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

UNDER THE AUSPICES of the European Federation of Catalysis Societies

FINANCIAL SUPPORT:

Russian Foundation for Basic Research, Moscow

OFFICIAL CONFERENCE SPONSOR:

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Information Supports, Journals:

«Kinetics and Catalysis»,  
«Catalysis in Industry»,  
«Supercritical Fluids: Theory and Practice»,  
«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).


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!

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Chairman,
Valentin N. Parmon,
Boreskov Institute of Catalysis
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O. V. Turova
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

<table>
<thead>
<tr>
<th>Oct., 21, Sunday</th>
<th>October 22, Monday</th>
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<tr>
<td>09.00 Registration</td>
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<tr>
<td>09.40 Summit hall</td>
<td>Conference Welcome, Parmon</td>
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<td></td>
<td>Chairmen: Bukhtiyarov, van Santen</td>
</tr>
<tr>
<td>10.00 PL-1 Bell</td>
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<tr>
<td>10.40 Coffee</td>
<td>Chairmen: Stakheev, Rupprechter</td>
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<tr>
<td>11.10 PL-2 Parmon</td>
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<tr>
<td>11.50 KL-1 van Santen</td>
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<tr>
<td>12.20 KL-2 Neyman</td>
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<tr>
<td>12.50 Lunch</td>
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<tr>
<td><strong>Registration 15.00-19.00</strong></td>
<td><strong>Summit hall</strong></td>
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<tr>
<td>Azimut hotel</td>
<td>Chairmen: Talsi, Selvam</td>
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<tr>
<td>14.30 KL-3 Ueda</td>
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<tr>
<td>15.00 Bukhtiyarov</td>
<td>(memory lecture Ipatieff)</td>
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<tr>
<td>15.20 Official sponsor SIBUR holding</td>
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<tr>
<td>15.50 Coffee</td>
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<tr>
<td><strong>Summit hall</strong></td>
<td><strong>Forum hall</strong></td>
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<tr>
<td>Chairmen: Ismayilov, Ueda</td>
<td>Chairmen: Neyman, Frenkel</td>
</tr>
<tr>
<td>16.20 OP-III-1 Sadykov</td>
<td>OP-I-1 Stakheev</td>
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<tr>
<td>16.40 OP-III-2 Dossumov</td>
<td>OP-I-2 Rösch</td>
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<tr>
<td>17.00 OP-III-3 Specchia</td>
<td>OP-I-3 Nasluzov</td>
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<tr>
<td>17.20 OP-III-4 Masalska</td>
<td>OP-I-4 Pichugina</td>
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<tr>
<td>17.40 OP-III-5 Bychkov</td>
<td>OP-I-5 Andrikopoulos</td>
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<td>18.00 OP-III-6 Lashina</td>
<td>OP-I-6 Gurevich</td>
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<tr>
<td>18.20 OP-III-7 Cholach</td>
<td>OP-I-7 Startsev</td>
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<tr>
<td>19.00 Welcome Party, Sovetskii hall (Azimut hotel)</td>
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<td>Time</td>
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<tr>
<td>09.00</td>
<td>PL-3 Que, Jr.</td>
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<tr>
<td>09.40</td>
<td>KL-4 Murzin</td>
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<tr>
<td>10.10</td>
<td>KL-5 Rupprechter</td>
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<tr>
<td>10.40</td>
<td>Coffee</td>
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<tr>
<td>11.10</td>
<td>OP-III-8 Zemlianov</td>
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<td>11.30</td>
<td>OP-III-9 Frenkel</td>
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<td>11.50</td>
<td>OP-III-10 Tsyganenko</td>
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<tr>
<td>12.10</td>
<td>OP-III-11 Kaichev</td>
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<td>12.30</td>
<td>OP-III-12 Pêna</td>
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<td>12.50</td>
<td>OP-III-13 Kovtunov</td>
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<tr>
<td>13.10</td>
<td>Lunch</td>
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<tr>
<td>14.30</td>
<td>OP-III-14 Palma</td>
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<td>14.50</td>
<td>OP-III-15 Dürr</td>
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<td>15.10</td>
<td>OP-III-16 Mishra</td>
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<td>15.30</td>
<td>OY-III-1 Gabrienko</td>
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<tr>
<td>15.40</td>
<td>OY-III-2 Meemken</td>
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<tr>
<td>15.50</td>
<td>OY-III-3 Kavalerskay</td>
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<tr>
<td>16.00</td>
<td>OY-III-4 Kazantsev</td>
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<tr>
<td>16.10</td>
<td>OY-III-5 Khudorozhkov</td>
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<tr>
<td>16.20</td>
<td>OY-III-6 Pakharukov</td>
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<tr>
<td>16.30</td>
<td>Coffee</td>
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<tr>
<td>17.00</td>
<td>Assambleya hall - POSTER SESSION</td>
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<td>– hanging of posters</td>
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<tr>
<td>17.00</td>
<td>– discussion</td>
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**TIMETABLE**

**October 24, Wednesday**

<table>
<thead>
<tr>
<th>Time</th>
<th>Summit hall</th>
<th>Forum hall</th>
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<tbody>
<tr>
<td></td>
<td>Chairmen: Margitfalvi, Masalska</td>
<td>Chairmen: Bryliakov, Palma</td>
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<tr>
<td>09.00</td>
<td>PL-4 Fokin</td>
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<td>09.40</td>
<td>KL-6 Özensoy</td>
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<td>10.10</td>
<td>KL-7 Ananikov</td>
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<tr>
<td>10.40</td>
<td><strong>Coffee</strong></td>
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<tr>
<td>11.10</td>
<td>Assambleya hall</td>
<td>Forum hall</td>
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<tr>
<td></td>
<td>Chairman: Sadykov, Dossumov</td>
<td>Chairmen: Bryliakov, Palma</td>
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<tr>
<td>11.10</td>
<td>OP-III-17 Lokteva</td>
<td>OP-V-1 Tompos</td>
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<tr>
<td>11.30</td>
<td>OP-III-18 Piccolo</td>
<td>OP-V-2 Shishido</td>
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<tr>
<td>11.50</td>
<td>OP-III-19 Mierzinski</td>
<td>OP-V-3 Saninno</td>
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<tr>
<td>12.10</td>
<td>OP-III-20 Tatsumi</td>
<td>OP-V-4 Kozlova</td>
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<tr>
<td>12.30</td>
<td>OP-III-21 Mishakov</td>
<td><strong>Sponsor -2- Donau lab</strong></td>
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<tr>
<td>12.50</td>
<td>OP-III-22 Selvam</td>
<td><strong>Sponsor-3- Promenergolab</strong></td>
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<tr>
<td>13.10</td>
<td><strong>Lunch</strong></td>
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<tr>
<td>14.30</td>
<td>Assambleya hall</td>
<td>Forum hall</td>
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<tr>
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<td>Chairman: Lokteva, Tatsumi</td>
<td>Chairmen: Kovtunov, Startsev</td>
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<tr>
<td>14.30</td>
<td>OP-III-23 Smirnov</td>
<td>OY-IV-1 Snytnikov P.</td>
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<td>14.50</td>
<td>OP-III-24 Gavrilov</td>
<td>OY-IV-3 Simakova</td>
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<td>15.10</td>
<td>OP-III-25 Vovk</td>
<td>OY-IV-4 Chistyakov</td>
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<td>15.30</td>
<td>OP-III-26 Requies</td>
<td>OY-IV-7 Bykova</td>
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<tr>
<td>15.50</td>
<td>OP-III-27 Stepanov</td>
<td>OY-IV-1 Tasseroul</td>
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<td>16.10</td>
<td>OP-III-28 Bruk</td>
<td>OY-V-2 Cherepanov</td>
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<td>OY-V-4 Maniecki</td>
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<td>OY-IV-2 Skobelev</td>
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<tr>
<td>16.30</td>
<td><strong>Coffee</strong></td>
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<tr>
<td>17.00</td>
<td>Assambleya hall</td>
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<td></td>
<td>Chairman: Tsyganov, Martyanov</td>
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<tr>
<td>17.00</td>
<td>RFBR Round-table (in Russian)</td>
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<td>18.00</td>
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<tr>
<td>19.00</td>
<td><strong>Banquet, restaurant Troika</strong></td>
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<tr>
<td>Time</td>
<td>Assambleya hall</td>
<td>Forum hall</td>
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<tr>
<td>09.00</td>
<td>Summit hall</td>
<td>PL-5 Kondratenko</td>
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<td>09.40</td>
<td>Summit hall</td>
<td>KL-8 Costas</td>
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<tr>
<td>10.10</td>
<td>Assambleya hall</td>
<td>KL-9 Talsi</td>
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<tr>
<td>10.40</td>
<td>Assambleya hall</td>
<td>Coffee</td>
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<tr>
<td>11.10</td>
<td>Assambleya hall</td>
<td>OP-III-29 Margitfalvi</td>
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<tr>
<td>11.30</td>
<td>Assambleya hall</td>
<td>OP-III-30 Jacquemin</td>
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<tr>
<td>11.50</td>
<td>Assambleya hall</td>
<td>OP-III-31 Kuznetsova L.</td>
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<tr>
<td>12.10</td>
<td>Assambleya hall</td>
<td>OP-III-32 Zolutarev</td>
</tr>
<tr>
<td>12.30</td>
<td>Assambleya hall</td>
<td>Closing</td>
</tr>
<tr>
<td>13.00</td>
<td>Assambleya hall</td>
<td>Lunch</td>
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<tr>
<td>15.00</td>
<td>Excursions</td>
<td>Hermitage Museum,</td>
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<tr>
<td>17.00</td>
<td>St. Isaac's Cathedral</td>
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</table>

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: Electro catalysis, 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
<table>
<thead>
<tr>
<th>Time</th>
<th>Session/Event</th>
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</table>
| 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<sub>3</sub>VO<sub>x</sub>  
Catalysis Research Center, Hokkaido University (Sapporo), Japan |
| 15.00 | Prof. Valerii I. Bukhtiyarov  
Memorial lecture 145th anniversary 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 CH₄ Dry Reforming on Nanocrystalline Doped Ceria-
Zirconia with Supported Pt, Ru, Ni and Ni–Ru
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk State University (Novosibirsk), Russia
³Institut de Recherches sur la catalyse et l’environnement de Lyon
(Lyon), France
⁴Gent 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
¹Institute of Combustion Problems, Al-Farabi Kazakh National
University (Almaty), Kazakhstan
²JSC “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/BaCeO₃·2ZrO₂ Catalyst For
Methane Combustion
¹Università di Genova, Department of Chemical and Process
Engineering (Genova), Italy
²Politecnico 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+Al₂O₃ Catalysts on \( n \)-Paraffins Transformation
Wroclaw University of Technology, Faculty of Chemistry (Wroclaw), 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+H₂ 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\(_2\)O\(_3\) 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.\textsuperscript{1,2}, Mukhamedzianova D.F.\textsuperscript{1}, Beletskaya A.V.\textsuperscript{1}, Ratmanova N.K.\textsuperscript{1}, Snyga Y.G.\textsuperscript{1}, Nikolaev S.A.\textsuperscript{1}, Askerka M.S.\textsuperscript{1}, Lanin S.N.\textsuperscript{1}, Shestakov A.F.\textsuperscript{2}, Kuz'menko N.E.\textsuperscript{1}

\textbf{Theoretical Insight on Catalytic Activity of Bimetallic Gold Catalysts}
\textsuperscript{1}Department of Chemistry, Lomonosov Moscow State University (Moscow), Russia
\textsuperscript{2}Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia

17.40  OP-I-5
Presenting author: Dr. Prokopis C. Andrikopoulos
Andrikopoulos P.C.\textsuperscript{1}, Michel C.\textsuperscript{1}, Chouzier S.\textsuperscript{2}, Sautet P.\textsuperscript{1}

\textbf{Oxidation of Alkanes: In Silico Catalyst Design}
\textsuperscript{1}University of Lyon, CNRS, Laboratoire de Chimie, ENS de Lyon (Lyon), France
\textsuperscript{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.\textsuperscript{1}, Kozhevin V.M.\textsuperscript{1}, Yavsin D.A.\textsuperscript{1}, Rostovshchikova T.N.\textsuperscript{2}, Lokteva E.S.\textsuperscript{2}

\textbf{Self-Induced Electric Fields in the System of Supported Metal Nanoparticles: The Impact on Heterogeneous Catalysis}
\textsuperscript{1}Ioffe Physical-Technical Institute of RAS (St. Petersburg), Russia
\textsuperscript{2}Lomonosov Moscow State University (Moscow), Russia

18.20  OP-I-7
Presenting author: Prof. Anatoliy N. Startsev

\textbf{Low Temperature Decomposition of Hydrogen Sulfide into Hydrogen and Diatomic Gaseous Sulfur}
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

19.00  \textit{Welcome Party, Sovetskii 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 University (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 CO₂ and MeOH  
Catalyzed By Sn(Ot-Bu)₄ with Acid-Base Additives, and its Reaction Mechanism  
¹Graduate School of Arts and Sciences, The University of Tokyo (Tokyo), Japan  
²Graduate 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
Diphenylphosphinoferroacenyl Thioether Diene Rh(I) and Ir(I)
Catalyzed Ketone Hydrogenation: Turning Precatalysts into Active
Species
¹Nesmeyanov Institute of Organoelement Compounds RAS (Moscow),
Russia
²Laboratoire de Chimie de Coordination CNRS (Toulouse), France
³Department 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
¹Dipartimento di Ingegneria Industriale, Università di Salerno, Fisciano (SA), Italy
²Tecnimont 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/Cs₂HPW₁₂O₄₀: Mechanism of the Reaction in the Presence of Methyl Iodide Promoter
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Department 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-Al₂O₃
1Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
2Novosibirsk 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 H₂O₂: Probing the Nature of Active Species by EPR Spectroscopic and Enantioselectivity Studies
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk 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 H₂O₂, Catalyzed by Aminopyridine Manganese Complexes
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk 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
¹St. Petersburg Department of Boreskov Institute of Catalysis SB RAS (St. Petersburg), Russia
²Vorozhtzov 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.\textsuperscript{1,2}, Chibiryaev A.M.\textsuperscript{2,3}, Nuzhdin A.L.\textsuperscript{1},
Bukhtiyarova G.A.\textsuperscript{1}, Martyanov O.N.\textsuperscript{1,2}
Catalytic Effect of Si-Containing Compounds on the C-Methylation of Indole in sc-MeOH
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{2}Novosibirsk State University (Novosibirsk), Russia
\textsuperscript{3}Vorozhtsov Institute of Organic Chemistry SB RAS (Novosibirsk), Russia

16.30  \textit{Coffee break}

\textit{Assambleya Hall, Azimut Hotel}

17.00-19.00  \textbf{POSTER SESSION}

11.00-16.00 - hanging posters
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 NOx 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
¹Lomonosov Moscow State University (Moscow), Russia
²Institute of Metal Physics UB RAS (Yekaterinburg), Russia
³School 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/SiO₂-Al₂O₃ 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 ZnAl₂O₄
Catalysts Used for Hydrogen Production from Methanol Steam
Reforming
¹Lodz University of Technology (Lodz), Poland
²University 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”
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk 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 Pt₃Sn/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., Furukawa S., Ohno Y., Teramura K., Tanaka T.
Reaction Mechanism of Selective Oxidation of Alcohols and Amines over Semiconductor Photocatalysts
¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University (Kyoto), Japan
²Precursory 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.
RuOₓ-VOₓ/TiO₂ as Very Highly Selective Photocatalysts for the Oxidative Dehydrogenation of Ethanol to Acetaldehyde
Department of Industrial Engineering, University of Salerno (Fisciano), Italy
Presenting author: Dr. Ekaterina A. Kozlova
Kozlova E.A.\textsuperscript{1}, Kozhevnikova N.S.\textsuperscript{2}, Lemke A.A.\textsuperscript{2}, Cherepanova S.V.\textsuperscript{1},
Lyubina T.P.\textsuperscript{1}, Gerasimov E.Yu.\textsuperscript{1}, Tsybulya S.V.\textsuperscript{1}, Shchipunov Yu.A.\textsuperscript{3},
Rempel A.A.\textsuperscript{2}

Design of the Nanocrystalline CdS/TiO\textsubscript{2} Photocatalyst
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{2}Institute of Solid State Chemistry UB RAS (Yekaterinburg), Russia
\textsuperscript{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 импульской 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.\textsuperscript{1,2}, Gavrilov M.S.\textsuperscript{1}, Volodin A.M.\textsuperscript{1}, Stoyanovskii V.O.\textsuperscript{1}, Slavinskaya E.M.\textsuperscript{1}, Mishakov I.V.\textsuperscript{1,2}, Shubin Yu.V.\textsuperscript{3}
Catalytic Purification of Exhaust Gases over Pd-Rh Alloy Catalysts: From Mechanism Understanding to High Temperature Stability
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{2}Novosibirsk State Technical University (Novosibirsk), Russia
\textsuperscript{3}Nikolaev Institute of Inorganic Chemistry SB RAS (Novosibirsk), Russia

15.10  OP-III-25
Presenting author: Dr. Evgeny I. Vovk
Say Z.\textsuperscript{1}, Vovk E.I.\textsuperscript{1,2}, Bukhtiyarov V.I.\textsuperscript{2}, Özensoy E.\textsuperscript{1}
Ce-O-Pt Active Sites in Ceria Promoted NO\textsubscript{x} Storage Reduction Catalysis
\textsuperscript{1}Department of Chemistry, Bilkent University (Ankara), Turkey
\textsuperscript{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 PdCl₂-CuCl₂/γ-Al₂O₃ Catalyst
¹Lomonosov Moscow University of Fine Chemical Technology (Moscow), Russia
²National Research Center "Kurchatov Institute" (Moscow), Russia
³N.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:
d.ф-м.н. С.А. Цыганов, начальник управления ориентированных исследований РФФИ, Москва;
d.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
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.\textsuperscript{1,2,3}, Shigarov A.B.\textsuperscript{1,2,3}, Snytnikov P.V.\textsuperscript{1,2,3}, Belyaev V.D.\textsuperscript{1}, Kirillov V.A.\textsuperscript{1,2,3}, Sobyanin V.A.\textsuperscript{1,2,3}
Modeling of Associated Petroleum Gas Steam Reforming Process
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{2}Novosibirsk State University (Novosibirsk), Russia
\textsuperscript{3}”UNICAT” Ltd, Pr. (Novosibirsk), Russia

14.40 OY-IV-3
Presenting author: Olga A. Simakova
Simakova O.A.\textsuperscript{1,2}, Murzina E.V.\textsuperscript{1}, Leino A.-R.\textsuperscript{3}, Mäki-Arvela P.\textsuperscript{1}, Willför S.M.\textsuperscript{4}, Murzin D.Yu.\textsuperscript{1}
Biomass Derived Lignan Hydroxymatairesinol Selective Oxidation over Au Catalysts
\textsuperscript{1}Laboratory of Industrial Chemistry and Reaction Engineering, Process Chemistry Centre, Åbo Akademi University (Åbo/Turku), Finland
\textsuperscript{2}Graduate School of Chemical Engineering, Åbo Akademi University (Åbo/Turku), Finland
\textsuperscript{3}Microelectronics and Materials Physics Laboratories, EMPART Research Group of Infotech Oulu, University of Oulu (Oulu), Finland
\textsuperscript{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., Pirard S.L., Lambert S.D., Páez C.A., Poelman D.,
Pirard J.-P., Heinrichs B.
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., Skorb E.V., Andreeva D.V.
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.\textsuperscript{1,2}, Simonov A.N.\textsuperscript{1}, Rudina N.A.\textsuperscript{1}, Parmon V.N.\textsuperscript{1,2}

Microstructure Effects in Catalysis of Oxygen Reduction Reaction over Electrodeposited Platinum: Influence of Intergrain Boundaries
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{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\textsubscript{2}O\textsubscript{3}-Al\textsubscript{2}O\textsubscript{3} Catalysts For Water Gas Shift Reaction And Methanol Synthesis

\textit{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.\textsuperscript{1,4}, Auezov A.B.\textsuperscript{2}, Konuspaev S.R.\textsuperscript{1}, Burkitbayev M.M.\textsuperscript{1}, Piccolo L.\textsuperscript{4}, Berhault G.\textsuperscript{4}, Shaimardan M.\textsuperscript{3}

Bimetallic Catalysts for Selective Benzene Hydrogenation for Environmental Gasoline Production
\textsuperscript{1}Al-Farabi Kazakh National University (Almaty), Kazakhstan
\textsuperscript{2}Scientific Research Institute of New Chemical Technology & Materials (Almaty), Kazakhstan
\textsuperscript{3}Kazakh British Technical University (Almaty), Kazakhstan
\textsuperscript{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.\textsuperscript{1}, Mukhamedzyanova D.F.\textsuperscript{1}, Pichugina D.A.\textsuperscript{1,2}, Kuz'menkov N.E.\textsuperscript{1}

The Theoretical Prediction of Structural and Electronic Effects of Gold-Based Systems in Selective Alkynes Activation
\textsuperscript{1}Lomonosov Moscow State University (Moscow), Russia
\textsuperscript{2}Institute of Problems of Chemical Physics RAS (Chernogolovka), Russia
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 O₂ Mediated by Fe- and Cr-MIL-101
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Institut de Recherches sur la Catalyse et l’Environnement de Lyon (Villeurbanne), France
³Nikolaev 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
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
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk 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?
¹Research Center for Natural Sciences (Budapest), Hungary
²Combitech-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
“MOleculcs, 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
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Mitsubishi 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
1Institute of Molecular Genetics RAS (Moscow), Russia
2Nesmeyanov Institute of Organoelement Compounds RAS (Moscow), Russia
3Shemyakin–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 H₂O₂ with Sulfuric Acid Catalyst under Mild Conditions
1Institute of Chemistry and Chemical Technology SB RAS (Krasnoyarsk), Russia
2Siberian Federal University (Krasnoyarsk), Russia
3Institut 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-CeZrO₂ Catalysts
1Università degli Studi di Torino, Department of Chemistry and NIS Centre of Excellence (Torino), Italy
2ISTEC, Centro Nazionale delle Ricerche (Torino), Italy
3ENEA, “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
**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 H₂O₂ Synthesis from H₂ and O₂ 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 H₂O₂ Through Pd(IV) Intermediates: A DFT Investigation**
*Lomonosov Moscow University of Fine Chemical Technologies, Moscow, Russia*

PP-I-5
**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., Gubaidullin I.M., Novichkova A.V.
**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
Ethylene to Benzene Catalytic Transformation Mechanism Performed at Nanocluster of Platinum Pt₄ 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 Ag₂₀ in Propylene Epoxidation
¹M.V. Lomonosov Moscow State University (Moscow), Russia
²Institute 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
¹Novosibirsk State University (Novosibirsk), Russia
²Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
³Institute 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
¹Institute of Structural Macrokinetics and Materials Science RAS (Chernogolovka), Russia
²N.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
¹Institute of Structural Macrokinetics and Materials Science RAS (Chernogolovka), Russia
²United Research and Development Center (Moscow), Russia

PP-II-7
Faingol’d E.E., Babkina O.N., Zharkov I.V., Bravaya N.M.
¹H 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 Catalytic Systems
Ph₂CCpFluMMe₂ (M = Zr, Hf) /TIBA/[Ph₃C⁺][B(C₆F₅)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
¹Institute of Organic Synthesis URAL Branch RAS (Yekaterinburg), Russia
²Ural Federal University (Yekaterinburg), Russia
³Institute 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
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²University 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
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., Kvoitunov K.V., Khudorozhkov A.K., Bukhtiyarov V.I., Koptyug I.V.
Selectivity Control of Pairwise Hydrogen Addition over Catalytic Hydrogenation of C₄ Hydrocarbons on Supported Pt and Pd Catalysts
1International Tomography Center SB RAS (Novosibirsk), Russia
2Novosibirsk State University (Novosibirsk), Russia
3Boreskov 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
Spectral and Catalytic Study of Silica Modified Cr\textsubscript{2}O\textsubscript{3}/Al\textsubscript{2}O\textsubscript{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\textsubscript{2}-C\textsubscript{3} Olefins over Nickel and Cobalt
Semenov Institute of Chemical Physics RAS (Moscow), Russia

PP-III-16
Chernikova V.S.\textsuperscript{1}, Erokhin A.V.\textsuperscript{1}, Golubina E.V.\textsuperscript{1}, Murzin V.Y.\textsuperscript{2}, Veligzhanin A.A.\textsuperscript{2}, Zubavichus Y.V.\textsuperscript{2}
Formation of Active Sites in NiZn/UDD Catalysts for the Selective Phenylacetylene Hydrogenation as Monitored by \textit{in situ} EXAFS
\textsuperscript{1}M.V.Lomonosov Moscow State University (Moscow), Russia
\textsuperscript{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\textsubscript{2}O\textsubscript{3} Catalysts Prepared by Polyol Method for Partial Oxidation of Methane
Department of Chemical Engineering, Istanbul University (Istanbul), Turkey
Hydrotalcite-Like Catalytic Materials Obtained from Industrial Wastes for Oxidation of Sulfur Compounds

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

Ni-Based Catalysts for Reforming of Methane with CO₂

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

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

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

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

Study of the Liquid-Phase Isobutane Alkylation with Butenes over Aluminum Chloride Complexes Synthesized in situ from Activated Aluminum and tert-C₄H₉Cl

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**
**Ba₀.₅Sr₀.₅Co₀.₈Fe₀.₂O₃₋δ**
¹Institute of High Temperature Electrochemistry UB RAS 
(Yekaterinburg), Russia  
²University of Twente (Twente), The Netherlands

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

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

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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**
¹Lomonosov Moscow State University (Moscow), Russia  
²LLC "SCN" (Snezhinsk), Russia
PP-III-34
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 La₁₋ₓSrₓFeO₃ Perovskites
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Institute of Solid State Chemistry SB RAS (Novosibirsk), Russia

PP-III-40
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
¹Leibniz-Institut für Katalyse e.V. an der Universität Rostock (Rostock), Germany
²Indian Institute of Chemical Technology (Hyderabad), India
³National Nanotechnology Research Center (Riyadh), Saudi Arabia
⁴Univ. 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

PP-III-53
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
PP-III-55
Kuzmina O.V., Dementeva E.V., Urtyakov P.V.
Diffusive Model of Isoamylene Dehydrogenation to Isoprene Using Ferric Potassium Catalysts
Kazan (Volga Region) Federal University (Kazan), Russia

PP-III-60
Lónyi F., Solt H.E., Valyon J.
Mechanism of NO-SCR with Methane over In,H- and Co,In,H-ZSM-5 Catalysts
Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences (Budapest), Hungary

PP-III-61
Lukiyanchuk I.V.¹, Chernykh I.V.¹, Rudnev V.S.¹, Tyrina L.M.¹, Ustinov A.Y.²
Binary Oxides of Transition Metals on Aluminum and Titanium in CO Oxidation
¹Institute of Chemistry FEB RAS (Vladivostok), Russia
²Far Eastern Federal University (Vladivostok), Russia

PP-III-65
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
¹Faculty of Sciences and Mathematics, University of Nis (Nis), Serbia
²Serbian Academy of Sciences and Arts (Belgrade), Serbia
³Institute of Nuclear Science "Vinca" (Belgrade), Serbia

PP-III-67
Massenova A.T., Zhumakanova A.S., Sassykova L.R., Rafikova Kh.
Study of Mechanism of Benzene Alkylation by Alkanes over Pt-Zeolite Catalysts
D.V. Sokolskii Institute of Organic Catalysis & Electrochemistry (Almaty), Kazakhstan
PP-III-68
Matveeva V.G.\textsuperscript{1}, Sapunov V.N.\textsuperscript{2}, Grigoriev M.E.\textsuperscript{1}, Sulman E.M.\textsuperscript{1}
\textbf{Non-Steady-State Kinetics of D-Glucose to D-Sorbitol on Ru-Containing Heterogeneous Catalyst}
\textsuperscript{1}Tver State Technical University (Tver), Russia
\textsuperscript{2}D. Mendeleev University of Chemical Technology of Russia (Moscow), Russia

PP-III-69
Mekhaev A.V.\textsuperscript{1}, Kvon R.I.\textsuperscript{2}, Taran O.P.\textsuperscript{2,3}, Yatluk Yu.G.\textsuperscript{1}
\textbf{Investigation of the Mechanism of Deactivation of Pd/Sibunit Catalyst Hydrodechlorination of Polychlorinated Biphenyls}
\textsuperscript{1}Postovsky Institute of Organic Synthesis UB RAS (Yekaterinburg), Russia
\textsuperscript{2}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{3}Novosibirsk State Technical University (Novosibirsk), Russia

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Mierczynski P.\textsuperscript{1}, Vasilev K.\textsuperscript{2}, Mierczynska A.\textsuperscript{3}, Maniecki T.P.\textsuperscript{1}
\textbf{Decomposition and Steam Reforming of Methanol over Pd, Cu - CNT Catalysts}
\textsuperscript{1}Lodz University of Technology, Institute of General and Ecological Chemistry Zeromskiego (Lodz), Poland
\textsuperscript{2}University of South Australia (Mawson Lakes Adelaide), Australia
\textsuperscript{3}Ian Wark Research Institute, University of South Australia (Mawson Lakes Adelaide), Australia

PP-III-73
Mota N.\textsuperscript{1}, Matus E.V.\textsuperscript{2}, Kuznetsov V.V.\textsuperscript{2}, Ismagilov I.Z.\textsuperscript{2}, Navarro R.M.\textsuperscript{1}, Kerzhentsev M.A.\textsuperscript{2}, Ismagilov Z.R.\textsuperscript{2,3}, Fierro J.L.G.\textsuperscript{1}
\textbf{Effect of B-Cation Substitution on the Activity of LaCrO\textsubscript{3} and LaNiO\textsubscript{3} Perovskites for Autothermal Reforming of Methane}
\textsuperscript{1}Instituto de Catálisis y Petroleoquímica, CSIC (Madrid), Spain
\textsuperscript{2}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{3}Institute of Coal Chemistry and Material Science SB RAS (Kemerovo), Russia
PP-III-74
Mounir Chamam\textsuperscript{1}, Laurence Pirault-Roy\textsuperscript{2}, Károly Lázár\textsuperscript{1}, Zoltán Paál\textsuperscript{1}
\textbf{MCP Transformation on Rh-M (M = Ge, Sn) Grafted Catalysts}
\textsuperscript{1}Institute of Isotopes (Budapest), Hungary
\textsuperscript{2}Université de Poitiers (Poitiers), France

PP-III-78
Nesmelov A.I., Kleiner V.I., Ivanuk A.V., Smetannikov O.V., Chinova M.S.
\textbf{Kinetic Regularities of 1-Decene Polymerization on Supported Titanium-Magnesium Nanocatalysts (TMNC) and Molecular Weight Characteristics of Obtained Polymers}
\textit{A.V. Topchiev Institute of Petrochemical Synthesis RAS (Moscow), Russia}

PP-III-79
Nikolaev S.A., Pichugina D.A., Golubina E.V., Majouga A.G.
\textbf{The Nature of Synergistic Effects in Catalysis by Au-NiO Nanoparticles}
\textit{Lomonosov Moscow State University (Moscow), Russia}

PP-III-80
Nindakova L.O., Ozolin D.V., Lubentzova K.V.
\textbf{Enantioselective Hydrogenation of C=C-Bound on Colloidal Palladium Catalyst Modified by (-)-Cinchonidine}
\textit{Irkutsk State Technical University (Irkutsk), Russia}

PP-III-81
Nizovskii A.I.\textsuperscript{1}, Kalinkin A.V.\textsuperscript{1}, Smirnov M.Yu.\textsuperscript{1}, Belskaya O.B.\textsuperscript{2}, Stepanova L.N.\textsuperscript{2}, Kazakov M.O.\textsuperscript{2}
\textbf{Influence of the Way of Active Sites Formation in Pt/MgAlO\textsubscript{x} Catalysts on their Catalytic Properties. XPS Study}
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
\textsuperscript{2}Institute of Hydrocarbons Processing SB RAS (Omsk), Russia
PP-III-82
Nizovskii A.I., Mikenas T.B., Kalinkin A.V., Smirnov M.Yu., Bukhtiyarov V.I.
New Capabilities for XPS Studies of Ziegler-Natta Catalysts Using a System of Sample Loading in Inert Atmosphere
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia

PP-III-83
Ollár T., Szarvas T., Tétényi P.
Mechanism of Butadiene Heterocyclization over Sulfideded HDS Catalysts
Centre of Energy Research, Hungarian Academy of Science (Budapest), Hungary

PP-III-85
Pavel O.D., Zavoianu R., Angelesc E., Neatu F.
MgAlY Layered Double Hydroxides as Catalysts for Organic Syntheses Catalysed by Base Sites
University of Bucharest, Faculty of Chemistry, Department of Organic Chemistry, Biochemistry and Catalysis (Bucharest), Romania

PP-III-86
Petrov S.N.¹, Tsyganenko A.A.¹, Rudakova A.V.¹, Smirnov K.S.²
FTIR Study of Adsorption and Transformations of HCN on Oxide Adsorbents
¹St. Petersburg State University (St. Petersburg), Russia
²UST de Lille Villeneuve d’Ascq Cedex (Lille), France

PP-III-88
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 CO₂ and n-Bu₂Sn(OR)₂
¹Institut de Sciences Analytiques, University of Lyon (Lyon), France
²Institut de Chimie Moléculaire, University of Burgundy (Dijon), France
**Oxygen Isotope Exchange of \((1-y)La_{1-x}Sr_xMnO_{3+\delta} \cdot yZr_{0.82}Y_{0.12}O_{1.91}\)**  
Institute of High Temperature Electrochemistry UB RAS  
(Yekaterinburg), Russia

Pylinina A.I., Povarova E.I., Mikhlenko I.I.  
**Features of the Alcohols’ Dehydrogenation on the NZP – Catalysts Depending on the Location of the Ion - Modifier**  
Peoples’ Friendship University of Russia (Moscow), Russia

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

Serov Y.M., Sheshko T.F.  
**Synthesis of Olefins from Carbon Oxides and Hydrogen on Iron-Manganese Nanosystems at Atmospheric Pressure**  
Peoples Friendship University of Russia (Moscow), Russia

Shilina M.I.\(^1\), Nevskaya S.M.\(^1\), Udalova O.V.\(^2\), Vasilevskii G.Y.\(^1\)  
**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
Impact of Activation Conditions on the State of the Active Cobalt Surface in Co-Al Catalysts of Fischer-Tropsch Synthesis

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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CO₂ Tolerance of Highly Productive Composite Fischer–Tropsch Co Catalyst

Sineva L.V.1,2, Ermolaev V.S.1,2, Mitberg E.B.1, Solomonik I.G.1, Khatkova E.Yu.1, Mordkovich V.Z.1,2

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

Results of Thermodynamic Modeling for Some Catalytic Processes

Sochagin A.A., Slobodov A.A.

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

Cr, V and Pt in O₂-Free Propane Dehydrogenation: Who Wins and Why?

Sokolov S., Stoyanova M., Rodemerck U., Linke D., Kondratenko E.V.

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

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

Solomonik I.G.1,2, Sineva L.V.1, Mordkovich V.Z.1,2

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2INFRA Technologies Ltd. (Moscow), Russia
PP-III-110
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
The Composition, Structure and Catalytic Activity of Some Metal-Oxide PEO-Coatings on Aluminum
1Far Eastern Federal University (Vladivostok), Russia
2Institute of Chemistry FEB RAS (Vladivostok), Russia

PP-III-111
Ustinova E.A.1, Shcheka O.L.2, Ustinov A.Yu.1,2
Cluster Modeling of Metal Oxide Structures on Al and their Interaction with CO
1Institute of Chemistry FEB RAS (Vladivostok), Russia
2Far Eastern Federal University (Vladivostok), Russia

PP-III-115
Wittine O., Matijašević L.J., Zrnčević S.
Phenol Oxidation by PP-CWAO Treatment with Cu/13X
Faculty of Chemical Engineering and Technology, University of Zagreb (Zagreb), Croatia

PP-III-118
Zakharov V.P.1, Mingaleev V.Z.2, Zakharova E.M.2
Modification of Heterogeneous Titanium Catalyst in Turbulent Microreactor at the Synthesis of (co)Polydiene
1Bashkir State University (Ufa), Russia
2Institute of Organic Chemistry of the URC RAS (Ufa), Russia

PP-III-119
Zemlyanov D.Y.
Atomic Layer Deposition for Water Gas Shift Reaction over Bimetallic Catalysts
Purdue University, Birck Nanotechnology Center (West Lafayette, IN), USA

PP-III-123
Simakova I.L., Troitskii S.Yu., Parmon V.N.
One-Pot Hydrodebenzylation – Acylation over Pd/C: Mechanistic View on Catalyst Deactivation
Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
PP-III-124
Cherepanov P., Andreeva D.
Sonochemical formation of mesoporous multi metal catalysts
Bayreuth University, Bayreuth, Germany

Section IV. Catalytic Processing of Renewables

PP-IV-1
AbdelDayem Hany M.1,2, Xiao T.3, Elshihy S.S.1
The Promoting Effect of Rare Earth Metals on Partial Oxidation of Methanol to Hydrogen over Ag and Cu Catalysts
1Chemistry Department, College of Science, King Faisal University (AlHofof), Saudi Arabia
2Chemistry Department, Faculty of Science, Ain Shams University (Cairo), Egypt
3Inorganic Chemistry Laboratory, Oxford University, United Kingdom

PP-IV-4
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/Al2O3 and NiMoS/Al2O3 Catalysts
1Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
2Novosibirsk State University (Novosibirsk), Russia

PP-IV-6
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
Application of the Concept of Interlayer Dynamics to Design of Novel TMS-Based Catalysts for Synthesis of Mixed Alcohols
1N.D. Zelinsky Institute of Organic Chemistry RAS (Moscow), Russia
2Samara State Technical University (Samara), Russia
PP-IV-8
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

PP-IV-9
Jaroszewska K., Masalska A., Grzechowiak J.R., Maniecki T., Mierczyński P.
Hydrocracking and Hydroisomerization of n-Alkanes over Ni Catalysts
1Faculty of Chemistry, Wrocław University of Technology (Wrocław), Poland
2Institute of General and Ecological Chemistry, Technical University of Łódź (Łódź), Poland

PP-IV-10
Khalaf M.M., Ibrahimov H.C., Yusifov Y.H., Ismailov E.H.
Novel Nanostructured Fe-, Co- Containing Materials as Heterogeneous Catalysts for the Decomposition of Heavy Oil Residue
1Institute of Petrochemical Processes, Azerbaijan National Academy of Sciences (Baku), Azerbaijan
2Chemistry Department, Faculty of Science, Sohag University (Sohag), Egypt

PP-IV-12
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
PP-IV-15
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/SiO₂ and La-Sr/CaO Catalysts
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³Institute of Coal Chemistry and Material Science SB RAS (Kemerovo), Russia

PP-IV-17
Okhlopkova L.B.¹, Matus E.V.¹, Kerzhentsev M.A.¹, Ismagilov I.Z.¹, Ismagilov Z.R.¹,²
Control of Metal Dispersion, Chemical Composition, Porous Structure and Thickness of Mesoporous PtSn/TiO₂ and PdZn/TiO₂ Coatings for Microcapillary Reactor
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Institute of Coal Chemistry and Material Science SB RAS (Kemerovo), Russia

PP-IV-18
Palma V., Barba D., Ciambelli P.
H₂S Purification from Biogas to Feed MCFC by Partial Oxidation on the V₂O₅-CeO₂ Catalyst
University of Salerno (Fisciano), Italy

PP-IV-19
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

PP-IV-21
Simonov M.N., Simakova I.L.
Mechanistic Study of Reaction Pathways in Butyl Lactate to Propylene Glycol Hydrogenolysis over Cu/SiO₂
Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
**PP-IV-22**

Sooknoi T.\(^1\), Ausavasukhi A.\(^2\)

**H\(_2\)-Least Approaches for Deoxygenation of Phenolic Compounds**

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**PP-IV-24**

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 Biodiesel Production over CaO Catalyst**

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\(^2\)Serbian Academy of Sciences and Arts (Belgrade), Serbia  
\(^3\)Institute of Nuclear Science "Vinca" (Belgrade), Serbia

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**Section V. Electrocatalysis, Photocatalysis, Biocatalysis**

**PP-V-2**


**Oxygen Exchange and Degradation of LSM—YSZ Cathode Materials**

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PP-V-3
Bakhtchadjian R.H.¹, Tsarukyan S.V.¹, Manucharova L.A.¹, Tavadyan L.A.¹, Barrault J.²
Dioxo-Mo(VI) - Complexes Anchored on Titania as Catalysts in Photo-Oxidative Decomposition of Some Aromatic Organochlorine Compounds by Dioxygen
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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 Na₂S–Na₂SO₃ Solutions under Visible Light
¹Boreskov Institute of Catalysis SB RAS (Novosibirsk), Russia
²Novosibirsk State University (Novosibirsk), Russia

PP-V-9
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
²Delft University of Technology (Delft), The Netherlands

PP-V-11
"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*
Knowledge of the mechanism of reactions occurring on the surface of heterogeneous catalysts is sought for the purpose of understanding what aspect of catalyst composition and structure limits 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 mechanisms, which can be used to derive and express 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 carboxylation 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.

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.

References:

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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 H₂O₂ as oxidant. Insights into the catalytic mechanism have been obtained from a combination of product distribution studies, ¹⁸O 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 O₂. 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.

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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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²Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands

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 probability. 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 CHx species is relatively slow. The dominant chain growth sites will be the step-edge type centers with efficient CHx 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.

References:

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.

References:
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$_3$VO$_x$ with unique crystal structures, orthorhombic phase and trigonal phase. Both of the Mo$_3$VO$_x$ 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$_3$VO$_x$ 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-membered 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.

References:
Mechanistic Aspects of Hydrogenation and Oxidation of Sugars
Åbo Akademi University, Turku, Finland

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.

References:

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 Ga2O3 and reactions on PdGa-Ga2O3 [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?
Understanding Thermal and Photocatalytic Chemical Routes for NOx 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 TiO2-promoted DeNOx catalysts with NOx storage capabilities will be discussed. The first genre of catalysts to be discussed is TiO2-promoted NOx-Storage Reduction (NSR, or Lean NOx Traps, LNT) catalysts which function through thermally activated surface processes. NSR catalysts are based on solid state storage of NOx(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 NOx during a short fuel-rich period. BaO/TiO2/Al2O3 based ternary mixed oxide NOx storage materials synthesized via sol-gel techniques reveal advantageous NOx storage and sulfur tolerance characteristics. Although the conventional BaO/Al2O3 binary mixed oxide system is prone to sulfur poisoning where it loses a significant portion of its NOx storage capacity in an irreversible fashion due to the formation of thermodynamically stable surface and bulk sulfate species, BaO/TiO2/Al2O3 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 TiO2 surface domains functioning as anchoring sites for BaO clusters, preventing the sintering of BaO sites and impeding the formation of large BaSO4 clusters that cannot be thermally regenerated efficiently. Along these lines, surface functionalization with TiO2 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\textsubscript{x} storage processes on NSR catalysts at the molecular level, planar model catalysts were prepared in the form of BaO/BaO\textsubscript{2}/Pt(111) and BaO\textsubscript{x}/TiO\textsubscript{2}/Pt(111). Structural characterization of these relatively well-defined model catalysts was performed via LEED and XPS while NO\textsubscript{x} adsorption characteristics were studied via XPS and TPD. It is observed that BaO\textsubscript{2} sites play a crucial role during the uptake and release of NO\textsubscript{x} species where the presence of exposed (open) Pt sites significantly enhance the BaO\textsubscript{2} formation and catalytically decrease the NO\textsubscript{x} desorption temperatures. Two different NO\textsubscript{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\textsubscript{2}-promoted NSR catalysts at elevated temperatures which include the formation of BaTiO\textsubscript{3} domains, sub-surface diffusion of BaO sites and the surface segregation of underlying TiO\textsubscript{2} domains. Influence of BaO domain size on the NO\textsubscript{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\textsubscript{2}-promoted DeNO\textsubscript{x} catalysts in the form of X/TiO\textsubscript{2}, and X/TiO\textsubscript{2}/Al\textsubscript{2}O\textsubscript{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\textsubscript{x}(g) oxidation and solid state NO\textsubscript{x} storage. Performance and the structural properties of these hybrid “Photocatalytic NO\textsubscript{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 interconversion 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.


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

References:

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
¹Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
²Novosibirsk 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 H₂O₂/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/H₂O₂. 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–FeV=O intermediate in the catalyst system 4/H₂O₂.[⁴] Direct correlation of VT-MS and EPR data shows that S = 1/2 intermediate 4e well corresponds to the oxoiron(V) species identified in the same system by VT-MS. Apparently, complexes 1e⁻⁴e are similar oxoiron(V) species. Comparative studies of asymmetric olefin epoxidation by Fe and Mn catalyst systems 3/H₂O₂/RCOOH and 5/H₂O₂/RCOOH have shown that 3 and 5 conduct enantioselective epoxidation of prochiral olefins with H₂O₂ 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⁻¹O(OC(O)R)]²⁺ (where M = Fe or Mn, R = alkyl, L = aminopyridine ligand).
References:

ORAL PRESENTATIONS
Section I. Catalysis: From First Principles

OP-I-1  Stakhveev 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 CH₄ Oxidation over Noble Metals: Comparison of Pt and Pd Catalysts
1Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia
2Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
Catalytic tests revealed different relationships between TOF in CH₄ 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
1Department Chemie and Catalysis Research Center, Technische Universität München, Garching, Germany
2Institute 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 SiO₂ and Al₂O₃ Surfaces. Embedded Cluster Scalar-Relativistic and Periodic Pseudopotential Density Functional Calculations
¹Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
²Technische Universität München, Catalysis Research Center, Garching, Germany

Formation energies and equilibrium structures of O₂ adsorption complexes with silver trimers and tetramers supported on α-Al₂O₃(0001) and MCM-41 surfaces have been calculated. The extent of O₂ activation is probed in surface NO oxidation reaction.

OP-I-4  Pichugina D.A.¹², 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
¹Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia
²Institute of Problems of Chemical Physics RAS, Chernogolovka, Russia

The scope of DFT in studying the active sites of AuₙNi and AuₙPd bimetallic particles will be presented. Ligand and ensemble effects in these systems will be considered in H₂O₂ 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
¹University of Lyon, CNRS, Laboratoire de Chimie, ENS de Lyon, Lyon, France
²Centre 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 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
¹Ioffe Physical-Technical Institute of RAS, St. Petersburg, Russia
²Lomonosov 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.


** ¶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 $2 \text{H}_2\text{S} \leftrightarrow 2 \text{H}_2 + \text{S}_2^{(\text{gas})}$ to produce hydrogen and gaseous diatomic sulfur. As calculated with DFT, $\text{S}_2$ 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., Haga S., Onaka M.

** Direct Synthesis of Dimethyl Carbonate from CO$_2$ and MeOH Catalyzed by Sn(Ot-Bu)$_4$ with Acid-Base Additives, and its Reaction Mechanism**

*Graduate School of Arts and Sciences, The University of Tokyo, Tokyo, Japan*

*Graduate School of Science, The University of Tokyo, Tokyo, Japan*

We discovered that Sn(Ot-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$_2$Sn(OMe)$_2$ catalyst. The high catalytic activity of Sn(Ot-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 $[\text{L}_2\text{TiMe}]^+[\text{MeMAO}]^-$ upon the interaction of bis(salicylaldimine), bis(enolatoimine) and related titanium precatalysts $\text{L}_2\text{TiCl}_2$ with methylalumoxane (MAO) has been followed by multinuclear NMR spectroscopy. The nature of chain-propagating species of the type $[\text{L}_2\text{TiP}]^+[\text{MeMAO}]^-$ (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.¹², Filippov O.A.¹, Fekete M.³, Duckett S.B.³, Manouy 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**  
¹Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia  
²Laboratoire de Chimie de Coordination CNRS, Toulouse, France  
³Department 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.
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 (H₄cdta = trans-1,2-cyclohexanediaminetetraacetic acid, C₁₄H₂₂O₈N₂; H₄pdta = 1,2-propanediaminetetraacetic acid, C₁₁H₁₈O₈N₂; TS = titanium silicalite). Degradation of thiocyanide and hydroxylation of phenol were monitored by ¹H and ¹³C NMR techniques.

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.

CH₄ 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 CH₄ and CO₂ 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
¹Institute of Combustion Problems, Al-Farabi Kazakh National University, Almaty, Kazakhstan
²JSC “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 CH₄ with O₂ because of the possible separate adsorption and activation of components in different parts of the cluster: CH₄ - on Ptᵐ⁺ (Ni⁺), and O₂ - on Ru⁰ (Cu⁰), 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/BaCeO₃·2ZrO₂ Catalyst for Methane Combustion
¹Università di Genova, Department of Chemical and Process Engineering, Genova, Italy
²Politecnico di Torino, Department of Applied Science and Technology, Torino, Italy

The ageing effect induced by S-compounds on 2% Pd/BaCeO₃·2ZrO₂ catalysts for CH₄ 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+Al₂O₃ 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, N₂ sorption, SEM, TEM, NH₃-TPD, PY-IR, TPR, H₂ 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.\textsuperscript{1,2}, Chumakova N.A.\textsuperscript{1,2}, Kaichev V.V.\textsuperscript{1,2}, Ustugov V.V.\textsuperscript{1}, Chumakov G.A.\textsuperscript{2,3}, Bukhtiyarov V.I.\textsuperscript{1,2}

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

\textsuperscript{1}Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
\textsuperscript{2}Novosibirsk State University, Novosibirsk, Russia
\textsuperscript{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 \textit{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\textsubscript{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\textsubscript{ad} species formation is the driving force of oscillations.

OP-III-8  Zemlyanov D.Y.\textsuperscript{1}, Klötzer B.\textsuperscript{2}

Does the Bulk Matter? Methane and Ethylene Oxidation on Palladium

\textsuperscript{1}Purdue University, Birck Nanotechnology Center, West Lafayette, USA
\textsuperscript{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.\textsuperscript{1,2}

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

\textsuperscript{1}Physics Department, Yeshiva University, New York, USA
\textsuperscript{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**
¹IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, Solaize, France
²Unité 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.
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.

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.

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. TPRReactions, 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.

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 Brønsted 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 ZnAl₂O₄ Catalysts Used for Hydrogen Production from Methanol Steam Reforming
¹Lodz University of Technology, Lodz, Poland
²University of South Australia, Mawson Lakes Adelaide, South Australia

The main goals of this study is to correlate the physicochemical properties of M/ZnAl₂O₄ (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-NH₃, TPR-H₂, 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 C₂H₄ reaction on H-ZSM-5 to produce C₃H₆. 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 C₂H₄ 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”
¹Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
²Novosibirsk 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%).

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 Al2O3, SiO2 and CeO2 with NOx and SOx are identified by XPS. The effect of the CO+O2 reaction on the size of Au nanoparticles supported on Al2O3 and Fe2O3 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
1Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2Novosibirsk State Technical University, Novosibirsk, Russia
3Nikolaev 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 (Al2O3) therefore initiating the phase transformation of the latter into α-Al2O3 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 NOx Storage Reduction Catalysis
1Department of Chemistry, Bilkent University, Ankara, Turkey
2Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

Influence of ceria on the NOx 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/BaO2/CeOx/CeO2 domains were observed leading to a complex redox interplay including oxidation of the precious metal sites, reduction of ceria, formation of BaO2 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 NOx 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 (H₂) 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/Al₂O₃ 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 Al₂O₃.

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.

Mechanism of Low-Temperature Carbon Monoxide Oxidation over PdCl₂-CuCl₂/γ-Al₂O₃ Catalyst
1Lomonosov Moscow University of Fine Chemical Technology, Moscow, Russia
2National Research Center “Kurchatov Institute”, Moscow, Russia
3N.D. Zelinsky Institute of Organic Chemistry RAS, Moscow, Russia

The state of the active constituents of the PdCl₂–CuCl₂/γ-Al₂O₃ 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 N₂–O₂–CO mixture pressure of 1 atm. A number of mechanistic hypotheses are discussed.

OP-III-29 Tálas E., Margitfalvi I.L.
Enantioselective Hydrogenation of Activated Ketones in the Presence of Pt–Cinchona Catalysts. Is the Proton Transfer Concept Valid?
1Research Center for Natural Sciences, HAS, Budapest, Hungary
2Combitech-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 an 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  
1Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia  
2Mitsubishi 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.

Solid State Isotope Exchange with Spillover Hydrogen in Organic Compounds  
1Institute of Molecular Genetics RAS, Moscow, Russia  
2Nesmeyanov Institute of Organoelement Compounds RAS, Moscow, Russia  
3Shemyakin–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.\textsuperscript{1,2}, Sudakova I.G.\textsuperscript{1}, Garyntseva N.V.\textsuperscript{1}, Djakovitch L.\textsuperscript{3}, Pinel C.\textsuperscript{3}

Kinetic Study of Aspen-Wood Delignification by H\textsubscript{2}O\textsubscript{2} with Sulfuric Acid Catalyst under Mild Conditions

\textsuperscript{1}Institute of Chemistry and Chemical Technology SB RAS, Krasnoyarsk, Russia
\textsuperscript{2}Siberian Federal University, Krasnoyarsk, Russia
\textsuperscript{3}Institut de Recherches sur la Catalyse et l’Environnement de Lyon (IRCELYON), Lyon, France

Kinetic study of aspen-wood delignification by H\textsubscript{2}O\textsubscript{2} with sulfuric acid catalyst under mild conditions is reported.

OP-IV-3 Berlier G.\textsuperscript{1}, Gopalakrishnan S.\textsuperscript{1,2}, Miletto I.\textsuperscript{1}, Coluccia S.\textsuperscript{1,2}, Caputo G.\textsuperscript{3}, Giaconia A.\textsuperscript{3}, Sau S.\textsuperscript{3}

Unravelling the Structure and Reactivity of Supported Ni Particles in Ni-CeZrO\textsubscript{2} Catalysts

\textsuperscript{1}Università degli Studi di Torino, Department of Chemistry and NIS Centre of Excellence, Torino, Italy
\textsuperscript{2}ISTEC, Centro Nazionale delle Ricerche, Torino, Italy
\textsuperscript{3}ENEA, “Casaccia” Research Center, Rome, Italy

The talk deals with Ni-CeZrO\textsubscript{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.


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\textsubscript{2}, CeO\textsubscript{2}, MgO, Al\textsubscript{2}O\textsubscript{3}, CeO\textsubscript{2}/ZrO\textsubscript{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 Pt₃Sn/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 Pt₃Sn (fcc) alloy phase over carbon support can be achieved. The bimetallic Pt₃Sn/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
¹Department of Molecular Engineering, Graduate School of Engineering, Kyoto University, Kyoto, Japan
²Precursory 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 Nb₂O₅ 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.
RuOₓ-VOₓ/TiO₂ 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 RuOₓ/TiO₂ and bimetallic RuOₓ-VOₓ/TiO₂ catalysts has been studied in a fluidized bed photoreactor at high illumination efficiency. For RuOₓ/TiO₂, by increasing ruthenium loading ethanol conversion decreased while acetaldehyde selectivity increased. With bimetallic RuOₓ-VOₓ/TiO₂ 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, Schipunov Yu.A.3, Remplel A.A.2

**Design of the Nanocrystalline CdS/TiO2 Photocatalyst**

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

Catalysts active under visible light on the basis of the composite of cadmium sulfide and titania CdS/TiO2 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**

1Lomonosov Moscow State University, Moscow, Russia
2Institute 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 Au12 cluster is accompanied by the formation of complexes, where the hydrocarbon is bonded with low-coordinated atoms of the cluster. The preferable adsorption of C2H2 over C2H4 on 3D isomer of Au12 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 C2H2 and C2H4 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.\textsuperscript{1}, Ottenbacher R.V.\textsuperscript{1,2}, Bryliakov K.P.\textsuperscript{1}, Talsi E.P.\textsuperscript{1}
Non-Heme Iron and Manganese-Catalyzed Asymmetric Olefin Epoxidations with H\textsubscript{2}O\textsubscript{2}: Probing the Nature of Active Species by EPR Spectroscopic and Enantioselectivity Studies
\textsuperscript{1}Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
\textsuperscript{2}Novosibirsk State University, Novosibirsk, Russia

Chiral bipyrrrolidine-pyridine-based Fe and Mn complexes have been found to efficiently catalyze olefin epoxidation with H\textsubscript{2}O\textsubscript{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)MV=O(OC(O)R)]\textsuperscript{2+} complexes (M = Fe, Mn; R = alkyl). A consistent mechanism for the active species formation has been proposed.

OY-II-3  Ottenbacher R.V.\textsuperscript{1,2}, Talsi E.P.\textsuperscript{1}, Bryliakov K.P.\textsuperscript{1}
Highly Efficient, Regioselective and Stereospecific Oxidation of Non-Activated Aliphatic C-H Groups with H\textsubscript{2}O\textsubscript{2}, Catalyzed by Aminopyridine Manganese Complexes
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\textsuperscript{2}Novosibirsk State University, Novosibirsk, Russia

Manganese(II) complexes [LMn\textsuperscript{II}(OTf)\textsubscript{2}] bearing non-heme tetradentate aminopyridine ligands catalyse the oxidation of non-activated aliphatic C-H groups with H\textsubscript{2}O\textsubscript{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.\textsuperscript{1}, Sanieva D.V.\textsuperscript{1}, Molev O.V.\textsuperscript{1}, Fedorov S.P.\textsuperscript{1}, Oleinik I.V.\textsuperscript{2}, Ivanchev S.S.\textsuperscript{1}
Self-Immobilizing Catalysts for Ethylene Polymerization Based on Derivatives of bis(Phenoxy-Imine) Titanium Halide Complexes
\textsuperscript{1}St. Petersburg Department of Boreskov Institute of Catalysis SB RAS, St. Petersburg, Russia
\textsuperscript{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(phenoxo-imine) titanium (IV) chloride complexes functionalized with an oxyallyl group containing different number of CH\textsubscript{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.
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.

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

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 feedstocks, and methylisobutyl and diisobutyl ketones obtained by condensation of acetone, the byproduct of biobutanol production.

Methane Activation and Conversion on Ag/H-MFI Catalyst

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.

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

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.
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 Al₂O₃. 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.

Carbonylation of Dimethyl Ether on Rh/Cs₂HPW₁₂O₄₀:
Mechanism of the Reaction in the Presence of Methyl Iodide Promoter

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

Using ¹³C 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.

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.

Concentration Hysteresis in the Oxidation of Methane over Pt/γ-Al₂O₃

1Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
2Novosibirsk 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 O₂:CH₄ 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**

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\(^{2}\)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.

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**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.

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**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
¹University of Bayreuth, Bayreuth, Germany
²Max 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  Oscheakov 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
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²Novosibirsk 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 O₂ electroreduction.