Boreskov Institute of Catalysis SB RAS, Russia
Lomonosov Moscow State University, Russia
Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

IX International Conference

MECHANISMS OF CATALYTIC REACTIONS

St. Petersburg, October 22- 25, 2012

SCIENTIFIC PROGRAM
INVITATION

Novosibirsk-2012

CONFERENCE ORGANIZERS

- Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
- Lomonosov Moscow State University, Moscow, Russia
- Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
- St. Petersburg Scientific Center RAS, St. Petersburg
- Scientific Council on Catalysis RAS, Russia

Санкт-Петербургский
научный центр РАН

UNDER THE AUSPICES of the European Federation of Catalysis Societies

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Russian Foundation for Basic Research, Moscow

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«World of Oil Products. Bulletin of Oil Companies»

GREETING

Dear Colleague,

We are pleased to invite you to participate in the IX International Conference "Mechanisms of Catalytic Reactions", which will take place in St. Petersburg, Russia, on October 22-25, 2012.

The Conference is organized under the auspices of the European Federation of Catalysis Societies (EFCATS).

The IX Conference "Mechanisms of Catalytic Reactions" follows an established tradition, with previous meetings held in Moscow (1974, 1979, 1986, 1990, 2002), Saint-Petersburg (2006), and Novosibirsk (1982, 2009).

Since 2009, the conferences of this series have a status of regular international events held every three years.

The IX Conference addresses challenging problems of catalysis and physical chemistry and welcomes researchers from across the globe, working in all fields of catalysis.

The venue of the Conference is St. Petersburg, which is reputed the cultural capital of Russia. An exclusive social program will allow further opportunities for the productive communication of the participants.

We wish you a fruitful work and a pleasant stay in St. Petersburg!

International Advisory Board
Chairman,
Valentin N. Parmon,
Boreskov Institute of Catalysis

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SCIENTIFIC PROGRAM

International Conferences “Mechanisms of Catalytic Reactions” have a status of regular international events devoted to challenging problems of modern physical chemistry and catalysis. Topics of the IX Conference will include:

I. Catalysis: from first principles
II. Mechanisms of heterogeneous catalysis
III. Mechanisms of homogeneous catalysis
IV. Catalytic processing of renewables
V. Electrocatalysis, photocatalysis, biocatalysis

Almost 230 participants from 30 countries applied for the conference. The conference program includes 5 plenary lectures, 9 key-notes, 56 oral (20 min) presentations, 23 oral (10 min) presentations of young scientists, 110 posters and 4 sponsor presentations.

English will be the official language of the Conference.

Round-table of the Russian Foundation for Basic Research will be held in Assambleya Hall on October 24, (5.00 p.m.). Russian participants are invited. The official language of the meeting is Russian.

EXHIBITION of promotional materials of conference sponsors will be organized. The exhibition will be held from 22 to 25 October in a hall, located near the conference halls at the hotel Azimut.

PRESENTATION

The time of presentation (including some time for questions) is 40 min for a plenary lecture, 30 min for a keynote lecture, 20 and 10 min for an oral presentation. Multimedia LCD projectors will be available. Organizers recommend the authors to prepare computer presentations in *.ppt format (Microsoft Office PowerPoint).

Space available for posters is 100 cm width × 100 cm height. The authors are requested to place their posters in Assambleya hall in the morning of October 23, and remove them at the end of the poster session.

CONFERENCE PUBLICATIONS

The final scientific program-brochure and the compact disk with the abstracts of all lectures, oral and poster presentations will be available at the registration desk.

Authors of plenary, keynote lectures and oral (20 min) presentations will are invited to publish full papers on their works in a special issue of "Topics in Catalysis" in 2013. The authors of preselected manuscripts should submit full texts, composed according to the Topics and Catalysis template before November, 1, 2012, to editorial@catalysis.ru (Prof. Dr. Konstantin P. Bryliakov). In the accompanying letter please indicate the names and contact details of two potential reviewers; it is best that one of those be a Conference participant.

Authors of 10 min oral presentation of young scientists are invited to publish full papers in a special issue of Kinetics & Catalysis. All manuscripts will be peer reviewed following the standard procedure. The full texts of 10 min oral contributions should not exceed 10-12 pages. All manuscripts of A4 format should be typed 1.5 line spaced using 12 points font. Full texts of manuscripts (in English for foreign authors; in English and Russian for Russian authors) should be submitted to the Kinetics & Catalysis both by e-mail: kincat@ioc.ac.ru and (2 hard copies) by regular post (“Kinetics and Catalysis”, Zelinsky IOC RAS, Leninsky Prospect 47, Moscow 119991, Russia) before November 15, 2012. Contact tel.: +7 (499) 135 53 58). The guidelines of the Kinetics & Catalysis for authors and a copyright transfer agreement form is available at the Conference website http://conf.nsc.ru/MCR-IX/en/scientific_program

Authors of poster presentations are invited to publish in Kinetics & Catalysis on a regular basis.

VENUE

St. Petersburg was founded by Peter the Great in the delta of the Neva River in 1703.

St. Petersburg is one of the most beautiful cities in the world. It is often referred to as the Venice of the North, but its beauty is really a brand all its own. Lavish interiors of the grandiose and skyline-dominating cathedrals, marvellous palaces and squares, fascinating suburbs present a unique monument of the Russian architecture. Many museums are world known due to their rich collections of art treasures.

ACCOMMODATION

The Conference will take place in Azimut*** Hotel (Lermontovskii prosp., 43/1; *http://www.azimuthotels.ru/en/hotels/st_peterburg/about_hotel/*).

The Hotel is located at a 10 minutes walking distance from Metro station "Tekhnologichesky Institute" and at a driving distance of 30 minutes from airports Pulkovo-1-local and Pulkovo-2-international. The Conference will be held in 3 conference halls at 18th floor of the hotel, which provides a fascinating panoramic view of the St. Isaac's Cathedral, the Neva River, the State Hermitage and other sights of St. Petersburg.

Accommodation is arranged at the Azimut*** Hotel at special rates strongly reduced for the Conference participants from 21st to 26th of October, 2012 (Check in: 2.00 p.m., Check out: 12.00 a.m.).

Bus No 39 runs from Airport Pulkovo-1-local to Metro station "Moskovskaya". Bus No 13 runs from Airport Pulkovo-2-international to Metro station "Moskovskaya".

Participants can get from Metro station "Tekhnologichesky Institute" to **Azimut Hotel** by electrobuses No 3 or 8 (please take second bus stop).

The Organizing Committee also reserved rooms for post-graduates and students at the hostel **"Gostevoi Fond"** (ul. 7th Krasnoarmeiskaya, 12; Check in: 12.00 a.m.). The hostel "Gostevoi Fond" is located 10 minutes on foot from the Azimut Hotel.

MEALS

Lunches will be served at the restaurant of the Azimut hotel, 1st floor. Vouchers for 4 lunches will be included in the participant package. Morning and afternoon coffee breaks will be provided.

REGISTRATION

Registration will take place at the Azimut hotel, 1st floor hall, on October 21 from 3 p.m. till 9 p.m. and on October 21 from 9 a.m. till 1 p.m.

BANK AND CURRENCIES EXCHANGE

Cash exchange is available in the bank not far from the hotel “Azimut hotel” (one U.S. dollar equals to ca. 31 roubles; one Euro equals to ca. 40 roubles in October, 2012). Eurocard, MasterCard and Visa credit cards are generally acceptable in automatic cash terminals of the Azimut hotel. Please note that personal cheques are not accepted.

SOCIAL PROGRAM

http://conf.nsc.ru/mcr-ix/en/cultural_program

The participants will be invited to the Welcome Reception on October 22, 7.00 p.m, at the restaurant “Sovetskii” of the Azimut Hotel. The Banquet will be held on October 24, 7.30. p.m., at the restaurant “Troika” (2700 Rub, including the price of variety show).

Excursions to **the State Hermitage** and **St. Isaac’s Cathedral** will be organized for the participants and accompany persons. The participants and guests are offered post-tour I **“Peterhof-Oranienbaum”**, post-tour-II **“Great Novgorod” (October 26)** and the optional excursion **"Tsarskoye Selo"** (**October 24).**

REGISTRATION FEE

The fee covers editorial expenditures, auditorium rent, participant bag, 4 lunches, coffee-breaks beverages, Welcome Party, excursions to the State Hermitage and St. Isaac’s Cathedral.

WEATHER

At the end of October, the weather in St. Petersburg is usually cool (8-10 ºC) and rainy; the Organizing Committee advises to bring umbrellas and warm suits.

TIMETABLE

Oct., 21, Sunday	**October 22, Monday**		
	09.00	*Registration*	
Arrival	**09.40**	**Summit hall** *Conference Welcome,* Parmon Chairmen: Bukhtiyarov, van Santen	
	10.00	PL-1 Bell	
	10.40	*Coffee*	
Regisration *15.00-19.00*		Chairmen: Stakheev, Rupprechter	
	11.10	PL-2 Parmon	
	11.50	KL-1 van Santen	
Azimut hotel	**12.20**	KL-2 Neyman	
	12.50	*Lunch*	
		Summit hall Chairmen: Talsi, Selvam	
	14.30	KL-3 Ueda	
	15.00	Bukhtiyarov (memory lecture Ipatieff)	
	15.20	***Official sponsor SIBUR holding***	
	15.50	*Coffee*	
		Summit hall Chairmen: Ismayilov, Ueda	**Forum hall** Chairmen: Neyman, Frenkel
	16.20	OP-III-1 Sadykov	OP-I-1 Stakheev
	16.40	OP-III-2 Dossumov	OP-I-2 Rösch
	17.00	OP-III-3 Specchia	OP-I-3 Nasluzov
	17.20	OP-III-4 Masalska	OP-I-4 Pichugina
	17.40	OP-III-5 Bychkov	OP-I-5 Andrikopoulos
	18.00	OP-III-6 Lashina	OP-I-6 Gurevich
	18.20	OP-III-7 Cholach	OP-I-7 Startsev
	19.00	***Welcome Party, Sovetskii hall (Azimut hotel)***	

	October 23, Tuesday	
	Summit hall Chairmen: Zlotin, Rösch	
09.00	PL-3 Que, Jr.	
09.40	KL-4 Murzin	
10.10	KL-5 Rupprechter	
10.40	*Coffee*	
	Summit hall Chairmen: Kondratenko, Özensoy	**Forum hall** Chairmen: Kozhevnikov I., Costas
11.10	OP-III-8 Zemlianov	OP-II-1 Masui
11.30	OP-III-9 Frenkel	OP-II-2 Bryliakov
11.50	OP-III-10 Tsyganenko	OP-II-3 Aubry
12.10	OP-III-11 Kaichev	OP-II-4 Belkova
12.30	OP-III-12 Pẽna	OP-II-5 Flid
12.50	OP-III-13 Kovtunov	***Sponsor- Bruker***
13.10	*Lunch*	
	Summit hall Chairmen: Kaichev, Zemlianov	**Forum hall** Chairmen: Aubry, Bruk
14.30	OP-III-14 Palma	OP-II-6 Suslov
14.50	OP-III-15 Dürr	OP-II-7 Zhou
15.10	OP-III-16 Mishra	OP-II-8 Zlotin
15.30	OY-III-1 Gabrienko	OY-II-1 Bocharova
15.40	OY-III-2 Meemken	OY-II-2 Lyakin
15.50	OY-III-3 Kavalerskay	OY-II-3 Ottenbacher
16.00	OY-III-4 Kazantsev	OY-II-4 Sanieva
16.10	OY-III-5 Khudorozhkov	OY-II-5 Gantman
16.20	OY-III-6 Pakharukov	OY-II-6 Kozhevnikov I.V.
16.30	*Coffee*	
11.00-16.30 **17.00-19.00**	**Assambleya hall - POSTER SESSION** **– hanging of posters** **– discussion**	

TIMETABLE

October 24, Wednesday			
	Summit hall Chairmen: Margitfalvi, Masalska		
09.00	PL-4 Fokin		
09.40	KL-6 Özensoy		
10.10	KL-7 Ananikov		
10.40	*Coffee*		
	Assambleya hall Chairmen: Sadykov, Dossumov	**Forum hall** Chairmen: Bryliakov, Palma	
11.10	OP-III-17 Lokteva	OP-V-1 Tompos	
11.30	OP-III-18 Piccolo	OP-V-2 Shishido	
11.50	OP-III-19 Mierzinski	OP-V-3 Saninno	
12.10	OP-III-20 Tatsumi	OP-V-4 Kozlova	
12.30	OP-III-21 Mishakov	***Sponsor -2- Donau lab***	
12.50	OP-III-22 Selvam	***Sponsor-3- Promenergolab***	
13.10	*Lunch*		
	Assambleya hall Chairmen: Lokteva, Tatsumi		**Forum hall** Chairmen: Kovtunov, Startsev
14.30	OP-III-23 Smirnov	**14.30**	OY-IV-1 Snytnikov P.
14.50	OP-III-24 Gavrilov	**14.40**	OY-IV-3 Simakova
15.10	OP-III-25 Vovk	**14.50**	OY-IV-4 Chistyakov
15.30	OP-III-26 Requies	**15.00**	OY-IV-7 Bykova
15.50	OP-III-27 Stepanov	**15.10**	OY-V-1 Tasseroul
16.10	OP-III-28 Bruk	**15.20**	OY-V-2 Cherepanov
		15.30	OY-V-3 Oschepkov
		15.40	OY-V-4 Maniecki
		15.50	OY-III-7 Konuspaeva
		16.00	OY-I-1 Mukhamedzyanova
		16.10	OY-IV-2 Skobelev
16.30	***Coffee***		
17.00 **18.00**	**Assambleya hall** Chairmen: Tsyganov, Martyanov RFBR Round-table (in Russian)		
19.00	***Banquet, restaurant Troika***		

October 25, Thursday			**October 26, Friday**
	Summit hall Chairmen: Murzin, Zhou		**post-tours**
09.00	PL-5 Kondratenko		
09.40	KL-8 Costas		
10.10	KL-9 Talsi		
10.40	*Coffee*		
	Assambleya hall Chairmen: Smirnov, Specchia	**Forum hall** Chairmen: Grove, Mishakov	
11.10	OP-III-29 Margitfalvi	OP-IV-1 Garyntseva	
11.30	OP-III-30 Jacquemin	OP-IV-2 Kozhevnikov I.	
11.50	OP-III-31 Kuznetsova L.	OP-IV-3 Berlier	
12.10	OP-III-32 Zolotarev	OP-IV-4 Simakova I.	
12.30	***Closing***		
13.00	*Lunch*		
 15.00 **17.00**	***Excursions*** ***Hermitage Museum,*** ***St. Isaac's Cathedral*** Section-I: Catalysis: from first principles; Section-II: Mechanisms of homogeneous catalysis; Section III: Mechanisms of heterogeneous catalysis; Section IV: Catalytic processing of renewables; Section V: Electrocatalysis, photocatalysis, biocatalysis ***Exhibition: October 22-25, hall, 18th floor*** *PL - Plenary lecture (40 min);* *KL - Keynote lecture (30 min);* *OP – oral (20 min);* *OY – oral of young scientists (10 min);*		

Scientific program

Monday, October 22

Summit Hall, Azimut Hotel

MORNING SESSION

Chairmen: Prof. Valerii I. Bukhtiyarov
Prof. Rutger Van Santen

09.40 ***Conference Welcome***

10.00 PL-1
Presenting author: Prof. Alexis T. Bell
Elucidating the Mechanism of Heterogeneously Catalyzed Reactions through Combined Experimental and Theoretical Studies
University of California (Berkeley), USA

10.40 *Coffee break*

Chairmen: Prof. Alexander Yu. Stakheev
Prof. Günther Rupprechter

11.10 PL-2
Presenting author: Prof. Valentin N. Parmon
Thermodynamics of Operating Catalyst: Some Approaches and Findings
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

11.50 KL-1
Presenting author: Prof. Rutger van Santen
Van Santen R.A.[1], Ghouri M.M.[2]
The Mechanism of the Fischer-Tropsch Reaction
[1]Institute for Complex Molecular Systems, Eindhoven University of Technology (Eindhoven), The Netherlands
[2]Schuit Institute of Catalysis, Eindhoven University of Technology (Eindhoven), The Netherlands

12.20 KL-2
Presenting author: Prof. Konstantin M. Neyman
Catalysis from First Principles: Is it Crucial to Account for the Effects of Nanostructuring?
ICREA and University of Barcelona (Barcelona), Spain

12.50 *Lunch*

AFTERNOON SESSION

Chairmen: Prof. Evgenii P. Talsi
Prof. Parasuraman Selvam

14.30 KL-3
Presenting author: Prof. Wataru Ueda
Konya T., Kobayashi D., Murayama T., Ueda W.
Catalytic Oxidation Mechanism Based on the High-Dimensional Structure of Mo_3VO_x
Catalysis Research Center, Hokkaido University (Sapporo), Japan

15.00 Prof. Valerii I. Bukhtiyarov
Memorial lecture 145th abbiversary of the pre-eminent Russian chemist Professor Vladimir N. Ipatieff
Boreskov Institute of Catalysis (Novosibirsk), Russia

15.20 Official sponsor SIBUR holding (in Russian)
Презентационный доклад
Официального спонсора конференции
Сергей С. Галибеев
Директор Центра «Сибур Технологии», Москва
СИБУР. Стратегия развития R&D

15.50 *Coffee break*

Summit Hall, Azimut Hotel

AFTERNOON SESSION

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Prof. Wataru Ueda
Prof. Etibar H. Ismayilov

16.20 OP-III-1
Presenting author: Prof. Vladislav A. Sadykov
Sadykov V.A.[1,2], Bobin A.S.[1], Rogov V.A.[1,2], Mezentseva N.V.[1,2], Alikina G.M.[1], Sadovskaya E.M.[1], Glazneva T.S.[1], Mirodatos C.[3], Galvita V.[4], Marin G.B.[4]
Mechanism of CH_4 Dry Reforming on Nanocrystalline Doped Ceria-Zirconia with Supported Pt, Ru, Ni and Ni–Ru
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia
[3]Institut de Recherches sur la catalyse et l'environnement de Lyon (Lyon), France
[4]Gent University (Gent), Belgium

16.40 OP-III-2
Presenting author: Prof. Kusman Dossumov
Dossumov K.[1], Tungatarova S.A.[2]
The Mechanism of Oxidative Conversion of Methane
[1]Institute of Combustion Problems, Al-Farabi Kazakh National University (Almaty), Kazakhstan
[2]JSC "D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry" (Almaty), Kazakhstan

17.00 OP-III-3
Presenting author: Prof. Stefania Specchia
Finocchio E.[1], Specchia S.[2]
Sulphur Ageing Mechanisms on $Pd/BaCeO_3{\cdot}2ZrO_2$ Catalyst For Methane Combustion
[1]Università di Genova, Department of Chemical and Process Engineering (Genova), Italy
[2]Politecnico di Torino, Department of Applied Science and Technology (Torino), Italy

17.20 OP-III-4
Presenting author: Prof. Aleksandra Masalska
Masalska A., Grzechowiak J., Jaroszewska K.
Effect of Metal-Support Interaction in Ni/ZSM-5+Al_2O_3 Catalysts on *n*-Paraffins Transformation
Wrocław University of Technology, Faculty of Chemistry (Wrocław), Poland

17.40 OP-III-5
Presenting author: Dr. Victor Yu. Bychkov
Bychkov V.Yu., Tyulenin Yu.P., Firsova A.A., Korchak V.N.
Effect of Carbonization on Dry Methane Reforming over Ni Catalysts
Semenov Institute of Chemical Physics RAS (Moscow), Russia

18.00 OP-III-6
Presenting author: Dr. Elena A. Lashina
Lashina E.A.[1,2], Chumakova N.A.[1,2], Kaichev V.V.[1,2], Ustugov V.V.[1], Chumakov G.A.[2,3], Bukhtiyarov V.I.[1,2]
Self-Oscillations in the Methane Oxidation on Ni: Mathematical Modelling
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia
[3]Sobolev Institute of Mathematics SB RAS (Novosibirsk), Russia

18.20 OP-III-7
Presenting author: Dr. Alexander R. Cholach
Cholach A.R., Bulgakov N.N.
A Single Model of Oscillations in the NO+H_2 Reaction on Noble Metals
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

19.00 *Welcome Party, Sovetskii Hall, Azimut Hotel*

Forum Hall, Azimut Hotel
AFTERNOON SESSION

ORAL PRESENTATIONS
Section I. Catalysis: From First Principles

Chairmen: Prof. Konstantin M. Neyman
Prof. Anatoly Frenkel

16.20 OP-I- 1
Presenting author: Prof. Alexander Yu. Stakheev
Stakheev A.Yu.[1], Batkin A.M.[1], Beck I.E.[2], Teleguina N.S.[1], Bragina G.O.[1], Zaikovsky V.I.[2], Larichev Yu.V.[2], Bukhtiyarov V.I.[2]
Particle Size Effect in CH_4 Oxidation over Noble Metals: Comparison of Pt And Pd Catalysts
[1]Zelinsky Institute of Organic Chemistry RAS (Moscow), Russia
[2]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

16.40 OP-I-2
Presenting author: Prof., Dr. Notker Rösch
Başaran D.[1], Chiu C.[1], Genest A.[1,2], Rösch N.[1,2]
Computational Insights into Aqueous Phase Processes for Biomass Reforming
[1]Department Chemie and Catalysis Research Center, Technische Universität München (Garching), Germany
[2]Institute of High Performance Computing, Singapore

17.00 OP-I-3
Presenting author: Dr. Vladimir A. Nasluzov
Nasluzov V.A.[1], Laletina S.S.[1], Shor A.M.[1], Shor E.A.[1], Rösch N.[2]
Activation of Oxygen on Microclusters of Silver Anchored on SiO_2 and Al_2O_3 Surfaces. Embedded Cluster Scalar-Relativistic and Periodic Pseudopotential Density Functional Calculations
[1]Institute of Chemistry and Chemical Technology SB RAS (Krasnoyarsk), Russia
[2]Technische Universität München (Garching), Germany

17.20 OP-I-4

Presenting author: Dr. Daria A. Pichugina

Pichugina D.A.[1,2], Mukhamedzianova D.F.[1], Beletskaya A.V.[1], Ratmanova N.K.[1], Snyga Y.G.[1], Nikolaev S.A.[1], Askerka M.S.[1], Lanin S.N.[1], Shestakov A.F.[2], Kuz'menko N.E.[1]

Theoretical Insight on Catalytic Activity of Bimetallic Gold Catalysts

[1]Department of Chemistry, Lomonosov Moscow State University (Moscow), Russia
[2]Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

17.40 OP-I-5

Presenting author: Dr. Prokopis C. Andrikopoulos

Andrikopoulos P.C.[1], Michel C.[1], Chouzier S.[2], Sautet P.[1]

Oxidation of Alkanes: In Silico Catalyst Design

[1]University of Lyon, CNRS, Laboratoire de Chimie, ENS de Lyon (Lyon), France
[2]Centre de Recherches et Technologies de Lyon, Laboratoire Intermédiaires Polyamide (Saint-Fons), France

18.00 OP-I-6

Presenting author: Prof. Sergey A. Gurevich

Gurevich S.A.[1], Kozhevin V.M.[1], Yavsin D.A.[1], Rostovshchikova T.N.[2], Lokteva E.S.[2]

Self-Induced Electric Fields in the System of Supported Metal Nanoparticles: The Impact on Heterogeneous Catalysis

[1]Ioffe Physical-Technical Institute of RAS (St. Petersburg), Russia
[2]Lomonosov Moscow State University (Moscow), Russia

18.20 OP-I-7

Presenting author: Prof. Anatoliy N. Startsev

Startsev A.N., Kruglyakova O.V., Chesalov Yu.A., Ruzankin S.F., Kravtsov E.A., Larina T.V., Paukshtis E.A.

Low Temperature Decomposition of Hydrogen Sulfide into Hydrogen and Diatomic Gaseous Sulfur

Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

19.00 ***Welcome Party, Sovetskii Hall, Azimut Hotel***

Tuesday, October 23

Summit Hall, Azimut Hotel

MORNING SESSION

Chairmen: Prof. Sergey G. Zlotin
Prof. Notker Rösch

09.00 PL-3
Presenting author: Prof. Lawrence Que, Jr.
Bio-Inspired Hydrocarbon Oxidations by Nonheme Iron Catalysts
Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota (Minneapolis), USA

09.40 KL-4
Presenting author: Prof. Dmitry Yu. Murzin
Mechanistic Aspects of Hydrogenation and Oxidation of Sugars
Åbo Akademi University (Turku), Finland

10.10 KL-5
Presenting author: Prof., Dr. Günther Rupprechter
The "True" Explanation is Typically rather Simple
Institute of Materials Chemistry, Vienna University of Technology (Vienna), Austria

10.40 *Coffee break*

Summit Hall, Azimut Hotel

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Prof. Evgenii Kondratenko
Prof. Emrah Özensoy

11.10 OP-III-8
Presenting author: Dr. Dmitry Yu. Zemlyanov
Zemlyanov D.Y.[1], Klötzer B.[2]
Does the Bulk Matter? Methane and Ethylene Oxidation on Palladium
[1]Purdue University, Birck Nanotechnology Center (West Lafayette), USA
[2]Institut für Physikalische Chemie, Universität Innsbruck (Innsbruck), Austria

11.30 OP-III-9
Presenting author: Prof. Anatoly I. Frenkel
In Situ X-Ray Studies of Model and Real Catalysts: Bridging the Complexity Gap
[1]Physics Department, Yeshiva University (New York), USA
[2]Synchrotron Catalysis Consortium, Brookhaven National Laboratory (Upton), USA

11.50 OP-III-10
Presenting author: Prof. Alexey A. Tsyganenko
FTIR Spectroscopy in the Studies of Catalytic Reaction Mechanisms
V.A. Fock Institute of Physics, St. Petersburg State Unversity
(St. Petersburg), Russia

12.10 OP-III-11
Presenting author: Dr. Vasily V. Kaichev
Kaichev V.V., Miller A.V., Prosvirin I.P., Bukhtiyarov V.I.
Decomposition and Oxidation of Methanol on Pt and Pd: *In Situ* XPS and Mass-Spectrometry Study
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

12.30 OP-III-12

Presenting author: Diego Alexander Peña

Diehl F.[1], Lecocq V.[1], Griboval-Constant A.[2], Khodakov A.Y.[2], Peña D.A.[2]

Different Carbon Species and Deactivation of Alumina Supported Cobalt Fischer-Tropsch Catalysts in Slurry Reactor

[1]IFP Energies nouvelles, Rond-point de l'échangeur de Solaize (Solaize), France

[2]Unité de Catalyse et de Chimie du solide (UCCS) Université de Lille 1 (Lille), France

12.50 OP-III-13

Presenting author: Dr. Kirill V. Kovtunov

Kovtunov K.V.[1,2], Barskiy D.A.[1,2], Zhivonitko V.V.[1,2], Salnikov O.G.[1,2], Khudorozhkov A.K.[3], Bukhtiyarov V.I.[3], Koptyug I.V.[1,2]

Heterogeneous Hydrogenation Reaction Mechanism Evaluation by Using Parahydrogen

[1]Institute "International Tomografic Center" SB RAS (Novosibirsk), Russia

[2]Novosibirsk State University (Novosibirsk), Russia

[3]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

13.10 *Lunch*

Forum Hall, Azimut Hotel

MORNING SESSION

ORAL PRESENTATIONS
Section II. Mechanisms of Homogeneous Catalysis

Chairmen: Prof. Ivan V. Kozhevnikov
Prof. Miquel Costas

11.10 OP-II-1
Presenting author: Yoichi Masui
Masui Y.[1], Haga S.[2], Onaka M.[1]
Direct Synthesis of Dimethyl Carbonate from CO_2 and MeOH Catalyzed By Sn(O*t*-Bu)$_4$ with Acid-Base Additives, and its Reaction Mechanism
[1]Graduate School of Arts and Sciences, The University of Tokyo (Tokyo), Japan
[2]Graduate School of Science, The University of Tokyo (Tokyo), Japan

11.30 OP-II-2
Presenting author: Prof. Konstantin P. Bryliakov
Talsi E.P., Bryliakov K.P.
Living Olefin Polymerization with Post-Titanocene Catalysts Containing *o*-Fluoroaryl Substituents: Role of Noncovalent Interactions
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

11.50 OP-II-3
Presenting author: Prof. Jean-Marie Aubry
Aubry J.M., Nardello-Rataj V.
Mechanism for the Reduction of Dioxygen by Diethylhydroxylamine (DEHA) Organocatalyzed by Natural Polyphenols
Université de Lille Nord de France (Villeneuve d'Ascq CEDEX), France

12.10 OP-II-4

Presenting author: Prof. Natalia V. Belkova

Belkova N.V.[1], Kozinets E.M.[1,2], Filippov O.A.[1], Fekete M.[3], Duckett S.B.[3], Manoury E.[2], Poli R.[2], Shubina E.S.[1]

Diphenylphosphinoferrocenyl Thioether Diene Rh(I) and Ir(I) Catalyzed Ketone Hydrogenation: Turning Precatalysts into Active Species

[1]Nesmeyanov Institute of Organoelement Compounds RAS (Moscow), Russia
[2]Laboratoire de Chimie de Coordination CNRS (Toulouse), France
[3]Department of Chemistry, University of York (York), United Kingdom

12.30 OP-II-5

Presenting author: Prof. Vitaly R. Flid

Flid V.R., Evstigneeva E.M., Shamsiev R.S.

Mechanisms of Catalytic Reactions of Norbornadiene

Lomonosov Moscow State Academy of Fine Chemical Technology (Moscow), Russia

12.50 Sponsor BRUKER ltd. (in Russian)

Презентационный доклад спонсора конференции

Олег И. Иванов

ООО БРУКЕР, Санкт-Петербург, Россия

Современный рентгеновский анализ в материаловедении

13.10 *Lunch*

Summit Hall, Azimut Hotel

AFTERNOON SESSION

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Dr. Vasily V. Kaichev
Dr. Dmitry Yu. Zemlyanov

14.30 OP-III-14
Presenting author: Prof. Vincenzo Palma
Palma V.[1], Castaldo F.[2], Ciambelli P.[1], Iaquaniello G.
Investigation on the Kinetic Behavior of Bio-Ethanol Steam Reforming over Bimetallic Catalysts Supported on Cerium Oxide
[1]Dipartimento di Ingegneria Industriale, Università di Salerno, Fisciano (SA), Italy
[2]Tecnimont KT S.p.A. (Roma), Italy

14.50 OP-III-15
Presenting author: Nadine Dürr
Dürr N., Menning N., Petzold T., Drochner A., Vogel H.
Mechanistic Studies on the Selective Oxidation of Acrolein to Acrylic Acid on Mo/V/W-Mixed Oxide Catalysts
Technische Universität Darmstadt, Ernst-Berl-Institut for Technical Chemistry and Macromolecular Science (Darmstadt), Germany

15.10 OP-III-16
Presenting author: Dr. Gopal S. Mishra
Machado K., Tavares P.B., Mishra G.S.
Scorpionate Gold Complexes Anchored on Nano-Size Magnetic Silica as Hybrid Catalysts for Oxyfunctionalization of Hydrocarbons
Department of Chemistry, University of Trás-os Montes and Alto Douro (UTAD) (Vila Real), Portugal

ORAL PRESENTATIONS OF YOUNG SCIENTISTS
Section III. Mechanisms of Heterogeneous Catalysis

15.30 OY-III-1
Presenting author: Dr. Anton A. Gabrienko
Gabrienko A.A., Arzumanov S.S., Stepanov A.G.
Methane Activation and Conversion on Ag/H-MFI Catalyst
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

15.40 OY-III-2
Presenting author: Fabian Meemken
Meemken F., Maeda N., Hungerbühler K., Baiker A.
Platinum-Catalyzed Asymmetric Hydrogenation: Spectroscopic Evidence for O-H-O Hydrogen Bond Interaction between Substrate and Modifier
Department of Chemistry and Applied Bioscience, ETH Zürich (Zurich), Switzerland

15.50 OY-III-3
Presenting author: Natalya E. Kavalerskaya
Kavalerskaya N.E., Rostovchshikova T.N., Lokteva E.S., Golubina E.V., Maslakov K.I.
Unusually Active Nanostructured Ni Catalysts with Low Metal Coverage for Chlorobenzene Hydrodechlorination
Lomonosov Moscow State University (Moscow), Russia

16.00 OY-III-4
Presenting author: Maxim S. Kazantsev
Kazantsev M.S.[1], Luzgin M.V.[1,2], Volkova G.G.[1], Stepanov A.G.[1,2]
Carbonylation of Dimethyl Ether on Rh/$Cs_2HPW_{12}O_{40}$: Mechanism of the Reaction in the Presence of Methyl Iodide Promoter
[1]*Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2]*Department of Natural Sciences, Novosibirsk State University (Novosibirsk), Russia*

16.10 OY-III-5

Presenting author: Alexander K. Khudorozhkov

Khudorozhkov A.K., Prosvirin I.P., Bukhtiyarov V.I.

Studying the Influence of Precursor and Promoter on the Activity and Stability of Methane Combustion Catalysts

Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

16.20 OY-III-6

Presenting author: Dr. Ilya Yu. Pakharukov

Pakharukov I.Yu.[1,2], Matrosova M.M.[1], Bukhtiyarov V.I.[1,2], Parmon V.N.[1,2]

Concentration Hysteresis in the Oxidation of Methane over Pt/γ-Al_2O_3

[1] *Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2] *Novosibirsk State University (Novosibirsk), Russia*

16.30 *Coffee break*

Assambleya Hall, Azimut Hotel

17.00-19.00 POSTER SESSION

11.00-16.00 - hanging posters

Forum Hall, Azimut Hotel

AFTERNOON SESSION

ORAL PRESENTATIONS
Section II. Mechanisms of Homogeneous Catalysis

Chairmen: Prof. Jean-Marie Aubry
Prof. Lev G. Bruk

14.30 OP-II-6
Presenting author: Dr. Dmitrii S. Suslov
Tkach V.S., Suslov D.S., Gubaidulina O.V., Bykov M.V.
Mechanism of the Dimerization of Propene in the Presence of the Ziegler-Natta Catalyst Based on Nickel and Aluminum Alkyl Halides
Irkutsk State University (Irkutsk), Russia

14.50 OP-II-7
Presenting author: Prof. Zhao-Hui Zhou
Yang Y.C., Zhou Z.H.
Catalytic Conversion of Phenol on Peroxo Edta-Type Titanate
State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University (Xiamen), China

15.10 OP-II-8
Presenting author: Prof. Segey G. Zlotin
Zlotin S.G., Kuherenko A.S., Maltsev O.V., Chizhov A.O.
Chiral Ionic Liquid/ESI-MS Methodology as an Efficient Tool for the Study of Transformations of Supported Organocatalysts
N.D. Zelinsky Institute of Organic Chemistry RAS (Moscow), Russia

ORAL PRESENTATIONS OF YOUNG SCIENTISTS
Section II. Mechanisms of Homogeneous Catalysis

15.30 OY-II-1
Presenting author: Viktoria V. Bocharova
Bocharova V.V., Kraikivskii P.B., Saraev V.V.
The role of Monovalent Nickel in Metalcomplex Catalysis
Federal State Budget Institution of Higher Education "Irkutsk State University" (Irkutsk), Russia

15.40 OY-II-2

Presenting author: Dr. Oleg Y. Lyakin

Lyakin O.Y.[1], Ottenbacher R.V.[1,2], Bryliakov K.P.[1], Talsi E.P.[1]

Non-Heme Iron and Manganese-Catalyzed Asymmetric Olefin Epoxidations with H_2O_2: Probing the Nature of Active Species by EPR Spectroscopic and Enantioselectivity Studies

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

15.50 OY-II-3

Presenting author: Roman V. Ottenbacher

Ottenbacher R.V.[1,2], Bryliakov K.P.[1], Talsi E.P.[1]

Highly Efficient, Regioselective and Stereospecific Oxidation of Non-Activated Aliphatic C-H Groups with H_2O_2, Catalyzed by Aminopyridine Manganese Complexes

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

16.00 OY-II-4

Presenting author: Dinara V. Sanieva

Ivancheva N.I.[1], Sanieva D.V.[1], Molev O.V.[1], Fedorov S.P.[1], Oleinik I.V.[2], Ivanchev S.S.[1]

Self-Immobilizing Catalysts for Ethylene Polymerization Based on Derivatives of bis(Phenoxy-Imine) Titanium Halide Complexes

[1]St. Petersburg Department of Boreskov Institute of Catalysis SB RAS (St. Petersburg), Russia
[2]Vorozhtzov Institute of Organic Chemistry SB RAS (Novosibirsk), Russia

16.10 OY-II-5

Presenting author: Dr. Mikhail G. Gantman

Tarkhanova I.G., Gantman M.G., Zelikman V.M.

Radical Processes Catalysed by Transition Metal Complexes with Grafted Ionic Liquids

M.V. Lomonosov Moscow State University (Moscow), Russia

16.20 OY-II-6

Presenting author: Dr. Ivan V. Kozhevnikov

Kozhevnikov I.V.[1,2], Chibiryaev A.M.[2,3], Nuzhdin A.L.[1], Bukhtiyarova G.A.[1], Martyanov O.N.[1,2]

Catalytic Effect of Si-Containing Compounds on the C-Methylation of Indole in *sc*-MeOH

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia
[3]Vorozhtsov Institute of Organic Chemistry SB RAS (Novosibirsk), Russia

16.30 *Coffee break*

Assambleya Hall, Azimut Hotel

17.00-19.00 POSTER SESSION

11.00-16.00 - hanging posters

Wednesday, October 24

Summit Hall, Azimut Hotel

MORNING SESSION

Chairmen: Prof. József Margitfalvi
Prof. Aleksandra Masalska

09.00 PL-4
Presenting author: Prof. Valery V. Fokin
Catalysis & Complexity: From Mechanism to Function
The Scripps Research Institute (La Jolla, California), USA

09.40 KL-6
Presenting author: Prof. Emrah Özensoy
Understanding Thermal and Photocatalytic Chemical Routes for NO_x Storage at the Molecular Level: From Advanced Realistic Catalysts to Planar Model Catalysts
Department of Chemistry, Bilkent University (Ankara), Turkey

10.10 KL-7
Presenting author: Prof. Valentine P. Ananikov
Transition-Metal-Catalyzed Carbon-Carbon and Carbon-Heteroatom Bonds Formation in Organic Synthesis
Zelinsky Institute of Organic Chemistry (Moscow), Russia

10.40 *Coffee break*

Assambleya Hall, Azimut Hotel
MORNING SESSION

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Prof. Vladislav A. Sadykov
Prof. Kusman Dossumov

11.10 OP-III-17
Presenting author: Prof. Ekaterina S. Lokteva
Lokteva E.S.[1], Erokhin A.V.[1], Yermakov A.Y.[2], Uimin M.A.[2], Bukhvalov D.[3]
Catalysis of Organic Reactions with Hydrogen on Graphene Activated by the Presence of Defects and Metal Sublayer
[1]Lomonosov Moscow State University (Moscow), Russia
[2]Institute of Metal Physics UB RAS (Yekaterinburg), Russia
[3]School of Computational Sciences, Korea Institute for Advanced Study (Seoul), Korea

11.30 OP-III-18
Presenting author: Dr. Laurent Piccolo
Piccolo L., Nassreddine S., Geantet C.
Mechanism of Tetralin Ring Opening and Ring Contraction over Bifunctional Ir/SiO_2-Al_2O_3 Catalysts
Institut de Recherches sur la Catalyse et l'environnement de Lyon (IRCELYON) (Villeurbanne), France

11.50 OP-III-19
Presenting author: Dr. Pawel Mierczynski
Mierczynski P.[1], Vasilev K.[2], Vasilev A.[2], Maniecki T.P.[1]
Comparative Studies of Pd, Ru, Ni and Cu Supported $ZnAl_2O_4$ Catalysts Used for Hydrogen Production from Methanol Steam Reforming
[1]Lodz University of Technology (Lodz), Poland
[2]University of South Australia (Mawson Lakes Adelaide), South Australia

12.10 OP-III-20

Presenting author: Prof. Takashi Tatsumi

Yamazaki H., Imai H., Yokoi T., Kondo J.N., Tatsumi T.

Reactivity of Methoxy Species in the Methanol to Olefin Reactions over H-ZSM-5

Chemical Resources Laboratory, Tokyo Institute of Technology (Yokohama), Japan

12.30 OP-III-21

Presenting author: Dr. Ilya V. Mishakov

Mishakov I.V.[1,2], Bauman Y.I.[1], Vedyagin A.A.[1,2]

Dechlorination of Chlorohydrocarbons on Bulk Ni-Alloyed catalysts: Mechanism of Carbon "Corrosion"

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State Technical University (Novosibirsk), Russia

12.50 OP-III-22

Presenting author: Prof. Parasuraman Selvam

Mahendran S., Selvam P.

Dehydration of Glycerol over Heteropoly Acid Supported Mesoporous Silica

National Centre for Catalysis Research, Department of Chemistry, Indian Institute of Technology Madras (Chennai), India

13.10 *Lunch*

Forum Hall, Azimut Hotel

MORNING SESSION

ORAL PRESENTATIONS
Section V. Electrocatalysis, Photocatalysis, Biocatalysis

Chairmen: Prof. Konstantin P. Bryliakov
Prof. Vincenzo Palma

11.10 OP-V-1
Presenting author: Dr. Andras Tompos
Borbáth I., Gubán D., Pászti Z., Sajó I., Tompos A.
Controlled Synthesis of Pt_3Sn/C Electrocatalysts with Exclusive Sn-Pt Interaction Designed for Use in Direct Methanol Fuel Cells
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences (Budapest), Hungary

11.30 OP-V-2
Presenting author: Prof. Tetsuya Shishido
Shishido T.[1], Furukawa S.[1], Ohno Y.[1], Teramura K.[1,2], Tanaka T.[1]
Reaction Mechanism of Selective Oxidation of Alcohols and Amines over Semiconductor Photocatalysts
[1]Department of Molecular Engineering, Graduate School of Engineering, Kyoto University (Kyoto), Japan
[2]Precursory Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST) (Saitama), Japan

11.50 OP-V-3
Presenting author: Prof. Diana Sannino
Sannino D., Vaiano V., Ciambelli P.
RuO_x-VO_x/TiO_2 as Very Highly Selective Photocatalysts for the Oxidative Dehydrogenation of Ethanol to Acetaldehyde
Department of Industrial Engineering, University of Salerno (Fisciano), Italy

12.10 OP-V-4

Presenting author: Dr. Ekaterina A. Kozlova

Kozlova E.A.[1], Kozhevnikova N.S.[2], Lemke A.A.[2], Cherepanova S.V.[1], Lyubina T.P.[1], Gerasimov E.Yu.[1], Tsybulya S.V.[1], Shchipunov Yu.A.[3], Rempel A.A.[2]

Design of the Nanocrystalline CdS/TiO$_2$ Photocatalyst

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Institute of Solid State Chemistry UB RAS (Yekaterinburg), Russia
[3]Institute of Chemistry FEB RAS (Vladivostok), Russia

12.30 Sponsor Donau Lab Moscow (in Russian)

Презентационный доклад спонсора конференции

Владимир Уголов

Быстрый и эффективный скрининг катализаторов
с использованием автоматизированных проточных реакторов

12.50 Sponsor Promenergolab Ltd., Moscow (in Russian)

Презентационный доклад спонсора конференции

Ольга М. Светлова

Автоматизированный прибор Thermo Scientific TPDRO1100 для исследования активности и удельной поверхности катализаторов методами ТПД, ТПО, ТПВ и импульсной хемосорбции

13.10 *Lunch*

Assambleya Hall, Azimut Hotel

AFTERNOON SESSION

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Prof. Ekaterina S. Lokteva
Prof. Takashi Tatsumi

14.30 OP-III-23
Presenting author: Dr. Mikhail Yu. Smirnov
Smirnov M.Yu., Kalinkin A.V., Vovk E.I., Pashis A.V., Bukhtiyarov V.I.
Application of Model Systems for XPS Studies of the Mechanism of Interaction of Supported Metal Catalysts with Gaseous Reaction Media
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

14.50 OP-III-24
Presenting author: Mikhail S. Gavrilov
Vedyagin A.A.[1,2], Gavrilov M.S.[1], Volodin A.M.[1], Stoyanovskii V.O.[1], Slavinskaya E.M.[1], Mishakov I.V.[1,2], Shubin Yu.V.[3]
Catalytic Purification of Exhaust Gases over Pd-Rh Alloy Catalysts: From Mechanism Understanding to High Temperature Stability
[1]*Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2]*Novosibirsk State Technical University (Novosibirsk), Russia*
[3]*Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk), Russia*

15.10 OP-III-25
Presenting author: Dr. Evgeny I. Vovk
Say Z.[1], Vovk E.I.[1,2], Bukhtiyarov V.I.[2], Özensoy E.[1]
Ce-O-Pt Active Sites in Ceria Promoted NO_x Storage Reduction Catalysis
[1]*Department of Chemistry, Bilkent University (Ankara), Turkey*
[2]*Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*

15.30 OP-III-26
Presenting author: Dr. Jesús Requies
Gandarias I., Fernández S.G., Requies J., Arias P.L.
Influence of the Hydrogen Source in the Mechanism of Glycerol Hydrogenolysis to 1,2-Propanediol
University of the Basque Country (UPV/EHU) (Bilbao), Spain

15.50 OP-III-27
Presenting author: Prof. Alexander G. Stepanov
Gabrienko A.A., Stepanov A.G.
Structure of Allylic Intermediates Formed from Olefins on Zinc Oxide
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

16.10 OP-III-28
Presenting author: Prof. Lev G. Bruk
Bruk L.G.[1], Titov D.N.[1], Zubavichus Ya.V.[2], Tkachenko O.P.[3], Ustugov A.V.[1], Oshanina I.V.[1], Veligzhanin A.A.[2], Kustov L.M.[3], Temkin O.N.[1]
Mechanism of Low-Temperature Carbon Monoxide Oxidation over $PdCl_2$-$CuCl_2$/γ-Al_2O_3 Catalyst
[1]Lomonosov Moscow University of Fine Chemical Technology (Moscow), Russia
[2]National Research Center "Kurchatov Institute" (Moscow), Russia
[3]N.D. Zelinsky Institute of Organic Chemistry RAS (Moscow), Russia

16.30 *Coffee break*

October 24, 2012

Assambleya Hall, Azimut Hotel

17.00-18.00 Russian Foundation for Basic Research
ROUND-TABLE (in Russian)

КРУГЛЫЙ СТОЛ

«Результаты конкурсов ориентированных фундаментальных исследований, поддержанных РФФИ в 2011 году, и пути их использования»

Рабочий язык – русский.

Председатели:
д.ф-м.н. С.А. Цыганов, начальник управления ориентированных исследований РФФИ, Москва;
д.х.н. О.Н. Мартьянов, зам. директора Института катализа СО РАН, Новосибирск

ПРОГРАММА

- к.т.н. Елена Р. Рудцкая, д.ф-м.н. Сергей А. Цыганов

Концепция конкурсов ориентированных исследований РФФИ
Отдел ориентированных фундаментальных исследований РФФИ, Москва

- д.х.н. О.Н. Мартьянов, член-корр. РАН С.С. Иванчев

Опыт выполнения инициативных проектов ориентированных фундаментальных исследований 2011-2012 гг.
Институт катализа им. Г.К. Борескова СО РАН, Новосибирск

19.00 ***Banquet, restaurant Troika***

Forum Hall, Azimut Hotel

AFTERNOON SESSION

ORAL PRESENTATIONS OF YOUNG SCIENTISTS
Section IV. Catalytic Processing of Renewables
Section V. Electrocatalysis, Photocatalysis, Biocatalysis
Section III. Mechanisms of Heterogeneous Catalysis
Section I. Catalysis: From First Principles

Chairmen: Prof. Kirill V. Kovtunov
Prof. Anatoliy N. Startsev

14.30 OY-IV-1
Presenting author: Dr. Pavel V. Snytnikov
Zyryanova M.M.[1,2,3], Shigarov A.B.[1,2,3], Snytnikov P.V.[1,2,3], Belyaev V.D.[1], Kirillov V.A.[1,2,3], Sobyanin V.A.[1,2,3]
Modeling of Associated Petroleum Gas Steam Reforming Process
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia
[3] "UNICAT" Ltd, Pr. (Novosibirsk), Russia

14.40 OY-IV-3
Presenting author: Olga A. Simakova
Simakova O.A.[1,2], Murzina E.V.[1], Leino A.-R.[3], Mäki-Arvela P.[1], Willför S.M.[4], Murzin D.Yu.[1]
Biomass Derived Lignan Hydroxymatairesinol Selective Oxidation over Au Catalysts
[1]Laboratory of Industrial Chemistry and Reaction Engineering, Process Chemistry Centre, Åbo Akademi University (Åbo/Turku), Finland
[2]Graduate School of Chemical Engineering, Åbo Akademi University (Åbo/Turku), Finland
[3]Microelectronics and Materials Physics Laboratories, EMPART Research Group of Infotech Oulu, University of Oulu (Oulu), Finland
[4]Laboratory of Wood and Paper Chemistry, Process Chemistry Centre, Åbo Akademi University (Åbo/Turku), Finland

14.50 OY-IV-4

Presenting author: Dr. Andrey V. Chistyakov

Chistyakov A.V., Murzin V.Yu., Gubanov M.A., Chudakova M.V., Yandieva F.A., Tsodikov M.V.

Direct Catalytic Treatment of Biomass Substrates Towards Hydrocarbon Fuel Components

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

15.00 OY-IV-7

Presenting author: Mariya V. Bykova

Bykova M.V., Ermakov D.Yu., Kaichev V.V., Smirnov A.A., Yakovlev V.A.

Novel Catalysts for Bio-Fuels Production from Biomass Fast Pyrolysis Oils

Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

15.10 OY-V-1

Presenting author: Dr. Ludivine Tasseroul

Tasseroul L.[1], Pirard S.L.[1], Lambert S.D.[1], Páez C.A.[1], Poelman D.[2], Pirard J.-P.[1], Heinrichs B.[1]

Kinetic Study of *p*-Nitrophenol Photodegradation with Modified TiO_2 Xerogels

[1]*University of Liège, Laboratoire de Génie chimique (Liège), Belgium*

[2]*University of Ghent, Department of Solid State Sciences (Ghent), Belgium*

15.20 OY-V-2

Presenting author: Pavel V. Cherepanov

Cherepanov P.V.[1], Skorb E.V.[2], Andreeva D.V.[1]

Ultrasonically Designed Metal / Polypyrrole Composite Catalysts for Fuel Cells

[1]*University of Bayreuth (Bayreuth), Germany*

[2]*Max Plank Institute of Colloids and Interfaces (Potsdam), Germany*

15.30 OY-V-3

Presenting author: Alexander Oschepkov

Oschepkov A.G.[1,2], Simonov A.N.[1], Rudina N.A.[1], Parmon V.N.[1,2]

Microstructure Effects in Catalysis of Oxygen Reduction Reaction over Electrodeposited Platinum: Influence of Intergrain Boundaries

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

15.40 OY-V-4

Presenting author: Dr. Tomasz P. Maniecki

Maniecki T.P., Kaczorowski P., Bawolak-Olczak K., Mierczynski P., Ura A.

Cu-Cr_2O_3-Al_2O_3 Catalysts For Water Gas Shift Reaction And Methanol Synthesis

Lodz University of Technology, Institute of General and Ecological Chemistry (Lodz), Poland

15.50 OY-III-7

Presenting author: Zere S. Konuspayeva

Konuspayeva Z.S.[1,4], Auezov A.B.[2], Konuspaev S.R.[1], Burkitbayev M.M.[1], Piccolo L.[4], Berhault G.[4], Shaimardan M.[3]

Bimetallic Catalysts for Selective Benzene Hydrogenation for Environmental Gasoline Production

[1]Al-Farabi Kazakh National University (Almaty), Kazakhstan
[2]Scientific Research Institute of New Chemical Technology & Materials (Almaty), Kazakhstan
[3]Kazakh British Technical University (Almaty), Kazakhstan
[4]Institut de Recherche sur la Catalyse et l'Environnement de Lyon (IRCELYON) (Lyon), France

16.00 OY-I-1

Presenting author: Dina F. Mukhamedzyanova

Ratmanova N.K.[1], Mukhamedzyanova D.F.[1], Pichugina D.A.[1,2], Kuz'menko N.E.[1]

The Theoretical Prediction of Structural and Electronic Effects of Gold-Based Systems in Selective Alkynes Activation

[1]Lomonosov Moscow State University (Moscow), Russia
[2]Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

16.10 OY-IV-2

Presenting author: Igor Y. Skobelev

Skobelev I.Y.[1], Sorokin A.B.[2], Kovalenko K.A.[3], Fedin V.P.[3], Kholdeeva O.A.[1]

Solvent-Free Allylic Oxidation of Alkenes with O_2 Mediated by Fe- and Cr-MIL-101

[1]*Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2]*Institut de Recherches sur la Catalyse et l'Environnement de Lyon (Villeurbanne), France*
[3]*Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk), Russia*

16.30 *Coffee break*

19.00 ***Banquet, restaurant Troika***

Thursday, October 25

Summit Hall, Azimut Hotel

MORNING SESSION

Chairmen: Prof. Dmitry Yu. Murzin
Prof. Zhao-Hui Zhou

09.00 PL-5
Presenting author: Prof. Evgenii V. Kondratenko
From Mechanistic and Kinetic Understanding of Heterogeneously Catalyzed Reactions to Tuning Catalysts Performance
Leibniz-Institut für Katalyse e. V. an der Universität Rostock (Rostock), Germany

09.40 KL-8
Presenting author: Prof. Miquel Costas
Costas M., Lloret-Fillol J., Prat I., Codolà Z., Gómez L., García-Bosch I., Company A., Cussó O., Canta M., Ribas X., Font D.
Selective Oxidation Catalysis with Non Porphyrinic Fe and Mn Complexes that Support High Oxidation States
Departament de Química,Universitat de Girona (Girona), Spain

10.10 KL-9
Presenting author: Prof. Evgenii P. Talsi
Bryliakov K.P.[1], Lyakin O.Y.[1], Ottenbacher R.V.[1,2], Talsi E.P.[1]
Active Species of Nonheme Iron- and Manganese-Catalyzed Oxidation
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

10.40 *Coffee break*

Assambleya Hall, Azimut Hotel

MORNING SESSION

ORAL PRESENTATIONS
Section III. Mechanisms of Heterogeneous Catalysis

Chairmen: Dr. Mikhail Yu. Smirnov
Prof. Stefania Specchia

11.10 OP-III-29
Presenting author: Prof. József Margitfalvi
Tálas E.[1], Margitfalvi J.L.[2]
Enantioselective Hydrogenation of Activated Ketones in the Presence of Pt-Cinchona Catalysts. Is the Proton Transfer Concept Valid?
[1]Research Center for Natural Sciences (Budapest), Hungary
[2]Combitech-Nanotech Kft. (Budapest), Hungary

11.30 OP-III-30
Presenting author: Marc Jacquemin
Jacquemin M., Hauwaert D., Gaigneaux E.M.
Mechanistic and Kinetic Studies of Aromatic Carbon-Carbon Coupling (Suzuki Reaction) with Heterogeneous Catalysts
Institute of Condensed Matter and Nanosciences – IMCN, Division "MOlecules, Solids and ReactiviTy - MOST, Université Catholique de Louvain (UCL) (Louvain-la-Neuve), Belgium

11.50 OP-III-31
Presenting author: Prof. Lidia I. Kuznetsova
Kuznetsova N.I.[1], Trebushat D.V.[1], Kuznetsova L.I.[1], Zudin V.N.[1], Kajitani H.[2], Utsunomiya M.[2], Takahashi K.[2]
On Mechanisms of Oxidation of 1,3-Butadiene on Pd-Te Catalysts in Polar Solvents
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Mitsubishi Chemical Corporation (Okayama), Japan

12.10 OP-III-32

Presenting author: Prof. Yurii A. Zolotarev

Zolotarev Yu.A.[1], Dadayan A.K.[1], Borisov Yu.A.[2], Nazimov I.V.[3], Vaskovsky B.V.[3], Myasoedov N.F.[1]

Solid State Isotope Exchange with Spillover Hydrogen in Organic Compounds

[1]*Institute of Molecular Genetics RAS (Moscow), Russia*
[2]*Nesmeyanov Institute of Organoelement Compounds RAS (Moscow), Russia*
[3]*Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry RAS (Moscow), Russia*

12.30 ***Closing***

12.50 ***Lunch***

15.00 ***Excursion – Hermitage Museum,***

17.00 ***Excursion – St. Isaac's Cathedral***

Forum Hall, Azimut Hotel

MORNING SESSION

ORAL PRESENTATIONS
Section IV. Catalytic Processing of Renewables

Chairmen: Dr. Jacobus J.C. Grove
Dr. Ilya V. Mishakov

11.10 OP-IV-1
Presenting author: Natalia V. Garyntseva
Kuznetsov B.N.[1,2], Sudakova I.G.[1], Garyntseva N.V.[1], Djakovitch L.[3], Pinel C.[3]
Kinetic Study of Aspen-Wood Delignification by H_2O_2 with Sulfuric Acid Catalyst under Mild Conditions
[1]Institute of Chemistry and Chemical Technology SB RAS (Krasnoyarsk), Russia
[2]Siberian Federal University (Krasnoyarsk), Russia
[3]Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON) (Lyon), France

11.30 OP-IV-2
Presenting author: Prof. Ivan V. Kozhevnikov
Alotaibi M., Kozhevnikova E.F., Kozhevnikov I.V.
Deoxygenation of Biomass-Derived Molecules over Multifunctional Polyoxometalate Catalysts in the Gas Phase
Department of Chemistry, University of Liverpool (Liverpool), United Kingdom

11.50 OP-IV-3
Presenting author: Dr. Gloria Berlier
Berlier G.[1], Gopalakrishnan S.[1,2], Miletto I.[1], Coluccia S.[1,2], Caputo G.[3], Giaconia A.[3], Sau S.[3]
Unravelling the Structure and Reactivity of Supported Ni Particles in Ni-$CeZrO_2$ Catalysts
[1]Università degli Studi di Torino, Department of Chemistry and NIS Centre of Excellence (Torino), Italy
[2]ISTEC, Centro Nazionale delle Ricerche (Torino), Italy
[3]ENEA, "Casaccia" Research Center (Rome), Italy

12.10 OP-IV-4

Presenting author: Dr. Irina L. Simakova

Zaytseva Yu.A., Simonov M.N., Simakova I.L., Shutilov A.A., Zenkovets G.A.

Ketonization of Valeric Acid over Metal Oxides as a First Step for Green Diesel Synthesis: Consideration from Mechanistic Viewpoint

Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

12.30 ***Closing***

12.50 *Lunch*

15.00 ***Excursion – Hermitage Museum,***

17.00 ***Excursion - St. Isaac's Cathedral***

POSTER SESSION

Section I. Catalysis: From First Principles

PP-I-1
Akhmetov I.V., Gubaydullin I.M., Bayguzina A.R., Muckminov R.R., Spivak S.I., Khusnutdinov R.I.
Discrimination between Reaction Mechanisms for the Synthesis of Methyl 5-Acetyl-2-Pyrrolecarboxylate
Institute of Petrochemistry and Catalysis RAS (Ufa), Russia

PP-I-2
Beletskaya A.V., Pichugina D.A., Kuz'menko N.E.
Mechanism of H_2O_2 Synthesis from H_2 and O_2 on Gold and Gold-Palladium Nanoclusters: DFT Approach
Lomonosov Moscow State University (Moscow), Russia

PP-I-4
Elena M. Evstigneeva
Oxidation of Allyl Complexes of Pd(II) by Aqueous H_2O_2 Through Pd(IV) Intermediates: A DFT Investigation
Lomonosov Moscow University of Fine Chemical Technologies, Moscow, Russia

PP-I-5
Gubaidullin I.M.[1], Ramazanov I.R.[1], Kadikova R.N.[1], Nurislamova L.F.[2]
Mathematical Modeling of Reactivity of Olefinic and Acetylenic Compounds in Catalytic Reaction of Cycloalumination
[1]Institute of Petrochemistry and Catalysis RAS (Ufa), Russia
[2]Bashkir State University (Ufa), Russia

PP-I-6
Koledina K.F.[1], Gubaidullin I.M.[2], Novichkova A.V.[2]
Development of the Kinetic Model of Detailed Mechanism of Olefin Hydroalumination
[1]Bashkir State University (Ufa), Russia
[2]Institute of Petrochemistry and Catalysis RAS (Ufa), Russia

PP-I-7
Molinari E., Tomellini M.
On the Role of Energy Distribution Functions of the Ad-Atoms in Recombinative Adsorption at Catalytic Surfaces
Dipartimento di Scienze e Tecnologie Chimiche Università di Rome Tor Vergata (Rome), Italy

PP-I-8
Mukhamedzyanova D.F., Pichugina D.A., Kuz'menko N.E.
Allylbenzene Double-Bond Migration in Gold-Containing Catalytic Systems: DFT Study
Lomonosov Moscow State University (Moscow), Russia

PP-I-9
Nikitenko N.G., Shestakov A.F.
Quantum Chemical Study of C-H Bond Activation in Methane and Methanol by Au(I) Complexes with Quercetin under Mild Conditions
Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

PP-I-10
Shamov A.G., Khrapkovskii G.M., Isakov D.R., Shamov G.A.
Ethylene to Benzene Catalytic Transformation Mechanism Performed at Nanocluster of Platinum Pt_4 Based on the Results of Quantum-Chemical Computations
Kazan National Research Technological University (Kazan), Russia

PP-I-11
Shamov A.G., Nikolaeva E.V., Tsyshevsky R.V., Khrapkovskii G.M.
Catalytic Transformations During Thermal Decomposition of Some Aliphatic Nitro Compounds
Kazan National Research Technological University (Kazan), Russia

PP-I-12

Slobodov A.A., Sochagin A.A., Radin M.A., Trenina M.V.

Thermodynamic Studying of Catalyst Processes and Systems – Possibilities and Efficiency

St. Petersburg State Institute of Technology (St. Petersburg), Russia

PP-I-13

Snyga Y.G.[1], Beletskaya A.V.[1], Pichugina D.A.[1,2], Kuz'menko N.E.[1]

Quantum-Chemical Investigation of Structural Effects of Ag_{20} in Propylene Epoxidation

[1]M.V. Lomonosov Moscow State University (Moscow), Russia
[2]Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

Section II. Mechanisms of Homogeneous Catalysis

PP-II-1

Antonov A.A.[1], Semikolenova N.V.[2], Zakharov V.A.[2], Zhang W.[3], Wang Y.[3], Sun W.-H.[3], Talsi E.P.[2], Bryliakov K.P.[2]

New Bis(imino)pyridine Nickel Catalysts: Polymerization of Norbornene and Investigation of the Active Species

[1]Novosibrsk State University (Novosibirsk), Russia
[2]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[3]Institute of Chemistry CAS (Beijing), China

PP-II-2

Bagrii E.I.

Chemistry Carbcations: β-Methyl Shift – A New Rearrangement of the Carbcations Bridged Alycyclic Hydrocarbons

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

PP-II-5

Chepaikin E.G.[1], Bezruchenko A.P.[1], Menchikova G.N.[1],
Moiseeva N.I.[2], Gekhman A.E.[2]

Mechanistic Scenarios for Homogeneous Catalytic Alkanes Oxidation

[1]Institute of Structural Macrokinetics and Materials Science RAS (Chernogolovka), Russia
[2]N.S. Kurnakov Institute of General and Inorganic Chemistry RAS (Moscow), Russia

PP-II-6

Chepaikin E.G.[1], Bezruchenko A.P.[1], Noskov Yu.G.[2]

Water-Gas Shift Reaction Catalyzed by Water Soluble Pd Complexes: Kinetics and Mechanism

[1]Institute of Structural Macrokinetics and Materials Science RAS (Chernogolovka), Russia
[2]United Research and Development Center (Moscow), Russia

PP-II-7

Faingol'd E.E., Babkina O.N., Zharkov I.V., Bravaya N.M.

^{1}H NMR Study of Activation of Dimethylated 2-Substituted Bisindenyl Zirconocenes with Triisobutylaluminum and Isobutylalumoxanes in Polymerization of Hexene-1

Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

PP-II-9

Galiullin A.N., Faingold E.E., Babkina O.N., Makhaev V.D.,
Bravaya N.M.

UV-Visible Spectroscopic Study of Catalystic Systems $Ph_2CCpFluMMe_2$ (M = Zr, Hf) /TIBA/$[Ph_3C_3]^+[B(C_6F_5)_4]^-$

Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

PP-II-12

Menshikov S.Yu.[1], Vazhenin V.A.[2], Valova M.S.[1], Sitnikov L.V.[3]

Preparation of Ionic Liquids on Base Methoxylpropylamine and Study Their Properties with $VO(acac)_2$ by ESR-Spectroscopy

[1]Institute of Organic Synthesis URAL Branch RAS (Yekaterinburg), Russia
[2]Ural Federal University (Yekaterinburg), Russia
[3]Institute of High Temperature Electrochemistry URAL Branch RAS (Yekaterinburg), Russia

PP-II-15

Soshnikov I.E.[1], Semikolenova N.V.[1], Osichow A.[2], Bryliakov K.P.[1], Zakharov V.A.[1], Mecking S.[2], Talsi E.P.[1]

NMR Spectroscopic Trapping of Nickel(II)-Alkyl Species in the Course of Polymerization of Ethylene with Neutral Ni(II) Complexes

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]University of Konstanz, Chair of Chemical Material Science, Department of Chemistry (Konstanz), Germany

PP-II-19

Zharkov I.V., Bravaya N.M.

Modeling of Tetraisobutylalumoxane Structures and its Complexes with Triisobutylaluminum

Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

PP-II-20

Konev V.N., Khlebnikova T.B., Pai Z.P.

A New Nitrogen-Containing Derivatives of Diterpenic Acids in Asymmetric Catalysis

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Section III. Mechanisms of Heterogeneous Catalysis

PP-III-7
Babayeva E.F., Soltanov R.I., Ahmedova R.H., Babayeva F.A., Ibrahimov H.J., Ismailov E.H.
Acid-Base Properties of Zn, Ga-Containing Zeolite Catalysts and their Activity in Associated Gas Conversion to Liquid Hydrocarbons
Institute of Petrochemical Processes of ANAS (Baku), Azerbaijan

PP-III-8
Bączkowska K., Grzechowiak J.R., Poźniak R.
New Silica-Alumina Supports for Pt Ring Opening Catalysts
Wrocław University of Technology, Faculty of Chemistry *(Wrocław), Poland*

PP-III-9
Baizhumanova T.S., Tungatarova S.A., Abdukhalykov D.B., Zhumabek M.
Research of Activity of the Pt-Ru Catalyst Supported on Metal Block Carriers in the Steam Oxygen Conversion of Methane
JSC "D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry" (Almaty), Kazakhstan

PP-III-10
Barskiy D.A.[1,2], Kovtunov K.V.[1,2], Khudorozhkov A.K.[3], Bukhtiyarov V.I.[3], Koptyug I.V.[1,2]
Selectivity Control of Pairwise Hydrogen Addition over Catalytic Hydrogenation of C_4 Hydrocarbons on Supported Pt and Pd Catalysts
[1] International Tomography Center SB RAS (Novosibirsk), Russia
[2] Novosibirsk State University (Novosibirsk), Russia
[3] Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

PP-III-11
Barthos R., Valyon J.
Heterogenization of Wacker Process over Palladium/Vanadium Catalysts
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences (Budapest), Hungary

PP-III-12
Bekmuhamedov G.E., Egorova S.R., Kataev A.N., Zalyaliev R.F., Lamberov A.A.
Spectral and Catalytic Study of Silica Modified Cr_2O_3/Al_2O_3 Dehydrogenation Catalyst
Kazan (Volga) Federal University (Kazan), Russia

PP-III-14
Bychkov V.Yu., Tyulenin Yu.P., Slinko M.M., Korchak V.N.
Oscillatory Behaviour during Oxidation of C_2-C_3 Olefins over Nickel and Cobalt
Semenov Institute of Chemical Physics RAS (Moscow), Russia

PP-III-16
Chernikova V.S.[1], Erokhin A.V.[1], Golubina E.V.[1], Murzin V.Y.[2], Veligzhanin A.A.[2], Zubavichus Y.V.[2]
Formation of Active Sites in NiZn/UDD Catalysts for the Selective Phenylacetylene Hydrogenation as Monitored by *in situ* EXAFS
[1]*M.V.Lomonosov Moscow State University (Moscow), Russia*
[2]*National Research Center "Kurchatov Institute" (Moscow), Russia*

PP-III-18
Çinar T., Altinçekiç T.G., Öksüzömer M.A.
Preparation and Characterization of Nanosized Ni-Co/Al_2O_3 Catalysts Prepared by Polyol Method for Partial Oxidation of Methane
Department of Chemical Engineering, Istanbul University (Istanbul), Turkey

PP-III-19

Cruceanu A.[1], Zavoianu R.[1], Pavel O.D.[1], Bradu C.[1], Dutu L.[1], Mara L.[2]

Hydrotalcite-Like Catalytic Materials Obtained from Industrial Wastes for Oxidation of Sulfur Compounds

[1]University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis (Bucharest), Romania
[2]National Institute for Research and Development for Nonferrous and rare metals, Bucharest, Romania (Bucharest), Romania

PP-III-20

Damyanova S.[1], Pawelec B.[2], Arishtirova K.[1]

Ni-Based Catalysts for Reforming of Methane with CO_2

[1]Institute of Catalysis of Bulgarian Academy of Sciences (Sofia), Bulgaria
[2]Institute of Catalysis and Petrochemistry, CSIC (Madrid), Spain

PP-III-24

Dossumov K., Tungatarova S.A., Yergazyeva G.Y.

The Study of Adsorption of Benzene by IR Spectroscopy

Kazakh National University of Al-Farabi «Center of Physical-Chemical Methods of Investigation and Analysis» (Almaty), Kazakhstan

PP-III-25

Douven S.[1], Pirard S.L.[1], Chan F.-Y.[2], Heyen G.[3], Pirard J.-P.[1]

Carbon Nanotube Synthesis by CCVD Process: Kinetic Study on a Ni-Mo/MgO Catalyst

[1]Laboratoire de Génie Chimique Université de Liège (Liège), Belgium
[2]Nanocyl S.A. (Sambreville), Belgium
[3]Laboratoire d'Analyse et de Synthèse des Systèmes Chimiques, Université de Liège, (Liège), Belgium

PP-III-26

Drozdov V.A., Arbuzov A.B., Kazakov M.O., Lavrenov A.V., Likholobov V.A.

Study of the Liquid-Phase Isobutane Alkylation with Butenes over Aluminum Chloride Complexes Synthesized *in situ* from Activated Aluminum and *tert*-C_4H_9Cl

Institute of Hydrocarbons Processing SB RAS (Omsk), Russia

PP-III-27

Eremin V.A.[1], Ananyev M.V.[1], Kurumchin E.Kh.[1], Yoo Ch.-Y.[2], Bouwmeester H.J.M.[2]

Oxygen Isotope Exchange and Pressure Relaxation of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$

[1]Institute of High Temperature Electrochemistry UB RAS (Yekaterinburg), Russia
[2]University of Twente (Twente), The Netherlands

PP-III-28

Federyaeva V.S.[1], Vitkovskaya R.F.[1], Petrov S.V.[1], Goralski J.[2]

Influence of Support Treatment with Inorganic Solutions on Properties of Glass and Basalt Fiber Catalysts

[1]St. Petersburg State University of Technology and Design (St. Petersburg), Russia
[2]Technical University of Lodz (Lodz), Poland

PP-III-30

Gatin A.K.[1], Grishin M.V.[1], Kirsankin A.A.[1], Kharitonov V.A.[1], Shub B.R.[1], Gurevich S.A.[2], Kozhevin V.M.[2], Yavsin D.A.[2]

Interaction of Single Metal Nanoparticles with Molecular Hydrogen and Oxygen

[1]Semenov Institute of Chemical Physics RAS (Moscow), Russia
[2]Ioffe Physical Technical Institute of Russian Academy of Sciences (Saint-Petersburg), Russia

PP-III-31

Golubina E.V.[1], Erokhin A.V.[1], Klezhina N.[1], Lokteva E.S.[1], Kharlanov A.N.[1], Petrov I.L.[2], Lunin V.V.[1]

Variation of Surface and Texture Nanodiamond Properties to Create Effective Hydrodechlorination Catalyst

[1]Lomonosov Moscow State University (Moscow), Russia
[2]LLC "SCN" (Snezhinsk), Russia

PP-III-34

Guliyev B.B., Ismailov E.H., Ibrahimov H.J., Babayeva F.A., Rustamov M.I.

Studies of the Thermal Decomposition of Methanol Adsorbed by Zeolite Based Catalyst Using TG/DSC and GC/MS Analysis

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

PP-III-37

Ilyasov I.R., Nazarov M.V., Laskin A.I., Mukhambetov I.N., Lamberov A.A.

Influence of the Electronic Properties of Palladium Particles Deposited on Alumina on the Reaction Mechanism of Hydrogenation of Vinylacetylene

Kazan (Volga) Federal University (Kazan), Russia

PP-III-39

Isupova L.A.[1], Prosvirin I.P.[1], Pavlyukhin Yu.T.[2]

Nature of Low Bond Oxygen Form in $La_{1-X}Sr_xFeO_3$ Perovskites

[1]*Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2]*Institute of Solid State Chemistry SB RAS (Novosibirsk), Russia*

PP-III-40

Kadirbekov K.A., Konuspaev S.R., Nurbaeva R.K., Zhambakin D.K.

Regularities of Formation of Hydrocarbon Cracking Catalysts for Modification of Natural Zeolite by Acids of Various Nature

JSC " A.B. Bekturov Institute of Chemical Sciences" (Almaty), Kazakhstan

PP-III-42

Kalevaru V.[1], Sri Hari Kumar A.[2], Qiao A.[1], Lingaiah N.[2], Alshammari A.[3], Sailu Ch.[4], Sai Prasad P.S.[2], Martin A.[1]

Catalytic Behavior of Decomposed Molybdophosphoric Acid Supported on Alumina for Oxidative Dehydrogenation of Ethane to Ethylene

[1]*Leibniz-Institut für Katalyse e.V. an der Universität Rostock (Rostock), Germany*
[2]*Indian Institute of Chemical Technology (Hyderabad), India*
[3]*National Nanotechnology Research Center (Riyadh), Saudi Arabia*
[4]*Univ. College of Technology, Osmania University (Hyderabad), India*

PP-III-43
Kalinkin A.V., Sorokin A.M., Smirnov M.Yu., Bukhtiyarov V.I.
XPS and STM Studies of Oxidation by NO_2 of Platinum Particles Supported on HOPG
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

PP-III-44
Karlsson E.A., Pericàs M.A.
Rationalisation of the Catalytic Role of Triazole-Linkers in Asymmetric Aldol Reactions in Water Catalysed by Polystyrene-Supported Hydroxyproline
Institute of Chemical Research of Catalonia (Tarragona), Spain

PP-III-45
Kavalerskaya N.E., Majouga A.G., Lokteva E.S., Golubina E.V., Maslakov K.I.
Au-Ni Synergism in the Alumina Supported Catalysts in the Hydrodechlorination of Chlorobenzene
Lomonosov Moscow State University (Moscow), Russia

PP-III-47
Kharlamova T.S.[1], Matveev A.S.[1], Sadykov V.A.[2]
Doped Apatite-Type Lanthanum Silicates as Catalysts for Oxidative Coupling of Methane
[1]Tomsk State University (Tomsk), Russia
[2]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

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Korchak V.N.[1], Bychkov V.Yu.[1], Falkevich G.S.[2], Shchankina V.G.[3], Sharkina V.I.[3]
Mechanism of Methanol Steam Reforming over Cu-Containing Catalyst in a High Excess of Water
[1]Semenov Institute of Chemical Physics RAS (Moscow), Russia
[2]Ltd. SAPR-NEFTECHIM (Moscow), Russia
[3]Ltd. NIAP-Katalizator (Novomoskovsk), Russia

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Kuzmina O.V., Dementeva E.V., Urtyakov P.V.
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Lukiyanchuk I.V.[1], Chernykh I.V.[1], Rudnev V.S.[1], Tyrina L.M.[1], Ustinov A.Y.[2]
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[1] *Institute of Chemistry FEB RAS (Vladivostok), Russia*
[2] *Far Eastern Federal University (Vladivostok), Russia*

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Marinkovic M.[1], Radulovic N.[1], Putanov P.[2], Momcilovic M.[3], Zarubica A.[1]
Physical-Chemical Properties of Phosphated Zirconia in the Reaction of *n*-Hexane Isomerization
[1] *Faculty of Sciences and Mathematics, University of Nis (Nis), Serbia*
[2] *Serbian Academy of Sciences and Arts (Belgrade), Serbia*
[3] *Institute of Nuclear Science "Vinca" (Belgrade), Serbia*

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Matveeva V.G.[1], Sapunov V.N.[2], Grigoriev M.E.[1], Sulman E.M.[1]

Non-Steady-State Kinetics of D-Glucose to D-Sorbitol on Ru-Containing Heterogeneous Catalyst

[1]Tver State Technical University (Tver), Russia
[2]D. Mendeleev University of Chemical Technology of Russia (Moscow), Russia

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Investigation of the Mechanism of Deactivation of Pd/Sibunit Catalyst Hydrodechlorination of Polychlorinated Biphenyls

[1]Postovsky Institute of Organic Synthesis UB RAS (Yekaterinburg), Russia
[2]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[3]Novosibirsk State Technical University (Novosibirsk), Russia

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Mierczynski P.[1], Vasilev K.[2], Mierczynska A.[3], Maniecki T.P.[1]

Decomposition and Steam Reforming of Methanol over Pd, Cu - CNT Catalysts

[1] Lodz University of Technology, Institute of General and Ecological Chemistry Zeromskiego (Lodz), Poland
[2]University of South Australia (Mawson Lakes Adelaide), Australia
[3]Ian Wark Research Institute, University of South Australia (Mawson Lakes Adelaide), Australia

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Effect of B-Cation Substitution on the Activity of $LaCrO_3$ and $LaNiO_3$ Perovskites for Autothermal Reforming of Methane

[1]Instituto de Catálisis y Petroleoquímica, CSIC (Madrid), Spain
[2]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[3]Institute of Coal Chemistry and Material Science SB RAS (Kemerovo), Russia

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[1]Institute of Isotopes (Budapest), Hungary
[2]Université de Poitiers (Poitiers), France

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Kinetic Regularities of 1-Decene Polymerization on Supported Titanium-Magnesium Nanocatalysts (TMNC) and Molecular Weight Characteristics of Obtained Polymers
A.V. Topchiev Institute of Petrochemical Synthesis RAS (Moscow), Russia

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Nikolaev S.A., Pichugina D.A., Golubina E.V., Majouga A.G.
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Influence of the Way of Active Sites Formation in Pt/MgAlOx Catalysts on their Catalytic Properties. XPS Study
[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Institute of Hydrocarbons Processing SB RAS (Omsk), Russia

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University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis (Bucharest), Romania

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FTIR Study of Adsorption and Transformations of HCN on Oxide Adsorbents

[1]*St. Petersburg State University (St. Petersburg), Russia*
[2]*UST de Lille Villeneuve d'Ascq Cedex (Lille), France*

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Poor Kalhor M.[1], Chermette H.[1], Ballivet-Tkatchenko D.[2]

A DFT Study of Electronic and Steric Effects of Alkoxy Ligands for Dialkyl Carbonate Formation from CO_2 and *n*-$Bu_2Sn(OR)_2$

[1]*Institut de Sciences Analytiques, University of Lyon (Lyon), France*
[2]*Institut de Chimie Moléculaire, University of Burgundy (Dijon), France*

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Porotnikova N.M., Ananyev M.V., Eremin V.A., Pankratov A.A., Kurumchin E.Kh.

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Features of the Alcohols' Dehydrogenation on the NZP – Catalysts Depending on the Location of the Ion - Modifier

Peoples' Friendship University of Russia (Moscow), Russia

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Rossi U.[1], Artiglia L.[2], Granozzi G.[2], Canu P.[1]

Direct Synthesis of Hydrogen Peroxide on Model Pd Surfaces

[1] *Dipartimento di Ingegneria Industriale (Padova), Italy*
[2] *Dipartimento di Scienze Chimiche (Padova), Italy*

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Serov Y.M., Sheshko T.F.

Synthesis of Olefins from Carbon Oxides and Hydrogen on Iron-Manganese Nanosystems at Atmospheric Pressure

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Different Catalytic Activity of Zeolites Modified by Transition Metal and Aluminum Chloride on Liquid- and Gas-Phase Conversion of Alkanes

[1] *Lomonosov Moscow State University (Moscow), Russia*
[2] *Semenov Institute of Chemical Physics RAS (Moscow), Russia*

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Simentsova I.I.[1,2], Khassin A.A.[1,2], Minyukova T.P.[1,2], Rogov V.A.[1,2], Davydova L.P.[1], Yurieva T.M.[1]

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[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University(Novosibirsk), Russia

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[1]Technological Institute for Superhard and Novel Carbon Materials (Troitsk), Russia
[2]INFRA Technologies Ltd. (Moscow), Russia

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Identification of Surface Structures Responsible for Activity and Selectivity of Cobalt-Based Catalyst in Fischer-Tropsch Synthesis

[1]Technological Institute for Superhard and Novel Carbon Materials (Troitsk), Russia
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Ustinov A.Yu.[1,2], Rudnev V.S.[1,2], Lukiyanchuk I.V.[2], Tyrina L.M.[2], Vasilyeva M.S.[1,2], Ustinova E.A.[2], Chernykh I.V.[2]
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[1]Far Eastern Federal University (Vladivostok), Russia
[2]Institute of Chemistry FEB RAS (Vladivostok), Russia

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[1]Institute of Chemistry FEB RAS (Vladivostok), Russia
[2]Far Eastern Federal University (Vladivostok), Russia

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[1]Bashkir State University (Ufa), Russia
[2]Institute of Organic Chemistry of the URC RAS (Ufa), Russia

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Purdue University, Birck Nanotechnology Center (West Lafayette, IN), USA

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The Promoting Effect of Rare Earth Metals on Partial Oxidation of Methanol to Hydrogen over Ag and Cu Catalysts
[1] *Chemistry Department, College of Science, King Faisal University (AlHofof), Saudi Arabia*
[2] *Chemistry Department, Faculty of Science, Ain Shams University (Cairo), Egypt*
[3] *Inorganic Chemistry Laboratory, Oxford University, United Kingdom*

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Deliy I.V.[1,2], Bukhtiyarova G.A.[1], Vlasova E.N.[1], Nuzhdin A.L.[1], Aleksandrov P.V.[1]
The Selectivity of Methyl Palmitate and Rapeseed Oil Hydroconversion on CoMoS/Al_2O_3 and NiMoS/Al_2O_3 Catalysts
[1] *Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia*
[2] *Novosibirsk State University (Novosibirsk), Russia*

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Dorokhov V.S.[1], Ishutenko D.I.[1,2], Nikulshin P.A.[2], Eliseev O.L.[1], Bondarenko T.N.[1], Lapidus A.L.[1], Kogan V.M.[1]
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[1] *N.D. Zelinsky Institute of Organic Chemistry RAS (Moscow), Russia*
[2] *Samara State Technical University (Samara), Russia*

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Grzechowiak J.R., Masalska A., Jaroszewska K., Zemska A.

Conversion of n-Paraffins Using Hybrid Catalysts Containing BEA Zeolite

Faculty of Chemistry, Wrocław University of Technology (Wrocław), Poland

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Jaroszewska K.[1], Masalska A.[1], Grzechowiak J.R.[1], Maniecki T.[2], Mierczyński P.[2]

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[1]*Faculty of Chemistry, Wrocław University of Technology (Wrocław), Poland*

[2]*Institute of General and Ecological Chemistry, Technical University of Łodź (Łodź), Poland*

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Khalaf M.M.[1,2], Ibrahimov H.C.[1], Yusifov Y.H.[1], Ismailov E.H.[1]

Novel Nanostructured Fe-, Co- Containing Materials as Heterogeneous Catalysts for the Decomposition of Heavy Oil Residue

[1]*Institute of Petrochemical Processes, Azerbaijan National Academy of Sciences (Baku), Azerbaijan*

[2]*Chemistry Department, Faculty of Science, Sohag University (Sohag), Egypt*

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Lapin N.V., Djankova N.J.

Catalytic Hydrolysis of Ammonia Borane with Iron and Nickel Oxides

Institute of Microelectronic Technology and High-Purity Materials RAS (Chernogolovka), Russia

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Matus E.V.[1], Kuznetsov V.V.[1], Ismagilov I.Z.[1], Mota N.[2],
Navarro R.M.[2], Kerzhentsev M.A.[1], Ismagilov Z.R.[1,3], Fierro J.L.G.[2]

Comparative Study of Oxidative Coupling of Methane to Ethane and Ethylene over Na-W-Mn/SiO_2 and La-Sr/CaO Catalysts

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Instituto de Catálisis y Petroleoquímica, CSIC (Madrid), Spain
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Ismagilov Z.R.[1,2]

Control of Metal Dispersion, Chemical Composition, Porous Structure and Thickness of Mesoporous PtSn/TiO_2 and PdZn/TiO_2 Coatings for Microcapillary Reactor

[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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Palma V., Barba D., Ciambelli P.

H_2S Purification from Biogas to Feed MCFC by Partial Oxidation on the V_2O_5-CeO_2 Catalyst

University of Salerno (Fisciano), Italy

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Palma V., Ricca A., Ciambelli P.

Methane Auto-Thermal Reforming in a Compact Thermal Integrated ATR Reformer: Monolithic Catalysts Performances

University of Salerno (Fisciano), Italy

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Simonov M.N., Simakova I.L.

Mechanistic Study of Reaction Pathways in Butyl Lactate to Propylene Glycol Hydrogenolysis over Cu/SiO_2

Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

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Sooknoi T.[1], Ausavasukhi A.[2]

H_2-Least Approaches for Deoxygenation of Phenolic Compounds

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[2]Program in Applied Chemistry, Faculty of Sciences and Liberal Arts, Rajamangala University of Technology Isan (Nakhon Ratchasima), Thailand

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Vasic M.[1], Ljupkovic R.[1], Radulovic N.[1], Putanov P.[2], Momcilovic M.[3], Zarubica A.[1]

Combined Methods for Mono-, Di- and Triglycerides Determination: A Biodisel Production over CaO Catalyst

[1]Faculty of Sciences and Mathematics, University of Nis (Nis), Serbia
[2]Serbian Academy of Sciences and Arts (Belgrade), Serbia
[3]Institute of Nuclear Science "Vinca" (Belgrade), Serbia

Section V. Electrocatalysis, Photocatalysis, Biocatalysis

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Ananyev M.V., Porotnikova N.M., Medvedev D.A., Eremin V.A., Yaroslavtsev I.Yu., Pankratov A.A., Kurumchin E.Kh.

Oxygen Exchange and Degradation of LSM—YSZ Cathode Materials

Institute of High Temperature Electrochemistry UB RAS (Yekaterinburg), Russia

PP-V-3

Bakhtchadjian R.H.[1], Tsarukyan S.V.[1], Manucharova L.A.[1],
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Dioxo-Mo(VI) - Complexes Anchored on Titania as Catalysts in Photo-Oxidative Decomposition of Some Aromatic Organochlorine Compounds by Dioxygen

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[2]Laboratoire de Catalyse en Chimie Organique, CNRS (Poitiers), France

PP-V-7

Lyubina T.P.[1], Kozlova E.A.[1,2]

New Photocatalysts Based on Cadmium and Zinc Sulfides for Hydrogen Evolution from Aqueous $Na_2S–Na_2SO_3$ Solutions under Visible Light

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

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Manea F.[1], Baciu A.[1], Pop A.[1], Remes A.[1], Pode R.[1], Schoonman J.[2]

Electrocatalytic Detection of Arsenic at Silver-Doped Zeolite-Carbon Nanostructured-Epoxy Composite Electrodes

[1]"Politehnica" University of Timisoara (Timisoara), Romania
[2]Delft University of Technology (Delft), The Netherlands

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Pode R., Manea F., Colar L.A., Jakab A.

Photocatalytic Degradation and Mineralization of Methylene Blue Dye onto Ag-Modified Natural Zeolite Catalyst

"Politehnica" University of Timisoara, Faculty of Industrial Chemistry and Environmental Engineering (Timisoara), Romania

PP-V-12

Samoilov A.V., Nikitich M.P., Vodyankin A.A., Vodyankina O.V.

Study of Free Charge Carrier Distribution on the Surface of Titania-Based Photocatalysts

Tomsk State University (Tomsk), Russia

PP-V-13
Sannino D., Vaiano V., Sacco O., Ciambelli P.
Mathematical Modelling of Photocatalytic Degradation of Methylene Blue under Visible Irradiation
University of Salerno, Department of Industrial Engineering (Fisciano), Italy

PP-V-15
Sintyureva M.M., Clarkson B.G, Creeth A.M.
Fuel Cells Powered by HPAs: FlowCath® Technology
ACAL Energy Ltd (Runcorn) United Kingdom

ANNOTATIONS OF PLENARY AND KEYNOTE LECTURES AND OF ORAL PRESENTATIONS

PLENARY LECTURES

PL-1 Bell A.T.

Elucidating the Mechanism of Heterogeneously Catalyzed Reactions through Combined Experimental and Theoretical Studies

University of California, Berkeley, USA

Knowledge of the mechanism of reactions occurring on the surface of heterogeneous catalysts is sought for the purpose of understand what aspect of catalyst composition and structure limit catalyst activity, selectivity, and stability. The first step is measurement of the reaction kinetics in order to understand how the rate of product formation depends on the reaction temperature and the reactant and product partial pressures. Such data can provide useful clues as to the mechanism by which the reaction proceeds. In the next step various spectroscopic techniques are used to probe the nature of adsorbed species and the relationship of their surface concentrations to the kinetics of product formation. In situ (or operando) IR or Raman spectroscopy are most often used for this purpose. Since both the bulk and surface composition and structure may change with reaction conditions, these properties are also probed using techniques such as UV-Visible spectroscopy, XANES, EXAFS, and in situ XPS. The deductions drawn from measurements of reaction kinetics and the characterization of adsorbed species are used to develop proposed reaction mechanism, which can be used to derive and an expression for the reaction kinetics. Agreement between the derived rate expression and the experimentally measured kinetics provides support for the proposed mechanism but does not prove that it is correct. Additional verification of deductions drawn from experimental findings is provided by the use of first principles theory to determine rate parameters for proposed elementary steps. If the activation energies and preexponential factors determined from theory agree with those deduced from experimental measurement, further confidence in the physical correctness of the proposed mechanism is gained. This talk will illustrate how experimental and theoretical methods can be used in conjunction to develop a better understanding of reaction mechanisms and the how catalyst composition and structure affect the kinetics of reactions catalyzed by heterogeneous catalysts. The examples considered will include the thermal dehydrogenation of alkanes, the carbonylation of olefins and ethers, and the electrochemical splitting of water. As a part of this discussion, we will also show how newly emerging experimental and theoretical techniques contribute to developing a deeper insights into the mechanism of catalyzed reactions.

PL-2 Parmon V.N.

Thermodynamics of Operating Catalyst: Some Approaches and Findings

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

In contrast to chemical kinetics, thermodynamics is so far not very actively used for describing the state and behavior of operating heterogeneous catalysts. The reason is indeed the non-equilibrium state of operating catalysts that does not allow common equilibrium thermodynamics to be used. In the last decade, however, there was a progress in understanding how the approaches of non-equilibrium thermodynamics could be applied to operating catalysts.

The presentation gives few examples of such applications. There are, first of all, explanation of superlow temperature of melting nanoparticles of metal catalysts active in carbon nanofiber production, semiquantitative description of the size effect for at least metal catalysts, possibility to couple or even convert direction of undesirable processes with the desirable ones, as well as ideas about possibility to change the stationary phase state of the operating catalytically active components via controlling the composition of the surrounding reactive mixture. It is also shown that a quite typical situation for catalytic processes is not coincidence of the rate-controlling step and the "bottle neck" (limiting step) of the overall process.

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Valentin Parmon, Thermodynamics of Non-Equilibrium Processes for Chemists with a Particular Application to Catalysis, Elsevier, 2010, 340 p.

PL-3 Que L.,Jr.

Bio-Inspired Hydrocarbon Oxidations by Nonheme Iron Catalysts

Department of Chemistry and Center for Metals in Biocatalysis,
University of Minnesota, Minneapolis, USA

Inspired by the versatile oxidation chemistry catalyzed by nonheme iron enzymes, we have been investigating the iron-catalyzed oxidations of hydrocarbons. Highly stereoselective *cis*-dihydroxylation of olefins has been observed with the use of nonheme iron(II) complexes with H_2O_2 as oxidant. Insights into the catalytic mechanism have been obtained from a combination of product distribution studies, ^{18}O labeling experiments, and kinetic analysis as well as DFT calculations. These results implicate a high-valent iron-based oxidant. Hydrocarbon oxidation can also be observed for iron complexes supported by tris(pyrazolyl)borate ligands that activate O_2. A high-valent iron-based oxidant is also postulated for these reactions, which exhibit shape selectivity. The unusual shape selectivity observed suggests that substrate recognition can be elicited even in a biomimetic complex of relatively simple design.

PL-4 Fokin V.V.

Catalysis & Complexity: From Mechanism to Function

The Scripps Research Institute, La Jolla, California, USA

Catalysis is at the heart of chemistry and disciplines that directly depend on it, for harnessing the complexity of catalytic processes offers unprecedented potential for making them useful on both laboratory and industrial scales. Investigation of complex catalytic systems requires methods that examine these processes under true bench top conditions in real time and throughout their course. This global profiling approach allows us to study critically important events, such as activation and deactivation of catalysts, unproductive off-cycle pathways, and provides insights into the dynamics of the changing environment of a catalytic reaction. We then use the resulting data-dense reaction profiles for the development of most efficient reaction conditions.

A key lesson that emerged from our work during the last decade is that one can achieve near perfect selectivity without relying on the classical lock and key enzymatic catalysis paradigm because highly dynamic mixtures of complexes that exist in rapid equilibria with each other can actually serve as exquisitely selective catalysts. A single, well-defined catalyst is not always required and may, in fact, be counterproductive. If allowed, the system will select, and will inescapably form, the right catalyst – and it does not need to dominate as far as population goes – as long as there is enough of it to effect the fastest catalytic turnover.

This approach will be exemplified using several case studies of the catalytic reactions of alkynes. Alkynes are among the most energetic hydrocarbons, and transition metals enable selective and controlled manipulation of the triple bond, opening the door to the wealth of reliable reactivity: transformations of alkynes into heterocycles and into a variety of molecules with new carbon–heteroatom bonds. The combination of catalytic alkyne functionalization followed by manipulation of the resulting products allows one to proceed from a system with high energy content to a system of lower energy in a stepwise fashion, thereby enabling controlled introduction of new elements of diversity in every step. Various architectures prepared using these methods are finding increased use in organic synthesis, nano- and biotechnology, and materials science.

PL-5 Kondratenko E.V.

From Mechanistic and Kinetic Understanding of Heterogeneously Catalyzed Reactions to Tuning Catalysts Performance

Leibniz-Institut für Katalyse e. V. an der Universität Rostock (Rostock), Germany

Heterogeneous catalysis is the basis of the majority of chemical processes in modern industry and affects our life in myriad ways. It helps to convert readily available raw materials to higher value-added products. Due to the scarcity of these materials and the requirements for treating/removal of side products, there is a high demand for more efficient and environmentally benign catalytic technologies. Yet, catalytic materials are too complex to predict their behaviour and to develop novel catalysts with desired performance (activity, selectivity, time-on-stream stability). Therefore it is highly desired to elaborate fundamental principles enabling to couple molecular knowledge about the structure and functioning of catalytically active sites with the reaction kinetics on the level as elementarily as possible. The relationships between the individual rate constants and catalytic sites can provide guidelines for the rational catalyst design and for the optimization of reactor operation.

To accomplish these objectives, various approaches are applied. This paper demonstrates the potential of steady-state, transient methods operating with sub-millisecond time resolution, time-resolved operando catalyst characterization and DFT calculations for monitoring and molecular understanding of various heterogeneously catalyzed reactions. The importance of micro-kinetic analysis will be especially highlighted. Finally, it will be shown that the sophisticated fundamental knowledge does really enable to tune catalysts performance for a number of gas-phase catalytic reactions such as functionalization of natural gas, Fischer-Tropsch, Ostwald and Deacon processes. This was, however, possible owing to the development of methods for controlled synthesis of catalysts with the uniformity of catalytically active species and their distribution on the support surface. Particularly the role of well-defined metal nanoparticles for establishing explicit structure-performance relationships will be discussed in this contribution.

KEYNOTE LECTURES

KL-1 Van Santen R.A.[1], Ghouri M.M.[2]

The Mechanism of the Fischer-Tropsch Reaction

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Due to the increasing detailed molecular information on the energetic and kinetics of elementary surface reactions that are part of the Fischer-Tropsch catalytic reaction cycle, the kinetics and selectivity can be probed in great detail. Using computational catalysis tools the relation between overall kinetics and structure of the catalytic reactive center can be probed in detail. The mechanism of the reaction is found to change with structure, which has important consequences for overall chain growth probabality. We will illustrate the state of affairs in detail for catalysis by Ruthenium.

To predict chain growth parameter and consumption rate, next to elementary kinetics data, available from first principle quantum-chemical data, microkinetics simulations are necessary. We will present a comparison of microkinetics simulations and Kinetic Monte Carlo simulations. Results of quantum-chemical calculations will be reported that are used as input to the kinetic simulations.

Three specific questions are addressed:

- the relation between activation energy of CO dissociation and chain growth probability;
- consequences to overall activity and selectivity of reaction centers with different CO dissociation sites and chain growth centers;
- the prediction of differences in CO consumption rate and selectivity for Ru and Co.

Most of current evidence indicates that the carbide mechanism is the most relevant for Fischer-Tropsch catalysis by metals as Co and Ru. It turns out that sites at the surface are selective that provide low energy paths to CHx intermediate formation. Such sites are similar to the step-edge sites known from transition metal surfaces that provide low barriers for CO dissociation.

Water removal and chain growth have to be fast reactions, whereas methane formation and also chain growth termination have to be slow.

The detailed mechanism of chain growth depends on the structure of the catalyst. We will discuss several possibilities.

We find that the optimum chain-growth probability not only requires a step-edge type of reaction center, but also a site that has a dual reaction center. In the latter case CO dissociation and chain growth do not interfere. A necessary condition is that Cads is generated initially in a four fold site and upon hydrogen addition moves to a three fold site. Whereas overall kinetics according to the single site model is limited by chain termination as slow step, in the dual site model the chain growth reaction has to be the slower elementary reaction step. This is in line with the general observation that chain growth parameters are different for the formation of short hydrocarbon chains versus the longer ones. Since particle size and shape will affect the relative stability of reactive centers, these results have important consequences for particle size dependence.

We predict low chain growth probabilities on the terraces, where formation of intermediate CH_x species is relatively slow. The dominant chain growth sites will be the step-edge type centers with efficient CH_x formation rates. When one compares the relative consumption rates of different metals it is important to establish whether comparisons are made for surfaces with CO dissociation as the slow step versus the rate of chain growth termination or the elementary rate of chain growth. In the comparison of Ru and Co, the terraces are found to be more reactive for Ru, but the step edge sites give the higher selectivity for Co.

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KL-2 Neyman K.M.

Catalysis from First Principles: Is it Crucial to Account for the Effects of Nanostructuring?

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Difference in the complexity of single crystal surfaces and “real” catalysts causes a problem known as material gap in catalysis. This major obstacle hinders the extension of profoundly understood processes on single crystal surfaces to equally good understanding of heterogeneous catalysis. Indeed, active components of most working catalysts are nanoparticles exposing defects and irregularities that often control the reactivity. To understand the reactivity of such systems, it is crucial to go beyond the still common single-crystal description. For that, model metal catalysts formed of well-characterized supported nanoparticles have been proven experimentally very fruitful [1]. Computational strategy to model experimentally studied catalysis-relevant nanoparticles will be outlined. Applications to metal [2-5], oxide [6, 7] and metal/oxide [8, 9] nanostructures will be discussed.

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KL-3 Konya T., Kobayashi D., Murayama T., Ueda W.

Catalytic Oxidation Mechanism Based on the High-Dimensional Structure of Mo_3VO_x

Catalysis Research Center, Hokkaido University, Sapporo, Japan

Mo-V-O-based complex oxides are one of the most important solid-state oxidation catalysts. However, it has been hard to understand the origin of catalytic function of these catalysts in molecular level. Now, we have two new crystalline solids of Mo_3VO_x with unique crystal structures, orthorhombic phase and trigonal phase. Both of the Mo_3VO_x catalysts have the same structure units of pentagonal ring, 6-membered ring [1-5], and 7-membered ring with different arrangements in *a-b* plane and in addition showed extremely high catalytic activities for the selective oxidation of acrolein to acrylic acid and the oxidation of ethane to ethene with molecular oxygen. Catalytic results indicated that the structural unit arrangement [2,4,5] in the *a-b* plane of the catalysts was dominant in the genesis of the oxidation activity and showed that the existence of the 7-membered ring site in the Mo_3VO_x catalysts was indispensable for the oxidation activity. It is proposed that the bridged lattice oxygen between highly distorted Mo and V octahedra forming the 7-memebered ring unit [2] is responsible for the catalytic oxidation, and the ring with Redox tunable pore diameter of about 0.4 nm [3,6] can capture the reactant molecules for effective oxidative activation.

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KL-4 Murzin D.Yu.

Mechanistic Aspects of Hydrogenation and Oxidation of Sugars

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In recent years, exploitation of renewable sources has gained considerable attention. In particular polyols and acids derived from respectively hydrogenation and oxidation of sugars are versatile molecules with a variety of applications. In the lecture these reactions occurring in the aqueous phase will be discussed.

Extensive kinetic studies on oxidation of arabinose, galactose and glucose combined with electrochemical potential measurements along with investigations of structure sensitivity and catalyst characterization were conducted over supported gold catalysts for the interpretation of the reaction mechanism [1]. The influence of the reaction parameters such as pH, temperature, and oxygen flow rate was investigated. In-situ catalyst potential measurements during oxidation gave information about the extent of the oxygen accumulation on the metal surface and a correlation to activity was obtained. An oxidative dehydrogenation mechanism was proposed and a kinetic model taking into account the catalyst potential changes was developed.

Hydrogenation of D–maltose, D–galactose, L–rhamnose and L–arabinose and some of their binary mixtures to corresponding polyols was carried out on a finely dispersed Ru/activated carbon catalyst with the objective of studying the kinetics and the reaction mechanism [2]. This work was supplemented with DFT investigations of five L-arabinose tautomers adsorption on a ruthenium surface allowing advancing a reaction mechanism. In particular it could be suggested that conformers of sugars are mostly adsorbed keeping the conformational properties and the most abundant tautomer, perpendicularly interacting with the metal surface, is the one, which is probably hydrogenated.

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KL-5 Rupprechter G.

The “True” Explanation is Typically rather Simple

Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria

We all know examples for that: people come up with models explaining mechanisms of surface reactions and, sometimes, the models may be rather fancy. When further results disagree with the originally proposed and disseminated model, the model is modified to become even more complex. However, in many cases, the original model may simply be wrong. The current contribution discusses 4 examples of this “phenomenon”:
i) the structure and selectivity of PdZn surface alloys [1,2], ii) hydrogen adsorption on Ga_2O_3 and reactions on PdGa-Ga_2O_3 [3,4], iii) CO dissociation on noble metals [5,6], and iv) CO oxidation on metallic vs. oxidic surfaces [7,8].

We show how a surface science approach utilizing *in situ* surface spectroscopy [9,10] and surface microscopy [11,12] on model catalysts, together with corresponding studies of technological catalysts, hopefully provides the right answers. Does it ?

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KL-6 Özensoy E.

Understanding Thermal and Photocatalytic Chemical Routes for NO_x Storage at the Molecular Level: From Advanced Realistic Catalysts to Planar Model Catalysts

Department of Chemistry, Bilkent University, Ankara, Turkey

In this talk, two different genres of TiO_2-promoted $DeNO_x$ catalysts with NO_x storage capabilities will be discussed. The first genre of catalysts to be discussed is TiO_2-promoted NO_x-Storage Reduction (NSR, or Lean NO_x Traps, LNT) catalysts which function through thermally activated surface processes. NSR catalysts are based on solid state storage of NO_x(g) in the exhaust stream on a catalytic component within a thermal window of 250 - 350 °C under oxidizing (lean) conditions followed by the reduction of the stored NO_x during a short fuel-rich period. $BaO/TiO_2/Al_2O_3$ based ternary mixed oxide NO_x storage materials synthesized via sol-gel techniques reveal advantageous NO_x storage and sulfur tolerance characteristics. Although the conventional BaO/Al_2O_3 binary mixed oxide system is prone to sulfur poisoning where it loses a significant portion of its NO_x storage capacity in an irreversible fashion due to the formation of thermodynamically stable surface and bulk sulfate species, $BaO/TiO_2/Al_2O_3$ ternary system displays significantly superior thermal regeneration characteristics at low temperatures and resists sulfur poisoning. This behavior can be attributed to the presence of small TiO_2 surface domains functioning as anchoring sites for BaO clusters, preventing the sintering of BaO sites and impeding the formation of large $BaSO_4$ clusters that cannot be thermally regenerated efficiently. Along these lines, surface functionalization with TiO_2 is presented as an effective strategy to *"fine-tune"* the surface dispersion of a particular oxide domain (i.e. BaO) on a complex mixed oxide system. These arguments are supported with experimental results obtained via XRD, BET, Raman spectroscopy, in-situ FTIR, TPD, XPS, TEM, SEM and EDX techniques.

In order to shed light on the fundamental surface phenomena taking place during the NO_x storage processes on NSR catalysts at the molecular level, planar model catalysts were prepared in the form of $BaO/BaO_2/Pt(111)$ and $BaO_x/TiO_2/Pt(111)$. Structural characterization of these relatively well-defined model catalysts was performed via LEED and XPS while NO_x adsorption characteristics were studied via XPS and TPD. It is observed that BaO_2 sites play a crucial role during the uptake and release of NO_x species where the presence of exposed (open) Pt sites significantly enhance the BaO_2 formation and catalytically decrease the NO_x desorption temperatures. Two different NO_x desorption mechanisms were proposed for model catalyst surfaces containing exposed Pt sites and surfaces lacking any exposed Pt sites. Furthermore, a mechanistic explanation was also provided for the thermally induced deactivation and the structural integrity loss of TiO_2-promoted NSR catalysts at elevated temperatures which include the formation of $BaTiO_3$ domains, sub-surface diffusion of BaO sites and the surface segregation of underlying TiO_2 domains. Influence of BaO domain size on the NO_x storage was also studied as a function of BaO surface coverage.

Inspired by the thermally-activated automotive catalysts given above, a second genre of photochemically-activated TiO_2-promoted $DeNO_x$ catalysts in the form of X/TiO_2, and $X/TiO_2/Al_2O_3$ (X=Li, Na, K, Cs, Ca, Sr or Ba) were also prepared via sol-gel techniques for indoor air purification purposes. These photochemically activated systems operate under ambient conditions (25 °C) and offer a hybrid platform combining photocatalytic NO_x(g) oxidation and solid state NO_x storage. Performance and the structural properties of these hybrid "Photocatalytic NO_x Oxidation and Storage" (PNOS) systems will also be discussed in the final part of the talk.

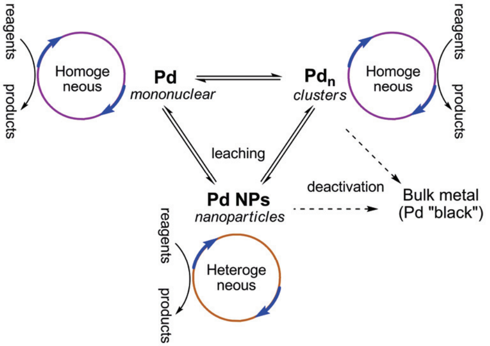
KL-7 Ananikov V.P.

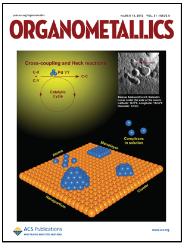
Transition-Metal-Catalyzed Carbon-Carbon and Carbon-Heteroatom Bonds Formation in Organic Synthesis

Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia

Carbon-carbon and carbon-heteroatom bonds formation are well-established and outstanding tools utilizing homogeneous catalysis in the areas of organic synthesis, pharmaceutical and medicinal chemistry, natural product synthesis, material science, and several other fascinating applications. Homogeneous catalysis in cross-coupling, Heck, carbonylation reactions, and also carbon-heteroatom bond formation has shown tremendous recent growth. Rapid methodology development in the areas of selective construction of C-C and C-Heteroatom bonds revealed unique features on the nature of metal catalysis: adaptive interconverion of different active species taking place during the catalytic transformation.

In the present study, the mechanism of transition-metal-catalyzed reactions are discussed in view of evolution of active species in solution and finding the relationship between the nature of catalyst active species to the efficiency and selectivity of the reaction (Scheme 1) [1].





Scheme 1. An example of interconversion of Pd catalyst active species in solution.

The questions of particular importance are catalytic properties related to mononuclear metal complexes and metal clusters in solution, interconversion between homogeneous and heterogeneous catalytic systems, leaching, and stability/recycling of the catalysts. The optimal strategy to select efficient catalytic system for C-C and C-Heteroatom bonds formation will be presented and discussed.

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KL-8 Costas M., Lloret-Fillol J., Prat I., Codolà Z., Gómez L., García-Bosch I., Company A., Cussó O., Canta M., Ribas X., Font D.

Selective Oxidation Catalysis with Non Porphyrinic Fe and Mn Complexes that Support High Oxidation States

Departament de Química, Universitat de Girona, Girona, Spain

The formation and cleavage of the O-O bond is arguably the most important reaction in living organisms. Reductive O-O breakage takes place in cytochrome C oxidase, during cellular respiration in aerobic organisms. [1] O-O cleavage also takes place in oxygenases, [2] and this reaction results in the generation of highly electrophilic high valent metal-oxo species, responsible for oxidative transformations. On the other hand, O-O bond formation takes place at a Mn4Ca cluster in the Oxygen Evolving Center of Photosystem II (PSII) of green plants. In both oxidative and respiration enzymes, metal ions adopting high oxidation states result from reductive O-O cleavage reactions, while in PSII they are responsible for O-O bond formation. [3] Selected coordination complexes catalyze analogous reactions, and some of these complexes have turned into very attractive tools for organic synthesis. [4] The study of the mechanisms of action of these catalysts has shed light into the molecular details of enzymatic systems. Our research group undertakes this approach and aims at studying the chemistry of iron and manganese coordination complexes which can sustain high oxidation states and that can act as catalysts for challenging oxidation reactions, such as the selective oxidation of alkyl C-H bonds, [5] the cis-dihydroxylation of alkenes, [6] stereoselective epoxidation [7] and the oxidation of water. [8] Recent progress from our group will be discussed.

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KL-9 Bryliakov K.P.[1], Lyakin O.Y.[1], Ottenbacher R.V.[1,2], Talsi E.P.[1]

Active Species of Nonheme Iron- and Manganese-Catalyzed Oxidation

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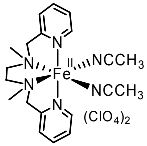
[2]*Novosibirsk State University, Novosibirsk, Russia*

Within biomimetic oxidation catalysts, aminopyridine complexes of such biologically important elements as Fe and Mn attract particular attention.[1] These complexes have been found to efficiently catalyze olefin epoxidation with percarboxylic acids or H_2O_2/AcOH in a chemo- and sometimes enantioselective fashion.[1,2] Electron paramagnetic resonance (EPR) spectroscopy has been used to characterize oxidizing species in the catalyst systems **1**-**4**/H_2O_2. It was found that very unstable intermediates **1c**-**4c** exhibiting similar rhombic $S = 1/2$ EPR signals and active towards epoxidation of olefins are formed in these systems.[3] Costas, Cronin, and co-workers have used cryospray-assisted variable temperature mass spectrometry (VT-MS), to detect an elusive HO–Fe^V=O intermediate in the catalyst system **4**/H_2O_2.[4] Direct correlation of VT-MS and EPR data shows that $S = 1/2$ intermediate **4c** well corresponds to the oxoiron(V) species identified in the same system by VT-MS. Apparently, complexes **1c**-**4c** are similar oxoiron(V) species. Comparative studies of asymmetric olefin epoxidation by Fe and Mn catalyst systems **3**/H_2O_2/RCOOH and **5**/H_2O_2/RCOOH have shown that **3** and **5** conduct enantioselective epoxidation of prochiral olefins with H_2O_2 in the presence of carboxylic acids, manganese catalyst **5** demonstrating much higher efficiency (1000 vs. 100 TON) and enantioselectivity (up to 93% *ee*: the highest value ever reported for aminopyridine manganese catalysts). The enantioselectivity drastically increases with rising steric bulk of the acid, thus indicating the presence of the carboxylic moiety in the active species. On the basis of EPR and enantioselectivity data, the active species can be assigned to complexes $[LM^V{=}O(OC(O)R]^{2+}$ (where M = Fe or Mn, R = alkyl, L = aminopyridine ligand).



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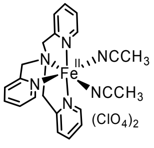

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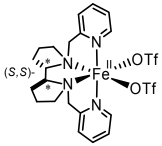

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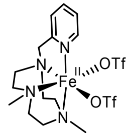

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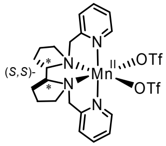

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ORAL PRESENTATIONS

Section I. Catalysis: From First Principles

OP-I-1 Stakheev A.Yu.[1], Batkin A.M.[1], Beck I.E.[2], Teleguina N.S.[1], Bragina G.O.[1], Zaikovsky V.I.[2], Larichev Yu.V.[2], Bukhtiyarov V.I.[2]

Particle Size Effect in CH_4 Oxidation over Noble Metals: Comparison of Pt and Pd Catalysts

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[2]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Catalytic tests revealed different relationships between TOF in CH_4 oxidation and the metal particle size for Pd and Pt catalysts. Particle size effect for Pd catalysts is significantly pronounced: TOF increases by more than one order of magnitude with increase in *d* Pd from 1 to 22 nm. This results in the most favourable performance for the catalyst with Pt particle size ~ 4 nm. On the other hand, over Pt catalysts TOF increases only by ~ 2-3 times with increasing particle size from 1 to 3-4 nm, and remains essentially constant when *d* Pt exceeds 4 nm. The observed differences stem from different reaction mechanisms over Pd and Pt.

OP-I-2 Başaran D.[1], Chiu C.[1], Genest A.[1,2], Rösch N.[1,2]

Computational Insights into Aqueous Phase Processes for Biomass Reforming

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Technische Universität München, Garching, Germany
[2]Institute of High Performance Computing, Singapore

Catalytic processes of alcohols in an aqueous phase were examined on the model systems 1- and 2-propanol over the surfaces Pt(111) and Pt(221). The reforming pathways were studied focusing on the C-C cleavage step and the difference in reactivity of 1- and 2-propanol. Possible alkane formation pathways are presented, for which the rate-limiting C-O cleavage step is discussed.

OP-I-3 Nasluzov V.A.[1], Laletina S.S.[1], Shor A.M. [1], Shor. E.A.[1], Rösch N.[2]
Activation of Oxygen on Microclusters of Silver Anchored on SiO_2 and Al_2O_3 Surfaces. Embedded Cluster Scalar-Relativistic and Periodic Pseudopotential Density Functional Calculations
[1]*Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia*
[2]*Technische Universität München, Catalysis Research Center, Garching, Germany*

Formation energies and equilibrium structures of O_2 adsorbtion complexes with silver trimers and tetramers supported on α-Al_2O_3(0001) and MCM-41 surfaces have been calculated. The extent of O_2 activation is probed in surface NO oxidation reaction.

OP-I-4 Pichugina D.A.[1,2], Mukhamedzianova D.F.[1], Beletskaya A.V.[1], Ratmanova N.K.[1], Snyga J.G.[1], Nikolaev S.A.[1], Askerka M.S.[1], Lanin S.N.[1], Shestakov A.F.[2], Kuz'menko N.E.[1]
Theoretical Insight on Catalytic Activity of Bimetallic Gold Catalysts

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[2]*Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia*

The scope of DFT in studying the active sites of Au_nNi and Au_nPd bimetallic particles will be presented. Ligand and ensemble effects in these systems will be considered in H_2O_2 formation and hydrocarbons isomerization.

OP-I-5 Andrikopoulos P.C.[1], Michel C.[1], Chouzier S.[2], Sautet P.[1]
Oxidation of Alkanes: In Silico Catalyst Design
[1]*University of Lyon, CNRS, Laboratoire de Chimie, ENS de Lyon, Lyon, France*
[2]*Centre de Recherches et Technologies de Lyon, Laboratoire Intermédiaires Polyamide, Saint-Fons, France*

Alkane C-H activation, and in particular, selective oxidation under mild conditions has been an enduring challenge in catalysis. Recently, attention has been drawn to metal-oxo systems that can mimic the effectiveness of biological systems. In the present DFT study, several heme and non-heme iron-oxo catalysts are in assessed in the H-abstraction/O-rebound mechanism. The effect of the equatorial or axial position of the ligands on the spin state and reactivity of the species is also taken into account.

OP-I-6 Gurevich S.A.[1], Kozhevin V.M.[1], Yavsin D.A.[1], Rostovshchikova T.N.[2], Lokteva E.S.[2]
¶Self-Induced Electric Fields in the System of Supported Metal Nanoparticles: The Impact on Heterogeneous Catalysis
[1]*Ioffe Physical-Technical Institute of RAS, St. Petersburg, Russia*
[2]*Lomonosov Moscow State University, Moscow, Russia*

We consider the appearance of self-induced electric fields in a system of supported metal nanoparticles. These fields are associated with fast-fluctuating charge dipoles arising due to thermally activated electron tunnel transitions between the nanoparticles or, in case of conducting support, between the particles and the support. Estimations show that the peak intensity of such fields can be up to 10^7 V/cm. The results of the catalytic experiments performed with supported metal nanoparticles confirm strong impact of these fields on the catalytic processes.

OP-I-7 Startsev A.N., Kruglyakova O.V., Chesalov Yu.A., Ruzankin S.F., Kravtsov E.A., Larina T.V., Paukshtis E.A.

¶Low Temperature Decomposition of Hydrogen Sulfide into Hydrogen and Diatomic Gaseous Sulfur

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

A new catalytic reaction of hydrogen sulfide decomposition is discovered, the reaction occurs on metal catalysts in gas phase at room temperature according to equation $2\ H_2S \leftrightarrow 2\ H_2 + S_2{}^{(gas)}$ to produce hydrogen and gaseous diatomic sulfur. As calculated with DFT, S_2 molecule is in the singlet state with energy 10.4 kcal/mol over the ground triplet state. “Fingerprints” of diatomic sulfur adsorbed on the solid surfaces and dissolved in different solvents are studied. When hydrogen sulfide is passing through the solid catalyst immersed in liquid solvent which is capable of dissolving sulfur generated, conversion of hydrogen sulfide at room temperature achieves 100 % producing hydrogen in gas phase.

Section II. Mechanisms of Homogeneous Catalysis

OP-II-1 Masui Y.[1], Haga S.[2], Onaka M.[1]

Direct Synthesis of Dimethyl Carbonate from CO_2 and MeOH Catalyzed by Sn(O*t*-Bu)$_4$ with Acid-Base Additives, and its Reaction Mechanism

[1]Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, Japan
[2]Graduate School of Science, The University of Tokyo, Tokyo, Japan

We discovered that Sn(O*t*-Bu)$_4$ was a user-friendly precatalyst for the direct synthesis of dimethyl carbonate from CO_2 and MeOH. It is far more active than the conventional $Bu_2Sn(OMe)_2$ catalyst. The high catalytic activity of Sn(O*t*-Bu)$_4$ is discussed in the light of the quantum chemical calculation and FT-IR analysis.

OP-II-2 Talsi E.P., Bryliakov K.P.

Living Olefin Polymerization with Post-Titanocene Catalysts Containing *o*-Fluoroaryl Substituents: Role of Noncovalent Interactions

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

In this work, formation of ion-pair intermediates of the type $[L_2TiMe]^+[MeMAO]^-$ upon the interaction of bis(salicylaldimine), bis(enolatoimine) and related titanium pre-catalysts L_2TiCl_2 with methylalumoxane (MAO) has been followed by multinuclear NMR spectroscopy. The nature of chain-propagating species of the type $[L_2TiP]^+[MeMAO]^-$ (where P is the growing polymeryl chain) is discussed.

OP-II-3 Aubry J.M., Nardello-Rataj V.

Mechanism for the Reduction of Dioxygen by Diethylhydroxylamine (DEHA) Organocatalyzed by Natural Polyphenols

Université de Lille Nord de France, Villeneuve d'Ascq CEDEX, France

The reduction of dioxygen dissolved in water by diethylhydroxylamine (DEHA) in the presence of synthetic or natural hydroquinones or benzoquinones as organocatalysts is investigated with regard to reaction rate and catalyst turnover. The rate-determining step is the regeneration of hydroquinones through the reduction of the corresponding benzoquinones by DEHA. A further improvement of the catalytic system is achieved by adding catalase to disproportionate the generated hydrogen peroxide, which is detrimental for the catalyst.

OP-II-4 Belkova N.V.[1], Kozinets E.M.[1,2], Filippov O.A.[1], Fekete M.[3], Duckett S.B.[3], Manoury E.[2], Poli R.[2], Shubina E.S.[1]

Diphenylphosphinoferrocenyl Thioether Diene Rh(I) and Ir(I) Catalyzed Ketone Hydrogenation: Turning Precatalysts into Active Species

[1]Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia
[2]Laboratoire de Chimie de Coordination CNRS, Toulouse, France
[3]Department of Chemistry, University of York, York, United Kingdom

The effect of the diene ligand and anion, solvent and added base (pyridine, MeONa) on the rate of hydrogenation of diphenylphosphinoferrocenyl thioether diene Rh(I) and Ir(I) precatalysts was studied by NMR and UV/Vis spectroscopies. Combined with DFT calculations these experimental data allow suggesting the precatalyst activation mechanism.

OP-II-6 Tkach V.S., Suslov D.S., Gubaidulina O.V., Bykov M.V.

Mechanism of the Dimerization of Propene in the Presence of the Ziegler-Natta Catalyst Based on Nickel and Aluminum Alkyl Halides

Irkutsk State University, Irkutsk, Russia

The role of the Ni(I) complexes in the dimerization of propylene in the presence of the Ziegler-Natta catalyst on the base of nickel and aluminum alkyl halides is discussed. Activity of the Ni(I) in the dimerization of propylene is assumed to proceed through dissociative oxidative addition of propylene and formation of Ni(III) at the first stage of the catalytic cycle.

OP-II-7 Yang Y.C., Zhou Z.H.

Catalytic Conversion of Phenol on Peroxo Edta-Type Titanate

State Key Laboratory for Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China

A series of peroxo pdta and cdta titanates have been isolated and characterized in the solid state and in solution, where hexadentate chelated pdta and cdta titanates(IV) were used as catalytic Ti(IV) species similar to those in constrained environment of TS-1 (H_4cdta = *trans*-1,2-cyclohexanediaminetetraacetic acid, $C_{14}H_{22}O_8N_2$; H_4pdta = 1,2-propanediaminetetraacetic acid, $C_{11}H_{18}O_8N_2$; TS = titanium silicalite). Degradation of thiocyanide and hydroxylation of phenol were monitored by ^{1}H and ^{13}C NMR techniques.

OP-II-8 Zlotin S.G., Kuherenko A.S., Maltsev O.V., Chizhov A.O.

Chiral Ionic Liquid/ESI-MS Methodology as an Efficient Tool for the Study of Transformations of Supported Organocatalysts

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

An efficient approach to the study of deactivation pathways of chiral organocatalysts in asymmetric Michael reactions by modifying original catalysts with ionic-liquid fragments followed by the ESI-MS analysis of recovered catalyst samples has been proposed.

Section III. Mechanisms of Heterogeneous Catalysis

OP-III-1 Sadykov V.A.[1,2], Bobin A.S.[1], Rogov V.A.[1,2], Mezentseva N.V.[1,2], Alikina G.M.[1], Sadovskaya E.M.[1], Glazneva T.S.[1], Mirodatos C.[3], Galvita V.[4], Marin G.B.[4]

Mechanism of CH_4 Dry Reforming on Nanocrystalline Doped Ceria-Zirconia with Supported Pt, Ru, Ni and Ni–Ru

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia
[3]Institut de Recherches sur la catalyse et l'environnement de Lyon, Lyon, France
[4]University of Gent, Gent, Belgium

CH_4 dry reforming mechanism was studied by using combination of transient kinetic methods (including TAP and SSITKA) with microcalorimetry and *in situ* FTIRS. Redox scheme with independent stages of CH_4 and CO_2 activation conjugated by fast oxygen transfer from support to Me-oxide interface was proved.

OP-III-2 Dossumov K.[1], Tungatarova S.A.[2]

The Mechanism of Oxidative Conversion of Methane

[1]Institute of Combustion Problems, Al-Farabi Kazakh National University, Almaty, Kazakhstan
[2]JSC "D.V. Sokolsky Institute of Organic Catalysis and Electrochemistry", Almaty, Kazakhstan

It was determined that the presence of PtRu and NiCu clusters in Pt-Ru and Ni-Cu-Cr catalysts facilitates the interaction of CH_4 with O_2 because of the possible separate adsorption and activation of components in different parts of the cluster: CH_4 - on Pt^o (Ni^o), and O_2 - on Ru^o (Cu^o), and the fact that the exchange and transfer of electrons in the clusters occur at high rates.

OP-III-3 Finocchio E.[1], Specchia S.[2]

Sulphur Ageing Mechanisms on $Pd/BaCeO_3{\cdot}2ZrO_2$ Catalyst for Methane Combustion

[1]Università di Genova, Department of Chemical and Process Engineering, Genova, Italy
[2]Politecnico di Torino, Department of Applied Science and Technology, Torino, Italy

The ageing effect induced by S-compounds on 2% $Pd/BaCeO_3{\cdot}2ZrO_2$ catalysts for CH_4 combustion was studied. Basic characterization, FT-IR studies and catalytic activity tests were performed. Prevailing ageing mechanisms after 500 h resulted in the oxidation of the surface Pd metal particles and surface-bulk sulfates formation, the latter destroying the starting crystallographic structure.

OP-III-4 Masalska A., Grzechowiak J., Jaroszewska K.

Effect of Metal-Support Interaction in Ni/ZSM-5+Al_2O_3 Catalysts on *n*-Paraffins Transformation

Wrocław University of Technology, Faculty of Chemistry, Wrocław, Poland

Examined were catalysts differing in metal-support interactions (controlled by the preparation methods) which influenced the metal-to-acid ratios. The catalysts were characterized by XRD, N_2 sorption, SEM, TEM, NH_3-TPD, PY-IR, TPR, H_2 chemisorption and XPS. Catalyst activity was tested during *n*-hexane conversion.

OP-III-5 Bychkov V.Yu., Tyulenin Yu.P., Firsova A.A., Korchak V.N.

Effect of Carbonization on Dry Methane Reforming over Ni Catalysts

Semenov Institute of Chemical Physics RAS, Moscow, Russia

Effects of carbonization of Ni catalysts on their reactivity and catalytic activity in dry methane reforming have been studied "in situ" using thermogravimetry and mass-spectrometry.

OP-III-6 Lashina E.A.[1,2], Chumakova N.A.[1,2], Kaichev V.V.[1,2], Ustugov V.V.[1], Chumakov G.A.[2,3], Bukhtiyarov V.I.[1,2]

Self-Oscillations in the Methane Oxidation on Ni: Mathematical Modelling

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[2]Novosibirsk State University, Novosibirsk, Russia
[3]Sobolev Institute of Mathematics SB RAS, Novosibirsk, Russia

We consider the mathematical model describing self-oscillations in the methane oxidation on Ni. Taking into account CH_4 dissociative adsorption as well as transformation of the adsorbed oxygen into NiO, we show that the kinetic model predicts the oscillatory behaviour under reaction conditions. Moreover, using the bifurcation theory and numerical methods, we specify the ranges of the inlet partial pressures and initial catalyst temperature, for which non-isothermal self-oscillations occur.

OP-III-7 Cholach A.R., Bulgakov N.N.

A Single Model of Oscillations in the NO+H_2 Reaction on Noble Metals

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Qualitative and quantitative descriptions of oscillatory phenomena are performed within a unified model consisting of two, the permanent and the temporal reaction pathways providing the steady-state and oscillatory mode, respectively. Enormous advantage of the adsorbed nitrogen atoms at the grain boundary over those at perfect terraces in activity of the key NH_{ad} species formation is the driving force of oscillations.

OP-III-8 Zemlyanov D.Y.[1], Klötzer B.[2]

Does the Bulk Matter? Methane and Ethylene Oxidation on Palladium

[1]Purdue University, Birck Nanotechnology Center, West Lafayette, USA
[2]Institut für Physikalische Chemie, Universität Innsbruck, Innsbruck, Austria

According to the traditional understanding, heterogeneous catalytic chemical reactions occur on the surface and the reaction rate mainly depends on a surface composition and a surface structure. However, dissolution of small molecules such as hydrogen, oxygen, carbon might take place and this might result in the changes of electronic and structure property of the surface. As the consequence, catalyst behavior could change. This will demonstrated for methane and ethylene oxidation over palladium. It was found that dissolution of carbon and oxygen could change catalytic activity of palladium, leading to passivation or activation of the catalyst.

OP-III-9 Frenkel A.I.[1,2]

In Situ X-ray Studies of Model and Real Catalysts:
Bridging the Complexity Gap

[1]Physics Department, Yeshiva University, New York, USA
[2]Synchrotron Catalysis Consortium, Brookhaven National Laboratory, Upton, USA

Rational design of catalysts requires understanding of correlations between geometric structure, thermal and electronic properties and their effects on catalytic activity, selectivity and stability. This task calls for a combination of techniques in the same experiment carried out in operando, i.e., when the catalyst is "working". At the synchrotrons, such innovations include combining X-ray absorption and scattering methods, and coupling them to vibrational spectroscopies (IR and Raman). I will describe recent advances at the Synchrotron Catalysis Consortium at Brookhaven National Laboratory, USA, in building instrumentation for operando studies. Examples will include investigation of the CO oxidation and Water Gas Shift reactions by combined techniques. Finally, I will demonstrate the feasibility of conducting experiments by XAS and TEM techniques using the same operando reactor cell for both probes.

OP-III-10 Tsyganenko A.A.

FTIR Spectroscopy in the Studies of Catalytic Reaction Mechanisms

V.A. Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russia

Advances in the studies of the reaction mechanisms, intermediates and the nature of active sites on oxide catalysts and zeolites by means of variable temperature FTIR spectroscopy are considered. The choice of test molecules for acid and basic site characterization, problems of their quantitative measurements, effect of lateral interactions, phenomenon of linkage isomerism, application of isotopic substitution for establishing the structure of surface species are discussed.

OP-III-11 Kaichev V.V., Miller A.V., Prosvirin I.P., Bukhtiyarov V.I.

Decomposition and Oxidation of Methanol on Pt and Pd:
***In situ* XPS and Mass-Spectrometry Study**

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Decomposition and oxidation of methanol on Pt(111) and Pd(111) were examined using *in situ* XPS and TPRS. It was found that even in the presence of oxygen, the methanol decomposition proceeds through two competitive routes: fast dehydrogenation to CO and slow decomposition of methanol via the C-O bond scission.

OP-III-12 Diehl F.[1], Lecocq V.[1], Griboval-Constant A.[2], Khodakov A.Y.[2], Peña D.A.[2]

Different Carbon Species and Deactivation of Alumina Supported Cobalt Fischer-Tropsch Catalysts in Slurry Reactor

[1]IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, Solaize, France
[2]Unité de Catalyse et de Chimie du solide (UCCS) Université de Lille 1, Lille, France

Carbon deposition seems to be one of the major deactivation mechanisms especially in long-term operations. Our work focuses on the identification and characterization of carbon species in cobalt catalyst, which form during FT reaction in a slurry reactor under different operating conditions, and their role in catalyst deactivation.

OP-III-13 Kovtunov K.V.[1,2], Barskiy D.A.[1,2], Zhivonitko V.V.[1,2], Salnikov O.G.[1,2], Khudorozhkov A.K.[3], Bukhtiyarov V.I.[3], Koptyug I.V.[1,2]

Heterogeneous Hydrogenation Reaction Mechanism Evaluation by Using Parahydrogen

[1]International Tomography Center SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia
[3]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

In this work it was shown that it is possible to study heterogeneous hydrogenation reactions catalyzed by immobilized as well as supported metal catalysts by parahydrogen-induced polarization (PHIP) method. The PHIP effects were demonstrated for heterogeneous hydrogenation reactions carried out in both liquid and gas phases and these results constitute the direct confirmation of the mechanism of the hydrogenation reactions.

OP-III-14 Palma V.[1], Castaldo F.[2], Ciambelli P.[1], Iaquaniello G.

Investigation on the Kinetic Behavior of Bio-Ethanol Steam Reforming over Bimetallic Catalysts Supported on Cerium Oxide

[1]Dipartimento di Ingegneria Industriale, Università di Salerno, Fisciano (SA), Italy
[2]Tecnimont KT S.p.A. (Roma), Italy

The performances of ceria supported bimetallic catalysts was investigated in the steam reforming reaction of simulated bio-ethanol in the low temperature range of 300-550°C in terms of activity, selectivity and stability. The products distribution was studied as function of contact time with the objective to identify the reaction behavior.

OP-III-15 Dürr N., Menning N., Petzold T., Drochner A., Vogel H.

Mechanistic Studies on the Selective Oxidation of Acrolein to Acrylic Acid on Mo/V/W-Mixed Oxide Catalysts

Technische Universität Darmstadt, Ernst-Berl-Institut for Technical Chemistry and Macromolecular Science, Darmstadt, Germany

In this work, partial oxidation of acrolein on Mo/V/W-mixed oxides was studied. A deeper insight into the effect of water on the catalytic mechanism could be obtained via transient kinetic methods (e.g. TPReactions, TPRed, TPOx) and especially by isotope exchange methods (SSITKA). Furthermore, the kinetics of the selective acrolein oxidation could be achieved. In particular performing SSITKA and mathematical modelling of the results deliver new insights into the reaction mechanism.

OP-III-18 Piccolo L., Nassreddine S., Geantet C.

Mechanism of Tetralin Ring Opening and Ring Contraction over Bifunctional Ir/SiO_2-Al_2O_3 Catalysts

Institut de Recherches sur la Catalyse et l'environnement de Lyon (IRCELYON), Villeurbanne, France

In the context of gas oil upgrading *via* selective ring opening, we have investigated the hydroconversion of tetralin over iridium nanoparticles supported on amorphous silica-alumina. This reaction leads to hydrogenation, ring contraction, and ring opening products. From the combination of catalytic tests at variable conversion and products identification by two-dimensional gas chromatography, a bifunctional mechanistic reaction scheme involving both metal and Brönsted acid sites has been established.

OP-III-19 Mierczynski P.[1], Vasilev K.[2], Vasilev A.[2], Maniecki T.P.[1]

Comparative Studies of Pd, Ru, Ni and Cu Supported $ZnAl_2O_4$ Catalysts Used for Hydrogen Production from Methanol Steam Reforming

[1]Lodz University of Technology, Lodz, Poland
[2]University of South Australia, Mawson Lakes Adelaide, South Australia

The main goals of this study is to correlate the physicochemical properties of $M/ZnAl_2O_4$ (M = Cu, Pd, Ru, Ni) catalysts with their activity in steam reforming of methanol reaction. To achieve the aims of this work, we prepared various monometallic catalysts by conventional impregnation method. The physicochemical properties of the catalysts were examined by BET, XRD, TPD-NH_3, TPR-H_2, XPS and chemisorption methods. The results of these characterizations were correlated with steam reforming of methanol (SRM) catalytic properties. Catalytic activity tests in SRM reaction were carried out under atmospheric pressure in the temperature range 120-420 °C using a flow quartz microreactor.

OP-III-20 Yamazaki H., Imai H., Yokoi T., Kondo J.N., Tatsumi T.

Reactivity of Methoxy Species in the Methanol to Olefin Reactions over H-ZSM-5

Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, Japan

We have closely investigated the reactivity of methoxy species on H-ZSM-5 by IR spectroscopy using isotopes, finding the promotional effect of methoxy species on the C_2H_4 reaction on H-ZSM-5 to produce C_3H_6. The isotope experiments suggested a concerted mechanism involving carbene-like species. Furthermore, the reaction of methoxy species with dimethyl ether is faster than that with C_2H_4 or methanol; dimethyl ether looks like a key intermediate in the methanol-to-olefin reaction over H-ZSM-5.

OP-III-21 Mishakov I.V.[1,2], Bauman Yu.I.[1], Vedyagin A.A.[1,2]

Dechlorination of Chlorohydrocarbons on Bulk Ni-Alloyed Catalysts: Mechanism of Carbon “Corrosion”

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State Technical University, Novosibirsk, Russia

This work describes the spontaneous in situ formation of the catalytic particles during the decomposition of chlorohydrocarbons on bulk Ni-based alloys used as precursors. These particles are characterized with an optimal chemical composition and size and act as sites for carbon nanofibers growth. The interaction mechanism resulting in formation of high-performance self-organizing catalyst will be discussed.

OP-III-22 Mahendran S., Selvam P.
Dehydration of Glycerol over Heteropoly Acid Supported Mesoporous Silica
National Centre for Catalysis Research, Department of Chemistry,
Indian Institute of Technology Madras, Chennai, India

In this work, a series of silicotungstic acid supported ordered mesoporous silica catalysts, designated as H-SiW/SBA-15, were tested for the dehydration reaction of glycerol. Among the different H-SiW loading (10-40 wt %), the one based on 30 wt. % showed higher activity in terms of glycerol conversion (> 99 %) and acrolein selectivity (~ 95%).

OP-III-23 Smirnov M.Yu., Kalinkin A.V., Vovk E.I., Pashis A.V., Bukhtiyarov V.I.
Application of Model Systems for XPS Studies of the Mechanism of Interaction of Supported Metal Catalysts with Gaseous Reaction Media
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

In this work, surface species formed under the reactions of model PGM catalysts supported on Al_2O_3, SiO_2 and CeO_2 with NO_x and SO_x are identified by XPS. The effect of the $CO+O_2$ reaction on the size of Au nanoparticles supported on Al_2O_3 and Fe_2O_3 is studied by XPS and TEM as well.

OP-III-24 Vedyagin A.A.[1,2], Gavrilov M.S.[1], Volodin A.M.[1], Stoyanovskii V.O.[1], Slavinskaya E.M.[1], Mishakov I.V.[1,2], Shubin Yu.V.[3]
Catalytic Purification of Exhaust Gases over Pd-Rh Alloy Catalysts:
From Mechanism Understanding to High Temperature Stability
[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State Technical University, Novosibirsk, Russia
[3]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

This work elucidates the main factors leading to deactivation of three-way Pd-Rh catalysts. Rhodium can readily diffuse from a surface inside the bulk of support (Al_2O_3) therefore initiating the phase transformation of the latter into α-Al_2O_3 where Rh ions become irreversibly encapsulated. The high temperature treatment of disperse Pd particles results in their significant sintering. Novel approach to catalyst stabilization based on the understanding of deactivation mechanism will be presented.

OP-III-25 Say Z.[1], Vovk E.I.[1,2], Bukhtiyarov V.I.[2], Özensoy E.[1]
Ce-O-Pt Active Sites in Ceria Promoted NO_x Storage Reduction Catalysis
[1]Department of Chemistry, Bilkent University, Ankara, Turkey
[2]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Influence of ceria on the NO_x storage and reduction behavior of NSR catalysts were investigated on Ba/Pt/Ce/Al. A strong metal support interaction (SMSI) between Pt sites and the $BaO/BaO_2/CeO_x/CeO_2$, domains were observed leading to a complex redox interplay including oxidation of the precious metal sites, reduction of ceria, formation of BaO_2 species as well as the formation of Pt-O-Ce interfacial sites on the 20Ba/Pt/20Ce/Al surface which seem to have a vital role in the NO_x storage and reduction chemistry.

OP-III-26 Gandarias I., Fernández S.G., Requies J., Arias P.L.

Influence of the Hydrogen Source in the Mechanism of Glycerol Hydrogenolysis to 1,2-Propanediol

University of the Basque Country (UPV/EHU), Bilbao, Spain

In most of literature works referred to glycerol hydrogenolysis, the latter is conducted under molecular hydrogen (H_2) atmosphere, which has some important drawbacks. In this presentation an alternative is presented: in situ generate the required hydrogen using hydrogen donors. The results obtained with in-situ generated hydrogen over Ni-Cu/Al_2O_3 catalyst are highly promising. A kinetic study performed revealed that the OH groups of glycerol and of the target product, 1,2-PDO, compete for adsorption on the acid sites of the Al_2O_3.

OP-III-27 Gabrienko A.A., Stepanov A.G.

Structure of Allylic Intermediates Formed from Olefins on Zinc Oxide

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Dissociative adsorption of propene on zinc oxide results in the formation of two equilibrium structures: σ,π-allyl and π-allyl, the former being a prevailing species. On the other hand, only σ,π-allyl was detected in case of *n*-butene adsorption.

OP-III-28 Bruk L.G.[1], Titov D.N.[1], Zubavichus Ya.V.[2], Tkachenko O.P.[3], Ustyugov A.V.[1], Oshanina I.V.[1], Veligzhanin A.A.[2], Kustov L.M.[3], Temkin O.N.[1]

Mechanism of Low-Temperature Carbon Monoxide Oxidation over $PdCl_2$-$CuCl_2$/γ-Al_2O_3 Catalyst

[1]Lomonosov Moscow University of Fine Chemical Technology, Moscow, Russia
[2]National Research Center "Kurchatov Institute", Moscow, Russia
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The state of the active constituents of the $PdCl_2$–$CuCl_2$/γ-Al_2O_3 catalyst for the low-temperature oxidation of the carbon monoxide by molecular oxygen was studied by XAS, XRD, SEM, and DRIFTS techniques. The kinetics of carbon monoxide oxidation with atmospheric oxygen on this catalyst was studied at T=27°C and a N_2–O_2–CO mixture pressure of 1 atm. A number of mechanistic hypotheses are discussed.

OP-III-29 Tálas E.[1], Margitfalvi J.L.[2]

Enantioselective Hydrogenation of Activated Ketones in the Presence of Pt-Cinchona Catalysts. Is the Proton Transfer Concept Valid?

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[2]Combitech-Nanotech Kft., Budapest, Hungary

In this contribution experimental evidences related to the proposed hydrogen (proton) transfer in the catalytic system Pt-Cinchona alkaloids used in the enantioselective hydrogenation of activated ketones were collected and analyzed. The analysis and new experimental results indicate that direct transfer of hydrogen (proton) from platinum to the substrate with the involvement of quinuclidine nitrogen can be questioned.

OP-III-30 Jacquemin M., Hauwaert D., Gaigneaux E.M.

Mechanistic and Kinetic Studies of Aromatic Carbon-Carbon Coupling (Suzuki Reaction) with Heterogeneous Catalysts

Institute of Condensed Matter and Nanosciences – IMCN,
Division "MOlecules, Solids and reactiviTy - MOST, Université Catholique de Louvain (UCL), Louvain-la-Neuve, Belgium

An experimental reaction rate expression of the Suzuki coupling has been determined by varying the concentration of the reactants and the reaction temperature. A theoretical rate expression has been also determined by making assumptions of the reaction pathway with a heterogeneous catalyst. By comparing these expressions, we were able to identify that the rate limiting step of the Suzuki coupling is the transmetallation of the phenylboronic acid on a intermediate species formed by the adsorption of the 4-bromotoluene onto the Pd.

OP-III-31 Kuznetsova N.I.[1], Trebushat D.V.[1], Kuznetsova L.I.[1], Zudin V.N.[1], Kajitani H.[2], Utsunomiya M.[2], Takahashi K.[2]

On Mechanisms of Oxidation of 1,3-Butadiene on Pd-Te Catalysts in Polar Solvents

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Mitsubishi Chemical Corporation, Okayama, Japan

Oxidation of 1,3-butadiene with molecular oxygen on supported Pd-Te catalysts in various organic polar media have been studied. We followed the oxidation peculiarities, products and mechanism depending on the reaction conditions.

OP-III-32 Zolotarev Yu.A.[1], Dadayan A.K.[1], Borisov Yu.A.[2], Nazimov I.V.[3], Vaskovsky B.V.[3], Myasoedov N.F.[1]

Solid State Isotope Exchange with Spillover Hydrogen in Organic Compounds

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[2]Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia
[3]Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry RAS, Moscow, Russia

This report summarizes data on the theoretical and experimental investigation of high temperature solid state catalytic isotope exchange (HSCIE) that takes place in organic compounds under the action of spillover hydrogen. The new one-center synchronous mechanism of hydrogen substitution in organic compounds has been studied. Kinetic isotope effect of solid state reaction of hydrogen exchange with SH is 1.2 – 1.4.

Section IV. Catalytic Processing of Renewables

OP-IV-1 Kuznetsov B.N.[1,2], Sudakova I.G.[1], Garyntseva N.V.[1], Djakovitch L.[3], Pinel C.[3]

Kinetic Study of Aspen-Wood Delignification by H_2O_2 with Sulfuric Acid Catalyst under Mild Conditions

[1]Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
[2]Siberian Federal University, Krasnoyarsk, Russia
[3]Institut de Recherches sur la Catalyse et l'Environnement de Lyon (IRCELYON), Lyon, France

Kinetic study of aspen-wood delignification by H_2O_2 with sulfuric acid catalyst under mild conditions is reported.

OP-IV-3 Berlier G.[1], Gopalakrishnan S.[1,2], Miletto I.[1], Coluccia S.[1,2], Caputo G.[3], Giaconia A.[3], Sau S.[3]

Unravelling the Structure and Reactivity of Supported Ni Particles in Ni-$CeZrO_2$ Catalysts

[1]Università degli Studi di Torino, Department of Chemistry and NIS Centre of Excellence, Torino, Italy
[2]ISTEC, Centro Nazionale delle Ricerche, Torino, Italy
[3]ENEA, "Casaccia" Research Center, Rome, Italy

The talk deals with Ni-$CeZrO_2$ catalysts, synthesized, characterized and tested for the low temperature methane steam reforming, with potential application in solar powered plants based on molten salt technology. Structural and surface properties of the samples were characterized, with particular focus on Ni particles morphology and redox behaviour. Catalytic tests showed good activity and stability also at low steam to carbon ratio.

OP-IV-4 Zaytseva Yu.A., Simonov M.N., Simakova I.L., Shutilov A.A., Zenkovets G.A.

Ketonization of Valeric Acid over Metal Oxides as a First Step for Green Diesel Synthesis: Consideration from Mechanistic Viewpoint

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

The ketonization of valeric acid and selectivity to 5-nonanone were investigated over ZrO_2, CeO_2, MgO, Al_2O_3, CeO_2/ZrO_2 at T= 573÷673 K. Methods of TEM, XRD, BET and XPS were applied to find correlation between structure of catalyst active component and its activity in order to elucidate the ketonization mechanism.

Section V. Electrocatalysis, Photocatalysis, Biocatalysis

OP-V-1 Borbáth I., Gubán D., Pászti Z., Sajó I., Tompos A.

Controlled Synthesis of Pt_3Sn/C Electrocatalysts with Exclusive Sn-Pt Interaction Designed for Use in Direct Methanol Fuel Cells

Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Budapest, Hungary

Upon tuning the conditions of Controlled Surface Reactions the exclusive formation of the desired Pt_3Sn (fcc) alloy phase over carbon support can be achieved. The bimetallic Pt_3Sn/C catalysts thus prepared displayed an outstanding performance in both the CO and methanol electrooxidation reactions.

OP-V-2 Shishido T.[1], Furukawa S.[1], Ohno Y.[1], Teramura K.[1,2], Tanaka T.[1]

Reaction Mechanism of Selective Oxidation of Alcohols and Amines over Semiconductor Photocatalysts

[1]Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyoto, Japan

[2]Precursory Research for Embryonic Science and Technology (PRESTO), Japan Science and Technology Agency (JST), Saitama, Japan

We investigated the reaction mechanisms of the photooxidation of alcohols and amines over Nb_2O_5 and revealed the reaction mechanisms of photooxidation of alcohols, and amines and that the surface complex consisting of adsorbed molecule and catalyst plays an important role in the photo-activation step. The effective wavelength is shifted to a longer wavelength by the formation of donor level derived from adsorbed molecule during a chemical reaction.

OP-V-3 Sannino D., Vaiano V., Ciambelli P.

RuO_x-VO_x/TiO_2 as Very Highly Selective Photocatalysts for the Oxidative Dehydrogenation of Ethanol to Acetaldehyde

Department of Industrial Engineering, University of Salerno, Fisciano, Italy

The gas-solid photocatalytic partial oxidation of ethanol to acetaldehyde on monometallic RuO_x/TiO_2 and bimetallic RuO_x-VO_x/TiO_2 catalysts has been studied in a fluidized bed photoreactor at high illumination efficiency. For RuO_x/TiO_2, by increasing ruthenium loading ethanol conversion decreased while acetaldehyde selectivity increased. With bimetallic RuO_x-VO_x/TiO_2 the highly selective yield to acetaldehyde of monometallic Ru based catalysts was enhanced by the highly active V species, reaching complete conversion of ethanol.

OP-V-4 Kozlova E.A.[1], Kozhevnikova N.S.[2], Lemke A.A.[2], Cherepanova S.V.[1], Lyubina T.P.[1], Gerasimov E.Yu.[1], Tsybulya S.V.[1], Shchipunov Yu.A.[3], Remplel A.A.[2]

Design of the Nanocrystalline CdS/TiO_2 Photocatalyst

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Institute of Solid State Chemistry UB RAS, Yekaterinburg, Russia
[3]Institute of Chemistry FEB RAS, Vladivostok, Russia

Catalysts active under visible light on the basis of the composite of cadmium sulfide and titania CdS/TiO_2 were obtained in an aqueous medium by a two-stage process. The highest photocatalytic activity in ethanol oxidation under visible light was exhibited by the samples obtained from solutions of ammine and citrate cadmium complexes.

ORAL PRESENTATIONS OF YOUNG SCIENTISTS

OY-I-1 Ratmanova N.K.[1], Mukhamedzyanova D.F.[1], Pichugina D.A.[1,2], Kuz'menko N.E.[1]

The Theoretical Prediction of Structural and Electronic Effects of Gold-Based Systems in Selective Alkynes Activation

[1]Lomonosov Moscow State University, Moscow, Russia
[2]Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia

The activation of C=C and C≡C bonds is a key step in the reactions of hydrocarbons conversion. The adsorption of ethylene and acetylene onto Au_{12} cluster is accompanied by the formation of complexes, where the hydrocarbon is bonded with low-coordinated atoms of the cluster. The preferable adsorption of C_2H_2 over C_2H_4 on 3D isomer of Au_{12} cluster was found out based on the calculated adsorption heats. It was shown that charge effect is more apparent than structural effect in hydrocarbons adsorption. Both C_2H_2 and C_2H_4 adsorb physically on the MgO(100) surface.

OY-II-1 Bocharova V.V., Kraikivskii P.B., Saraev V.V.

The Role of Monovalent Nickel in Metalcomplex Catalysis

Federal State Budget Institution of Higher Education "Irkutsk State University", Irkutsk, Russia

It is shown that the counter-disproportionation reaction occurs at the joint presence of Ni(0) and Ni(II) in the system, to form complexes of Ni(I). Metallocyclic mechanism of polymerization of norbornene involving Ni(I) and Ni(III) complexes is proposed.

OY-II-2 Lyakin O.Y.[1], Ottenbacher R.V.[1,2], Bryliakov K.P.[1], Talsi E.P.[1]

Non-Heme Iron and Manganese-Catalyzed Asymmetric Olefin Epoxidations with H_2O_2: Probing the Nature of Active Species by EPR Spectroscopic and Enantioselectivity Studies

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia

Chiral bipyrrolidine-pyridine-based Fe and Mn complexes have been found to efficiently catalyze olefin epoxidation with H_2O_2 in the presence of carboxylic acids with up to 93% enantioselectivity (*ee*). The *ee* rises with rising steric bulk of the acid. The nature of active epoxidizing species has been probed by EPR and enantioselectivity studies, and they were assigned to $[(L)M^V{=}O(OC(O)R)]^{2+}$ complexes (M = Fe, Mn; R = alkyl). A consistent mechanism for the active species formation has been proposed.

OY-II-3 Ottenbacher R.V.[1,2], Talsi E.P.[1], Bryliakov K.P.[1]

Highly Efficient, Regioselective and Stereospecific Oxidation of Non-Activated Aliphatic C-H Groups with H_2O_2, Catalyzed by Aminopyridine Manganese Complexes

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia

Manganese(II) complexes $[LMn^{II}(OTf)_2]$ bearing non-heme tetradentate aminopyridine ligands catalyse the oxidation of non-activated aliphatic C-H groups with H_2O_2 in the presence of acetic acid, demonstrating excellent efficiency (up to 970 TON), site-selectivity and stereospecificity (up to > 99 %).

OY-II-4 Ivancheva N.I.[1], Sanieva D.V.[1], Molev O.V.[1], Fedorov S.P.[1], Oleinik I.V.[2], Ivanchev S.S.[1]

Self-Immobilizing Catalysts for Ethylene Polymerization Based on Derivatives of bis(Phenoxy-Imine) Titanium Halide Complexes

[1]St. Petersburg Department of Boreskov Institute of Catalysis SB RAS,
St. Petersburg, Russia
[2]Vorozhtzov Institute of Organic Chemistry SB RAS, Novosibirsk, Russia

The catalysis features and ethylene polymerization mechanism depending on the structure are studied for the bis(phenoxy-imine) titanium (IV) chloride complexes functionalized with an oxyallyl group containing different number of CH_2 units located in the para- or meta-position in the phenyl ring relating to the imine nitrogen and different substituents in the phenoxy-group. The characterized catalyst systems feature significant activity and can be effectively applied in the production of polyethylenes for various purposes.

OY-II-5 Tarkhanova I.G., Gantman M.G., Zelikman V.M.

Radical Processes Catalysed by Transition Metal Complexes with Grafted Ionic Liquids

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

Catalysts of two environmentally important processes (thiols oxidative coupling and C-H C-Cl bonds metathesis) have been obtained and characterized. The catalysts are copper complexes with immobilized ionic liquids. The main factors influencing the catalytic activity have been determined.

OY-II-6 Kozhevnikov I.V.[1,2], Chibiryaev A.M.[2,3], Nuzhdin A.L.[1], Bukhtiyarova G.A.[1], Martyanov O.N.[1,2]

Catalytic Effect of Si-Containing Compounds on the C-Methylation of Indole in *sc*-MeOH

[1]Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia
[3]Vorozhtsov Institute of Organic Chemistry, SB RAS, Novosibirsk, Russia

Biomass-derived oxygenates are attractive as renewable raw materials for the production of value-added chemicals and biofuel components. For fuel applications, they require reduction in their oxygen content, i.e., deoxygenation. Here various reaction pathways of (hydro)deoxygenation of carboxylic acids and ketones in the gas phase over multifunctional catalysts based on polyoxometalates (POMs) are discussed. Amongst the substrates are C3-C6 carboxylic acids, representing the carboxylic acids derived from carbohydrate feedctocks, and methylisobutyl and diisobutyl ketones obtained by condensation of acetone, the byproduct of biobutanol production.

OY-III-I Gabrienko A.A., Arzumanov S.S., Stepanov A.G.

Methane Activation and Conversion on Ag/H-MFI Catalyst

Boreskov Institute of Catalysis, SB RAS, Novosibirsk, Russia

Methoxy species have been observed as surface intermediates of methane conversion to aromatics on Ag/H-MFI by ^{13}C CP/MAS NMR. Mechanism of methane-to-aromatic conversion on Ag-modified catalyst has been suggested.

OY-III-2 Meemken F., Maeda N., Hungerbühler K., Baiker A.

Platinum-Catalyzed Asymmetric Hydrogenation: Spectroscopic Evidence for O-H-O Hydrogen Bond Interaction between Substrate and Modifier

Department of Chemistry and Applied Bioscience, ETH Zürich, Switzerland

Using in situ attenuated total reflection infrared (ATR-IR) spectroscopy in combination with modulation excitation spectroscopy and phase-sensitive detection we uncovered a new hydrogen bonding between ketopantolactone and modifier on the Pt-surface, i.e. C9-O··H··O=C which so far has been overlooked in the literature.

OY-III-3 Kavalerskaya N.E., Rostovchshikova T.N., Lokteva E.S., Golubina E.V., Maslakov K.I.

Unusually Active Nanostructured Ni Catalysts with Low Metal Coverage for Chlorobenzene Hydrodechlorination

Lomonosov Moscow State University, Moscow, Russia

Laser electrodispersion technique was used for preparation of nanostructured Ni catalysts containing highly uniform (about 2 nm) metal particles on Sibunit and Al_2O_3. Catalysts with extremely low metal loadings were unusually active in the hydrodechlorination of chlorobenzene at 250-350 °C in the gas-phase flow type system. Such activity could be explained in terms of charge transfer between the closely situated Ni particles or between the Ni particle and support.

OY-III-4 Kazantsev M.S.[1], Luzgin M.V.[1,2], Volkova G.G.[1], Stepanov A.G.[1,2]

Carbonylation of Dimethyl Ether on $Rh/Cs_2HPW_{12}O_{40}$: Mechanism of the Reaction in the Presence of Methyl Iodide Promoter

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Department of Natural Sciences, Novosibirsk State University, Novosibirsk, Russia

Using ^{13}C solid-state NMR the surface methoxy-group and Rh-carbonyl have been shown to be the main intermediates of the reaction. The use of methyl iodide promoter decreases the reaction temperature due to opening new reaction pathway *via* Rh-methyl and Rh-acetyl intermediates.

OY-III-5 Khudorozhkov A.K., Prosvirin I.P., Bukhtiyarov V.I.

Studying the Influence of Precursor and Promoter on the Activity and Stability of Methane Combustion Catalysts

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

This report is devoted to the problem of palladium on alumina catalysts low stability in the methane full oxidation reaction. One of the ways to increase the tolerance of palladium to the water vapor is reviewed. This method consists in some metal oxides addition to the catalyst composition in order to change the palladium charge state, thereby changing catalyst stability. It is shown that nickel or cobalt oxides addition leads to the increase of catalyst activity, whereas platinum oxide addition leads to the increase of both catalyst activity and stability. Some assumptions about the role of Pt, Co and Ni oxides in the palladium catalytic properties changing are made.

OY-III-6 Pakharukov I.Yu.[1,2], Matrosova M.M.[1], Bukhtiyarov V.I.[1,2], Parmon V.N.[1,2]

Concentration Hysteresis in the Oxidation of Methane over $Pt/\gamma\text{-}Al_2O_3$

[1]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
[2]Novosibirsk State University, Novosibirsk, Russia

It was found that there are two stable stationary states of the catalytic system with low and high catalytic activity, which are realized at the same external conditions depending on the direction of change of O_2:CH_4 ratio from fuel-lean to fuel-rich.

OY-IV-3 Simakova O.A.[1, 2], Murzina E.V.[1], Leino A.-R.[3], Mäki-Arvela P.[1], Willför S.M.[4], Murzin D.Yu.[1]

Biomass Derived Lignan Hydroxymatairesinol Selective Oxidation over Au Catalysts

[1]Laboratory of Industrial Chemistry and Reaction Engineering, Process Chemistry Centre, Åbo Akademi University, Åbo/Turku, Finland
[2]Graduate School of Chemical Engineering, Åbo Akademi University, Åbo/Turku, Finland
[3]Microelectronics and Materials Physics Laboratories, EMPART Research Group of Infotech Oulu, University of Oulu, Oulu, Finland
[4]Laboratory of Wood and Paper Chemistry, Process Chemistry Centre, Åbo Akademi University, Åbo/Turku, Finland

The liquid-phase aerobic oxidation of the biomass-derived lignan hydroxymatairesinol (HMR) was studied. The reaction product is another lignan oxomatairesinol (oxoMAT), which can be applied as an active component in the pharmaceutical, textile and cosmetic industry. Gold catalysts have demonstrated a complete selectivity towards oxomatairesinol. The dependence of oxoMAT yield on the reaction parameters, as well as reaction kinetics and catalyst deactivation was investigated.

OY-IV-4 Chistyakov A.V., Murzin V.Yu., Gubanov M.A., Chudakova M.V., Yandieva F.A., Tsodikov M.V.

Direct Catalytic Treatment of Biomass Substrates Towards Hydrocarbon Fuel Components

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

Current paper presents the results concerning to development of nanosized heterometallic catalysts suitable for primary biomass products direct treatment towards fuels and chemicals. The genesis of the most active and stable nanosized catalytic systems was studied. Active clusters structure effect on considering reactions pathways and selectivity is under discussion.

OY-IV-7 Bykova M.V., Ermakov D.Yu., Kaichev V.V., Smirnov A.A., Yakovlev V.A.

Novel Catalysts for Bio-Fuels Production from Biomass Fast Pyrolysis Oils

Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

A new type of non-sulfided Ni-based catalysts for fast pyrolysis oil hydrotreatment (HDO) has been proposed. The catalysts produced by sol-gel technique were tested in HDO of model compound guaiacol and characterized by a number of physicochemical methods.

OY-V-2 Cherepanov P.V.[1], Skorb E.V.[2], Andreeva D.V.[1]

Ultrasonically Designed Metal / Polypyrrole Composite Catalysts for Fuel Cells

[1]University of Bayreuth, Bayreuth, Germany
[2]Max Plank Institute of Colloids and Interfaces, Potsdam, Germany

Investigation of electrochemical properties of mesoporous materials, namely metal (aluminum /cobalt and aluminum/cobalt and iron alloys) polypyrrole composite systems, prepared by electrochemical deposition of polymer (polypyrrole) on ultrasonically modified metal alloy surface, is reported.

OY-V-3 Oschepkov A.G.[1,2], Simonov A.N.[1], Rudina N.A.[1], Parmon V.N.[1,2]

Microstructure Effects in Catalysis of Oxygen Reduction Reaction over Electrodeposited Platinum: Influence of Intergrain Boundaries

[1]Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
[2]Novosibirsk State University (Novosibirsk), Russia

Activity of electrocatalysts is known to be strongly influenced by the presence of defects in their structure. Electrodeposition is one of the most efficient methods for the preparation of defective catalysts. We demonstrate, for the first time, the enhanced activity of electrodeposited Pt catalysts with high concentration of defective intergrain boundaries for the O_2 electroreduction.