P25 with platinum and palladium. The developed catalysts were about three-fold more active than traditionally best photocatalyst Degussa P25. Kinetic curves of DMMP oxidation on TiO<sub>2</sub> and Pt/TiO<sub>2</sub> are well approximated by the Langmuir–Hinshelwood model with competitive adsorption of oxygen and organophosphorus compound. The increase of activity of Pt/TiO<sub>2</sub> is linked with higher oxygen adsorption constant or reaction rate coefficient. Photocatalytic oxidation can be scaled up to a larger reactor with the same reaction rates expressed as mmol l<sup>-1</sup> min<sup>-1</sup> in mineralization of DMMP. The batch recirculating reactor with total volume 3 l utilizes photocatalyst deposited over porous support and demonstrated higher oxidation rate and catalyst stability compared to suspended photocatalyst. Main criteria for mass-transfer process in the batch recirculating reactor were calculated to understand how concentration cross gradient depends on flow rate. The concentration of oxygen in reaction mixture changed with the stirring or recirculation rate and exerts strong influence on the oxidation rate.

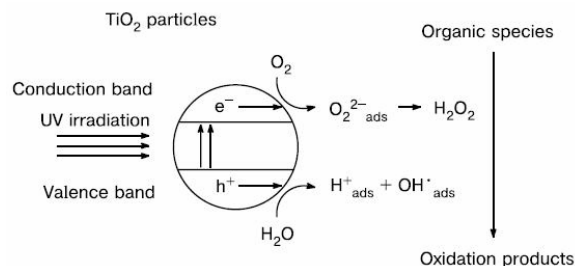
## REGULARITIES OF DECOMPOSITION OF ORGANIC VAPORS USING A PHOTOCATALYTIC AIR CLEANER

I.A. Baturov, A.V. Vorontsov, D.V. Kozlov

*Russ. Chem. Bull.*,  
54(8) (2005) pp. 1866-1873.

The kinetics of oxidation of vapors of model air contaminants, viz., acetone, ethanol, and heptane, was studied using a photocatalytic air cleaner. The composition of the oxidation products was determined, and the rates of oxidation of the starting substances were measured. The deep oxidation of the starting substrates to CO<sub>2</sub> and H<sub>2</sub>O occurs until their concentration achieves a limiting value. At higher concentrations a "breakthrough" of the starting

substrate is observed. Ethanol is oxidized with the formation of intermediate products. The experimental data obtained were approximated by a kinetic model, which includes stages of formation of intermediates and their competitive adsorption. The results of the approximation agree well with the experimental data.



## Electrocatalysis and Electrochemical Processes

### ELECTROCATALYTIC PROPERTIES OF Au(111)-Pd QUASI-SINGLE-CRYSTAL FILM ELECTRODES AS PROBED BY ATR-SEIRAS

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*Russ. J. Electrochem.*,  
42(11) (2006) pp. 1177-1192.

Electrochemical and electrocatalytic properties of thin films Au(111-25 nm), which are quasi-single-crystal electrodes 25 nm thick made of gold with the (111) preferential orientation, and same electrodes modified with a monolayer (ML) of palladium are studied in 0.1 M solutions of HClO<sub>4</sub> and H<sub>2</sub>SO<sub>4</sub> employing voltammetric techniques and surface enhanced infrared reflection absorption spectroscopy (ATR-SEIRAS). Spectroscopic experiments demonstrate strong adsorption of electrolyte species (H<sub>2</sub>O, OH<sub>ads</sub>, anions) on the Pd surface. The weak and reversible adsorption of CO on Au(111-25 nm) does not change the interfacial-water structure. Adsorption of CO on the Pd-modified film results in an irreversibly adsorbed CO adlayer stabilized by co-adsorbed isolated water species. Various electrooxidation mechanisms are discussed. Electrochemical and spectroscopic investigations on the adsorption and electrooxidation of HCOOH on bare and 1 ML Pd-Au(111-25 nm) electrodes reveal that electrooxidation proceeds in both cases via a direct or dehydrogenation pathway. This mechanism involves the formation of formate as intermediate, which is detected by *in situ* ATR-SEIRAS. The reactivity on Pd-modified surfaces is higher than on

bare gold. The specifically adsorbed anions (sulfate/bisulfate) and the oxide formation on the substrate surface lower the reactivity for CO and HCOOH on both surfaces.

### ELECTROCRYSTALLIZATION OF Pt LAYERS ONTO Au SUBSTRATES; AN X-RAY DIFFRACTION STUDY

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E.R. Savinova, G.A. Tsirlina\* (\*Moscow Lomonosov  
State University, Moscow, Russia)

*Z. Kristallogr. Suppl.*,  
23 (2006) pp. 293-298.

An X-ray diffraction study of the structural features of Pt electrodeposited on Au substrates was performed. The influence of the deposition potential, electrochemical ageing and model catalytic reactions on the structural characteristics of deposits has been analysed. It has been shown that under the conditions employed highly defective electrolytic deposits are formed composed of nm-sized particles (10–30 nm). Electrochemical ageing and model electrochemical reactions lead to the relaxation of the defect structure of electrodeposited Pt, which is expressed in an increase of lattice parameter and particle size and decrease in the values of strains and density of randomly distributed dislocations. The data obtained showed that the deposition potential is a key parameter determining structural characteristics of Pt electrolytic deposits, and allowed to reveal the minimum of intergrowth degree of Pt nano-particles.

## ELECTRODEPOSITED PLATINUM REVISITED: TUNING NANOSTRUCTURE VIA THE DEPOSITION POTENTIAL

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*Electrochem. Acta*,  
51(21) (2006) pp. 4477-4488.

Pt nanostructured materials composed of nm-sized Pt crystallites interconnected via grain boundaries are prepared by electrochemical deposition on Au and glassy carbon substrates from aqueous chloride solutions of hexachloroplatinic acid under potentiostatic mode at various potentials (0.025–0.550 V versus RHE). These samples may be considered as model electrode materials for the investigation of the influence of structural defects in electrocatalysis. Nanostructure and morphology of electrodeposited materials are analyzed with X-ray diffractometry and scanning electron microscopy. Considerable distortions of Pt lattice are detected, which are revealed by the decreased lattice parameter and significant microstrains. These lattice distortions increase with the decrease of the deposition overvoltage, and are the highest in the region of kinetically controlled electrodeposition. The deposition potential can be thus used as a tool to tune the nanostructure of supported Pt. Defectiveness is found to correlate with the degree of surface screening estimated from the difference of the calculated and the experimental surface areas. Screening is found to result from both the crystal coalescence and the existence of nanopores. Continuous potential cycling is accompanied by restructuring of both nanoparticles and intergrain boundaries, but does not fully relax lattice compression.

## TEMPERATURE DEPENDENCE OF THE OXYGEN REDUCTION KINETICS ON Ru<sub>x</sub>Se<sub>y</sub>/C CATALYSTS

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*Fuel Cells*,  
6(3-4) (2006) pp. 203–207.

The temperature dependence of the oxygen reduction kinetics on carbon-supported Ru<sub>x</sub>Se<sub>y</sub> catalysts is studied using a rotating disc electrode in 0.5 M H<sub>2</sub>SO<sub>4</sub> in the temperature interval from 25°C to 65°C. When the absolute value of the overpotential is below ca. 0.65 V, the reaction is limited by a one-electron charge transfer step, where the transfer coefficient is independent of the temperature and equal to 0.44. The apparent activation enthalpy at zero

overpotential is 0.49 eV and the pre-exponential factor is independent of the temperature.

## SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF Se-MODIFIED CARBON-SUPPORTED Ru NANOPARTICLES FOR THE OXYGEN REDUCTION REACTION

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*J. Phys. Chem. B*,  
110(13) (2006) pp. 6881-6890.

This work is part of a continued research aimed at the understanding of the promoting role of Se in the enhancement of the electrocatalytic activity of Ru in the oxygen reduction reaction. The objective of this paper is to systematically investigate the transformation of Ru nanoparticles upon their modification with the increasing amounts of Se. The Se-modified Ru/C samples with Se:Ru ratio from 0 to 1 were prepared by reacting carbon-supported Ru nanoparticles with SeO<sub>2</sub> followed by reductive annealing and characterized using high-resolution transmission electron microscopy, energy-dispersive X-ray, X-ray diffraction analysis, X-ray photoelectron spectroscopy, and extended X-ray absorption fine structure. The results suggest that Se strongly interacts with Ru, resulting in the chemical bond between Ru and Se and formation of Ru selenide clusters whose core at low Se content can be described as Ru<sub>2</sub>Se<sub>2</sub>O<sub>0.5</sub>. At Se:Ru = 1, high-resolution electron microscopy shows evidence of formation of core-shell particles, comprising a hexagonally packed Ru core and a Ru selenide shell with lamellar morphology. Modification of Ru nanoparticles with Se enhances their electrocatalytic activity in the oxygen reduction reaction, which is explained by the role of Se in inhibiting surface oxidation.

## IMPROVEMENT OF THE PERFORMANCE OF A DIRECT METHANOL FUEL CELL USING A PULSE TECHNIQUE

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*J. Electrochem. Soc.*,  
153(6) (2006) pp. A997-A1003.

A pulse method is suggested for the improvement of the performance of a direct methanol fuel cell



operated with PtRu anode and Pt cathode. The pulse method can be realized either in a potentiostatic or in a galvanostatic mode. In the galvanostatic regime of low current densities it allows for a temporary hoist of the cell voltage by up to 150 mV. It is suggested that by periodically applying a pulse to the fuel cell, the anode potential is shifted to positive values at which the otherwise high CO<sub>ads</sub> coverage on the PtRu anode is decreased by oxidation. After the pulse, the methanol oxidation rate is enhanced until the previous CO<sub>ads</sub> coverage is re-established and a new pulse is then applied. Differential electrochemical mass spectroscopy data reveal that an appreciable voltage gain can be obtained at a reduction of only ca. 10–15% of the CO<sub>ads</sub> saturation coverage.

#### KINETIC MODELING OF CO<sub>ad</sub> MONOLAYER OXIDATION ON CARBON-SUPPORTED PLATINUM NANOPARTICLES

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*J. Phys. Chem. B*,  
110(42) (2006) pp. 21028-21040.

A theoretical study of CO<sub>ad</sub> electrooxidation on Pt nanoparticles is presented. Effects of size and surface texture of nanoparticles on the interplay of relevant kinetic processes are investigated. Thereby, strong impacts of particle size on electrocatalytic activities, observed in experiments, are rationalized. Theoretical approach employs the active site concept to account for the heterogeneous surface of nanoparticles. It, moreover, incorporates finite rates of surface mobility of adsorbed CO. As demonstrated, the model generalizes established mean field or nucleation and growth models. Very good agreement of our model with chronoamperometric current transients at various particle sizes and electrode potentials was found (Maillard, F.; Savinova, E.R.; Stimming, U. *J. Electroanal. Chem.*, in press). The full interplay of on-site reactivity at active sites and low surface mobility of CO<sub>ad</sub> unfolds on the smallest nanoparticles (~2 nm). In this case, the solution of the model requires kinetic Monte Carlo simulations specifically developed for this problem. For larger nanoparticles (>4 nm) the surface mobility of CO<sub>ad</sub> is high compared to the reaction rate constants, and the kinetic equations can be solved in the limiting case of infinite surface mobility. The analysis provides an

insight into the prevailing reaction mechanisms and allows for the estimation of relevant kinetic parameters.

#### CO MONOLAYER OXIDATION ON Pt NANOPARTICLES: FURTHER INSIGHTS INTO THE PARTICLE SIZE EFFECTS

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*J. Electroanal. Chem.*, 599(2) (2007) pp. 221-232.

This paper provides further insights into the particle size effects in CO monolayer oxidation. Strong particle size effects are confirmed in the size range from 1.8 to 5 nm. The discrepancies in the literature concerned with the particle size effects in CO monolayer oxidation are reconciled by exploring the influence of the experimental conditions on the stripping voltammograms and chronoamperograms. Evidence supporting the contribution of slow non-electrochemical step to the overall mechanism of CO oxidation is presented. The particle size effects in CO monolayer oxidation are attributed to the size-dependent CO<sub>ads</sub> + OH<sub>ads</sub> interaction as well as to the size-dependent CO<sub>ads</sub> surface diffusion coefficient.

#### HIGH-TEMPERATURE EFFECTS ON THE ELECTRICAL PROPERTIES AND MACROSTRUCTURE OF CARBON COMPOSITES

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*Inorg. Mater.*,  
41(6) (2006) pp. 609-616.

The electrical conductivity of MPG-6 and MPG-7 carbon composites has been measured before and after 1.4-MeV electron irradiation and ac resistive heating up to degradation temperatures (above 2500°C). The results demonstrate that both heating and electron irradiation reduce the resistivity of the materials and increase the defect density at the macrostructural level, while X-ray diffraction analysis reveals no significant structural changes in the temperature range studied. Detailed characterization of the composites suggests that their strength is limited by crystallite or grain boundaries.

## Polymerization Catalysts and Polymer Materials

### Cu(II) AND Cu(I) COMPLEXES WITH 2-(3,5-DIPHENYL-1H-PYRAZOLE-1-yl)-4,6-DIPHENYLPYRIMIDINE: SYNTHESIS AND STRUCTURE. CATALYTIC ACTIVITY OF Cu(II) COMPOUNDS IN REACTION OF ETHYLENE POLYMERIZATION

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*Russ. J. Coord. Chem.*, 32(3) (2006) pp. 199-207.

The Cu(II) and Cu(I) complexes with 2-(3,5-diphenyl-1H-pyrazole-1-yl)-4,6-diphenylpyrimidine (L) of the composition  $\text{CuLX}_2$  (X = Cl, Br) and  $\text{CuL}(\text{MeCN})\text{Br}$  are synthesized. According to X-ray diffraction data, the complexes have molecular structures. The molecules L are coordinated to the copper atom in bidentate-cyclic mode, i.e., through the  $\text{N}^2$  atom of pyrazole and  $\text{N}^1$  atom of pyrimidine rings. The coordination polyhedron of the  $\text{Cu}^{2+}$  ion in  $\text{CuLX}_2$  compounds is completed to a distorted tetrahedron with halide ions, that of the  $\text{Cu}^+$  ion in  $\text{CuL}(\text{MeCN})\text{Br}$  compounds, with the bromide ion and the nitrogen atom of acetonitrile molecule. The  $\text{CuLX}_2$  complexes (X = Cl, Br) in combination with cocatalysts (methylaluminoxane and triisobutylaluminium) exhibit catalytic activity in ethylene polymerization.

### ACTIVATION OF BIS(PYRROLYLALDIMINATO) AND (SALICYLALDIMINATO) (PYRROLYLALDIMINATO) TITANIUM POLYMERIZATION CATALYSTS WITH METHYLALUMOXANE

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*Organometal.*, 26(2) (2007) pp. 288-293.

Cationic intermediates formed upon activation of an olefin polymerization catalyst based on bis[*N*-phenylpyrrolylaldiminato]titanium(IV) dichloride ( $\text{L}_2\text{TiCl}_2$ , I) and [*N*-(3-*tert*-butylsalicylidene)-2,3,4,5,6-pentafluoroanilinato-*N'*-phenylpyrrolylaldiminato]titanium(IV) dichloride

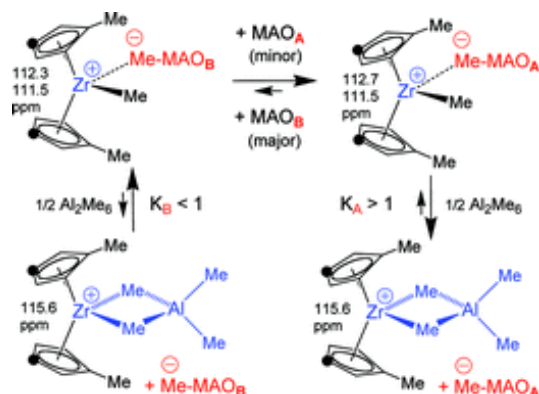
( $\text{L}'\text{TiCl}_2$ , II) with methylaluminoxane (MAO) have been identified. Outer-sphere ion pairs of the type  $[\text{L}_2\text{TiMe}(\text{S})]^+[\text{MeMAO}]^-$  and  $[\text{L}'\text{TiMe}(\text{S})]^+[\text{MeMAO}]^-$  capable of ethene polymerization have been characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy. Unlike methyl metallocenium cations, the barrier of the first ethene insertion into the Ti-Me bonds of these species is not significantly higher than that of subsequent insertions. Surprisingly, whereas homoligated catalyst precursors  $\text{L}_2\text{TiCl}_2$  in the presence of MAO are prone to ligand transfer to aluminum, under the same conditions the heteroligated system  $\text{L}'\text{TiCl}_2/\text{MAO}$  proved resistant to ligand scrambling.

### DISTINCT METHYLALUMOXANE(MAO)-DERIVED Me-MAO(-) ANIONS IN CONTACT WITH A ZIRCONOCENIUM CATION - A $^{13}\text{C}$ -NMR STUDY

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*Dalton Trans.*, 38 (2006) pp. 4539-4544.

Zirconocenium cations of the type  $[(\text{MeC}_5\text{H}_4)_2\text{ZrMe}]^+$ , formed by excess methylaluminoxane (MAO) from  $(\text{MeC}_5\text{H}_4)_2\text{ZrCl}_2$  or  $(\text{MeC}_5\text{H}_4)_2\text{ZrMe}_2$  with  $^{13}\text{C}$ -labelled ring ligands, are found to form ion pairs with two types of anions,  $\text{Me-MAO}_A^-$  and  $\text{Me-MAO}_B^-$ , which differ in their coordinative strengths. More strongly coherent ion pairs  $[(\text{MeC}_5\text{H}_4)_2\text{ZrMe}^{+\dots}\text{Me-MAO}_B^-]$  are converted to more easily separable ion pairs  $[(\text{MeC}_5\text{H}_4)_2\text{ZrMe}^{+\dots}\text{Me-MAO}_A^-]$  by a sufficient excess of MAO. These react with  $\text{Al}_2\text{Me}_6$  to form outer-sphere ion pairs containing the cationic  $\text{AlMe}_3$  adduct  $[(\text{MeC}_5\text{H}_4)_2\text{Zr}(\mu\text{-Me})_2\text{AlMe}_2]^+$ ; formation of the more easily separable ion pairs might be required also for polymerisation catalysis.



**FORMATION AND STRUCTURES OF  
CATIONIC ZIRCONIUM COMPLEXES IN  
TERNARY SYSTEMS  
rac-(SBI)ZrX<sub>2</sub>/ABu<sup>i</sup><sub>3</sub>/[CPh<sub>3</sub>][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] (X= Cl, Me)**

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*J. Organomet. Chem.*,  
692(4) (2007) pp. 859-868.

Using <sup>13</sup>C, <sup>1</sup>H and <sup>19</sup>F NMR spectroscopy, formation of cationic species was studied in ternary systems (SBI)ZrX<sub>2</sub>/AlBu<sub>3</sub><sup>i</sup>/[CPh<sub>3</sub>][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>], where X = Cl, Me [(SBI) = *rac*-Me<sub>2</sub>Si(Ind)<sub>2</sub>]. In the first system (X = Cl), the ion pair [(SBI)Zr(μ-Cl)<sub>2</sub>Zr(SBI)][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>]<sub>2</sub> (IV) predominates at low Al/Zr ratios (Al/Zr < 10), whereas at higher Al/Zr ratios (≥20) in the absence of monomer mainly [(SBI)Zr(μ-H)(μ-C<sub>4</sub>H<sub>7</sub>) AlBu<sub>2</sub><sup>i</sup>] [B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] (V) is formed. The binuclear complex [(SBI)Zr(μ-Cl)<sub>2</sub>Zr(SBI)][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>]<sub>2</sub> has been characterized crystallographically. Species V is also formed in the system X = Me at high Al/Zr ratios. In the presence of AlBu<sub>3</sub><sup>i</sup>, IV displays activity in propylene polymerization and is the most likely precursor of the polymerizing species. Consistent mechanisms have been proposed for the reactions in these catalytic systems.

**SUPPORTED TITANIUM-MAGNESIUM  
CATALYSTS WITH DIFFERENT TITANIUM  
CONTENT: KINETIC PECULIARITIES AT  
ETHYLENE HOMOPOLYMERIZATION AND  
COPOLYMERIZATION AND MOLECULAR  
WEIGHT CHARACTERISTICS OF  
POLYETHYLENE**

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*J. Appl. Polym. Sci.*, 102(6) (2006) pp. 5436-5442.

The effect of Ti content on the activity of titanium-magnesium catalysts (TMC) and molecular weight distribution (MWD) of polyethylene (PE) produced has been studied. It was found that the activity enhances sharply as Ti content decreases from 0.6 to 0.07 wt %, and shows no significant changes in the Ti content range of 0.6-5.0 wt %. The maximum activity (36 kg PE/mmol Ti·h·bar C<sub>2</sub>H<sub>4</sub>) was observed for TMC with the lowest Ti content. The catalyst with low titanium content (~0.1 wt % of Ti) produced PE with narrower MWD ( $M_w/M_n = 3.1-3.5$ ) as compared to catalysts with higher titanium content (3-5 wt % of

Ti;  $M_w/M_n = 4.8-5.0$ ). New data on the effect of hydrogen on MWD of PE have been found. Increasing hydrogen concentration results in broadening the MWD of PE, especially in the case of TMC with high titanium content. The data presented indicate the heterogeneity of active centers of TMC in the reaction of chain transfer with hydrogen. The data on the ethylene-hexene-1 copolymerization over TMC with different titanium content are presented. Comonomer reactivity ratios were shown to be independent of the Ti content in TMC. Presumably the difference in activity of these catalysts is mainly caused by the difference in the number of active centers.

**DRIFT STUDY OF INTERNAL DONORS IN  
SUPPORTED ZIEGLER-NATTA CATALYSTS**

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*J. Mol. Catal.*,  
246(1-2) (2006) pp. 248-254.

The state of internal donor (ID) in the supported titanium-magnesium (TiCl<sub>4</sub>/ID/MgCl<sub>2</sub>) catalysts for stereospecific propylene polymerization has been studied by diffuse reflectance infrared spectroscopy (DRIFT). The samples were prepared via interaction of highly dispersed MgCl<sub>2</sub> with different IDs (ethyl benzoate, EB; di-*n*-butyl phthalate, DBP) and TiCl<sub>4</sub>. It was found that the DRIFT spectra of carbonyl groups of IDs adsorbed on MgCl<sub>2</sub> could be best described as a superposition of several overlapping vibration bands from a variety of surface complexes. Within this model the content of individual EB and DBP complexes on the MgCl<sub>2</sub> surface was calculated. In the case of EB, three main complexes were found on the MgCl<sub>2</sub> support in about equal proportions. In the case of DBP, only one of three complexes was preferentially formed. The surface content of both EB and DBP was found to decrease in presence of TiCl<sub>4</sub>. At the same time TiCl<sub>4</sub> had influenced the distribution pattern of EB but not DBP complexes. The most likely scenario of competitive adsorption of TiCl<sub>4</sub> and IDs on the MgCl<sub>2</sub> support is discussed. A model describing surface distribution of TiCl<sub>4</sub> on MgCl<sub>2</sub> is proposed for TiCl<sub>4</sub>/EB/MgCl<sub>2</sub> and TiCl<sub>4</sub>/DBP/MgCl<sub>2</sub> catalysts.

## MOLECULAR MASS CHARACTERISTICS OF POLYETHYLENE PRODUCED WITH SUPPORTED VANADIUM-MAGNESIUM CATALYSTS

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*Polym. Int.*, 55(2) (2006) pp. 165-170.

Highly active supported vanadium-magnesium catalysts (VMC) produce polyethylene (PE) with broad and bimodal molecular mass distribution (MMD) in comparison with the famous titanium-magnesium catalysts (TMC). The effect of hydrogen as an efficient chain-transfer agent on the MMD of PE has been studied. Increasing hydrogen concentration causes a considerable broadening of MMD of PE due to the shift of the low molecular weight peak on the MMD curve. At the same time, the high molecular weight shoulder stays at the same position even at high hydrogen concentration. This means that VMC contain two types of active centre. One type is very reactive in the chain-transfer reaction with hydrogen. These centres produce low molecular weight PE in polymerization in the presence of hydrogen. The other type of active centre is not active in chain transfer with hydrogen. These centres produce high molecular weight PE  $((1-3) \cdot 10^6)$  and hydrogen does not affect the position of the high molecular weight shoulder. MMD data were used to analyze the kinetics of the chain-transfer reaction with hydrogen and to calculate the rate constants of this reaction.

## DETERMINATION OF THE MOLECULAR CHARACTERISTICS OF POLYOLEFINS WITH THE USE OF THE TOMS EFFECT

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*J. Eng. Phys. Thermophys.*, 79(1) (2006) pp. 168-172.

The interrelation between the physicochemical properties of macromolecules and the hydrodynamic parameters of a turbulent flow of diluted polymer solutions in a cylindrical channel has been analytically determined. The possibility of estimating of the molecular characteristics of high-molecular polymers with the use of the turborheometric method has been considered. The antiturbulence efficiency of polyhexane used in energy-conserving technologies of pipeline transport of hydrocarbon materials has been

analyzed on the basis of comparison of the molecular masses of polymers determined by different methods.

## DRIFTS AND DRS STUDIES OF PHILLIPS ETHYLENE POLYMERIZATION CATALYSTS

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*Appl. Catal., A*, 313(2) (2006) pp. 130-136.

Formation of the  $\text{CrO}_3/\text{SiO}_2$  catalyst prepared by the reaction of  $\text{CrO}_3$  vapor with silica pre-dehydroxylated at 250–800°C was studied by the DRIFT and DRS methods. It was found that  $\text{CrO}_3$  reacts with the silica OH-groups at 250°C to produce various chromate species and water. The latter is removed from the catalyst surface by vacuumation at 250°C. It was found the nature of  $\text{CrO}_3$  interaction with silica and the structure and composition of the surface species depend on silica dehydroxylation temperature. The reactions of  $\text{CrO}_3$  with the silica dehydroxylated at 250, 400 and 800°C yielded, respectively, monochromates; mono- and dichromates; polychromates. The catalyst activity at ethylene polymerization strongly increases with increasing dehydroxylation temperature, especially in the range of 250–400°C. The results obtained prove di- and polychromates to be the active components of the Phillips type chromium-oxide catalysts from which the active centers are formed at interaction of the active component with co-catalyst ( $\text{AlEt}_3$ ) and ethylene. Active centers contain the surface organochromium compounds with chromium ions in low oxidation states (lower than Cr(VI)).

## KINETIC STUDY OF ETHYLENE POLYMERIZATION OVER SUPPORTED BIS(IMINO)PYRIDINE IRON (II) CATALYSTS

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*Macromol. Chem. Phys.*, 207(15) (2006) pp. 1368-1375.

The number of active centers ( $C_p$ ) and propagation rate constants ( $k_p$ ) for polymerization of ethylene with supported catalysts  $\text{LFeCl}_2/\text{SiO}_2$ ,  $\text{LFeCl}_2/\text{Al}_2\text{O}_3$  and  $\text{LFeCl}_2/\text{MgCl}_2$  ( $\text{L} = 2,6-(2,6-(\text{Me})_2\text{C}_6\text{H}_3\text{N} \text{ CMe})_2\text{C}_5\text{H}_3\text{N}$ ), activated by an  $\text{Al}(i\text{-Bu})_3$  co-catalyst, were determined by a method of polymerization inhibition with radioactive  $^{14}\text{CO}$ . In contrast to homogeneous systems based on  $\text{LFeCl}_2$ , the supported catalysts are highly active and stable in ethylene polymerization at 70-80°C. In the presence of hydrogen, the activity of the supported catalysts substantially increases (2-4 fold). The data

obtained on the effect of hydrogen on the calculated  $C_p$  and  $k_p$  values suggests that for ethylene polymerization without hydrogen, the “dormant” active centers are formed in the catalytic systems. A scheme for the formation of these “dormant” centers and their reactivation in presence of hydrogen is suggested. For the investigated supported catalysts the  $C_p$  values were found to be only 2 to 4% of the total iron complex content in the catalysts. The  $k_p$  value for the catalysts prepared using different supports ( $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$  and  $\text{MgCl}_2$ ) were close ( $3.2 \cdot 10^4$  to  $4.5 \cdot 10^4 \text{ L} \cdot (\text{mol} \cdot \text{s})^{-1}$  at  $70^\circ\text{C}$ ). The support composition affects neither the molecular mass (MM) nor the molecular mass distribution (MMD) of the polymers produced. The obtained  $C_p$  and  $k_p$  values and data on the polymer MM and MMD lead to conclusion that the nature of the support has almost no effect on the structure of the active centers and the distribution of their reactivity.

#### **HOMOGENEOUS AND SUPPORTED CATALYSTS BASED ON BIS(IMINO)PYRIDYL IRON(II) COMPLEXES FOR ETHYLENE POLYMERIZATION**

**V.A. Zakharov, N.V. Semikolenova, T.B. Mikenas, A.A. Barabanov, G.D. Bukatov, L.G. Echevskaya, M.A. Matsko**

*Kinet. Catal.*,  
47(2) (2006) pp. 303-309.

Data on ethylene polymerization on homogeneous and supported catalysts based on 2,6-bis(imino)pyridyl Fe(II) complexes activated by trialkylaluminums are considered (activity, the molecular-weight characteristics of polymers, the number of active sites, and the propagation rate constants). Unlike homogeneous systems, the supported catalysts prepared with the use of various carriers ( $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{MgCl}_2$ ) exhibited high stability and activity at  $70\text{--}80^\circ\text{C}$  and produced high-molecular-weight polyethylene with a broad molecular-weight distribution (MWD). The molecular weights and MWDs of polymers and the propagation rate constant depended on the nature of the carrier only slightly. The reasons for an unusual effect of an increase in the activity of the supported catalysts in ethylene polymerization in the presence of hydrogen are discussed.

#### **NEW REACTION FOR PREPARATION OF LIQUID RUBBER**

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*J. Polym. Sci., Part A: Polym. Chem.*,  
44(8) (2006) pp. 2510-2520.

The article reports on the noncatalytic transformation of a polybutadiene (number-average molecular weight = 128,000) into a functionalized liquid rubber via the carboxidation of the polymer C=C bonds by nitrous oxide. The reaction was conducted in a benzene solution at  $160\text{--}230^\circ\text{C}$  and a pressure of 3-6 MPa. The carboxidation mechanism was determined. The main route (95%) of the reaction proceeded without cleavage of C=C bonds and led to the formation of ketone groups in the polymer backbone. A minor route (5%) of the reaction proceeded with the cleavage of C=C bonds, yielding two smaller fragments containing aldehyde and vinyl end groups. The availability of the cleavage route could lead to a dramatic decrease in the molecular weight, which, depending on the carboxidation degree, could be 1-2 orders of magnitude less than that of the initial material. Thus, the carboxidation of more than 15% of the polybutadiene C=C bonds transformed it into a C=O-functionalized liquid rubber with a narrow molecular weight distribution.

#### **POLYMERIZATION OF ETHYLENE BY $\text{SiO}_2$ -SUPPORTED TWO-COMPONENT CATALYTIC SYSTEMS CONTAINING BIS(IMINO)PYRIDINE AND BIS(IMINE) LIGANDS**

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*Polymer Sci., Ser A*,  
48(3) (2006) pp. 251-256.

The polymerization of ethylene initiated by  $\text{SiO}_2$ -supported two-component catalytic systems based on 2,6-bis[1-(2,4-dimethyl-6-cyclohexylphenylimino)ethyl]pyridine iron (II) chloride (**I**) and 1,2-bis(2-cyclohexyl-4,6-dimethylphenylimino)acenaphthene] nickel bromide (**II**) was studied. Methylaluminoxane was used as a cocatalyst during support. It was shown that the activity of two-component catalytic systems and the molecular mass and short-chain branching of polyethylene samples depend on the supporting procedure: simultaneous immobilization of components **I** and **II**, separate immobilization of

components on the support (first **I**, then **II**, and vice versa), and the use of a mixture of components **I** and **II** immobilized separately on SiO<sub>2</sub>.

## NANOSTRUCTURES IN POLYMER SYSTEMS

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*Polymer Sci., Ser B,*  
48(7-8) (2006) pp. 213-225.

General concepts concerning the formation, structure, and some properties of nanosized structural elements in polymers and polymeric materials are summarized from the standpoint of feasibility of formation of nanoparticles and nanoreactors in such systems and practical use of advantages offered by these structures. The familiar concepts are complemented with the results obtained recently. Examples are given to illustrate the implementation of elements of nanotechnology based on the principles of creation of nanostructures in amorphous and crystalline polymers, copolymers, and molecular composites. Practicable methods for the preparation of polymeric nanostructures by controlled crystallization, microphase and nanophase separation of components, and their dispersion, as well as the formation of interfaces, are discussed.

## TRANSEETHERIFICATION OF MELAMINE-FORMALDEHYDE RESIN METHYL ETHERS AND COMPETING REACTION OF SELF-CONDENSATION

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*J. Appl. Polym. Sci.,*  
110(5) (2006) pp. 2977-2985.

Transeetherification of methyl ethers of melamine-formaldehyde resin (MER) with monophenyl ethers of ethylene glycol or propylene glycol (ROH) and competing reaction of self-condensation are studied depending on MER composition (amounts of CH<sub>3</sub>O-, -CH<sub>2</sub>OH, and NH<sub>2</sub>-groups, ROH type, MER/ROH molar ratio), presence or absence of acid catalysts, and temperature. High rates of self-condensation processes prevent a complete conversion of CH<sub>3</sub>O- into RO-groups. It turned out MER free of methylol groups were not able to be transeetherified with high yields due to a premature gelation taking place prior to attaining 50% conversion of methoxy groups (~ 4 mol/kg) even at low MER/ROH ratios. In contrast, transeetherification of MER with methylol groups content up to 3 mol/kg affords the

incorporation of RO-groups into the resin up to 8 mol/kg owing to direct etherification of -CH<sub>2</sub>OH groups. The following factors are responsible for the growth of etherified product yield: presence of methylol groups in MER in some amounts without deterioration of MER-ROH compatibilization; CH<sub>3</sub>O-/ROH molar ratio no higher than 1; primary alcohols (ROH) is more preferable compared to secondary ones; thermal activation of the process is more efficient in comparison with acidic catalysis.

## POLYMER HYDROGELS BASED ON 2-HYDROXYETHYL METHACRYLATE: MODIFICATION, SORPTION, AND DESORPTION OF AMINOGLYCOSIDES

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*Russ. J. Appl. Chem.,*  
79(4) (2006) pp. 584-589.

Methods of modification of polymer hydrogels based on 2-hydroxyethyl methacrylate with the aim to improve their hydrophilic characteristics are described. The absorption of antibiotics such as aminoglycosides and the kinetics of their liberation from modified hydrogels are studied.

## NEW METHODS FOR PRODUCTION OF THERAPEUTIC SOFT CONTACT LENSES

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New polymer hydrogel material is synthesized and methods for production of soft contact lenses (SCL) is developed.

1. The developed silicon-hydrogel medical soft contact lenses (MSCL) possess high oxygen permeability (Dk/t > 125) and can be applied for effective relief of the corneal syndrome.

2. MSCL are developed based on synthetic polymer hydrogels with a high water content (70-94.5 wt %). They feature an enhanced sorbability for medical products and capability of releasing them at a controlled rate.

3. The developed biopolymer (gelatin) based MSCL with water content of 80-90 wt % demonstrate a high biological activity and are applicable as wound healing agents in cases of eye damage or diseases.

## MEDICAL SOFT CONTACT LENSES BASED ON POLYMER HYDROGELS

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*The Eye*, 5 (2006).

Under discussion is the therapeutic effect of new soft contact lenses (MSCL) synthesized on the basis of polymer hydrogels with high water content (polyacrylamide, cross-linked gelatin, alkali-modified poly-2-hydroxyethylmetacrylate), as well as a new highly oxygen-permeable silicon-hydrogel. The new MSCL are demonstrated to be effective bandage to relieve the corneal syndrome and to accelerate reparative processes on treating endothelial and epithelial dystrophias and postoperative complications. In order to estimate the MSCL efficiency, several factors are proposed to consider simultaneously; these factors are sorbability of the polymer hydrogel with respect to an antibiotic, antibacterial activity of the antibiotic, the antibiotic capability of crossing the hemiophthalmic barrier. Optimal hydrogel-antibiotic combinations are identified.

## QUANTUM-CHEMICAL STUDIES OF THE STRUCTURE AND CATALYTIC ACTIVITY OF BIS(PHENOXYIMMINE) COMPLEXES OF TITANIUM AND ZIRCONIUM

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*Doklady Chem.*, 410(2) (2006) pp. 217-219.

Quantum chemical calculations were performed to establish regularities of the influence of structures of bis(phenoxyimine) complexes of titanium and zirconium on the process energy during the formation of catalytically active species and their complexes with ethylene, growth of the polymer chains, as well as on the energy of concurrent catalyst deactivation and decomposition processes.

## ELECTRON RADIATION EFFECTS ON THE STRUCTURE OF ULTRADISPERSE POLYTETRAFLUOROETHYLENE

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*J. Struct. Chem.*, 46(5) (2005) pp. 848-855.

Electron radiation effects (40 mrad, 70 mrad, and 100 mrad) on the molecular and supramolecular structure and morphology of ultradisperse polytetrafluoroethylene obtained by the thermogas dynamic (TGD) method were studied by IR and EPR spectroscopy, X-ray phase analysis, and atomic force microscopy. Irradiation of ultradisperse powder in air leads to oxidized polymer forms due to the terminal carbonyl groups and stable peroxide radicals that appear in the structure. Fast electron radiation in doses of up to 100 mrad did not change the polymer crystallinity and particle entity, while thin films on the surface of ultradisperse polytetrafluoroethylene powder decomposed.

## OPTICAL ISOTROPIC MESOPHASE IN SIDE CHAIN COPOLYMERS CONTAINING ISOPHTHALIC ACID GROUPS

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*Liq. Cryst.*, 33(5) (2006) pp. 621-624.

Random side chain copolymers, containing cyanobiphenyl mesogenic units and 37-58 mol% of isophthalic acid monomer units, possess an unusual ability to produce optically isotropic mesophases. This is demonstrated by the absence of birefringence and by high optical transparency of their films. At the same time, corresponding DSC curves show a well pronounced first order transition with a heat of fusion of 1.5-2.34 kJ mol<sup>-1</sup>. A key reason behind the formation of an optically isotropic mesophase is likely to be related to the microphase separation between side groups of the copolymers.



## **INFLUENCE OF SILVER NANOPARTICLES ON THE ORDER PARAMETER OF LIQUID CRYSTALLINE POLYMERS**

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*Liq. Cryst.*, 33(9) (2006) pp. 1059-1063.

New polymer nematic nanocomposites are prepared containing 1.43-4.64 wt% of silver nanoparticles whose mean dimensions are 2-4 nm.

According to H<sub>2</sub> NMR spectroscopic measurements, on increasing the content of metallic nanoparticles, the orientational order parameter S<sub>zz</sub> of the nematic phase shown by the nanocomposites increases.

## **Composite Sorbents**

### **NEW COMPOSITE ADSORBENTS FOR CONVERSION AND STORAGE OF LOW TEMPERATURE HEAT: ACTIVITY IN THE BORESKOV INSTITUTE OF CATALYSIS**

**Yu.I. Aristov**

*J. Heat Transfer Soc. Jpn.*,  
45(192) 2006) pp. 12-19.

In this communication it is discussed how to design new solid sorbents with sorption properties close or even equal to those perfectly fitting the cycle. In the first part the mentioned requirements are formulated for a particular single-effect non-regenerative cycle driven by low temperature heat. The conclusion has been made that solid sorbents which match in the best way the theoretical requirements for mentioned cycle are those with a monovariant equilibrium, specifically, salts and their crystalline hydrates capable of exchanging water due to chemical reaction with the salt. The second part of the paper is devoted to practical tools, which are available to design and synthesise an optimal composite sorbent of water for a particular ATH cycle. It was proved that the sorption properties of SWSs can be monitored by a proper choice of the chemical nature and content of the confined salt, the average size of pores of the host matrix and synthesis conditions. Thus, this part reviews the current state-of-the art on the new family of the SWS composites.

### **A NEW APPROACH TO HEAT AND MOISTURE REGENERATION IN THE VENTILATION SYSTEM OF ROOMS. I. LABORATORY PROTOTYPE OF THE REGENERATOR**

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*J. Engin. Phys. Thermophys.*,  
79(3) (2006) pp. 569-576.

A new heat-and-mass transfer device that a) permits simultaneous heat and moisture regeneration in the ventilation system, b) provides anti-icing at the heat-exchanger outlet, and c) maintains comfortable humidity in a room is proposed. In this unit a composite sorbent is used for moisture exchange and a heat accumulating medium for heat exchange between income and outcome air fluxes. First part presents experimental results on cyclic heat exchange and its optimization to reach a high degree of heat regeneration. Proper heat storing material and its grain size were chosen. The affect of the air residence time and half cycle time on regeneration degree was studied.

### **A NEW APPROACH TO HEAT AND MOISTURE REGENERATION IN THE VENTILATION SYSTEM OF ROOMS. II. PROTOTYPE OF THE REAL DEVICE**

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*J. Engin. Phys. Thermophys.*,  
79(3) (2006) pp. 577-584.

This paper presents the results of investigations conducted on the real prototype of a regenerator

whose operating conditions depended on the weather conditions during the testing (winter of 2004). It has been shown that the heat and moisture recovery coefficients can be purposefully and independently regulated in a wide range by proper adsorbent and heat-accumulating medium selection. The use of the proposed device in the ventilation system of a standard two-room apartment can lead to a 44% reduction of heating costs annually.

#### KINETICS OF WATER ADSORPTION ON SILICA FUJI DAVISON RD

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*Microporous Mesoporous Mater.*, 96(1-3) (2006) pp. 65-71.

The kinetics of water adsorption on loose grains of Fuji Davison RD silica gel was studied by a TG differential step method in the temperature range 29–64°C and in the pressure range 6.5–34 mbar. Three grain sizes were selected, 0.3–0.325, 0.355–0.425 mm and 0.8–1.0 mm. Furthermore, adsorption isobars at  $P_{H_2O} = 9, 18$  and 48 mbar were measured over the temperature range of 30–150°C by a TG technique to determine pertinent equilibrium parameters which are used to calculate the coefficients of diffusion. The equilibrium uptake was described as a linear function of the Dubinin–Polanyi adsorption potential.

It was found that the influence of particle size, temperature and pressure on the adsorption kinetics can be well described in terms of the Fickian diffusion model. The apparent water diffusivity  $D_{ap}$  was found to be an Arrhenius function of temperature with the apparent activation energy  $E_a = 41.5$  kJ/mol and the pre-exponential factor  $D_{ap0} = 2.9 \times 10^{-4}$  m<sup>2</sup>/s. The apparent diffusivity of water in silica pores was measured to be  $D_e = (3.7–4.7) \times 10^{-7}$  m<sup>2</sup>/s and possessed a slight increase with temperature. This value is close to the Knudsen diffusivity, calculated for a cylindrical pore of radius  $r_p = 1.0$  nm.

For smaller grains at  $T > 39^\circ\text{C}$  the contribution of thermal effects was revealed, which decreases the rate of water sorption. In this case, application of non-isothermal kinetic model of Lee and Ruthven allowed good description of experimental uptake curves as well as the estimation of parameters which determine simultaneous heat and mass transfer.

#### KINETICS OF WATER SORPTION ON SWS-1L (CALCIUM CHLORIDE CONFINED TO MESOPOROUS SILICA GEL): INFLUENCE OF GRAIN SIZE AND TEMPERATURE

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*Chem. Eng. Sci.*, 61(5) (2006) pp. 1453-1458.

Kinetics of water sorption on loose grains of composite sorbent CaCl<sub>2</sub> confined to mesoporous silica (SWS-1L) was measured at  $T=33-69^\circ\text{C}$  and  $P_{(H_2O)}=8-70$  mbar over water uptake range 0–0.47 g/g for various particle sizes  $R_p$  (between 0.355 and 1.4 mm). The measurements were performed in a constant pressure unit based on a CAHN microbalance under isothermal external conditions. The results obtained evidence an enhancement of the sorption rate and apparent diffusion constant with the decrease in the particle size (approximately as  $R_p^{-2}$  at  $R_p > 0.71$  mm). Contribution of thermal effects was found for water sorption on smaller SWS particles (0.355–0.425 mm), which decreases the sorption rate. The apparent water diffusivity was found to depend on the local slope of the SWS water sorption isotherm. The pore diffusivity of water in the temperature range 33–69°C was calculated from experimental data  $D_e = (0.12 \pm 0.06) \times 10^{-6}$  m<sup>2</sup>/s that is approximately 10 times lower than the Knudsen pore diffusivity estimated for pores of silica KSK. The possible reasons of the diffusivity reduction are discussed.

#### KINETICS OF WATER SORPTION ON A CaCl<sub>2</sub>-IN-SILICA-GEL-PORES SORBENT: THE EFFECTS OF THE PELLET SIZE AND TEMPERATURE

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*Kinet. Catal.*, 47(5) (2006) pp. 770-775.

Kinetics of water vapor sorption on the CaCl<sub>2</sub>-in-KSK-pores composite (SWS-1L) have been studied at  $T = 33-69^\circ\text{C}$  and vapor pressures of 8–70 mbar for pellet sizes of  $2R_{pel} = 0.355-0.425, 0.71-0.85,$  and 1.2–1.4 mm. Sorption has been measured under isothermal conditions on a thermobalance by abruptly raising the vapor pressure in the measurement cell by a small value and then maintaining the new pressure. In the initial portion of the kinetic curves, the amount of sorbed water ( $\Delta m$ ) increases in proportion to the sorption time ( $t$ ) to the power 1/2. From the slope of the  $\Delta m$  versus  $t^{1/2}$  curve, it is possible to derive the sorption rate constant  $k_D = D_{eff}/R_{pel}^2$  and the effective diffusivity  $D_{eff}$ . The latter is independent of  $R_{pel}$  for

$2R_{\text{pel}} \geq 0.71$  mm. The rate of water sorption on smaller (0.355-0.425 mm) pellets grows less rapidly, apparently because of the effect of the heat of sorption. The effective diffusivity is determined by the local slope of the water vapor sorption isotherm for SWS-1L. Applying an appropriate correction enables one to calculate the effective diffusivity for water vapor in the sorbent pores, which appears to be  $D_e = (0.35 \pm 0.17) \cdot 10^{-6}$  m<sup>2</sup>/s. This value is approximately 10 times smaller than the Knudsen water diffusion coefficient calculated for a single cylindrical pore with a size equal to the average pore size of the composite. Two possible causes of this discrepancy are discussed, specifically, an increase in the pore tortuosity because of the presence of the salt and the interaction between water and the salt.

#### DYNAMICS OF HYDRATION WATER IN CaCl<sub>2</sub> COMPLEXES

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*Chem. Phys. Lett.*, 419(1-3) (2006) pp. 111-114.

The measurement of unusually well-defined vibrational modes of water are reported. Calcium chloride forms complexes made of different amounts of water, namely 1/3, 2 or 4 water per CaCl<sub>2</sub> molecule. Based on the crystallographic structure, normal mode calculations from first principles were performed, and the neutron scattering spectra were simulated. A very good agreement between calculation and experiment, without any parameter refinement, confirms and completes the intuitive assignment of vibrational excitations of water. A closer look at the calculation enables to investigate the anharmonicity of the system and the dispersion of the excitations along the hydrogen bonds.

#### DYNAMICS OF WATER VAPOR SORPTION IN A CaCl<sub>2</sub>/SILICA GEL/BINDER BED: THE EFFECT OF THE BED PORE STRUCTURE

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*Kinet. Catal.*, 47(5) (2006) pp. 776-781.

The dynamics of water vapor sorption in a compact, binder-containing bed of a CaCl<sub>2</sub>-in-silica-gel-pores sorbent has been investigated by NMR microscopy. The procedure suggested for the preparation of this bed allows the porous structure of the bed to be modified in a wide range. The bed pore structure and water transfer in the bed have been studied in relation to the particle size of the initial

silica gel, the size of mesopores in the sorbent particles, and the binder content. By varying these parameters, it is possible to optimize the ratio of the diffusion resistance of the interparticle macropores to that of the internal mesopores of the particles. If sorption is controlled by water diffusion in the macropores, a sorption front forms in the sample to move inside the bed. The distance traveled by the front is proportional to the sorption time to the power 1/2. The effective diffusion coefficient of water in the macropores is estimated from the front motion dynamics to be between  $0.8 \times 10^{-9}$  and  $3.0 \times 10^{-9}$  m<sup>2</sup>/s, depending on the porous structure of the bed.

#### DYNAMICS OF WATER SORPTION ON COMPOSITES "CaCl<sub>2</sub> IN SILICA": SINGLE GRAIN, GRANULATED BED, CONSOLIDATED LAYER

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*Fluid Transport in Nanoporous Materials: Proceedings of the NATO Advanced Study Institute, NATO Science Series II: Mathematics, Physics and Chemistry, Springer, Eds. W.C. Conner, J. Fraissard, 2006, pp. 553-565.*

In the paper results on kinetics of water sorption on composite "CaCl<sub>2</sub> in mesoporous silica KSK" are presented. Three adsorbent configurations are considered, namely, a single grain, a granulated layer and a consolidated layer prepared with a binder and pore-forming additives.

Three methods have been used to study the water transport and sorption: a) <sup>1</sup>H NMR microimaging experiments on the spatial distribution of sorbed water in the sorbent and its temporal evolution, b) the PFG NMR method and c) the kinetics of water sorption under constant volume-variable pressure conditions.

#### IMPACT OF PHASE COMPOSITION ON WATER ADSORPTION ON INORGANIC HYBRIDS "SALT/SILICA"

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*J. Colloid Interface Sci.*, 301(2) (2006) pp. 685-691.

The effect of a "guest-host" interaction on the phase composition and sorption properties of the composite sorbents "salt in a porous host matrix" has been studied. The matrix was a mesoporous silica of KSK type, while the confined salts were CaCl<sub>2</sub>,

CuSO<sub>4</sub>, MgSO<sub>4</sub>, and Na<sub>2</sub>SO<sub>4</sub>. Both structure and properties of the composites were studied by X-ray diffraction, titration in the pH range of 2–9, differential dissolution, and TG techniques. Chemical interaction between the silica surface and the salt during preparation results in the formation of the salt surface complexes and stabilization of the dispersed salt in two phases, namely, a crystalline phase and an X-ray amorphous phase. The water sorption properties of the composites depend on the phase composition and can be intently modified by using variation of the preparation conditions.

#### **AMMONIA SORPTION ON COMPOSITES "CaCl<sub>2</sub> IN INORGANIC HOST MATRIX": ISOSTERIC CHART AND ITS PERFORMANCE**

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*Int. J. Low Carbon Techn.*,  
1(3) (2006) pp. 191-200.

The isosteres of ammonia sorption on new composite sorbents "CaCl<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub>" and "CaCl<sub>2</sub>/vermiculite" were measured at T = 20-90°C and P = 0.08-9 bar. It was found that the modification of host matrices by the salt dramatically increases the ammonia uptake due to the formation of CaCl<sub>2</sub>·nNH<sub>3</sub> complexes. The isobaric enthalpy and entropy of ammonia sorption by the salt confined to alumina pores were significantly lower respect to those for the bulk one. For a basic cycle, the values of COP = 0.40-0.48 were calculated at T<sub>e</sub> = -18°C, T<sub>c</sub> = 36-42°C and T<sub>g</sub> = 117-120°C. High COP could make these sorbents promising for application in cooling units driven by relatively low temperature heat.

#### **ASSESSMENT OF THE OPERATION OF A LOW-TEMPERATURE ADSORPTION REFRIGERATOR**

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*Therm. Eng.*,  
53(3) (2006) pp. 240-244.

A simple algorithm is proposed, based on Polanyi's temperature invariance principle, for selecting adsorbents that hold promise for the development of adsorption refrigerators using sources of low-grade heat (industrial heat wastes, solar energy, etc.). It is shown that, among the materials considered, those holding most promise for the development of adsorption systems for cooling water are new composite selective water sorbents, primarily KSKG silicagel modified with calcium chloride.

#### **NEW COMPOSITE WATER AND AMMONIA SORBENTS FOR CHEMICAL AND ADSORPTION HEAT PUMPS**

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*J. Engin. Phys. Thermophys.*,  
79(6) (2006) pp. 531-552.

Review of new composite water and ammonia sorbents - composites "salt in a porous host matrix" is given. Possibility of monitoring sorption properties of composites on the nanophase level by proper choice of their composition, size of pores of the host matrix and synthesis conditions is shown. The use of new materials in devices for storage of low temperature heat is considered.

## Catalysts for Organic Products Synthesis

### COPPER AND SILVER ACTIVITY IN THE COURSE OF PARTIAL ETHYLENE GLYCOL OXIDATION

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*Catal. Ind.*,  
5 (2006) pp. 25-30.

The partial ethylene glycol oxidation allows producing glyoxal – valuable product used in a number of organic syntheses. The process is not realized commercially in Russia that is caused by the lacking of proper domestic catalytic systems. Activities of polycrystalline Cu- and Ag-catalysts for the ethylene glycol oxidation process proposed for production are compared. Copper and silver activities are studied under the comparable conditions with variation of temperature and oxygen content in the reaction mixture. A possibility was shown to improve the given value for both metals by introducing phosphor-containing promoters to facilitate the formation of dispersed metal particles on the surface, which act as highly active centers of ethylene glycol to glyoxal conversion. The catalysts studied may be recommended to be used as active systems of industrial synthesis of glyoxal.

### LIQUID PRODUCTS OF THE PROCESSES OF HYDROGENATION AND HYDROLYSIS OF BARZAS SAPROMIXITE

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*Chem. Sustain. Devel.*,  
14(1) (2006) pp. 73-80.

Liquid products of the processes of hydrogenation and hydrolysis of Barzas sapromixite under autoclave conditions are studied. The application of mechanochemically activated iron-ore catalyst in the processes of hydrogenation and hydrolysis of sapromixite allows one to increase the content of distillate fractions in liquid products, and low-molecular hydrocarbons in low-boiling fraction with boiling point 180°C.

### CATALYTIC HYDROLIQUEFACTION OF BARZASS LIPTOBIOLITIC COAL IN A PETROLEUM RESIDUE AS A SOLVENT

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*Fuel*, 85(7-8) (2006) pp. 918-922.

Hydrogenation of liptobiolitic coal from the Barzas Pit (Russia) in a petroleum residue as a solvent was investigated in the presence of an iron containing ore catalyst at 400-430°C and working pressure 7.1 MPa. Near 94-97% of the coal organic mass was converted into gaseous and liquid products. The addition of the catalyst in amount of 5% to the coal mass increases the degree of the coal conversion by 21-23 wt%. Under these conditions, the yield of hydrocarbon light liquid products (bp<200°C) was increased up to 24-28 wt%. The distillate products consist mainly of paraffins, while most part of the aromatic hydrocarbons are alkylbenzenes.

### SYNTHESIS OF METHYLMERCAPTAN FROM METHANOL AND HYDROGEN SULFIDE AT ELEVATED PRESSURE ON AN INDUSTRIAL CATALYST

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*Petr. Chem.*,  
46(1) (2006) pp. 28-33.

The catalytic reaction of methanol with hydrogen sulfide at a total pressure of 0.1–1.8 MPa was investigated. The main product at different values of total pressure in the system was methylmercaptan, and the by-products were dimethyl sulfide, dimethyl ether, carbon oxides. An increase in the contact time increased the yields of methylmercaptan and dimethyl sulfide, whereas the yields of dimethyl ether and gases changed slightly. The selectivity for methylmercaptan was approximately constant up to a ~95% conversion of methanol. The elevation in temperature increased the reaction rate but barely affected the product formation selectivity. The rate of methanol conversion increases linearly with the hydrogen sulfide concentration and depends on the methanol concentration raised to a power of 0.4–0.5; water retards the process. The selectivity for methylmercaptan decreases, and that for dimethyl sulfide and dimethyl ether increases at an H<sub>2</sub>S to methanol molar ratio below 1.4 : 1, regardless of the

value of total pressure. The reaction rate increases with the total pressure raise to a power 0.4–0.5; however, the selectivities for methylmercaptan and by-products remain unchanged.

#### **METHANE OXIDATION BY LATTICE OXYGEN OF CeNbO<sub>4+d</sub>**

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*Catal. Commun.*,  
8(3) (2007) pp. 335-339.

The reactivity of methane with lattice oxygen of cerium niobate, CeNbO<sub>4+δ</sub>, was studied by temperature-programmed reduction (TPR) in dry CH<sub>4</sub> flow at 523–1073 K. Phase transformations and reduction of cerium niobate at 900–1023 K lead to a massive release of hyperstoichiometric oxygen, in amounts determined by the intermediate-temperature phase composition dependent on thermal history. In this temperature range, CH<sub>4</sub>-TPR shows prevailing formation of carbon monoxide and steam, suggesting that the synthesis gas generation occurs in parallel with extensive oxidation of H<sub>2</sub> on the cerium niobate surface. At 1073 K when  $\delta \rightarrow 0$ , the reaction of methane with CeNbO<sub>4+δ</sub> selectively yields synthesis gas with H<sub>2</sub>/CO ratio close to two.

#### **CATALYSTS FOR NON-OXIDATIVE METHANE CONVERSION**

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*Stud. Surf. Sci. Catal.*,  
162 (2006) pp. 913-920.

In the last few years the researchers give considerable attention to the process of the Non-Oxidative Methane Conversion into aromatic hydrocarbons over zeolite catalysts modified by the ions of transient metals. Generally, the catalysts are produced via mechanical mixing of a zeolite with metal oxide or via zeolite impregnation by metal salt solution followed by drying and calcination.

The present paper cites the data on the production of Mo-containing catalysts of methane dehydroaromatization both by conventional methods and using a nanosized powder (NSP) of molybdenum (0.5–6.0 wt%) produced via wire electroexplosion in argon medium. The tests of the catalytic activity of Mo/ZSM-5

catalysts produced were performed in a flow type installation at 750°C, gas hourly space velocity 1000 h<sup>-1</sup> and atmospheric pressure.

The methods of high-resolution transmission electron microscopy (HRTEM), energy-dispersive X-ray (EDX) spectroscopy were used to study the state of active sites of the catalysts produced. In accordance with the data of HRTEM and EDX analysis, Mo is present in the catalysts in two forms. The first Mo form is stabilized on the zeolite surface as the 2–10 nm particles and identified as a phase of Mo<sub>2</sub>C carbide. In the inner zeolite channels the second form of Mo stabilization as Mo-containing clusters less than 1 nm was found. The increase in the Mo content in a zeolite to 6 wt% results in the increase in the size of intravolume clusters to ~ 2 nm.

Using HRTEM, it was established that during the preparation and reaction two kinds of mesopores are formed in the porous zeolite texture: extended mesopores 3–10 nm in diameter having the exit to the external surface and mesopores formed as a result of zeolite dealumination in the reaction course followed by the formation of Mo aluminates or its carbided forms. The development of the mesoporous zeolite structure is an important factor promoting the activity of Mo-HZSM in the reactions of the formation of high-molecular aromatic compounds. A higher activity and stability of the catalysts produced using Mo NSP as compared with other samples were established.

#### **METHANOL DEHYDROGENATION OVER COPPER-CONTAINING CATALYSTS MODIFIED BY ZINC OXIDE**

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*Catal. Ind.*, 3 (2006) pp. 29-33.

The aim of the work is improvement of catalytic properties of copper-containing methanol-to-methyl formate dehydrogenation catalysts, methyl formate being industrially important semiproduct in the organic synthesis processes. The effect of modifying zinc oxide additive on activity and selectivity to methyl formate of 5%Cu/SiO<sub>2</sub> and 5%Cu/Sibunit catalysts was investigated. It was found that its introduction results in increasing the yield of methyl formate up to 1.2–1.5 times for silica gel-based samples but the opposite dependence for Sibunit-based one. The X-ray phase analysis was used to study the nature of observed differences: it was found the dispersion of copper particles in the case of SiO<sub>2</sub> and

their coarsening in the case of Sibunit using. The modified catalyst with Cu/ZnO = 2/1 ratio may be recommended for operation at the semi-industrial scale.

#### **DIMERIZATION OF $\alpha$ -METHYLSTYRENE ON HIGH-SILICA ZEOLITES**

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*Petrol. Chem.*,  
46(5) (2006) pp. 332-337.

$\alpha$ -Methylstyrene dimerization was studied on high-silica  $\beta$ , ZSM-12, and TsVN zeolites. The acid properties of the zeolites were studied by IR spectroscopy. It was revealed that the catalytic properties of the zeolites in  $\alpha$ -methylstyrene dimerization depend on both the acidic and structural characteristics of the catalysts. The highest activity in the reaction was exhibited by zeolite  $\beta$ , as the maximum amount of acid sites were found in its structural units (inside channels, on the outer surface). Zeolite ZSM-12 had the highest selectivity for linear dimers.

#### **ZrFe INTERMETALLIDES FOR FISCHER-TROPSCH SYNTHESIS: PURE AND ENCAPSULATED INTO ALUMINA-CONTAINING MATRICES**

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*Stud. Surf. Sci. Catal.*,  
163 (2006) pp. 125-128.

Performance of the bulk hydrogenated ZrFe intermetallides both pure and encapsulated into

alumina-containing matrix ( $\text{Al}_2\text{O}_3/\text{Al}$ ,  $\text{Al}_2\text{O}_3$ ) was studied in catalysis of Fischer-Tropsch synthesis. Their structural, textural and surface properties were characterized by combination of such methods as XRD, SEM, TEM, nitrogen adsorption-desorption isotherms and XPS, and impact of these properties on catalytic activity and selectivity was analyzed. The highest activity per the surface Fe atom ( $\sim 5 \cdot 10^{-19}$   $\text{CH}_x/\text{at.Fe}\cdot\text{h}$ ) was obtained for pure active component, while the highest activity per the unit of volume ( $\sim 168$   $\text{g C}_{5+}/\text{l}\cdot\text{h}$ ) was revealed for a composite catalyst at 300°C, 3 MPa and space velocity  $\sim 7000$   $\text{h}^{-1}$ .

#### **HYDROGENATION OF SOME NATURAL TERPENES OVER $\text{CuO-Al}_2\text{O}_3$ AND $\text{NiO-Cr}_2\text{O}_3$ CATALYSTS**

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*Chem. Sustain. Devel.*, 14(5) (2006) pp. 523-528.

Reaction of catalytic hydrogenation of natural compounds (limonene,  $\alpha$ -pinene,  $\beta$ -pinene, camphene, 3-carene) is studied over  $\text{CuO-Al}_2\text{O}_3$ ,  $\text{NiO-Cr}_2\text{O}_3$  and for comparison over  $\text{Pt}/\gamma\text{-Al}_2\text{O}_3$  catalysts at high temperatures (180-350°C) and under the pressure 2.5-3 atm in catalytic flow reactor. Reaction products were analyzed by chromatomass spectrometry quantitatively and qualitatively. The highest efficiency and high selectivity were observed on  $\text{CuO-Al}_2\text{O}_3$  catalyst. Isomeric mixture of *para*-mentanes, or *para*-1-menten is formed from limonene depending on catalyst activity;  $\alpha$ - and  $\beta$ -pinenes gives a mixture of *cis*- and *trans*-pinanes with prevalence of the last isomer; camphene gives isomeric mixture of *exo*- and *endo*-isocamphenes in equal quantities; 3-carene gives 1,1,4-trimethylcycloheptane.

# Mathematical Simulation of Processes and Reactors. Chemical Engineering

## EFFECT OF OXYGEN MOBILITY IN SOLID CATALYST ON TRANSIENT REGIMES OF CATALYTIC REACTION OF METHANE PARTIAL OXIDATION AT SHORT CONTACT TIMES

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*Catal. Lett.*,  
110(3-4)(2006) pp. 235-242.

Mathematical modeling of the effect of the oxygen mobility in a solid oxide catalyst on the dynamics of transients of fast catalytic reactions has been carried out. The analysis was based upon the redox mechanistic scheme with a due regard for diffusion of oxygen from the bulk of catalyst to its surface. Parameters of kinetic and mathematical models were selected via fitting of the experimental data for methane selective oxidation into syngas on 1.4%Pt/Gd<sub>0.2</sub>Ce<sub>0.4</sub>Zr<sub>0.4</sub>O<sub>x</sub> catalyst. The range of the Thiele parameter ( $\phi$ ) where the oxygen bulk diffusion affects the most strongly reaction transients corresponds to  $\phi \in [0.3-7]$ . For high-surface-area oxide catalysts, the bulk oxygen diffusion coefficients corresponding to this range of the Thiele parameter are in the range of  $10^{-18}$ - $10^{-13}$  cm<sup>2</sup>/s.

## EXPERIMENTAL STUDY OF THE GAS-PHASE HYDROFLUORINATION OF PERCHLOROETHYLENE OVER A CHROMIUM-BASED CATALYST

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*React. Kinet. Catal. Lett.*,  
88(2) (2006) pp. 399-404.

Gas-phase hydrofluorination of perchloroethylene to pentafluoroethane in the presence of a chromium-magnesium catalyst at 0.4 MPa and 330–390°C has been studied. A reaction scheme taking into account the formation of by-products is suggested.

## KINETIC BEHAVIOR OF BENZENE HYDROGENATION AND THIOPHENE HYDROGENOLYSIS ON SULFIDE Ni-Mo/Al<sub>2</sub>O<sub>3</sub> CATALYST

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*React. Kinet. Catal. Lett.*,  
88(2) (2006) pp. 325-332.

An unsteady-state kinetic model of both benzene hydrogenation (HDA) and thiophene hydrogenolysis

(HDS) on a sulfide hydrotreating catalyst Ni-Mo/Al<sub>2</sub>O<sub>3</sub> has been developed. The model adequately describes experimental data obtained at the pressure 2 MPa, temperature 573 K and at various contact times and ratios of benzene/thiophene. The model is based on the assumption that the catalyst surface contains only one type of active sites, *i.e.*, Ni atoms in the sulfide bimetallic species, which are responsible for both hydrogenolysis and hydrogenation reactions.

## MATHEMATICAL MODEL OF UNSTEADY STATE PROCESSES IN A MULTI-SECTIONAL SYMMETRIC CATALYTIC REACTOR

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*Siberian J. Ind. Appl. Math.*,  
VIII, 3(23) (2005) pp. 48-57.

Mathematical model of unsteady state processes in a multi-sectional symmetric catalytic reactor with periodic changes of the input gas flow direction is developed. The peculiarity of this apparatus is as follows: the fixed bed consists of six granular layers, in the outer layers of an inert material, there are no chemical reactions proceeding, while in two next layers the catalytic reactions take place, and in two central layers of an inert granular substance the homogeneous reactions proceed. Moreover, after the third part of the fixed bed a part of the gas flow is directed out from the reactor into an outer heat exchanger. In the case in hands, the coefficients of the two-phase one-dimensional model are step functions. The significant difference in the intensity of the homogeneous and catalytic reactions leads to some high gradients which propagate along the computational region in the dynamical operation. In the paper an efficient algorithm is suggested for numerical studies of the model. It is based on the balanced monotonic difference schemes. The dynamics of periodic solution formation is described and the periodic operation parameters are studied.



### **MODELING OF STEAM REFORMING OF NATURAL GAS USING CATALYSTS WITH GRAINS OF COMPLEX SHAPES**

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N.V. Vernikovskaya, E.I. Smirnov, V.A. Kuzmin,  
N.A. Chumakova**

*Theor. Found. Chem. Eng.*,  
40(2) (2006) pp. 155-167.

A mathematical model is developed to describe steam reforming of natural gas in a catalyst grain and a catalyst bed. The model differs from the published ones by a detailed description of the processes in a catalyst grain and the mechanisms of radial heat and mass transfer, including for catalyst grains of complex shape. The model parameters are numerically analyzed, and the efficiencies of catalyst grains of different shapes and sizes are compared.

### **REGENERATION OF A CATALYTIC FILTER IN THE PRESENCE OF HIGHLY FLAMMABLE HYDROCARBONS IN SOOT**

**T.L. Pavlova, N.V. Vernikovskaya,  
N.A. Chumakova, A.S. Noskov**

*Combust., Explosion, Shock Waves*,  
42(4) (2006) pp. 396-402.

The dynamical process of oxidative regeneration of a catalytic particulate filter made of a fibrous material is analyzed theoretically by mathematical modeling. The model describes the dynamics of temperature and concentrations of gaseous composition and soot particles in the filter wall. The effect of the controlled rate of the input temperature increase and the presence of highly flammable hydrocarbons in exhaust gases entering the filter is demonstrated.

### **AUTOMATION OF CALCULATIONS OF CHEMICAL-TECHNOLOGICAL SCHEMES OF CATALYTIC PROCESSES**

**I.V. Bukreeva, Yu.V. Malozemov, V.S. Kharitonov,  
A.S. Shmelyov, S.I. Reshetnikov, I.A. Zolotarsky**

*Catal. Ind.*, 4 (2006) pp. 24-29.

Application of information-computer complexes has been considered for implementation of computer calculations of complex chemical-technological schemes of catalytic processes. The most general principles of their formulation and architecture are given. Taken one of them (FLOCAS) as an example, its structure and the main directions of use are shown, for example, the development of new chemical-technological productions and optimization of current

ones, analysis of technical proposals, searching the optimal operations of equipment operation, and others.

### **APPLICATION OF THE CHEMPAK PACKAGE FOR MODELING OF GAS-DYNAMICS REACTOR**

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*Comput. Technol.*, 11(1) (2006) pp. 35-51.

The ChemPAK program package for solving the direct problems of chemical kinetics with arbitrary number of chemical reactions is suggested. The package contains an expandable library of computational modules and provides a function of data transfer to multiprocessor. The process of  $C_1$ - $C_2$  hydrocarbon's pyrolysis in gas-dynamics reactor with emission has been numerically simulated using the ChemPak software package.

### **SIMULATION OF THE THREE-DIMENSIONAL DYNAMICS OF MATTER IN THE GRAVITATIONAL FIELD USING MULTIPROCESSOR COMPUTERS**

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*Comput. Technol.*, 11(1) (2006) pp. 15-27.

A numerical model for investigation of the 3D motion of matter in a gravitational field is proposed. The model satisfies all fundamental conservation laws. For acceleration of computations an effective parallel algorithm for use on multiprocessor computers with distributed memory is implemented. The results of the numerical experiments with the initial distribution of matter in the form of a plane disk are presented. These experiments are aimed to define the parameters' values, which lead to the stability of the disk with respect to asymmetrical disturbances directed along the axis of rotation and to the spiral gravity waves.

## INVESTIGATION OF FINE GRANULAR MATERIAL FLOW THROUGH A PACKED BED

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*Chem. Eng. Sci.*, 61(8) (2006) pp. 2394-2405.

Three different methods cut-off, time-of-flight, and Pulsed Field Gradient Nuclear Magnetic Resonance were used to study downstream flow of fine granular material through the fixed bed reactor. For describing the transport of solid particles within a fixed granular bed, a model has been developed. In time-of-flight and cut-off techniques the highest average velocity of filtration is observed at the lowest mass flow rate in all experimental traces, while upon the flow rate increase it tends to an asymptotic value. Experimental results obtained by pulsed field gradient nuclear magnetic resonance technique have revealed the bimodal character of particles velocities distribution. The average filtration velocity has a maximum at an intermediate mass flow rate close to the bed flooding, in contrast to the results obtained by cut-off and time-of-flight methods. The velocities measured using all three techniques were compared by converting them into dimensionless values. From the experimental results, the values of model parameters have been evaluated which allowed to describe particle velocities within a bed.

## MATHEMATIC MODELING OF THE PROCESS OF PRODUCTION OF NANOFIBROUS CARBON FROM METHANE IN AN ISOTHERMAL REACTOR WITH A FIXED BED OF THE Ni–Al<sub>2</sub>O<sub>3</sub> CATALYST

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*Chem. Eng. J.*, 120(3) (2006) pp. 139-147.

The process of synthesis of nanofibrous carbon from methane achieved in an isothermal plug flow reactor with a fixed bed of catalyst 90 wt.% Ni–Al<sub>2</sub>O<sub>3</sub> is considered. It is shown that the equations allow a solution in the form of a progressive wave of deactivation that moves at a constant rate and has a stationary profile. Analytic dependencies are obtained to calculate the wave rate and carbon content in the deactivated catalyst. The process parameters are calculated at 823 K and specific methane consumption 120 l/h g. The process parameters are compared for two types of reactors operating at identical conditions: a plug flow reactor with the fixed catalyst bed and a

reactor with perfect mixing of catalyst particles and gas. The specific carbon yield is shown to be higher in the latter.

## OXYGEN DIFFUSION IN NANOSTRUCTURED PEROVSKITES

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*Catal. Today*, 118(1-2) (2006) pp. 151-157.

Nonstoichiometric perovskite-related oxides (e.g. ferrites and cobaltites, etc.) are characterized by fast oxygen transport at ambient temperatures, which relates to the microstructural texturing of these materials, consisting wholly of nanoscale microdomains.

A heterogeneous diffusion model to describe the kinetics of oxygen incorporation into nanostructured oxides have been developed. Nanodomain boundaries are assumed to be the high diffusivity paths for oxygen transport whereas diffusion into the ordered domains proceeds much slower. The model has been applied for qualitative evaluation of oxygen diffusion parameters from the data on wet electrochemical oxidation of nanostructured perovskite SrCo<sub>0.5</sub>Fe<sub>0.2</sub>Ta<sub>0.3</sub>O<sub>3-y</sub> samples.

Using Laplace transform methods, an exact solution is found for a ramped step-wise potential, allowing fitting of the experimental data to theoretical curves (in Laplace transforms). A further model generalization is considered by introducing additional parameters for the size distribution of domains and particles.

## DEVELOPMENT OF PORTABLE HYDROGEN GENERATOR USING CHEMICAL HYDRIDE

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*Int. Sci. J. Alternative Energy Ecol.*, 7 (2006) pp. 29-30.

Application of portable fuel cells raises the problem of creation of hydrogen compact sources. At present several types of portable hydrogen generators for fuel cells are offered, including the perspective generators based on hydrolysis of hydrides – sodium

borohydride and ammonia-borane. Joint efforts of State Research Institute of Chemistry and Technology of Organoelement Compounds and Boreskov Institute of Catalysis allow to develop portable systems for hydrogen generation on the basis of sodium borohydride hydrolysis with optimized mass and size properties.

In this study was found that Ru and Rh catalysts supported on untraditional LiCoO<sub>2</sub> carrier and TiO<sub>2</sub> show the highest activity in NaBH<sub>4</sub> hydrolysis in comparison with catalysts prepared using traditional supports -  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, carbonaceous material.

Carried out studies have permitted to develop the optimized design of portable hydrogen generator with automatic control system.

#### **THERMOLYSIS OF $\alpha$ -PINENE IN SUPERCRITICAL LOWER ALCOHOLS**

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*Russ. Chem. Bull.*,  
54(8) (2005) pp. 987-992.

Thermal isomerization of  $\alpha$ -pinene in supercritical solvents, viz., ethanol, methanol, and propan-1-ol, was carried out, and differences in the rate and selectivity of the process were revealed. In supercritical ethanol the reaction rate increases sharply and the selectivity remains unchanged with an increase in the temperature (from 290 to 390°C) or pressure (from 90 to 270 atm). The main reaction products are limonene, isomeric alloocimenes, and pyronenes. The selectivity for limonene in propan-1-ol is higher than in other alcohols when the conversion of  $\alpha$ -pinene is not higher than 50%. In supercritical ethanol (430°C, 120 atm, 140 s) limonene is more stable than  $\alpha$ -pinene (conversion 8%).

#### **RESULTS OF TESTING THE PLANT FOR SUPERCRITICAL WATER OXIDATION OF NITROGLYCERIN AND DIETHYLENE GLYCOL DINITRATE**

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*Ind. Eng. Chem. Res.*,  
45(24) (2006) pp. 7977-7981.

In Russia, the first stationary supercritical water oxidation (SCWO) pilot plant for the oxidation of

industrial wastes at an operating factory with a tubular flow reactor and a capacity of about 40 kg/h wastewater has been created on the basis of fundamental investigations. It allowed for the elimination of a mixture of nitroglycerin and diethylene glycol dinitrate in the wastewater with very high efficiency. Acetone was used as the fuel, and hydrogen peroxide or air was used as the oxidant.

#### **PURIFICATION OF DETONATION PRODUCTS FROM TOXIC COMPOUNDS**

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In "*Shock-Assisted Synthesis and Modification of Materials*",  
Eds. A.A. Deribas, Yu.B. Scheck, Moscow:  
Torus Press Ltd., 2006, 176 pp.

In this work, various systems for purification of gaseous detonation products from toxic constituents are tested. Ammonite and hexogen charges were exploded in a blasting camera. Hexogen contained the admixture of Cu and Al<sub>2</sub>O<sub>3</sub> powders. Purification of gases from solid particles was performed with a centrifugal bubble apparatus containing a gas-liquid layer wetted with a cuprammonium solution. This technique turned out effective for entrapping carbon compounds and dust but insufficient for nitrogen- and sulfur-containing compounds. For this reason, also was tested the absorber based on phosphor ammonium salts developed at the Boreskov Institute of Catalysis. The content of hazardous gases was detected with a portable chromatograph AkhG-002-01.

#### **HYDROGEN-RICH GAS PRODUCTION FROM GASOLINE IN A SHORT CONTACT TIME CATALYTIC REACTOR**

**L.N. Bobrova, I.A. Zolotarsky, V.A. Sadykov, V.A. Sobyenin**

In "*Materials in Clean Power Systems: Applications, Corrosion, and Protection*",  
Eds. Z.G. Yang, K.S. Weil, M.P. Brady,  
TMS (The Minerals, Metals & Materials Society),  
2006, pp. 25-38.

The research concerns the problems emerged from a short contact time adiabatic reactor operation in a pilot plant scale. Hydrogen-rich gas was generated by selective catalytic oxidation of gasoline over monolithic catalysts with the composite ceramometal and metallic supports. For the purpose of thermodynamic consideration of the process gasoline was simulated by a mixture of 28 organic compounds.

It was demonstrated, that over the range of operational parameters required for syngas generation nearly equilibrium synthesis gas was produced. Some bottlenecks of the process performance are considered. Pre-reforming of fuel with releasing of some chemical energy before the catalyst can be observed in the monolith reactor. Breakthrough of the feed could arise near the reactor wall in a certain case. Feed composition, superficial velocity and design factors affect the phenomena mentioned.

#### **THERMODYNAMIC ANALYSIS OF A SOLID OXIDE FUEL CELL POWER SYSTEM WITH EXTERNAL NATURAL GAS REFORMING**

**V.D. Meshcheryakov, V.A. Kirillov, V.A. Sobyantsev**

*Theor. Found. Chem. Eng.*,  
40(1) (2006) pp. 51-58.

A thermodynamic analysis of a solid oxide fuel cell power system is performed using conditions of thermodynamic equilibrium in a prereformer of natural gas to synthesis gas and a solid oxide fuel cell battery. It is shown that a thermally coupled steam reformer of natural gas provides a significantly higher efficiency of conversion of fuel energy to electric energy than other types of reformers.

#### **PHENOL OXIDATION IN SUPERCRITICAL WATER IN A WELL-STIRRED CONTINUOUS REACTOR**

**A. Yermakova, P.E. Mikenin, V.I. Anikeev**

*Theor. Found. Chem. Eng.*,  
40(2) (2006) pp. 168-174.

A well-stirred reactor for phenol and acetic acid oxidation in supercritical water is considered. A mathematical model of an adiabatic reactor is formulated. A numerical algorithm for solving the model equations using the homotopy method is developed. The model takes into account specific features of processes under supercritical conditions, namely, the changes in the thermodynamic properties (enthalpy, heat capacity, and critical parameters) of mixtures with a change in pressure and temperature. The thermodynamic properties are calculated by methods of nonideal thermodynamics. It is shown that there is a multiplicity of steady-state solutions at various reactor performances. The results of numerical analysis of the effect of the inlet flow temperature, the amount of methanol (fuel) fed, and the total pressure on the reactor performance are presented.

#### **MASS TRANSFER IN A MEDIUM WITH A RAPIDLY RENEWED INTERFACE**

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*Theor. Found. Chem. Eng.*,  
40(2) (2006) pp. 225-232.

Specific features of the mass transfer in a medium with a rapidly renewed interface are theoretically analyzed. It is shown that, in the case of intense renewal of the interface, if the adsorption of gas molecules on the liquid surface is taken into account, an additional number of molecules of the substance being dissolved are transferred to the bulk of the liquid by convective transfer of surface adsorption layers. If this process is taken into account, there is an additional mass flux into the liquid and, consequently, the mass-transfer rate is higher. In particular, this allows one to increase the concentration of the substance being dissolved above the thermodynamically equilibrium value in the absence of chemical reaction. Types of mass-transfer apparatuses in which the considered mode can be realized are discussed.

#### **MULTICAPILLARY COLUMNS FOR CHROMATOGRAPHY**

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*Am. Lab.*, 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  $\mu\text{m}$ . However, capillary columns with a diameter smaller than 100  $\mu\text{m}$  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.

## **SOL-GEL MULTICAPILLARY COLUMNS FOR GAS-SOLID CHROMATOGRAPHY**

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(\*ChromBA, Inc., State College, USA)

*J. Chromatography A*,  
1101 (2006) pp. 315-318.

In this work, the method is reported for the preparation of multicapillary columns (MCCs) for gas-solid chromatography. The porous layer adsorbent is formed on capillary walls by the hydrolysis of aluminum alkoxide in the presence of polypropylene glycol (PPG) and HCl. Porosity and selectivity of the adsorbent depend on reaction conditions and the concentration of PPG. Sol-gel MCCs are well suited for high-speed chromatographic analysis of light hydrocarbons by gas-solid chromatography. Nine-component mixtures of C1-C4 hydrocarbons are separated within 8-12 s. The efficiency of 25-30 cm long alumina sol-gel MCCs consisting of approximately 1400 capillaries of 40 microm diameter is up to 2500-3000 theoretical plates.

## **SUPERFAST CHROMATOGRAPHY AND ITS POTENTIALITIES IN CATALYTIC STUDIES**

**V.N. Sidelnikov**

In "*Industrial Catalysis. Lectures*",  
Ed. A.S. Noskov, Moscow, Kalvis, 2006, pp. 7-29.

The paper deals with approaches to accelerating processes of chromatographic analysis. The application of short capillary columns with a small (10 to 50  $\mu\text{m}$ ) diameter of capillaries is shown to be most efficient for shortening the separation time. There are limitations in employing the columns, the principal one being the necessity of injection of a very small sample volume. This limitation can be circumvented using not one but a great bunch of small-diameter capillaries; the bunch behaves like a chromatographic column referred to as polycapillary column (PCC). In this case the sample injected to the column can be increased in volume to allow the operation over a wide concentration range. Under discussion are the PCC properties and the mechanism of broadening of the chromatographic peak. The PCC applications for gas-liquid and gas adsorption chromatography are exemplified. An example of catalytic application of PCC also is considered.

## **THE STATE AND PROSPECTS OF DEVELOPMENT OF CATALYST SUBINDUSTRY AND CATALYTIC DEVELOPMENTS IN RUSSIA**

**V.N. Parmon, A.S. Noskov, N.P. Anfimova,  
V.P. Shmachkova**

*Catal. Ind.*, 1 (2006) pp. 6-20.

An analysis of the current state of the catalytic production in Russia has been carried out compared with the world one. The attention is paid to the cardinal reorganization in the national economy that has resulted in the catastrophic cutting down of application of domestic catalysts in the key branches of the industry, thereby endangering the economical and, in some instances, political safety of our country. The main reasons of reducing the portion of the domestic catalysts in the processes of chemical, oil-refining, and petrochemical productions are generalized. The proposals are formulated that are related to the restructuring of the RF catalytic subindustry. The priorities in creation of new generations of catalysts and the development of the catalytic technologies for a period of 2006–2015 are considered. It is shown that the innovative factors in the catalyst producing subindustry, being the most science-intensive one among the other branches of the chemical complex, are determinant mainly for the resource saving and energy efficiency of the base large-scale productions. The changeover to the new generations of catalysts appreciably improves the depth of fresh raw material processing and decreases the quantity of waste being formed.

## **FIBERGLASS CATALYSTS FOR DIESEL EXHAUST-GAS PURIFICATION**

**D.A. Arendarskii, A.N. Zagoruiko,  
B.S. Bal'zhinimaev**

*Chem. Sustain Devel.*,  
13(6) (2005) pp. 731-735.

Results of laboratory and pilot tests of fiberglass catalysts for diesel exhaust-gas purification are presented. It is shown that such catalysts provide high oxidation level of CO and hydrocarbons, and also reduction of nitrogen oxides in exhaust gases of real diesel engines.

## NITROGEN OXIDES REMOVAL FROM EXHAUSTS GASES OF DIESEL ENGINES: PROBLEMS AND PROSPECTS

V.A. Sadykov, T.G. Kuznetsova, R.V. Bunina, G.M. Alikina, L.Ch. Batuev, V.A. Sobyenin, V.A. Kirillov, V.P. Doronin\*, V.A. Matyshak\*\*, A.Ya. Rozovskii\*\*\*, V.F. Tretyakov\*\*\*, T.N. Burdeinaya\*\*\*, V.V. Lunin\*\*\*\*, J. Ross\*\*\*\*\* (\*Institute of Hydrocarbons Processing, Omsk, Russia; \*\*Semenov Institute of Chemical Physics, Moscow, Russia; \*\*\*Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; Moscow Lomonosov State University, Moscow, Russia; \*\*\*\*\*University of Limerick, Limerick, Ireland)

*Chem. Sustain. Devel.*,  
13(6) (2005) pp. 713-724.

The paper presents estimation of opportunities of application of new technologies for nitrogen oxides removal from diesel exhaust gases based on stationary and non-stationary processes of nitrogen oxides reduction by diesel fuel or products of its selective conversion to syn-gas or olefins in package generators. Using syn-gas in the mixture with main fuel for gasoline engine or diesel allows sharply reduce the emissions of harmful substances and increase the efficiency of engines, especially upon using of ultra-poor mixtures. Availability of using complex oxide systems with high oxygen mobility as catalysts for the processes of soot particles oxidation with nitrogen oxides, promoting removal of both types of harmful impurities, is shown.

## CATALYSTS ON THE BASE OF COMPLEX OXIDES WITH PEROVSKITE- AND FLUORITE-LIKE STRUCTURES FOR SOOT REMOVAL FROM DIESEL EXHAUSTS

T.G. Kuznetsova, V.A. Sadykov, V.A. Matyshak\*, L.Ch. Batuev, V.A. Rogov (\*Semenov Institute of Chemical Physics, Moscow, Russia)

*Chem. Sustain. Devel.*, 13(6) (2005) pp. 779-785.

Reaction of soot oxidation in mixture  $O_2 + He$  and  $O_2 + NO_2 + He$  is studied over substituted perovskites based on lanthanum manganites, and modified fluorites based on solid solution Ce-Zr-O, including those doped with Pt. It is shown, that efficiency of soot oxidation is higher for the mixture, containing  $NO_2$ . It is established, that necessary condition for initiation of soot oxidation is the presence of weakly bonded surface oxygen, and for the process of developed soot oxidation – mobility of lattice oxygen.

## FORMATION AND DECOMPOSITION OF ETHANE, PROPANE, AND CARBON DIOXIDE HYDRATES IN SILICA GEL MESOPORES UNDER HIGH PRESSURE

E.Y. Aladko\*, Y.A. Dyadin\*, V.B. Fenelonov, E.G. Larionov\*, A.Y. Manakov\*, M.S. Melgunov, F.V. Zhurko\* (\*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia)

*J. Phys. Chem. B*,  
110(39) (2006) pp. 19717-19725.

The experimental data on decomposition temperatures for the gas hydrates of ethane, propane, and carbon dioxide dispersed in silica gel mesopores are reported. The studies were performed at pressures up to 1 GPa. It is shown that the experimental dependence of hydrate decomposition temperature on the size of pores that limit the size of hydrate particles can be described on the basis of the Gibbs-Thomson equation only if one takes into account changes in the shape coefficient that is present in the equation; in turn, the value of this coefficient depends on a method of mesopore size determination. A mechanism of hydrate formation in mesoporous medium is proposed. Experimental data providing evidence of the possibility of the formation of hydrate compounds in hydrophobic matrixes under high pressure are reported. Decomposition temperature of those hydrate compounds is higher than that for the bulk hydrates of the corresponding gases.

## EQUILIBRIUM CONDITIONS FOR DECOMPOSITION OF GAS HYDRATES, DISPERSED IN MESOPOROUS MEDIUM

E.Ya. Aladko\*, Dyadin\*, F.V. Zhurko\*, E.G. Larionov\*, M.S. Melgunov, A.Yu. Manakov\*\*, A.N. Nesterov\*\*, V.B. Fenelonov (\*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia)

*Gas Indust.*,  
*Special Edition: Gas Hydrates* (2006) pp. 18-27.

Considerable part of natural gas hydrates localized in permafrost or in near-bottom sea and ocean areas are the inclusions in the space between average and fine fractions of sediments. Equilibrium thermodynamic conditions of such hydrate decomposition may depend on the size of enclosing rocks. The influence of medium pore size on the decomposition temperatures for the dispersed gas hydrates is discussed quantitatively in the work.

### **HYDROGEN PURIFICATION FOR FUEL CELLS BY CARBON MONOXIDE SELECTIVE METHANATION**

**T.P. Minyukova, I.Sh. Itenberg, M.P. Demeshkina, N.V. Shtertser, T.M. Yurieva**

*Chem. Sustain. Devel.*, 13(6) (2005) pp. 793-796.

Possibility of fine hydrogen cleaning from CO by method of preferential hydrogenation of carbon oxide (II) to methane up to residual CO content 1000 ppm is studying. Efficient nickel-containing catalyst is suggested for creation of package unit for hydrogen treatment for fuel cells providing desired cleaning result ( $\leq 1000$  ppm CO at the outlet), selectivity ( $\geq 70$  % of methane forms from CO) and activity (contact time  $\leq 6000$  h<sup>-1</sup>).

### **STUDIES OF THE REACTION BETWEEN CF<sub>2</sub>Cl<sub>2</sub> AND NANOCRYSTALLINE MgO USING A TEOM MICROANALYZER**

**I.V. Mishakov, A.A. Vedyagin, A.F. Bedilo, M.S. Melgunov, R.A. Buyanov**

*Doklady Phys. Chem.*,  
410(1) (2006) pp. 251-254.

Potentialities of the new approach to mass measuring provided in a TEOM microanalyzer are demonstrated with the topochemical reaction of Freon CF<sub>2</sub>Cl<sub>2</sub> with nanodispersed MgO conducted in the flow mode. The induction period of 5 min (375°C) to two hours (300°C) is established to occur; after that

the reaction is the fast phase of magnesia to fluoride transformation. The nature of the induction period and the mechanism of the topochemical reaction until its accomplishment are elucidated. Unordinary profiles of temperature and reaction rate of MgO to MgF<sub>2</sub> transformation are discovered and interpreted; these are accounted for by variations in the molar volume of the solid phase and by its cracking during the chemical phase transformations.

Application of the TEOM microanalyzer makes it possible to determine the activation energy of the reaction. As the first approximation, the mechanism is a combination of topochemical stages involving cleavage of chemical bonds and exchange between oxygen and fluorine atoms. The obtained activation energy is an apparent quantity; it characterizes a total of energetic set of stages.

### **POTENTIALITIES OF GRAVIMETRY FOR ECOLOGICAL AIR MONITORING**

**A.A. Vedyagin, I.V. Mishakov, A.I. Nizovskii**

*Omsk Sci. Bull.*, 2(35) (2006) pp. 144-147.

Authors considered the contemporary ways to monitor an atmospheric contaminations by gravimetric method based on TEOM analyzer. An examples of using the said method to determine continuously aerosol and PM concentration in air as well as micro-impurities and vapors of organic compounds are discussed.





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