

Boreskov Institute of Catalysis, Novosibirsk, Russia
Immanuel Kant Baltic Federal University, Kaliningrad, Russia
Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
Lomonosov Moscow State University, Moscow, Russia

X International Conference
“Mechanisms of Catalytic Reactions”

Svetlogorsk, Kalinigrad Region, Russia
October 2 - 6, 2016

SCIENTIFIC PROGRAM

Kaliningrad-2016

CONFERENCE ORGANIZERS

ФЕДЕРАЛЬНОЕ
АГЕНСТВО
НАУЧНЫХ
ОРГАНИЗАЦИЙ



IKBFU



UNDER THE AUSPICES OF

EFCATS

European Federation of Catalysis Societies

European Federation
of Catalysis Societies



National Catalytic
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CONFERENCE ORGANIZERS

- Federal Agency for Scientific Organizations, Russia
- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Immanuel Kant Baltic Federal University, Kaliningrad, Russia
- Zelinsky Institute of Organic Chemistry, Moscow, Russia
- Lomonosov Moscow State University, Moscow, Russia
- Novosibirsk State University, Novosibirsk, Russia
- Scientific Council on Catalysis RAS, Moscow, Russia
- Mendeleev Chemical Society of Republic of Tatarstan, Kazan, Russia

Dear Colleague,

The X Conference “Mechanisms of Catalytic Reactions”, organized under the auspices of the European Federation of Catalysis Societies (EFCATS) and the National Catalytic Society of Russia, welcomes researchers from across the globe.

The Conference follows the established tradition, with previous meetings held in Moscow (1974, 1979, 1986, 1990, 2002), Saint-Petersburg (2006, 2012), and Novosibirsk (1982, 2009).

The scope of the Conference covers all aspects of research on the mechanisms of homogeneous and heterogeneous catalytic reactions.

We are pleased to welcome you in Svetlogorsk, one of the most picturesque resort cities of the Russian Baltic coast. We believe that the unique location will foster both scientific and social communication and wish you a fruitful work and a pleasant stay in Svetlogorsk!

*Organizing Committee Chairman
Valerii Bukhtiyarov,
Boreskov Institute of Catalysis*



Scientific Committee

- Valentin P. Ananikov**, Zelinsky Institute of Organic Chemistry, RAS,
Moscow, Russia
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Organizing Committee

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Kaliningrad, Russia

M.S. Suvorova, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

SCIENTIFIC PROGRAM

The X Conference “Mechanisms of Catalytic Reactions” is the event in the series of International MCR-Conferences started in 1974 in Moscow. Traditionally, the Conferences on the Mechanisms of Catalytic Reactions focus on advances in understanding the mechanisms of chemical reactions occurring in the presence of catalysts, ranging from homogeneous molecular catalysts (inorganic, organic, metal complex based) to heterogeneous catalysts.

The scientific program of MCR X includes four plenary lectures (40 min) and seven keynote lectures (30 min); 46 oral presentations (20 min) and 30 short oral presentations (10 min) are scheduled in three parallel sessions. The Conference Program also includes 100 poster presentations. The main topics are:

- First-principles approach, theory and simulation in catalysis;
- Advanced methods for studies of mechanisms of catalyzed reactions;
- In-situ and operando studies of model and real catalysts;
- Kinetics and reaction intermediates of catalyzed processes;
- From mechanistic studies to design of advanced catalyst systems.

The official language of the Conference is English.

The Conference is accompanied by the School-Symposium of young scientists "Quantum-mechanical modeling of catalytic processes". The Program of the School includes two keynote lectures (30 min) and 8 short oral presentations (10 min).

Conference Exhibition of compact installations and devices, as well as promotional materials, will be held throughout the Conference, on October 3-5.

Presentation

The duration of presentation (including time for questions) is 40 min for plenary lectures, 30 min for keynote lectures, 20 min for oral presentations, and 10 min for short oral presentations.

Multimedia LCD projectors will be available. The organizers recommend the authors to prepare computer presentations in *.ppt format (Microsoft Office PowerPoint).

Poster size is the following: vertical, 100 cm x 65 cm. The authors are requested to place their posters on October 3 from 9.00 to 17.00, and remove them after 19.00 the same day, at the end of poster session.

Conference publications

The final Scientific Program brochure and Book of Abstracts of lectures, oral and poster presentations on a USB key will be available at the registration desk.

Special issue of Kinetics and Catalysis

Authors of keynote lectures and oral presentations (20 and 10 min) are invited to submit manuscripts related to their presentations, to be published in a special issue of Kinetics and Catalysis (no. 5 in 2017).

Manuscripts will be peer reviewed following the standard procedure.

The manuscript text of keynote lecture should not exceed 16 pages; 20 min oral contribution, 12 pages; and 10 min oral contribution, 10 pages. A4 page format, Times New Roman 12 pt, 1.5 line spaced.

The texts (in English for foreign authors; in English and Russian for Russian authors) should be submitted to Kinetics and Catalysis before October 25, 2016 both by e-mail (*kincat@ioc.ac.ru*) and regular post (Kinetics and Catalysis, Zelinsky IOC RAS, Leninsky Prospect 47, Moscow 119991, Russia).

Contact tel.: +7 (499)135 53 58.

*Please see attached the guidelines for Kinetics and Catalysis:
http://conf.nsc.ru/MCR-X/en/mcr-x_MCR-Conference_publication*

Venue

The Conference will take place in three conference halls at the business center of the Volna hotel*** (Kaliningradskiy prospect, 68 B, Svetlogorsk, <http://www.hotelvolna.ru>): Atlantika, Baltika and Belyi.

Transportation

Representatives of the Organizing Committee will meet all participants at the Airport “Khrabrovo” and provide transportation from Kaliningrad to the Volna and Universal hotels (Svetlogorsk). Shuttle bus transportation “Airport – Hotels – Airport” during arrival and departure days will be provided.

Accommodation

Accommodation is arranged by the Organizing Committee at the Volna and Universal hotels at special rates.

The Universal hotel (ul. Nekrasova, 3) is close to the Volna hotel.

Meals

Lunches will be served at the restaurant “Siniy” of the Volna hotel, 1st floor. Vouchers for 3 lunches will be included in the participant package. Morning and afternoon coffee breaks will be provided.

Registration

Registration will take place at the Volna hotel, 2nd floor hall, on October 2 from 11.00 till 16.30 and on October 3 from 8.30 till 13.00.

Bank and Currencies exchange

Cash exchange is available at Sberbank next to the Volna hotel (in September 2016, one Euro equals ca. 70 roubles and one U.S. dollar equals ca. 63 roubles). Eurocard, MasterCard and Visa credit cards are acceptable in banks and cash machines. Please note that personal cheques are not accepted.

Social events

http://conf.nsc.ru/MCR-X/en/mcr-x_socev

The participants are invited to the Welcome reception at 19.30 on October 2 (the Siniy restaurant of the Volna hotel). The Conference banquet will be held at the Hercules restaurant, Kaliningrad, on October 4 at 19.30 (*ticket, 2500 Rub*).

Sightseeing excursion: *the excursion “Kaliningrad – Koenigsberg. From the past to the present” will be organized for the participants and accompany persons on October 4, 2016 (14.30 – 18.30, included in the Conference fee).*

The participants and guests are offered a special sightseeing program:

City sightseeing walk “Svetlogorsk is the pearl of the Baltic”

October 2 and 3, 2016 (extra fee)

Excursion “Yantarny – Meeting sun stone”

October 5, 2016 (14.30 – 18.30, extra fee)

Post-Tour “Curonian Spit”:

Visit to the Museum of the National Park

October 6, 2016 (10.00-17.00, extra fee)

The excursion and the tour start from the Volna hotel and end at the Khrabrovo Airport of Kaliningrad.

Registration fee

The fee covers registration for the Conference, editorial expenditures, delegate bag, auditorium rent, coffee-breaks, three lunches, Welcome Party, transfer airport-hotel-airport, and sightseeing excursion to Kaliningrad.

Weather

In early October, the weather in Svetlogorsk is usually 14-16 °C. The Organizing Committee advises the Conference participants to bring umbrellas and warm suits.

Sunday, October 2, 2016

*The Volna hotel,
Kalinigradskiy prospekt, 68 B*

11.00-16.30 Registration: 2nd floor hall, the Volna hotel

Atlantika Hall

AFTERNOON SESSION

17.00-17.30 Opening session

Chairmen: Prof. Valerii I. Bukhtiyarov
Prof. Alexander Yu. Stakheev

PLENARY LECTURE

17.30-18.10 Global Energy Award Lecture (2016), PL-1

Presenting author: Prof. Valentin N. Parmon

**Catalysis and Energetics: Experience of the Boreskov Institute
of Catalysis**

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

18.30-22.00 Welcome Reception

(the Siniy restaurant, 1st floor of the Volna hotel)

Monday, October 3

The Volna hotel

8.30-13.00 Registration: 2nd floor hall, the Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Prof. Valerii I. Bukhtiyarov
Prof. Valentin N. Parmon

PLENARY LECTURE

8.30 PL-2

Presenting author: Prof. Stig Helveg

Electron Microscopy Advances in Catalysis

Haldor Topsøe A/S, Haldor Topsøes Allé 1, Kgs. Lyngby, Denmark

KEYNOTE LECTURES

9.10 KN-1

Presenting author: Dr. Axel Knop-Gericke

Pfeifer V.^{1,4}, Arrigo R.³, Velasco J.², Jones T.¹, Schlögl R.^{1,2},
Knop-Gericke A.¹

How to Extend In Situ Photoelectron Spectroscopy Studies of Electrochemically Active Gas-Solid Interfaces to Liquid-Solid Interfaces?

1 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. Inorganic Chemistry, Berlin, Germany

2 – Max-Planck-Institut für Chemische Energiekonversion, Dept. Heterogeneous Reactions, Mülheim, Germany

3 – Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, UK

4 – Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Berlin, Germany

9.40 KN-2

Presenting author: Dr. Evhenii V Kondratenko.

Hahn T., Kondratenko V.A., Linke D., Kondratenko E.V.

Metathesis of C_2H_4 and 2- C_4H_8 to C_3H_6 : Effect of Support and Kind of MoO_x and WO_x Species on Selectivity and Reaction Pathways

Leibniz Institute for Catalysis at the University of Rostock, Rostock, Germany

10.10 *Coffee break*

Atlantika Hall

Section 3. In-situ and operando studies of model and real catalytic sites

Chairmen: Dr. Axel Knop-Gericke

Prof. Svetlana Schauermann

ORAL PRESENTATIONS

10.40 S3 OP₂₀₋₀₂

Presenting author: Dr. Mikhail Yu. Smirnov

Smirnov M.Yu., Vovk E.I., Kalinkin A.V., Klembovskii I.O.,

Bukhtiyarov V.I.

The Formation of Dissolved and Oxidic Oxygen in Supported Platinum Particles and Their Reactivity towards Hydrogen

Boriskov Institute of Catalysis SB RAS, Novosibirsk, Russia

11.00 S3 OP₂₀-03

Presenting author: Dr. Elise Berrier

Berrier E., Mamede A.-S., Blanck D., Schön A., Dacquín J.-P.,
Dujardin C., Granger P., Paul J.-F.

Iron Oxide Nanophases Mobility in and out LaFeO₃ Perovskite Lattice in Three-Ways Catalysis Probed by *In Situ* Raman Spectroscopy and Surface Analyses

*University Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181
- UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France*

11.20 S3 OP₂₀-04

Presenting author: Prof. Vladimir A. Zakharov

Zakharov V.^{1,2}, Mikenas T.¹, Koshevoi E.¹, Nikolaeva M.¹, Matsko M.¹,
Shubin A.^{1,2}

Formation and Structure of Active Centres in Supported Ziegler-Natta Catalysts for Olefin Polymerization on the Base of New Experimental Data

*1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 – Novosibirsk State University, Novosibirsk, Russia*

11.40 S3 OP₂₀-05

Presenting author: Prof. Etibar H. Ismailov

Abbasov Y.A., Ismailov E.H.

Para-, Superpara/Ferromagnetic Particles in the Ziegler Type Catalytic Systems: Structure and Reactivity

Institute of Petrochemical Processes, NANA, Baku, Azerbaijan

12.00 S3 OP₂₀-06

Presenting author: Dr. Andrey V. Bukhtiyarov

Bukhtiyarov A.V.^{1,2}, Prosvirin I.P.^{1,3}, Saraev A.A.¹, Klyushin A.Yu.⁴,
Knop-Gericke A.⁴, Schlögl R.⁴, Bukhtiyarov V.I.^{1,2,3}

CO Oxidation on the Bimetallic Pd-Au/HOPG Catalysts: NAP XPS and MS Investigation

*1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia
2 – Research and Educational Center for Energy Efficient Catalysis in
Novosibirsk State University, Novosibirsk, Russia
3 – Novosibirsk State University, Novosibirsk, Russia
4 – Fritz-Haber-Institute der Max Planck Society, Berlin, Germany*

12.20 S3 OP₂₀-07

Presenting author: Prof. Boris N. Kuznetsov

Kuznetsov B.N.^{1,2}, Chesnokov N.V.^{1,2}, Taraban'ko V.E.^{1,2},

Garyntseva N.V.¹, Sudakova I.G.¹

**Kinetic Studies of Green Catalytic Processes of Wood Oxidative
Delignification**

1 – Institute of Chemistry and Chemical Technology SB RAS,

Krasnoyarsk, Russia

2 – Siberian Federal University, Krasnoyarsk, Russia

13.00 Lunch

AFTERNOON SESSION

Atlantika Hall

Chairman: Prof. Dionisios G. Vlachos

PLENARY LECTURE

14.30 PL-3

Presenting author: Prof. Javier Pérez-Ramírez

Halogen Chemistry on Catalytic Surfaces

Institute for Chemical and Bioengineering, ETH Zurich, Switzerland

Atlantika Hall

Section 4. Kinetics and reaction intermediates of catalyzed processes

Chairmen: Prof. Vladimir A. Zakharov

Prof. Leino Reko

ORAL PRESENTATIONS

15.10 S4 OP₂₀-01

Presenting author: Dr. Tatiana Yu. Kardash

Kardash T.Yu.^{1,2}, Vinokurov Z.S.^{1,2}, Stonkus O.A.^{1,2},
Svintsitskiy D.A.^{1,2}

***In Situ* Time-resolved XRD Study of Red/Ox Transformations in Copper Oxide-based Systems**

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Russia

15.30 S4 OP₂₀-02

Presenting author: Dr. Roman V. Ottenbacher

Talsi E.P.^{1,2}, Ottenbacher R.V.^{1,2}, Bryliakov K.P.^{1,2}

Aminopyridine Manganese Complexes Catalyzed Asymmetric Epoxidation with Various Oxidants: Evidence for Multiple Mechanisms

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

15.50 S4 OP₂₀-03

Presenting author: Prof. Oxana P. Taran

Gromov N.V.^{1,2,3}, Kolinko P.A.^{1,4}, Aymonier C.², Taran O.P.^{1,3}

“One-Pot” Hydrolytic-Dehydration of Cellulose into Glucose and 5-Hydroxymethylfurfural over Solid Acid Catalysts. Kinetics and Reaction Intermediates Study

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institut de Chimie de la Matière Condensée de Bordeaux, CNRS, Pessac, France

3 – Université Bordeaux, ICMCB, Pessac, France

4 – Novosibirsk State Technical University, Novosibirsk, Russia

5 – Novosibirsk State University, Novosibirsk, Russia

16.10 S4 OP₂₀-04

Presenting author: Dr. Alina Tirsoaga

Jurca B.¹, Tirsoaga A.¹, Granger P.², Parvulescu V.I.¹

Catalytic Behaviour of Supported Cu₂O in Gas-Phase C-N Coupling Reaction: Influence of Deactivation Phenomena from Continuous-Flow Kinetic Observations

1 – Faculty of Chemistry, University of Bucharest, Bucharest, Romania

2 – Unité de Catalyse et de Chimie du Solide, UMR CNRS 8181,

Université Lille 1, Sciences et Technologies, Villeneuve d'Ascq, France

16.30 Coffee break

17.00-19.00 Poster Session, 2nd floor, the Volna hotel

Monday, October 3

The Volna hotel

8.30-13.00 Registration: 2nd floor, the Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Prof. Valerii I. Bukhtiyarov
Prof. Valentin N. Parmon

PLENARY LECTURE

8.30 PL-2

Presenting author: Dr. Stig Helveg

Electron Microscopy Advances in Catalysis

Haldor Topsøe A/S, Haldor Topsøes Allé 1, Kgs. Lyngby, Denmark

KEYNOTE LECTURES

9.10 KN-1

Presenting author: Dr. Axel Knop-Gericke

Pfeifer V.^{1,4}, Arrigo R.³, Velasco J.², Jones T.¹, Schlögl R.^{1,2},
Knop-Gericke A.¹

How to Extend In Situ Photoelectron Spectroscopy Studies of Electrochemically Active Gas-Solid Interfaces to Liquid-Solid Interfaces?

1 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. Inorganic Chemistry, Berlin, Germany

2 – Max-Planck-Institut für Chemische Energiekonversion, Dept. Heterogeneous Reactions, Mülheim, Germany

3 – Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, UK

4 – Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Berlin, Germany

9.40 KN-2

Presenting author: Dr. Evhenii V Kondratenko.

Hahn T., Kondratenko V.A., Linke D., Kondratenko E.V.

Metathesis of C₂H₄ and 2-C₄H₈ to C₃H₆: Effect of Support and Kind of MoO_x and WO_x Species on Selectivity and Reaction Pathways

Leibniz Institute for Catalysis at the University of Rostock, Rostock, Germany

10.10 *Coffee break*

Belyi Hall

Section 1. First-principles approach, theory and simulation in catalysis

Chairmen: Prof. Konstantin Neyman

Prof. Stefano Fabris

ORAL PRESENTATIONS

10.40 S1 OP₂₀-01

Presenting author: Dr. Lyudmila V. Moskaleva

Moskaleva L.V., Bäumer M.

Catalytic Activity of Nanoporous Gold: Insights from a Computational DFT Study

Institute for Applied and Physical Chemistry and Center for Environmental Research and Sustainable Technology, Universität Bremen, Bremen, Germany

11.00 S1 OP₂₀-02

Presenting author: Dr. Daria A. Pichugina

Pichugina D.A., Polynskaya Yu.G., Utkin A.G., Kuz'menko N.E.

Structure, Spin and Doping Effects in Oxygen Dissociation on Gold Clusters

Department of Chemistry, M.V. Lomonosov Moscow State University, Moscow, Russia

11.20 S1 OP₂₀-03

Presenting author: Dr. Elena A. Shor

Nasluzov V.A.¹, Shor A.M.¹, Ivanova-Shor E.A.¹, Laletina S.S.¹,
Neyman K.M.^{2,3}

A Density Functional Study of Active Oxygen Species at Ceria-supported Silver Clusters

1 – *Institute of Chemistry and Chemical Technology SB RAS,
Krasnoyarsk, Russia*

2 – *Universitat de Barcelona, Barcelona, Spain*

3 – *Institució Catalana de Recerca i Estudis Avançats (ICREA),
Barcelona, Spain*

11.40 S1 OP₂₀-04

Presenting author: Dr. Igor Yu. Skobelev

Skobelev I.Y.^{1,2}, Carbó J.J.³, Poblet J.M.³, Kholdeeva O.A.^{1,2}

Mechanistic Insights into Oxidation of Organic Compounds with H₂O₂ Catalyzed by Ti-containing Polyoxometalates

1 – *Boreshkov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

3 – *Universitat Rovira i Vigili, Marcel·lí Domingo s/n, Tarragona, Spain*

12.00 S1 OP₂₀-05

Presenting author: Dr. Andrey V. Matveev

Cholach A.R., Bryliakova A.A., Matveev A.V.

Correlation between Structure and Activity of Catalytic Centres

Boreshkov Institute of Catalysis SB RAS, Novosibirsk, Russia

12.20 S1 OP₂₀-06

Presenting author: Dr. Tatiana V. Tyumkina

Tyumkina T.V., Idrisova S.M., Khafizova L.O., Khusainova L.I.,
Parfenova L.V., Khalilov L.M., Dzhemilev U.M.

Mechanistic Aspects of Transmetallation in Three- and Five- membered Metallacyclic Intermediates

Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

12.40 S1 OP₂₀₋₀₇

Presenting author: Dr. Elena A. Lashina

Hysteresis Effect and Coexistence of the Steady State and Self-oscillations under CO Oxidation over Pd Foil

Lashina E.A.^{1,3}, Slavinskaya E.M.^{1,3}, Chumakova N.A.^{1,3},
Chumakov G.A.^{2,3}, Stadnichenko A.I.^{1,3}, Boronin A.I.^{1,3}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia

3 – Novosibirsk State University, Novosibirsk, Russia

13.00 Lunch

AFTERNOON SESSION

Atlantika Hall

Chairman: Prof. Dionisios G. Vlachos

PLENARY LECTURE

14.30 PL-3

Presenting author: Prof. Javier Pérez-Ramírez

Halogen Chemistry on Catalytic Surfaces

Institute for Chemical and Bioengineering, ETH Zurich, Switzerland

Belyi Hall

Section 5. From mechanistic studies to design of advanced catalyst systems

Chairmen: Prof. Vladislav Sadykov

Dr. Yulia Demidova

ORAL PRESENTATIONS

15.10 S5 OP₂₀₋₀₁

Presenting author: Dr. Olga B. Belskaya

Belskaya O.B.^{1,2}, Mironenko R.M.^{1,3}, Talsi V.P.¹, Likholobov V.A.^{1,2}

The Pathways of 2,4,6-Trinitrobenzoic Acid Transformation in the Aqueous-Phase Hydrogenation. Development of Advanced Pd/Sibunit Catalysts for Exhaustive Hydrogenation

1 – Institute of Hydrocarbons Processing, SB RAS, Omsk, Russia

2 – Omsk State Technical University, Omsk, Russia

3 – Omsk F.M. Dostoevsky State University, Omsk, Russia

15.30 S5 OP₂₀-02

Presenting author: Dr. Irina Delidovich

Delidovich I., Palkovits R.

Phosphate-catalyzed Isomerization of Aldoses into Ketoses and Their Recovery Using Anionic Extraction

1 – Chair of Heterogeneous Catalysis and Chemical Technology, RWTH Aachen University, Aachen, Germany

15.50 S5 OP₂₀-03

Presenting author: Prof. Ekaterina S. Lokteva

Lokteva E.S.^{1,2}, Golubina E.V.^{1,2}, Erokhin A.V.¹, Klokov S.V.^{1,2}, Maslakov K.I.^{1,2}, Yermakov A.Ye.³, Likholobov V.A.²

Catalytic Activity of Carbon-encapsulated Metal Nanoparticles

1 – Lomonosov Moscow State University, Moscow, Russia

2 – Institute of Hydrocarbon Processing SB RAS, Omsk, Russia

3 – Institute of Metal Physics UrO RAS, Yekaterinburg, Russia

16.10 S5 OP₂₀-04

Presenting author: Prof. Konstantin P. Bryliakov

Bryliakova A.A.¹, Talsi, E.P.^{1,2}, Rybalova T.V.^{2,3}, Bryliakov K.P.^{1,2}

Ti-Salan/Salalen Based Catalyst Systems for the Environmentally Benign Asymmetric Oxidation of Thioethers to Sulfoxides with H₂O₂

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia

16.30 *Coffee break*

17.00-19.00 **Poster Session**, 2nd floor, the Volna hotel

Monday, October 3

The Volna hotel

8.30-13.00 Registration, 2nd floor, the Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Prof. Valerii I. Bukhtiyarov
Prof. Valentin N. Parmon

PLENARY LECTURE

8.30 PL-2

Presenting author: Dr. Stig Helveg

Electron Microscopy Advances in Catalysis

Haldor Topsoe A/S, Haldor Topsøes Allé 1, Kgs. Lyngby, Denmark

KEYNOTE LECTURES

9.10 KN-1

Presenting author: Dr. Axel Knop-Gericke

Pfeifer V.^{1,4}, Arrigo R.³, Velasco J.², Jones T.¹, Schlögl R.^{1,2},
Knop-Gericke A.¹

How to Extend In Situ Photoelectron Spectroscopy Studies of Electrochemically Active Gas-Solid Interfaces to Liquid-Solid Interfaces?

1 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Dept. Inorganic Chemistry, Berlin, Germany

2 – Max-Planck-Institut für Chemische Energiekonversion, Dept. Heterogeneous Reactions, Mülheim, Germany

3 – Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, UK

4 – Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Berlin, Germany

9.40 KN-2

Presenting author: Dr. Evhenii V Kondratenko

Hahn T., Kondratenko V.A., Linke D., Kondratenko E.V.

Metathesis of C₂H₄ and 2-C₄H₈ to C₃H₆: Effect of Support and Kind of MoO_x and WO_x Species on Selectivity and Reaction Pathways

Leibniz Institute for Catalysis at the University of Rostock, Rostock, Germany

10.10 *Coffee break*

Baltika Hall

Chairmen: Dr. Marcus Rose

Dr. Evgeny I. Vovk

SHORT ORAL PRESENTATIONS

10.40 OP₁₀-01

Presenting author: Sergei A. Chernyak

Chernyak S.A., Suslova E.V., Egorov A.V., Maslakov K.I.,

Savilov S.V., Lunin V.V.

CO/CO₂ Hydrogenation and CO Disproportionation over Small Co Particles Supported on Carbon Nanotubes

Lomonosov Moscow State University, Department of Chemistry, Moscow, Russia

10.50 OP₁₀-02

Presenting author: Dr. Stanislav S. Yakushkin

Yakushkin S.S.^{1,2}, Nuzhdin A.L.^{1,2}, Bukhtiyarova G.A.¹, Martyanov O.N.^{1,2}

ESR Investigation of Nitrobenzene Hydrogenation over Au/Al₂O₃ Catalyst

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Research and Educational Center for Energy Efficient Catalysis, Novosibirsk State University, Novosibirsk, Russia

11.00 OP₁₀-03

Presenting author: Dr. Lidia S. Kibis

Kibis L.S.^{1,2}, Stadnichenko A.I.^{1,2}, Koscheev S.V.^{1,2},
Slavinskaya E.M.^{1,2}, Ivanova A.S.^{1,2}, Boronin A.I.^{1,2}

XPS Study of Oxidized Rhodium Species Active in CO Oxidation Reaction

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Russia

11.10 OP₁₀-04

Presenting author: Dr. Kirill V. Semikin

Semikin K.V.¹, Smirnova D.A.¹, Sladkovskiy D.A.¹, Sladkovskaya E.V.¹

Insights on the Mechanism for the Heterogeneous Iso-Butane/Butene Alkylation over Solid Catalyst

*1 – St. Petersburg State Technological Institute (Technical University),
Laboratory of Catalytic Technologies, St.Petersburg, Russia*

11.20 OP₁₀-05

Presenting author: Dr. Mikhail A. Salaev

Salaev M.A., Vodyankina O.V.

Metal-Promoter Interface in Selective Alcohol Oxidation: Understanding the Synergetic Effects of P-promoted Ag Catalysts

National Research Tomsk State University, Tomsk, Russia

11.30 OP₁₀-06

Presenting author: Dr. Andrey V. Vorotyntsev

Vorotyntsev A.V., Petukhov A.N., Vorotyntsev V.M., Kadomtseva A.V.

Catalytic Hydrogenation of Silicon and Germanium Tetrachloride

*Nizhny Novgorod State Technical University n.a. R.E. Alekseev, Nizhny
Novgorod, Russia*

11.40 OP₁₀-07

Presenting author: Valeriya V. Grinenko

Grinenko V.V., Khrizanforov M.N., Strekalova S.O.,
Khrizanforova V.V., Gryaznova T.V., Budnikova Y.H.

Regularities of Electrochemical Aromatic C-H Fluoroalkylation Using Ni and Fe Complexes

A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center, Russian Academy of Sciences, Kazan Russia

11.50 OP₁₀-08

Presenting author: Alexandra M. Zima

Zima A.M., Lyakin O.Y., Ottenbacher R.V., Bryliakov K.P., Talsi E.P.

Bioinspired Nonheme Iron Catalysts for Oxidation: Remarkable Effect of Carboxylic Acid Additive on the Electronic Structure of the Active Oxoferryl Species

*Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Novosibirsk State University, Novosibirsk, Russia*

12.00 OP₁₀-09

Presenting author: Vasily Yu. Evtushok

Evtushok V.Yu.^{1,2}, Skobelev I.Y.¹, Maksimchuk N.V.^{1,2}, Carbó J.J.³,
Poblet J.M.³, Kholdeeva O.A.^{1,2}

Mechanistic Studies of Selective Oxidation of Alkylarenes with H₂O₂ Catalyzed by γ -Keggin Divanadium-substituted Phosphotungstate

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Universitat Rovira i Virgili, Tarragona, Spain

12.10 OP₁₀-10

Presenting author: Viktoriia V. Torbina

Torbina V.V.¹, Nedoseykina N.S.¹, Ivanchikova I.D.^{1,2},
Kholdeeva O.A.^{1,2}, Vodyankina O.V.¹

Propylene Glycol Oxidation with Hydrogen Peroxide over UiO-66

1 – Tomsk State University, Tomsk, Russia

2 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

12.20 OP₁₀₋₁₁

Presenting author: Yulia A. Chumachenko

Chumachenko Yu.A., Lavrenov A.V., Gulyaeva T.I., Arbuzov A.B.,
Leontieva N.N., Trenikhin M.V., Drozdov V.A.

Influence of Platinum Precursor on the Formation of Active Sites of Bifunctional Catalysts of One-Step Vegetable Oil Hydrocracking

Institute of Hydrocarbons Processing SB RAS, Omsk, Russia

12.30 OP₁₀₋₁₂

Presenting author: Sofia O. Strekalova

Strekalova S.O., Khrizanforov M.N., Grinenko V.V.,
Khrizanforova V.V., Gryaznova T.V., Budnikova Y.H.

Metal-induced Oxidative Phosphorylation of Aromatic Compounds

A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan

13.00 Lunch

AFTERNOON SESSION

Atlantika Hall

Chairman: Prof. Dionisios G. Vlachos

PLENARY LECTURE

14.30 PL-3

Presenting author: Prof. Javier Pérez-Ramírez

Halogen Chemistry on Catalytic Surfaces

Institute for Chemical and Bioengineering, ETH Zurich, Switzerland

Baltika Hall

Chairmen: Dr. Vasily V. Kaichev

Dr. Ekaterina A. Kozlova

SHORT ORAL PRESENTATIONS

15.10 OP₁₀₋₁₃

Presenting author: Kirill A. Lomachenko

Lomachenko K.A.¹, Borfecchia E.², Falsig H.³, Beato P.³,
Janssens T.V.W.³, Soldatov A.V.¹, Bordiga S.², Lamberti C.^{1,2}

In Situ and Operando X-ray Absorption and Emission Spectroscopy: Probing SCR-relevant Cu Species in Cu-CHA Zeolite

1 – Southern Federal University, Rostov-on-Don, Russia

2 – University of Turin, Turin, Italy

3 – Haldor Topsøe, Kgs. Lyngby, Denmark

15.20 OP₁₀₋₁₄

Presenting author: Aram L. Bugaev

Bugaev A.L.^{1,2}, Guda A.A.¹, Lomachenko K.A.¹, Lazzarini A.²,
Grosso E.², Pellegrini R.³, Soldatov A.V.¹, Bugaev L.A.¹,
Dmitriev V.P.⁴, van Bokhoven J.A.⁵, Lamberti C.^{1,2}

In Situ Palladium Hydride and Carbide Formation in the Palladium Nanoparticles during Catalytic Reactions

1 – IRC “Smart Materials”, Southern Federal University, Rostov-on-Don, Russia

2 – University of Turin, Turin, Italy

3 – Chimet SpA - Catalyst Division, Viciomaggio Arezzo, Italy

4 – European Synchrotron Radiation Facility, Grenoble, France

5 – Swiss Light Source, Paul Scherrer Institute, Villigen, and ETH Zurich, Switzerland

15.30 OP₁₀₋₁₅

Presenting author: Dr. Olga A. Bulavchenko

Bulavchenko O.A.^{1,2}, Vinokurov Z.S.^{1,2}, Afonassenko T.N.³,
Tsyrl'nikov P.G.³, Tsybulya S.V.^{1,2}, Saraev A.A.^{1,2}, Kaichev V.V.^{1,2}

In Situ XPS and XRD Study of Mixed Mn-Zr Oxide Catalysts Reduction

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Institute of Hydrocarbon Processing SB RAS, Omsk, Russia

15.40 OP₁₀₋₁₆

Presenting author: Dr. Dmitriy I. Potemkin

Uskov S.I.^{1,2}, Enikeeva L.V.³, Potemkin D.I.^{1,2}, Snytnikov P.V.^{1,2},
Gubaydullin I.M.^{3,4}, Sobyenin V.A.¹

Kinetic Study of the Low-Temperature Steam Reforming of Light Hydrocarbons in the Presence of Methane over the Ni-based Catalyst

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Institute of Petrochemistry and Catalysis RAS, Ufa, Russia

4 - Ufa State Petroleum Technological University, Ufa, Russia

15.50 OP₁₀₋₁₇

Presenting author: Dr. Anna V. Nartova

Nartova A.V.^{1,2,3}, Semikolenov S.V.¹, Bukhtiyarov A.V.^{1,3},
Kovtunova L.M.^{1,2}, Shterk G.V.^{1,2}, R.I. Kvon¹, Bukhtiyarov V.I.^{1,2}

The Role of Oxygen in Deactivation of DeNO_x Platinum catalysts. In Situ XPS and N¹⁵O Kinetic Study

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Research and Educational Center for Energy Efficient Catalysis in Novosibirsk State University, Novosibirsk, Russia

16.00 OP₁₀₋₁₈

Presenting author: Valerii V. Dutov

Dutov V.V.¹, Mamontov G.V.¹, Zaykovskii V.I.², Vodyankina O.V.¹

Ethanol and CO Oxidation over Ag/SiO₂ Catalysts: Effect of Hydroxyl Coverage of the Support

1 – Tomsk State University, Tomsk, Russia

2 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

16.10 OP₁₀₋₁₉

Presenting author: Oleg G. Salnikov

Salnikov O.G.^{1,2}, Burueva D.B.^{1,2}, Kovtunov K.V.^{1,2}, Bukhtiyarov V.I.^{2,3}, Koptuyug I.V.^{1,2}

Mechanisms of Heterogeneous Hydrogenation of α,β -unsaturated Carbonyl Compounds and Thiophene Hydrodesulfurization Studied Using Parahydrogen-induced Polarization Technique

1 – International Tomography Center SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

16.20 OP₁₀₋₂₀

Presenting author: Dr. Andrey A. Saraev

Saraev A.A.^{1,2}, Kaichev V.V.^{1,2}, Bukhtiyarov A.V.^{1,2}, Zemlyanov D.Yu.³, Bukhtiyarov V.I.^{1,2}

Preparation of Model VO_x/TiO₂ Catalysts by Atomic Layer Deposition

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Birck Nanotechnology Center, Purdue University, West Lafayette, USA

16.30 *Coffee break*

17.00-19.00 **Poster Session, 2nd floor, the Volna hotel**

Tuesday, October 4

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Alexander Sorokin
Dr. Evhenii V Kondratenko

PLENARY LECTURE

8.30 PL-4

Presenting author: Prof. Dionisios G. Vlachos
Vlachos D.G.^{1,2}, Patet R.^{1,2}, Caratzoulas S.², Dauenhauer P.^{2,3}

Mechanisms and Kinetics in Complex Systems: Application to Biomass Processing

1 – Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, USA

2 – Catalysis Center for Energy Innovation, USA

3 – Department of Chemical and Materials Science, University of Minnesota, Minneapolis, MN, USA

KEYNOTE LECTURES

9.10 KN-3

Presenting author: Prof. Reko Leino

Combinations of Catalytic and Kinetic Tools for Small Molecule Synthesis

Johan Gadolin Process Chemistry Centre, Laboratory of Organic Chemistry, Åbo Akademi University, Åbo, Finland

9.40 KN-4

Presenting author: Dr. Ilya V. Yudanov

Yudanov I.V.¹, Mamatkulov M.M.¹, Laletina S.S.²

Size Effects in Adsorption Properties of Metal Nanoparticles: an Insight from the DFT Computational Modeling

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia

10.10 Coffee break

Atlantika Hall

Chairmen: Prof. Ekaterina S. Lokteva

Dr. Pavel Nikulshin

Section2. Advanced methods for studies of mechanisms of catalyzed reactions

ORAL PRESENTATIONS

10.40 S2 OP₂₀-01

Presenting author: Dr. Masatoshi Nagai

Nagai M., Ishiwatari N., Ikeda W., Ishiguro K., Suzaki K.

Active Sites of the Functionalized Coals and Carbons for Oxygen Reduction in Fuel Cell and Friedel-Crafts Reaction

Tokyo University of Agriculture and Technology, Koganei, Japan

11.00 S2 OP₂₀-02

Presenting author: Prof. Vladislav A. Sadykov

Mechanism of Ethanol Reforming into Syngas on Complex Oxides Promoted by Pt/Ni+Ru

Sadykov V.A.^{1,2}, Simonov M.N.^{1,2}, Rogov V.A.^{1,2}, Mezentseva N.V.^{1,2},

Chub O.V.¹, Chesalov Yu.A.¹, Sadovskaya E.M.^{1,2}, Pavlova S.N.¹,

Arapova M.V.¹, Smal E.A.¹, Lukashevich A.I.¹, Roger A.-C.³, van Veen A.C.⁴

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – University of Strasbourg, Strasbourg, France

4 – University of Warwick, UK

11.20 S2 OP₂₀-03

Presenting author: Dr. Olga A. Stonkus

Stonkus O.A.^{1,2}, Slavinskaya E.M.^{1,2}, Kibis L.S.^{1,2}, Podyacheva O.Yu.^{1,2}, Grayfer E.V.³, Fedorov V.E.^{2,3}, Zaikovskii V.I.^{1,2}, Boronin A.I.^{1,2}

The Self-sustained Oscillations in CO Oxidation and Structural Transformations of Platinum Metals Supported on Carbon Materials

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

11.40 S2 OP₂₀-04

Presenting author: Dr. Vladimir L. Kuznetsov

Kuznetsov V.L.^{1,2}, Krasnikov D.V.^{1,2}, Shmakov A.N.^{1,2}, Lapina O.B.¹, Andreev A.S.^{1,2}, Ishchenko A.V.¹, Prosvirin I.P.¹, Kalinkin A.V.¹, Selyutin A.G.¹, Kazakova M.A.^{1,2}

In Situ Study of the Activation Bimetallic Catalyst for Multi-walled Carbon Nanotubes Growth

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

12.00 S2 OP₂₀-05

Presenting author: Dr. Vladimir V. Zhivonitko

Zhivonitko V.V.^{1,2}, Telkki V.V.³, Koptyug I.V.^{1,2}

Parahydrogen Enhanced NMR for Mechanistic Studies: from Exploring New Catalytic Systems to Microfluidic Reactor Imaging

1 – International Tomography Center SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – University of Oulu, Oulu, Finland

12.20 S2 OP₂₀-07

Presenting author: Dr. Maria L. Gringolts

Denisova Yu.I.¹, Gringolts M.L.¹, Peregudov A.S.², Kudryavtsev Y.V.¹,
Krentsel L.B.¹, Shandryuk G.A.¹, Litmanovich A.D.¹,
Finkelshtein E.Sh.¹

**Cross-Metathesis between Polynorbornenes and Poly (1-octylene)
Mediated by Grubbs' Catalysts**

*1 – A.V. Topchiev Institute of Petrochemical Synthesis,
RAS, Moscow, Russia*

*2 – Nesmeyanov Institute of Organoelement Compounds,
RAS, Moscow, Russia*

13.00-14.30 *Lunch*

15.00-19.00 **Excursion to Kaliningrad**

19.30-23.00 **Banquet (Herkules restaurant, Kaliningrad)**

Tuesday, October 4

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Alexander Sorokin
Dr. Evhenii V Kondratenko

PLENARY LECTURE

8.30 PL-4

Presenting author: Prof. Dionisios G. Vlachos
Vlachos D.G.^{1,2}, Patet R.^{1,2}, Caratzoulas S.², Dauenhauer P.^{2,3}

Mechanisms and Kinetics in Complex Systems: Application to Biomass Processing

1 – Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, USA

2 – Catalysis Center for Energy Innovation, USA

3 – Department of Chemical and Materials Science, University of Minnesota, Minneapolis, MN, USA

KEYNOTE LECTURES

9.10 KN-3

Presenting author: Prof. Reko Leino

Combinations of Catalytic and Kinetic Tools for Small Molecule Synthesis

Johan Gadolin Process Chemistry Centre, Laboratory of Organic Chemistry, Åbo Akademi University, Åbo, Finland

9.40 KN-4

Presenting author: Dr. Ilya V. Yudanov

Yudanov I.V.¹, Mamatkulov M.M.¹, Laletina S.S.²

Size Effects in Adsorption Properties of Metal Nanoparticles: an Insight from the DFT Computational Modeling

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia

10.10 Coffee break

Beliy Hall

Chairmen: Dr. Alina Tirsoaga

Prof. Oxana Taran

Section 4. Kinetics and reaction intermediates of catalyzed processes

ORAL PRESENTATIONS

10.40 S4 OP₂₀-05

Presenting author: Prof. Gunther Kolb

Wichert M.¹, Zapf R.¹, Ziogas A.¹, Kolb G.^{1,2}, Klemm E.³

Detailed Kinetic Study of Methanol Steam Reforming over Novel Pt/In₂O₃/Al₂O₃ Catalyst in a Microstructured Recycle Reactor

1 – Fraunhofer ICT-IMM, Mainz, Germany

2 – Eindhoven University of Technology, Eindhoven, The Netherlands

3 – Universität Stuttgart, ITC, Stuttgart, Germany

11.00 S4 OP₂₀-06

Presenting author: Dr. Alexander M. Khenkin

Mechanism of Oxidation of C-H Bonds by Homogeneous Vanadium Substituted Polyoxomolybdates

Weizmann Institute of Science, Rehovot, Israel

11.20 S4 OP₂₀-07

Presenting author: Dr. Andreas Martin

Reining S., Kondratenko E.V., Kalevaru V.N., Martin A.

Mechanistic Aspects of the Gas Phase Acetoxylation of Toluene over Pd-Sb/TiO₂ Catalyst

Leibniz Institute for Catalysis, Rostock, Germany

11.40 S4 OP₂₀-08

Presenting author: Prof. Mikhail Yu. Sinev

Lomonosov V.I., Gordienko Yu.A., Fattakhova Z.T., Sinev M.Yu.

Reactive Oxygen Species and Kinetics of Oxidative Coupling of Methane over NaWMn/SiO₂ Mixed Oxide Catalyst

Semenov Institute of Chemical Physics RAS, Moscow, Russia

12.00 S4 OP₂₀-09

Presenting author: Dr. Evgeny E. Faingol'd

Faingol'd E.E., Panin A.N., Babkina O.N., Saratovskikh S.L.,

Bravaya N.M.

Sterically Hindered Isobutylaluminum Aryloxides as Metallocene Activators in Homo- and Copolymerization of Olefins

Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region, Russia

12.20 S4 OP₂₀-10

Presenting author: Dr. Marcus Rose

Pfützenreuter R., Rose M.¹

A Kinetic and Mechanistic Study on the Heterogeneously Catalysed Aqueous Phase Amination and Isomerization of Biogenic Alcohols

1 – Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Aachen, Germany

12.40 S4 OP₂₀₋₁₁

Presenting author: Dr. Yulia S. Demidova

Demidova Yu.S.^{1,2}, Simakova I.L.^{1,2}, Wärnä J.³, Simakov A.⁴,
Murzin D.Yu.³

Kinetic Modelling of One-Pot Alcohol Amination over Gold Catalyst

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Åbo Akademi University, Turku/Åbo, Finland

4 – Centro de Nanociencias y Nanotecnología de la Universidad Nacional Autónoma de México, México

13.00-14.30 *Lunch*

15.00-19.00 **Excursion to Kaliningrad**

19.30-23.00 **Banquet (Herkules restaurant, Kaliningrad)**

Tuesday, October 4

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Alexander Sorokin
Dr. Evhenii V Kondratenko

PLENARY LECTURE

8.30 PL-4

Presenting author: Prof. Dionisios G. Vlachos
Vlachos D.G.^{1,2}, Patet R.^{1,2}, Caratzoulas S.², Dauenhauer P.^{2,3}

Mechanisms and Kinetics in Complex Systems: Application to Biomass Processing

1 – Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, USA

2 – Catalysis Center for Energy Innovation, USA

3 – Department of Chemical and Materials Science, University of Minnesota, Minneapolis, MN, USA

KEYNOTE LECTURES

9.10 KN-3

Presenting author: Prof. Reko Leino

Combinations of Catalytic and Kinetic Tools for Small Molecule Synthesis

Johan Gadolin Process Chemistry Centre, Laboratory of Organic Chemistry, Åbo Akademi University, Åbo, Finland

9.40 KN-4

Presenting author: Dr. Ilya V. Yudanov

Yudanov I.V.¹, Mamatkulov M.M.¹, Laletina S.S.²

Size Effects in Adsorption Properties of Metal Nanoparticles: an Insight from the DFT Computational Modeling

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia

10.10 *Coffee break*

Baltika Hall

School-Symposium "Quantum-mechanical modeling of catalytic processes"

Chairmen: Dr. Ilya V. Yudanov

Dr. Elena A. Shor

KEYNOTE LECTURES

10.40 KIs-1

Presenting author: Prof. Konstantin M. Neyman

Neyman K.M.^{1,2}, Kovács G.¹, Kozlov S.M.¹

Innovative Computational Design of Advanced Nanoalloy Materials for Catalysis and Beyond

1 – Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional, Universitat de Barcelona, Barcelona, Spain

2 – Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain

11.10 KIs-2

Presenting author: Prof. Stefano Fabris

Bonding and Reactivity at Catalytic Interfaces: Modelling Novel Electrodes from Ideal to Realistic Reaction Environments

CNR-IOM DEMOCRITOS Simulation Center and SISSA - Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

ORAL PRESENTATIONS

11.40 SOP₁₀-01

Presenting author: Dr. Svetlana S. Laletina

Laletina S.S.¹, Shor E.A.¹, Mamatkulov M.², Kaichev V.V.²,
Bukhtiyarov V.I.²

DFT Study of Methanol Decomposition on Platinum Clusters

*1 – Institute of Chemistry and Chemical Technology SB RAS,
Krasnoyarsk, Russia*

2 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

11.50 SOP₁₀-02

Presenting author: Maria N. Golosnaya

Golosnaya M.N., Pichugina D.A., Kuz'menko N.E

Phosphine-protected Gold Clusters: from Structure Prediction to Catalytic Reaction Study

Lomonosov Moscow State University, Moscow, Russian Federation

12.00 SOP₁₀-03

Presenting author: Nadezhda A. Nikitina

Nikitina N.A., Oleynichenko A.V., Pichugina D.A., Majouga A.G.,
Kuz'menko N.E.

DFT Study of the Active Sites of Gold Clusters Anchored by Thiolate, Selenolate and Tellurolate Ligands

*Department of Chemistry, Lomonosov Moscow State University,
Moscow, Russia*

12.10 SOP₁₀-04

Presenting author: Vladimir V. Gogol

Gogol V.V., Pichugina D.A., Kuzmenko N.E.

DFT Insight into CO Oxidation Catalyzed by Gold-Copper Nanoclusters

*Department of Chemistry, Lomonosov Moscow State University,
Moscow, Russian Federation*

12.20 SOP₁₀-05

Presenting author: Dr. Sergei E. Malykhin

Malykhin S.E.^{1,2}, Ivanov D.I.¹, Dubkov K.A.¹

Mechanism of the Selective Oxidation of Olefins with Nitrous Oxide

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Department of Natural Science, National Research University - Novosibirsk State University, Novosibirsk, Russia

12.30 SOP₁₀-06

Presenting author: Yulia G. Polynskaya

Polynskaya Yu.G., Pichugina D.A., Kuz'menko N.E.

Propylene Epoxidation over Silver and Bimetallic Gold-Silver Clusters

Lomonosov Moscow State University, Moscow, Russia

12.40 SOP₁₀-07

Presenting author: Grigory Yu. Zhigulin

Zhigulin G.Yu.¹, Sanyal R.², Ketkov S.Yu.¹, Das D.²

Theoretical Investigation of Solvent Influence on Catalytic Activity of New di- and tetraNuclear Copper(II) Complexes with Mannich-Base Ligands

1 – Razuvaev Institute of Organometallic Chemistry RAS,

Nizhny Novgorod, Russia

2 – University of Calcutta, Calcutta, India

12.50 SOP₁₀-08

Presenting author: Dr. Andrey V. Matveev

Lysova A.A.¹, Bryliakova A.A.², Tantardini C.¹, Matveev A.V.^{1,2},

Benassi E.^{1,3}

Study of Adsorption and Diffusion of Atomic Oxygen on the Surface and in Subsurface Region of Pd Nanoparticles and Pd(110) Single Crystal

1 – Novosibirsk State University, Novosibirsk, Russia

2 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

3 – Scuola Normale Superiore di Pisa, Pisa, Italy

13.00-14.30 *Lunch*

15.00-19.00 **Excursion to Kaliningrad**

19.30-23.00 **Banquet (Herkules restaurant, Kaliningrad)**

Wednesday, October 5

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Stig Helveg
Prof. Konstantin P. Bryliakov

KEYNOTE LECTURES

8.30 KN-5

Presenting author: Dr. Alexander B. Sorokin

High-valent Diiron Oxo Species: Key Intermediates in Challenging Oxidations

Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, UMR 5256, CNRS – Université Lyon 1, Villeurbanne, France

9.00 KN-6

Presenting author: Prof. Igor V. Koptug I

Koptug I.V., Kovtunov K.V., Zhivonitko V.V.

Signal Enhancement with Parahydrogen for Operando NMR in Catalysis

International Tomography Center, SB RAS, Novosibirsk, Russia

9.30 KN-7

Presenting author: Prof. Svetlana Schauer mann

Elementary Steps in Surface Reactions: Mechanisms, Kinetics and Thermodynamics

1 – Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

2 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

10.00 *Coffee break*

Atlantika Hall

Section2. Advanced methods for studies of mechanisms of catalyzed reactions

Chairmen: Dr. Alexander Khenkin
Prof. Gunther Kolb

ORAL PRESENTATIONS

10.30 S2 OP₂₀₋₀₈

Presenting author: Dr. Galina A. Bukhtiyarova

Synergetic Effect of Ni₂P/SiO₂ and γ -Al₂O₃ Physical Mixture in Hydrodeoxygenation of Methyl Palmitate

Deliy I.V., Shamanaev I.V., Pakharukova V.P., Gerasimov E.Yu.,
Bukhtiyarova G.A.

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

10.50 S2 OP₂₀₋₀₉

Presenting author: Prof. Sema L. Ioffe

New Approach to Reactivity Umpolung of Aliphatic Nitro Compounds. The Mechanistic Consideration

Ioffe S.L., Khoroshutina Yu.A., Smirnov V.O., Mikhaylov A.A.

N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

11.10 S2 OP₂₀₋₁₀

Presenting author: Dr. Ekaterina A. Kozlova

Photocatalytic Hydrogen Evolution under Visible Light over Me/Cd_{0.3}Zn_{0.7}S (Me = Au, Pt, Pd): Transformation of Metal co-Catalysts During the Irradiation

Kozlova E.^{1,2,3}, Kolinko P.^{1,2,3}, Kurenkova A.^{1,2}, Saraev A.^{1,2},
Gerasimov E.^{1,2,3}, Cherepanova S.^{1,2,3}

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Educational Center for Energy Efficient Catalysis in Novosibirsk State University, Novosibirsk, Russia

11.30 S2 OP₂₀₋₁₁

Presenting author: Dr. Elena V. Golubina

Active Sites in Ni-containing Catalysts for Selective Phenylacetylene Hydrogenation

Golubina E.V.^{1,2}, Lokteva E.S.^{1,2}, Maslakov K.I.^{1,2}, Erokhin A.V.¹,
Murzin V.Y.³, Zubavichus Y.V.³

1 – Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

2 – Institute of Hydrocarbon Processing SB RAS, Omsk, Russia

3 – National Research Centre “Kurchatov Institute”, Moscow, Russia

11.50 S2 OP₂₀₋₁₂

Presenting author: Prof. Olga T. Kasaikina

Effects of Magnetic Field and Oxygen on Catalytic Hydroperoxide Decomposition in Mixed Micelles with Cationic Surfactants

Kasaikina O.T., Pisarenko L.M., Potapova N.A.

Semenov Institute of Chemical Physics, Moscow, Russia

Atlantika Hall

12.10-13.00 **Closing session**

13.00-14.30 *Lunch*

14.30-18.30 **Excursion to Yantarnyi**

(The Excursion starts at 14:30 from the Volna hotel and ends at 18:30 at the Khrabrovo Airport of Kaliningrad)

Wednesday, October 5

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Stig Helveg
Prof. Konstantin P. Bryliakov

KEYNOTE LECTURES

8.30 KN-5

Presenting author: Dr. Alexander B. Sorokin

High-valent Diiron Oxo Species: Key Intermediates in Challenging Oxidations

Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, UMR 5256, CNRS – Université Lyon 1, Villeurbanne, France

9.00 KN-6

Presenting author: Prof. Igor V. Koptug

Koptug I.V., Kovtunov K.V., Zhivonitko V.V.

Signal Enhancement with Parahydrogen for Operando NMR in Catalysis

International Tomography Center, SB RAS, Novosibirsk, Russia

9.30 KN-7

Presenting author: Prof. Svetlana Schauer mann

Elementary Steps in Surface Reactions: Mechanisms, Kinetics and Thermodynamics

1 – Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

2 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

10.00 *Coffee break*

Belyi Hall

Section 5. From mechanistic studies to design of advanced catalyst systems

Chairmen: Prof. Mikhail Yu. Sinev
Prof. Igor V. Koptuyug

ORAL PRESENTATIONS

10.30 S5 OP₂₀₋₀₅

Presenting author: Dr. Pavel A. Nikulshin

Highly Active Ternary NiCoMoS/Al₂O₃ Hydrotreating Catalysts Based on Co₂Mo₁₀-Heteropolyacid and Nickel Citrate

Nikulshin P.A.¹, Mozhaev A.V.¹, Maslakov K.I.², Pimerzin A.A.¹

1 – Samara State Technical University, Russia

2 – Chemistry Department, M.V. Lomonosov Moscow State University, Russia

10.50 S5 OP₂₀₋₀₆

Presenting author: Dr. Svetlana A. Yashnik

Design of Pt,Pd-doped Mn-Hexaaluminate Catalyst with High Efficiency and Stability in Methane Oxidation

Yashnik S.A.¹, Vinokurov Z.S.¹, Saraev A.A.¹, Ishchenko A.V.¹,

Kaichev V.V.¹, Ismagilov Z.R.^{1,2}

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia

11.10 S5 OP₂₀₋₀₇

Presenting author: Prof. Vladimir A. Sobyenin

Mechanism of Dimethoxymethane Steam Reforming to Hydrogen-Rich Gas over Alumina Supported CuO-ZnO and CuO-CeO₂ Catalysts

Pechenkin A.A.^{1,2}, Badmaev S.D.^{1,2}, Belyaev V.D.^{1,2}, Sobyenin V.A.¹

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

11.30 S5 OP₂₀-08

Presenting author: Dr. Irina L. Simakova

Simakova I.L.^{1,2}, Panchenko V.N.¹, Guliaeva Yu.A.¹, Simonov M.N.^{1,2}

Kinetic and Mechanistic Aspects of One-Pot Valeric Acid Transformation into Alkane over Pd (Pt)/MO_x

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

11.50 S5 OP₂₀-09

Presenting author: Dr. Ilia V. Mishakov

Prompt Metal Dusting of Model Ni-based Alloys:

Mechanism of Active Sites Formation Followed by CNM Growth

Mishakov I.V.^{1,2}, Bauman Yu.I.¹, Vedyagin A.A.¹, Buyanov R.A.¹

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

Atlantika Hall

12.10-13.00 **Closing session**

13.00-14.30 *Lunch*

14.30-18.30 **Excursion to Yantarnyi**

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Wednesday, October 5

The Volna hotel

MORNING SESSION

Atlantika Hall

Chairmen: Dr. Stig Helveg
Prof. Konstantin P. Bryliakov

KEYNOTE LECTURES

8.30 KN-5

Presenting author: Dr. Alexander B. Sorokin

High-valent Diiron Oxo Species: Key Intermediates in Challenging Oxidations

Institut de Recherches sur la Catalyse et l'Environnement de Lyon, IRCELYON, UMR 5256, CNRS – Université Lyon 1, Villeurbanne, France

9.00 KN-6

Presenting author: Prof. Igor V. Koptug

Koptug I.V., Kovtunov K.V., Zhivonitko V.V.

Signal Enhancement with Parahydrogen for Operando NMR in Catalysis

International Tomography Center, SB RAS, Novosibirsk, Russia

9.30 KN-7

Presenting author: Prof. Svetlana Schauer mann

Elementary Steps in Surface Reactions: Mechanisms, Kinetics and Thermodynamics

1 – Institute of Physical Chemistry, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

2 – Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

10.00 *Coffee break*

Baltika Hall

Chairmen: Dr. Olga Belskaya
Dr. Lyudmila Moskaleva

SHORT ORAL PRESENTATIONS

10.30 OP₁₀₋₂₁

Presenting author: Prof. Marco Piumetti

Piumetti M., Bensaïd S., Fino D., Russo N., Andana T., Pirone R.

CO and Soot Oxidation with CeO₂-ZrO₂ Mixed Oxides in the Absence of Oxygen

Department of Applied Science and Technology, Politecnico di Torino, Turin, Italy

10.40 OP₁₀₋₂₂

Presenting author: Dr. Dmitry A. Svintsitskiy

Svintsitskiy D.A.^{1,2}, Kardash T.Yu.^{1,2}, Slavinskaya E.M.^{1,2},
Koscheev S.V.^{1,2}, Avdeev A.V.¹, Izaak T.I.³, Boronin A.I.^{1,2}

Paramelaconite-based Catalysts of Low-Temperature CO Oxidation

1 – Borskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Tomsk State University, Tomsk, Russia

10.50 OP₁₀₋₂₃

Presenting author: Mabuatsela V. Maphoru

Maphoru M.V.¹, Heveling J.¹, Kesavan Pillai S.²

Oxidation of Naphthols on Nanocrystalline Pt-Group Metal Catalysts

1 – Tshwane University of Technology, Pretoria, South Africa

2 – Council for Scientific and Industrial Research, Pretoria, South Africa

11.00 OP₁₀-24

Presenting author: Ekaterina I. Shuvarakova

The Effect of Electron-Acceptor Sites on Catalytic Shuvarakova E.I.^{1,2},
Bedilo A.F.^{1,2}, Chesnokov V.V.¹, Kenzhin R.M.¹

Dehydrochlorination of 1-Chlorobutane over Metal Oxide Catalysts

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

*2 – Novosibirsk Institute of Technology, Moscow State University of
Design and Technology, Novosibirsk, Russia*

11.10 OP₁₀-25

Presenting author: Dr. Mikhail N. Khrizanforov

Electrocatalytic Functionalization of Biologically Important Substrates of Different Classes of Arenes

Khrizanforov M.N., Strelakova S.O., Grinenko V.V., Khrizanforova
V.V., Kholin K.V. Gryaznova T.V., Budnikova Y.H.

*A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan
Scientific Center, Russian Academy of Sciences, Kazan, Russia*

11.20 OP₁₀-27

Presenting author: Prof. Lusegen A. Bugaev

Bimetallic PtCu Nanoparticles in PtCu/C Electro-Catalysts

Bugaev L.A., Srabionyan V.V., Pryadchenko V.V., Bugaev A.L.,
Avakyan L.A., Belenov S.V., Guterman V.E.

*Southern Federal University, Physical and Chemical Faculties,
Rostov-on-Don, Russia*

11.30 OP₁₀-28

Presenting author: Dr. Evgeny I. Vovk

Vovk E.I.^{1,2}, Karatok M.², Shah A.A.², Bukhtiyarov V.I.¹, Ozensoy E.²

Atomic Oxygen on Ag(111) Generated via Ozone Decomposition and Its Reactivity towards Methanol

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Chemistry Department, Bilkent University, Ankara, 06800, Turkey

11.40 OP₁₀-29

Presenting author: Dr. Oleg V. Potapenko

Potapenko O.V., Bukin K.A., Doronin V.P., Sorokina T.P., Talzi V.P.,
Likholobov V.A.

**Investigation of Hydrogen Transfer Reactions between C₆-
Hydrocarbons**

on the Catalysts with Different Natures

Institute of Hydrocarbons processing SB RAS, Omsk, Russia

11.50 OP₁₀-30

Presenting author: Tapas Rajkhowa

Evaluation of Cu Based Catalysts for Glycerol Hydrogenolysis

Rajkhowa T., Lauwaert J., Thybaut J.W.

*Laboratory for Chemical Technology, Ghent University,
Technologiepark 914, Gent, Belgium*

Atlantika Hall

12.10-13.00 **Closing session**

13.00-14.30 *Lunch*

14.30-18.30 **Excursion to Yantarnyi**

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ends at 18:30 at the Khrabrovo Airport of Kaliningrad)*

Poster Presentations

PP-01

Conjugation of Carbon Monoxide Steam Conversion with Ethylbenzene to Styrene Dehydrogenation in the Presence of CO₂

Abasov S.I., Mamedova M.T., Zarbaliyev R.R., Agayeva S.B.,
Iskenderova A.A., Nasibova A.R., Tagiev D.B.

Institute of Petrochemical Processes named after Yu.G.Mamedaliyev, ANAS, Baku, Azerbaijan

PP-02

Eco-friendly High-Octane Petrol Extracting from Straight-run Gasoline by Low Temperature Reforming

Tagiyev D.B., Abasov S.I., Agayeva S.B., Mamedova M.T., Starikov R.V.,
Iskenderova A.A., Imanova A.A.

Institute of Petrochemical Processes named after Yu.G.Mamedaliyev, ANAS, Baku, Azerbaijan

PP-04

Nickel Supported on MOF-5 and UiO-66 in Vapor-Phase Hydrodechlorination of Chlorobenzene

Agafonov A.A.^{1,2}, Lokteva E.S.^{1,2}, Strokova N.E.¹, Ivakin Yu.D.¹

1 – Lomonosov Moscow State University, Moscow, Russia

2 – Institute of Hydrocarbons Processing SB RAS, Omsk, Russia

PP-06

Development of Kinetic Models of Catalytic Reactions with the Use of Parallel Computing

Akhmetov I.V.¹, Gubaydullin I.M.²

1 – Ufa State Petroleum Technological University, Ufa, Russia

2 – Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

PP-08

Effect of Support of Ternary KCoMoS Catalysts on the Morphology of Active Phase Species and Their Properties in Selective FCC Gasoline Hydrotreating

Anashkin Yu.V., Ishutenko D.I., Nikulshin P.A.

Samara State Technical University, Samara, Russia

PP-10

Isotopic Methods to Study Little-known Catalytic Activity of Solid Alkaline Hydroxides for Energy Conversion and Storage

Baikov Yu.M., Nikulin E.I, Egorov V.M.

Ioffe Institute, St-Petersburg, Russia

PP-16

Ring-opening Metathesis Polymerization of Fullerene-containing α,ω -bis-Norbornenes by Catalyst Grubbs 1st Generation

Biglova Yu.N.¹, Nuriahmetova Z.F.¹, Torosyan S.A.², Mustafin A.G.¹, Miftakhov M.S.²

1 – Bashkir State University, Department of Chemistry, Ufa, Russia

2 – Ufa Institute of Chemistry, RAS, Ufa, Russia

PP-17

Metathesis Homopolymerization of Fullerene-containing 7-thia-bicyclo[2.2.1]hept-2-ene by Catalyst Grubbs 1st Generation

Biglova Yu.N.¹, Zagitov V.V.¹, Mustafin A.G.¹, Miftakhov M.S.²

1 – Bashkir State University, Department of Chemistry, Ufa, Russia

2 – Ufa Institute of Chemistry, RAS, Ufa, Russia

PP-18

Influence of the Electronic Properties of Palladium Particles Deposited on Alumina on the Reaction Mechanism of Hydrogenation of 1,3-Butadiene

Boretskaya A.V., Lamberov A.A., Ilyasov I.R., Laskin A.I.

Kazan Federal University, Kazan, Russia

PP-19

Parahydrogen-induced Polarization for Mechanistic Investigation of Heterogeneous Hydrogenation Reactions

Burueva D.B., Salnikov O.G., Kovtunov K.V., Koptuyug I.V.

International Tomography Center SB RAS, Novosibirsk, Russia

Novosibirsk State University, Novosibirsk, Russia

PP-20

Mechanistic Aspects of the Activation of Silica-supported Iron Catalysts for Fischer–Tropsch Synthesis in Carbon Monoxide and Syngas

Chernavskii P.A., Pankina G.V., Kazak V.O.

Chemistry Department, Lomonosov Moscow State University, Moscow, Russia

PP-24**Nickel Based Catalysts for Combined Steam and Carbon Dioxide Reforming of Methane**

Danilova M.M., Fedorova Z.A., Zaikovskii V.I., Porsin A.V., Kirillov V.A., Krieger T.A.

Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

PP-25**Selective Carvone Hydrogenation to Dihydrocarvone over Au Catalyst**

Demidova Yu.S.^{1,2}, Suslov E.V.³, Simakova O.A.⁴, Simakova I.L.^{1,2}, Volcho K.P.^{2,3}, Salakhutdinov N.F.^{2,3}, Murzin D.Yu.⁵

1 – *Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

3 – *Novosibirsk Institute of Organic Chemistry, Novosibirsk, Russia*

4 – *Georgia Institute of Technology, Atlanta, USA*

5 – *Åbo Akademi University, Turku/Åbo, Finland*

PP-27**On a Mechanism of Catalytic Combustion of Soot:****Evaluating “Extra-tight” Catalyst-Soot Contact Condition**

Dubkov A.A., Kovtunova L.M., Bukhtiyarov V.I.

Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

PP-28**Effect of Pore Size of Zeolites on Olefin Oligomerization**

Efimov A.V., Popov A.G.

Moscow State University, Moscow, Russia

PP-32**Tri-Reforming of Methane to Synthesis Gas over Porous Nickel Based Catalysts**

Fedorova Z.A., Danilova M.M., Zaikovskii V.I., Krieger T.A., Bukhtiyarov A.V., Porsin A.V.

Borekov Institute of Catalysis, SB RAS, Novosibirsk, Russia

PP-34

Different Activity of Zn²⁺ and ZnO Species for Methane Activation and Conversion at Zn-modified Zeolites

Gabrienko A.A., Arzumanov S.S., Toktarev A.V., Stepanov A.G.

1 – *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Department of Natural Sciences, Novosibirsk State University, Novosibirsk, Russia*

PP-36

Mechanism of n-Hexane Isomerization over Palladium Catalysts

Luu Cam Loc¹, Nguyen Tri¹, Gaidai N.A.², Agafonov Yu.A.²,

Dao Thi Kim Thoa³, Ha Cam Anh³, Hoang Tien Cuong¹, Lapidus A.L.²

1 – *Institute of Chemical Technology, Vietnam Academy of Science and Technology, Ho Chi Minh City, Vietnam*

2 – *N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Science, Moscow, Russia*

3 – *University of Technology, Vietnam National University, Ho Chi Minh City, Vietnam*

PP-39

Kinetics of Cross-Metathesis between Polynorbornene and Polyoctenamer in the Presence of 1st and 2nd Generation Grubbs' Catalysts

Denisova Yu.I., Gringolts M.L., Shandryuk G.A., Krentsel L.B.,

Litmanovich A.D., Finkelshtein E.Sh., Kudryavtsev Y.V.

A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Moscow, Russia

PP-40

Synthesis of (Me)₃Si-Norbornene–Cyclooctene Multiblock Copolymers with the Cross-Metathesis of Poly(Me₃Si-Norbornene) and Polyoctenamer Using Grubbs 1st Catalyst

Denisova Yu.I., Gringolts M.L., Shandryuk G.A., Krentsel L.B.,

Litmanovich A.D., Finkelshtein E.Sh., Kudryavtsev Y.V.

A.V. Topchiev Institute of Petrochemical Synthesis, RAS, Moscow, Russia

PP-41

Catalysis of Hydrogen Atom Transfer in KBr Matrix

Grinvald I.I., Kalagaev I.Yu., Petukhov A.N., Vorotyntsev I.V., Spirin I.A., Salkina S.V.

Alekseev State Technical University, Nizhniy Novgorod, Russia

PP-42

Influence of Electric Field on the Chemical Properties of Nanoparticles

Grishin M.V., Gatin A.K., Kharitonov V.A., Kolchenko N.N., Sarvadiy S. Yu., Shub B.R., Slutsky V.G.

Semenov Institute of Chemical Physics RAS, Moscow, Russia

PP-43

Modeling of the Electrochemical Impedance in Anodic Dissolution of Iron Using a Heuristic Algorithms

Enikeev A.R.¹ Maleeva M.A.², Gubaydullin I.M.¹

1 – Institute of Petrochemistry and Catalysis RAS, Ufa, Russia

2 – A.N. Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Moscow, Russia

PP-44

Identification of Corrosion Processes by Morphology of Metal Surface Using Computer Vision

Enikeev M.R.¹, Gubaydullin I.M.^{1,2}, Koledina K.F.^{1,2}, Maleeva M.A.³

1 – Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

2 – Ufa State Petroleum Technical University, Ufa, Russia

3 – Frumkin Institute of Physical Chemistry and Electrochemistry RAS, Moscow, Russia

PP-45

Study of the Mechanism of the Catalytic Reaction of Alcohols with Dimethyl Carbonate

Koledina K.F.^{1,2}, Koledin S.N.¹, Gubaydullin I.M.^{1,2}

1 – Institute of Petrochemistry and Catalysis, Russian Academy of Sciences, Ufa, Russia

2 – Ufa State Petroleum Technological University, Ufa, Russia

PP-46

Catalytic Activity and Charge State of Supported Metal Nanoparticles

Gurevich S.A.¹, Kozhevnikov V.M.¹, Yavsin D.A.¹, Il'yuschenkov D.S.¹, Rostovshchikova T.N.², Lokteva E.S.²

1 – Ioffe Physical-Technical Institute of RAS, St-Petersburg, Russia

2 – Lomonosov Moscow State University, Moscow, Russia

PP-48

Selective Oxidation of Alcohols to Aldehydes over Pt-Sb/C Catalysts

Heveling J., Langa S., Nyamunda B.C.

Tshwane University of Technology, Pretoria, South Africa

PP-49

Pt₂₄ Subnanoparticle as a Prospective Nanocatalyst for Regioselective Hydrogenation. DFT Study of Its Structural, Thermodynamic and Adsorption Properties

Ignatov S.K.¹, Gadzhiev O.B.¹, Okhapkin A.I.¹, Razuvaev A.G.¹, Kunz S.², Bäumer M.²

1 – N.I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia

2 – University of Bremen, Bremen, Germany

PP-50

DFT Study of Pt Catalyzed Hydrogenation: Adsorption, Surface Diffusion, and Subsurface Migration of Molecular and Atomic Hydrogen on the Pt₂₄ Subnanoparticle

Ignatov S.K.¹, Gadzhiev O.B.¹, Okhapkin A.I.¹, Razuvaev A.G.¹, Kunz S.², Bäumer M.²

1 – N.I. Lobachevsky State University of Nizhny Novgorod, Nizhny Novgorod, Russia

2 – University of Bremen, Bremen, Germany

PP-51

Effect of Reaction Conditions on Ethane Oxidative Conversion over MoVTeNbO Catalyst

Bondareva V.M.¹, Ishchenko E.V.^{1,2}, Kardash T.Yu.^{1,2}, Ovchinnikova E.V.¹, Sobolev V.I.¹

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

PP-52

K_x-CoMoS/Al₂O₃ Catalysts with Low Metal Loadings for Selective Hydrotreating of FCC Gasoline

Ishutenko D.I., Nikulshin P.A., Mozhaev A.V., Pimerzin A.A.

Samara State Technical University, Samara, Russia

PP-53

DFT Study on MAO Effect in Alkene Hydrometalation as Stage of Ziegler-Natta Type Catalytic Processes

Tyumkina T.V.¹, Islamov D.N.¹, Kovyazin P.V.¹, Parfenova L.V.¹,
Ivchenko P.V.^{2,3}, Nifant'ev I.E.^{2,3}

1 – Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

2 – Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

3 – A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

PP-54

La_{1-x}Ca_xCoO₃ Perovskites for Methane Oxidation

Isupova L.A., Gerasimov E.Yu., Kulikovskaya N.A., Saputina N.F.

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

PP-55

The Role of Cs Promoters on N₂O Decomposition over Ni-Co-Spinel Catalyst

Ivanova Yu.A., Sutormina E.F., Isupova L.A.

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

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Theoretical and Experimental Aspects of Zirconocene-catalyzed α -Olefin Dimerization and Oligomerization

Ivchenko P.V.^{1,2}, Nifant'ev I.E.^{1,2}, Tyumkina T.V.³, Parfenova L.V.³

1 – A.V. Topchiev Institute of Petrochemical Synthesis RAS, Moscow, Russia

2 – Lomonosov Moscow University, Department of Chemistry, Moscow, Russia

3 – Institute of Petrochemistry and Catalysis of RAS, Ufa, Russia

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Oxidation of Propane over Pd(111): *In situ* XPS and Mass Spectrometry Study

Kaichev V.V.^{1,2}, Saraev A.A.^{1,2}, Matveev A.V.^{1,2}, Knop-Gericke A.³,

Bukhtiyarov V.I.^{1,2}

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Fritz Haber Institute of the Max Plank Society, Berlin, Germany

PP-58**XPS and STM Study of Model Au/C and Pt/C Samples Oxidation by Nitrogen Dioxide**

Kalinkin A.V., Smirnov M.Yu., Sorokin A.M., Bukhtiyarov A.V., Bukhtiyarov V.I.

Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

PP-59**X-ray-induced Reduction of $\text{H}_2\text{Pt}(\text{OH})_6$ and K_2PtCl_6 Studied by XPS**

Kalinkin A.V., Smirnov M.Yu., Nizovskii A.I., Bukhtiyarov V.I.

Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

PP-60**CO Oxidation on $\text{Ce}_x\text{Zr}_{(1-x)}\text{O}_2$ and $\text{CuO}/\text{Ce}_x\text{Zr}_{(1-x)}\text{O}_2$ Catalysts Prepared Using CTAB and Sawdust as a Template**

Kaplin I.Y., Lokteva E.S., Golubina E.V., Levanov A.V., Maslakov K.I.

Lomonosov Moscow State University, Chemistry Department, Moscow, Russia

PP-61**Influence of Potassium on the Activation Process of Silica-Supported Iron Catalysts for Fischer–Tropsch Synthesis in Carbon Monoxide and Syngas**

Kazak V.O., Pankina G.V., Chernavskii P.A.

Chemistry Department, Lomonosov Moscow State University, Moscow, Russia

PP-62**Autothermal Reforming of Ethanol over Ni Catalysts Supported on Ceria-based Mixed Oxides**

Kerzhentsev M.A.¹, Matus E.V.¹, Okhlopko L.B.¹, Ismagilov I.Z.¹, Sukhova O.B.¹, Kuznetsov V.V.¹, Yashnik S.A.¹, Prosvirin I.P.¹, Bharali P.², Ismagilov Z.R.^{1,3}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Tezpur University, Napaam, Tezpur, India

3 – Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia

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Quantum-chemical Modeling of the Active Center of MnNaW/SiO₂ Catalyst for Oxidative Coupling of Methane

Zilberberg I.L.¹, Shubin A.A.¹, Ismagilov I.Z.¹, Matus E.V.¹, Kerzhentsev M.A.¹, Ismagilov Z.R.^{1,2}

1 – *Borsov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia*

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Hydrodechlorination of Chlorobenzene on PdCo/C Catalyst Produced by Pyrolysis of Sawdust Impregnated with a Solution of Pd(NO₃)₂ and Co(NO₃)₂

Klokov S.V.^{1,2}, Lokteva E.S.^{1,2}, Maslakov K.I.^{1,2}, Trenikhin M.V.², Likholobov V.A.²

1 – *Lomonosov Moscow State University, Moscow, Russia*

2 – *Institute of Hydrocarbons Processing SB RAS, Omsk, Russia*

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Transition Metal Sulfide Catalysts for Synthesis Gas Conversion into Alcohols and Other Oxygenates

Kogan V.M., Dorokhov V.S., Permyakov E.A.

Zelinsky Institute of Organic Chemistry, RAS, Moscow, Russia

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Selective CO Methanation in the Presence of CO₂ over Nickel-Ceria Catalysts: from Mechanistic Studies to Catalyst Design

Konishcheva M.V.^{1,2}, Potemkin D.I.^{1,2}, Snytnikov P.V.^{1,2}, Sobyenin V.A.^{1,2}

1 – *Borsov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

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Understanding the Key Intermediate of Aromatic Nitration Mechanism Catalyzed by Lewis Acids

Koskin A.P.¹, Borodin A.O.^{2,3}, Malykhin S.E.^{1,4}, Mishakov I.V.^{1,4}, Vedyagin A.A.^{1,3}

1 – *Borsov Institute of Catalysis, Novosibirsk, Russia*

2 – *Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia*

3 – *Novosibirsk State Technical University, Novosibirsk, Russia*

4 – *Novosibirsk State University, Novosibirsk, Russia*

PP-69**Mechanistic Insights in Aldol Condensation of n-Butanal over ZrBEA Catalyst**

Kots P.A., Zabilskaya A.V., Ivanova I.I.

Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

PP-70**Mechanistic Studies of Heterogeneous Reaction and NMR Imaging of Catalytic Hydrogenation by Using Parahydrogen**

Kovtunov K.V.^{1,2}, Salnikov O.G.^{1,2}, Burueva D.B.^{1,2}, Romanov A.S.^{1,2}, Koptyug I.V.^{1,2}

1 – International Tomography Center SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

PP-72**Effect of the Preparation Method of GdFeO₃ Perovskites on Their Catalytic Properties**

Sheshko T.F.¹, Kryuchkova T.A.¹, Zimina V.D.¹, Serov Y.M.¹, Yafarova L.V.², Zvereva I.A.²

1 – Peoples Friendship University of Russia, Faculty of Science, Physical and Colloidal Chemistry Department, Moscow, Russia

2 – Saint-Petersburg State University, Petrodvorets, Saint-Petersburg, Russia

PP-74**Epoxidation of Fatty Acid Methyl Esters of Vegetable Oils by Air Oxygen**

Kulazhskaya A.D., Larina S.O., Amirkhanov I.R., Voronov M.S., Sapunov V.N.

Dmitry Mendeleev University of Chemical Technology of Russia, Moscow, Russia

PP-75**Effect of Water on Hydrocarbons Formation from CO and H₂ over Co/H-Zeolite Catalysts**

Kulchakovskaya E.V.¹, Mordkovich V.Z.^{1,2}, Sineva L.V.^{1,2}

1 – Technological Institute for Superhard and Novel Carbon Materials, Troitsk, Moscow, Russia

2 – INFRATEchnology Ltd., Moscow, Russia

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The Investigation of the Mechanism of Heck Reaction with Aromatic Carboxylic Anhydrides Using Advanced Methods of Competing Reactions

Larina E.V., Yarosh E.V., Lagoda N.A., Kurokhtina A.A., Schmidt A.F.

Chemical Department of Irkutsk State University, Irkutsk, Russia

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Peroxide Oxidation of Hydrocarbons Mediated by Heteropolycompounds and Affected by Ionic Liquids

Kuznetsova N.I., Kuznetsova I.L.

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

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Detailed Characteristic of the Pt-HPA-IL Catalytic System Applied to Oxidation by O₂/H₂ Gases

Kuznetsova N.I.¹, Kuznetsova L.I.¹, Koscheeva O.S.², Larina T.V.¹,

Maksimovskaya R.I.¹

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

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In-Situ SAXS Study of Sol-Gel Process to Prepare Ag/P₂O₅/SiO₂ Catalysts

Larichev Yu.V.^{1,2}, Vodyankina O.V.³

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Tomsk State University, Tomsk, Russia

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Self-oscillating Dynamics in the Partial Oxidation of Methane over a Ni Foil in Relations with Reversible Oxidation and Carbonization of the Catalyst Bulk

Lashina E.A.^{1,2}, Saraev A.A.^{1,2}, Ustugov V.V.¹, Chumakova N.A.^{1,2},

Kaichev V.V.^{1,2}, Bukhtiyarov V.I.^{1,2}

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

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Design of Mixed CeO₂-ZrO₂/SiO₂ Supports and Ag Catalysts on the Basis Thereof for Low-Temperature CO Oxidation

Litvyakova N.N., Sadlivskaya M.V., Mamontov G.V.

Tomsk State University, Tomsk, Russia

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Lignosulfonate Destruction with Ozone-Catalyst Systems

Mitrofanova A.N., Mamleeva N.A., Lunin V.V.

M.V. Lomonosov Moscow State University, Chemistry Department, Moscow, Russia

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Oxidative Destruction of DDT Photocatalyzed by Dioxo-Mo(VI) Complex Anchored on TiO₂

Manucharova L.A., Bakhtchadjian R.A., Tavadyan L.A.

Nalbandyan Institute of Chemical Physics NAS RA, Yerevan, Republic of Armenia

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Dimers Intermediates in Chlorophenols Oxidation over Ti Supported Electrocatalysts

Saleh M.M. (Yemen), Zaev D.A., Mikhalenko I.I.

Peoples` Friendship University of Russia, Moscow, Russia

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Microkinetic Model Explaining CO Oxidation Activity and CORPOX Selectivity of CuO-CeO₂ Catalyst

Mitrichev I.I., Jhensa A.V., Kol'tsova E.M.

Dmitry Mendeleev University of Chemical Technology of Russia, Moscow, Russia

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Mechanisms of the Phase Transitions of Gibbsite and χ -Al₂O₃ into Boehmite under Hydrothermal Treatment in an Aqueous Suspension

Egorova S.R., Mukhamed'yarova A.N., Lamberov A.A., Kurbangaleeva A.Z.

Kazan (Volga region) Federal University, Kazan, Russia

PP-96

Development of XPS Method for Study of Supported Metal Catalysts

Nizovskii A.I.¹, Kalinkin A.V.¹, Smirnov M.Yu.¹, Belskaya O.B.²,
Mikenas T.B.¹, Bukhtiyarov V.I.¹

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Hydrocarbons Processing SB RAS, Omsk, Russia

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Design of PdZn/(Ti,Ce)O₂ Coating Doped with Cerium and Comparative Kinetic Study in the Selective Hydrogenation of 2-Methyl-3-butyn-2-ol in Microcapillary Reactor

Okhlopko L.B.¹, Prosvirin I.P.^{1,2}, Kerzhentsev M.A.¹, Ismagilov Z.R.^{1,3}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

3 – Institute of Coal Chemistry and Material Science, Kemerovo, Russia

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Isomerization of n-Butane on Pd-SZ Catalyst. Effect of Reaction Conditions

Ovchinnikova E.V., Urzhuntsev G.A., Chumachenko V.A., Echevsky G.V.

Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

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In-Situ XPS Study of a New Phenomenon of Kinetic Hysteresis over Pt, Rh Catalysts in Selective Methane Oxidation

Pakharukov I.Yu.^{1,2}, Prosvirin I.P.^{1,2}, Chetyrin I.A.^{1,2}, Kovtunova L.M.^{1,2},
Bukhtiyarov V.I.^{1,2}, Parmon V.N.^{1,2}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

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The Influence of Preparation of Co-Fe/Spinel FTS Catalysts on Physico-chemical Properties: Mossbauer Spectroscopy and XPS

Pankina G.V., Kazak V.O., Lunin V.V.

Chemistry Department, Lomonosov Moscow State University, Moscow, Russia

PP-105**The Kinetics of Glycidol Obtaining by Allyl Alcohol Epoxidation by Hydrogen Peroxide on Titanium-containing Zeolite Catalyst TS-1**

Pastukhova Z.Y., Bruk L.G., Flid V.R.

M.V. Lomonosov Moscow State Academy of Fine Chemical Technology, Moscow, Russia

PP-106**Kinetics of Allyl Chloride Epoxidation with Hydrogen Peroxide Catalyzed by Extruded Titanium Silicalite**

Sulimov A.V.¹, Ovcharova A.V.¹, Flid V.R.², Pastukhova Zh.Yu.², Leontieva S.V.², Flid M.R.³, Trushechkina M.A.³

1 – Nizhni Novgorod State Technical University, Nizhni Novgorod, Russia

2 – Moscow Technological University (Institute of Fine Chemical Technologies), Moscow, Russia

3 – R&D Engineering Centre “Syntez”, Moscow, Russia

PP-107**Catalytic Properties of Sulfur-containing Compounds on the Gold Nanoparticles Surface**

Pervezentseva D.O.¹, Gorchakov E.V.², Petrushin M.S.¹, Hisamutdinov I.S.¹

1 – Tomsk Polytechnic University, Tomsk, Russia

2 – Stavropol State Agrarian University, Stavropol, Russia

PP-108**Effect of Potassium Modification on Electronic and Absorption Properties of Active centers of CoMoS Catalyst: A DFT Study**

Permyakov E.A., Dorokhov V.S., Kogan V.M.

Zelinsky Institute of Organic Chemistry, Moscow, Russia

PP-109**Effect of Co/Mo Ratio on the Mo- and S-Edge Reactivity**

Permyakov E.A., Kogan V.M.

Zelinsky Institute of Organic Chemistry, Moscow, Russia

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Catalytic Activity of Anion-Exchange Resins in Disproportionation of Trichlorosilane

Petukhov A.N., Vorotyntsev A.V., Vorotyntsev V.M.

Nizhny Novgorod State Technical University n.a. R.E. Alekseev, Nizhny Novgorod, Russia

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Structure-sensitive Reactions over Ceria-based Nanocatalysts: The Catalytic Oxidation of Soot and Carbon Monoxide

Piumetti M., Bensaïd S., Fino D., Russo N.

Department of Applied Science and Technology, Politecnico di Torino, Turin, Italy

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Simultaneous Reduction of Hexachloroplatinic Acid and Graphene Oxide for Fuel Cell Electrocatalyst Preparation

Pushkarev A.S.^{1,2}, Pushkareva I.V.^{1,2}, Grigoriev S.A.¹

1 – National Research University “Moscow Power Engineering Institute”, Moscow, Russia

2 – National Research Center “Kurchatov Institute”, Moscow, Russia

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Structure and Catalytic Behavior of Ni-containing Catalysts Produced by Laser Electrodispersion Technique

Rostovshchikova T.N.¹, Lokteva E.S.¹, Maslakov K.I.¹, Golubina E.V.¹, Yermakov A.Ye.², Gurevich S.A.³, Kozhevnikov V.M.³, Yavsin D.A.³

1 – Lomonosov Moscow State University, Moscow, Russia

2 – Institute of Metal Physics of UB of RAS, Yekaterinburg, Russia

3 – Ioffe Physical-Technical Institute of RAS, St. Petersburg, Russia

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Study of Key Stages of Gas Phase Oxidative Desulfurization of Diesel Fuel on CuZnAlO Catalyst

Yashnik S.A.¹, Salnikov A.V.¹, Kerzhentsev M.A.¹, Kaichev V.V.¹,

Kozlova G.S.², Khitsova L.M.², Ismagilov Z.R.^{1,2}, Yaming J.³, Koseoglu O.R.³

1 – Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Institute of Coal Chemistry and Material Science FRS CCC SB RAS, Kemerovo, Russia

3 – Saudi Aramco, Research and Development Center, Dhahran, Kingdom of Saudi Arabia

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Oxidation of Ethanol over Pt(111): *In Situ* XPS and PM IRAS Study

Saraev A.A.^{1,2}, Bukhtiyarov A.V.^{1,2}, Laletina S.S.³, Bespalov Ya.R.^{1,2},
Zemlyanov D.Yu.⁴, Kaichev V.V.^{1,2}, Bukhtiyarov V.I.^{1,2}

1 – *Boriskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

3 – *Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia*

4 – *Birck Nanotechnology Center, Purdue University, West Lafayette, USA*

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The Mechanism of 5-Vinyl-2-norbornene Selective Oxidation with Nitrous Oxide into 1-Pyrazoline Derivative

Ivanov D.P.¹, Babushkin D.E.¹, Semikolenov S.V.¹, Nartova A.V.^{1,2},
Dubkov K.A.¹, Kharitonov A.S.¹

1 – *Boriskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

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Structural Peculiarities and Catalytic Properties of Perovskite

(Gd,Sr)_{n+1}Fe_nO_{3n+1}

Dementieva M.V.¹, Sheshko T.F.¹, Serov Y.M.¹, Yafarova L.V.², Zvereva I.A.²

1 – *Peoples Friendship University of Russia, Moscow, Russia*

2 – *Saint-Petersburg State University, Russia*

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Mixed-valence Co⁺/Co²⁺ Structures in Carbon Monoxide Oxidation on Co-modified ZSM-5

Shilina M.I., Rostovshchikova T. N., Seredina V.O.

Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia

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New Chemical Models for Non-Heme Oxygenases

Shteinman A.A.¹, Das B.², Mitra M.², Nordlander E.²

1 – *Institute of Problems of Chemical Physics, RAS, Chernogolovka, Russia*

2 – *Chemical Physics, Department of Chemistry, Lund University, Lund, Sweden*

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Oxidative Carbonilation of Methanol over Copper-Aluminum Delafossite

Shtertser N.V.^{1,2}, Dokuchits E.V.^{1,2}, Khassin A.A.^{1,2}

1 – Novosibirsk National Research University, Novosibirsk, Russia

2 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

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XRD PDF *Operando* – A Promising Tool for Catalyst Diagnostics

Shmakov A.N.^{1,2,3}, Vinokurov Z.S.¹, Selyutin A.G.¹, Kuper K.E.²

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Budker Institute of Nuclear Physics SB RAS, Novosibirsk, Russia

3 – Research and Educational Center for Energy Efficient Catalysis, Novosibirsk National Research State University, Russia

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Two Directions of Chain Propagation in Methyl Methacrylate and Styrene Polymerization in the Presence of Metallocenes

Kolesov S.V., Sigaeva N.N., Nasibullin I.I., Friesen A.K.

Federal State Institution of Science Institute of Chemistry of Ufa, Ufa, Russia

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Hydrodeoxygenation of Pentanoic Acid Catalyzed by Pt(Re)/TiO₂

Simakova I.L.^{1,2}, Demidova Y.S.^{1,2}, Simonov M.N.^{1,2}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

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Nitrous Oxide Decomposition over Supported Nickel and Cobalt Catalyst as a Method for the Evaluation of the Metallic Phase Surface Area

Simentsova I.I.¹, Minyukova T.P.¹, Khassin A.A.^{2,1}

1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia

2 – Novosibirsk State University, Novosibirsk, Russia

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Catalytic Advantages of Solid Solutions, Based on Transient Metal Oxides

Sinitsin S.A., Petrov A.Yu., Glebov M.B.

D.Mendeleev University of Chemical Technology of Russia (MUCTR), Moscow, Russia

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Alkyne and Alkene Hydrogenations on Immobilized Iridium Complexes Investigated by PHIP Technique

Skovpin I.V.^{1,2}, Zhivonitko V.V.^{1,2}, Prosvirin I.P.^{2,3}, Khabibulin D.F.³,
Koptyug I.V.^{1,2}

1 – *International Tomography Centre SB RAS, Novosibirsk, Russia*

2 – *Novosibirsk State University, Novosibirsk, Russia*

3 – *Borshchov Institute of Catalysis SB RAS, Novosibirsk, Russia*

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Innovative TMR-GC/MS System for Rapid Characterization of Catalysts: Ethanol and Citrus Unshui Peel Conversion

Soll M.¹, Ito K.², Teramae N.^{2,3}, Kim Y.-M.^{2,4}, Watanabe C.², Park U.-K.⁵

1 – *Frontier Laboratories Europe, Germany, Essen*

2 – *Frontier Laboratories, Japan, Koriyama*

3 – *Department of Chemistry, Tohoku University, Sendai, Japan*

4 – *Department of Environ. Sciences and Biotechn., Hallym Univ., Chuncheon, Korea*

5 – *School of Environmental Engineering, University of Seoul, Seoul, Korea*

PP-138

Multifunctional Combined Catalyst for Diesel Engine Exhaust Aftertreatment System

Mytareva A.I., Bokarev D.A., Baeva G.N., Stakheev A.Yu.

Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

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“Polyfunctional” Mn-Ce/Beta Catalysts for Simultaneous NH₃-DeNO_x and CO/HC Oxidation

Krivoruchenko D.S., Bokarev D.A., Telegina N.S., Stakheev A.Yu.

N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

PP-140

Selective Liquid-Phase Hydrogenation of Internal and Terminal Alkynes over Novel Pd-In Bimetallic Catalysts

Markov P.V.¹, Bragina G.O.¹, Rassolov A.V.¹, Baeva G.N.¹, Mashkovsky I.S.¹,
Yakushev I.A.², Vargaftik M.N.², Stakheev A.Yu.¹

1 – *Zelinsky Institute of Organic Chemistry RAS (ZIOC RAS), Moscow, Russia*

2 – *Kurnakov Institute of General and Inorganic Chemistry (IGIC RAS), Moscow, Russia*

PP-141**The Reaction Thermodynamics and Mechanisms of H₂S Decomposition into Hydrogen and Elemental Sulfur**

Startsev A.N.

*Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia***PP-142****C4-C5 Alcohols Condensation Reactions over VIII Group Metals**Simakova I.L.^{1,2}, Demidova Y.S.^{1,2}, Simonov M.N.^{1,2}*1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia**2 – Novosibirsk State University, Novosibirsk, Russia***PP-145****Methane Combustion over Mn-containing Cordierites**Sutormina E.F., Isupova L.A.*Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia***PP-146****Biomimetic Catalytic Oxidation of Water with Ru(bpy)₃³⁺ in the Presence of Colloidal Cobalt (III) Hydroxide. Kinetics and Mechanism Study**Taran O.P.^{1,2}, Chikunov A.S.¹, Koval V.V.³, Parmon V.N.^{1,4}*1 – Borekov Institute of Catalysis SB RAS, Novosibirsk, Russia**2 – Novosibirsk State Technical University, Novosibirsk, Russia**3 – Institute of Chemical Biology and Fundamental Medicine SB RAS, Novosibirsk, Russia**4 – Novosibirsk State University, Novosibirsk, Russia***PP-149****Catalyst Systems of Desulfurization of Motor Fuels Based on Vanadium and Molybdenum Oxides**Vishnetskaya M.V.¹, Tomskii I.S.², Vahrushin P.A.¹, Tomskaia L.A.²*1 – Gubkin Russian State University of Oil and Gas, Moscow, Russia**2 – Mirny Polytechnic Institute (branch) of North-Eastern Federal University, Mirny, Russia***PP-156****Non-oxidative Conversion of Methane and n-Pentane in the Presence of Supported Oxide Catalysts**Vinichenko N.V.^{1,2}, Golinsky D.V.¹, Pashkov V.V.¹, Belyi A.S.^{1,2}, Krol O.V.¹, Trenikhin M.V.¹, Shilova A.V.¹, Zatolokina E.V.¹*1 – Institute of Hydrocarbons Processing SB RAS, Omsk, Russia**2 – Omsk State Technical University, Omsk, Russia*

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Chemical Aspect of Regulation of Active Site Structure in Cu-ZSM-5

Yashnik S.A.¹, Khitsova L.M.², Furiga R.², Parmon V.N.¹, Ismagilov Z.R.^{1,2}

1 – *Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia*

2 – *Institute of Coal Chemistry and Material Science SB RAS, Kemerovo, Russia*

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¹H NMR and Quantum Chemistry Study of Hydrolysis of

Isobutylaluminium Aryloxides

Zharkov I.V., Faingold E., Bravaya N.M., Chernyak A.V.

Institute of Problems of Chemical Physics of the RAS, Chernogolovka, Russia

PP-168

DFT Studies of Interrelations between Structures of New Nickel(II)

Complexes with N,O-coordinating Ligands and Their Catecholase Activity

Rychagova E.A.¹, Ketkov S.Yu.¹, Zhigulin G.Yu.¹, Das D.²

1 – *G.A. Razuvaev Institute of Organometallic Chemistry of RAS, Nizhny Novgorod, Russia*

2 – *University of Calcutta, Calcutta, India*

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Electrocatalytic Properties of Rhenium-Nickel Electrodes Prepared by Electrodeposition from Aqueous Solution in the Hydrogen Evolution Reaction

Zhulikov V.V.¹, Gamburg Yu.D.¹, Krutsikh V.M.¹, Kuznetsov V.V.², Zhalnerov M.V.²

1 – *Institute of Physical Chemistry and Electrochemistry Russian Academy of Science, Moscow, Russia*

2 – *Moscow University Chemical Technology of Russia, Moscow, Russia*

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Theoretical Foundations Catalytic Synthesis of Aromatic Acetylene Alcohols

Ziyadullaev O.E., Abdurakhmanova S.S., Turabdzhanov S.M.

Tashkent Chemical Technological Institute, Tashkent, Uzbekistan

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Relativistic Electrons of sp^2 Nanocarbons

Sheka E.F.

Department of Theoretical Physics and Mechanics, Peoples' Friendship University of Russia, Moscow, Russia