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OVERVIEW PLENARY LECTURES

Monday, July 2, 2012
09:30  Water splitting on heterogeneous photocatalysts
K. Domen, University of Tokyo/J

13:50  Computational chemistry: a guide for understanding catalysts structure and function
P. Sautet, Ecole Normale Supérieure de Lyon and CNRS/F

Tuesday, July 3, 2012
09:00  Engineering polyolefin solutions using advanced catalysis
C. Kresge, Dow Chemical Company, Midland, MI/USA

Wednesday, July 4, 2012
09:00  Models in heterogeneous catalysis: what has been learned?
H. Freund, Fritz-Haber-Institute, Berlin/D

Thursday, July 5, 2012
09:00  Progress towards understanding the relationships between catalyst composition and structure and catalyst activity and selectivity
A. Bell, University of California, Berkeley, CA/USA

Friday, July 6, 2012
09:00  Design and study of molecular catalysts for small molecule activation and conversion
R. Periana, The Scripps Research Institute, Jupiter, FL/USA
Dear colleagues,

On behalf of the Conference Organizing Committee, I welcome you to the 15th International Congress on Catalysis, 28 years after the 8th Congress was held in Berlin. We hope that this meeting will reflect successfully the long tradition and current dynamics of the catalysis community in academia and industry. We have chosen Munich, because it is a vibrant center of research and technology and the home of two major universities and many academic centers and research institutes. Munich offers, however, also a lively cultural life ranging from Opera and Ballet to numerous museums combined with a wide variety of possibilities to sample local cuisine and last but not least the beer, that quintessential practical example of catalytic chemistry and engineering. We hope that the program that we have assembled will allow you to experience these unique traits of our city during a week filled with exciting catalysis science and technology.

Throughout its history, but specially so over the last four years, catalysis has emerged as the enabling technology in our transition towards sustainable utilization of energy resources and synthesis of chemicals, and in doing so will allow significant reductions of our carbon footprint and the elimination of the negative environmental impacts of chemical processes. We look forward to a week of intense discussion and free exchange of knowledge about all aspects of catalysis. The theme of the congress, „From fundamental understanding to catalyst design and novel processes“, highlights the rational approach to these developments by grounding industrial applications firmly on fundamental science, a tradition that has proved tremendously successful. The honorary chairman of the Congress, Prof. Gerhard Ertl, the 2007 Nobel Laureate stands as an excellent example of an approach that brings essential understanding into industrial processes and developments.

This 15th International Congress on Catalysis aims to provide a forum to show the transdisciplinary relations among theory, fundamental and applied research, as well as their realization in industry. The format and contents of the program offers the participants cross-disciplinary lecture threads that emphasize developments in diverse fields such as biocatalysis and organocatalysis, organometallic catalysis, but also photocatalysis and practical deployments of catalytic processes in industry. We have also introduced a new forum for presenting and exchanging ideas in more focused topics that are presented in parallel as posters. It is hoped that this will allow enhancing the level of involvement beyond what is possible with presenting posters.

We thank you for sharing your science, as we thank our industrial sponsors for their generous support. Without your input and without their help it would not have been possible to realize the program ahead of us. Whatever your area of expertise, we expect that knowledge will flourish and be shared during these next few days and that your new results and concepts will challenge alternate interpretations and change the way that we carry out our science in the future. We hope that you will enjoy this week with us, that you will renew the bonds with old friends and that you will leave Munich with new friends.

Johannes A. Lercher
(Chair, Organizing Committee of the 15th ICC)
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<td>C7A</td>
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### PROGRAM OVERVIEW

#### Sunday, July 1, 2012

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<tr>
<th>Time</th>
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<tr>
<td>15:00</td>
<td>Exhibitors stand assembly</td>
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<tr>
<td>17:00</td>
<td>Registration open</td>
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<tr>
<td>19:00</td>
<td>Welcome reception</td>
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#### Monday, July 2, 2012

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<tr>
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<td>PLENARY: Domen</td>
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<td>13 a</td>
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<tr>
<td>13 b</td>
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<td>14 a</td>
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<tr>
<td>14 c</td>
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<td>11a, 11b, 12a, 12b</td>
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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>10:50</td>
<td>KEYNOTE Apesteguia</td>
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<tr>
<td>11:10</td>
<td>KEYNOTE Li</td>
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<td>12:10</td>
<td>LUNCH BREAK</td>
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<td>13:50</td>
<td>Room Saal 1, PLENARY: Sautet</td>
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<td>KEYNOTE Ryoo</td>
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<td>15:10</td>
<td>KEYNOTE Olsenbye</td>
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<td>15:30</td>
<td>COFFEE BREAK</td>
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<td>17:50</td>
<td>KEYNOTE Beller</td>
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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>19:30</td>
<td>Poster party</td>
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<table>
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**subject to change**
### PROGRAM OVERVIEW

#### Tuesday, July 3, 2012

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<thead>
<tr>
<th>Time</th>
<th>Room Saal 1</th>
<th>Subject</th>
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<tr>
<td>9:00</td>
<td>PLENARY: Kresge</td>
<td>Fine chemicals and pharmaceuticals</td>
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<tr>
<td>10:00</td>
<td>COFFEE BREAK</td>
<td>Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster symposia 13-16</td>
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<tr>
<td>12:00</td>
<td>LUNCH BREAK</td>
<td>Room Saal 1 Awardee Fine chemicals and pharmaceuticals Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster session 1 for posters with even numbers</td>
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<tr>
<td>13:20</td>
<td>Room Saal 1</td>
<td>KEYNOTE Coles-Hamilton</td>
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<td>Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster symposia 17-20</td>
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<tr>
<td>17:20</td>
<td>Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster symposia 17-20</td>
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<tr>
<td>19:00</td>
<td>Free evening</td>
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#### Wednesday, July 4, 2012

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<th>Subject</th>
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<tr>
<td>9:00</td>
<td>PLENARY: Freund</td>
<td>Green synthesis Advances in computational catalysis Synthesis gas generation and conversion Organo-metallic catalysis Poster symposia 21-24</td>
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<td>10:00</td>
<td>COFFEE BREAK</td>
<td>Room 13 a 13 b 14 a 14 c 11a, 11b, 12a, 12b</td>
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<tr>
<td>10:20</td>
<td>KEYNOTE Sauer</td>
<td>Room Saal 1 Awardee Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster session 1 for posters with even numbers</td>
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<tr>
<td>13:20</td>
<td>Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster symposia 25-28</td>
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<tr>
<td>17:20</td>
<td>Mobile source emission Hydrotreating, hydrocracking and CC-coupling Industrial implementation Poster symposia 29-32</td>
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<tr>
<td>19:00</td>
<td>Bavarian evening at Paulaner am Nockherberg</td>
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### Thursday, July 5, 2012

**9:00** PLENARY: Bell

**10:00** COFFEE BREAK

**13 a** Platform and specialty chemicals from renewables

**13 b** Catalysis in CO₂ capture, sequestration and utilization

**14 a** Fuel cell catalysis

**14 b** Organo-catalysis/biocatalysis

**14 c** Poster symposia 33-36

**10:20** KEYNOTE Neurock

**10:40** Room Saal 1

**11:00** LUNCH BREAK

**12:00** Room Saal 1

**13:20** Awardee

**14:20** KEYNOTE Reetz

**14:40** ROADMAP CATALYSIS MILs

**15:00** Room Saal 1

**15:20** KEYNOTE Davis

**15:40** COFFEE BREAK

**16:20** Room Saal 1

**17:00** COFFEE BREAK

**17:20** KEYNOTE Bukhtiyarov

**18:00** Congress Dinner

**18:20** Poster symposia 37-40

**18:40** Poster symposia 41-44

**20:00** 24:00

**20:30** Students party

### Friday, July 6, 2012

**9:00** PLENARY: Penina

**10:00** COFFEE BREAK

**13 a** Selective oxidation

**13 b** From mechanistic insights to advances in reactor technology

**14 a** Catalysts for clean fuels production

**14 b** Green synthesis

**10:20** KEYNOTE Gladden

**10:40** Room Saal 1

**11:00** LUNCH BREAK

**12:00** Room Saal 1

**13:20** KEYNOTE Marin

**14:20** KEYNOTE Neurock

**14:40** ROADMAP CATALYSIS MILs

**15:00** Room Saal 1

**15:20** KEYNOTE Reetz

**15:40** COFFEE BREAK

**16:20** Room Saal 1

**17:00** COFFEE BREAK

**17:20** KEYNOTE Davis

**18:00** Congress Dinner

**18:20** Poster symposia 33-36

**18:40** Poster symposia 41-44

**20:00** 24:00

**20:30** Students party

**21:00** Congress Dinner

**24:00** 01:00

**01:00** Students party
Catalysts accelerate change – and together, so do we.

Catalysts enable us to efficiently convert hydrocarbons into the fuels and chemicals our customers need. BP continuously strives to understand and develop new catalysts to improve our processes and products.

We believe in exploring innovative solutions, with our research partners, scientists and engineers through our global university programmes. Together we are developing novel catalysts and processes as well as biocatalysis for the generation of new energy resources.

Find out more about BP at www.bp.com
### Lecture Program

**Monday, July 2, 2012**

#### Room Saal 1

<table>
<thead>
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<th>Event</th>
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<tr>
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<tr>
<td>09:10</td>
<td><strong>PLENARY LECTURE</strong></td>
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#### Room 13 b

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<tr>
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<td><strong>Novel routes to catalysis via nanotechnology</strong></td>
</tr>
<tr>
<td>12:10</td>
<td>Lewis-acid catalysis using metallocalixarenecomplexes: Bridging the heterogeneous-homogeneous gap</td>
</tr>
<tr>
<td>13:50</td>
<td><strong>PLENARY LECTURE</strong></td>
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<tr>
<td>15:30</td>
<td>COFFEE BREAK</td>
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### Event Details

**Novel routes to catalysis via nanotechnology**

- Chairs: A. Endoheyt, University of Szegez/H; V. Karazhev, UDP LLC a Honeywell Company, Des Plains, IL/USA
- **Catalyst design at the subnanometer scale: the role of size, composition, support and structural fluctuonality**
  - S. Lee, C. Yin, G. Koran, G. Ferguson, J. Greeley, L. Curtis, B. Lee, S. Sefert, R. Winans, Argonne National Laboratory, IL/USA; M. di Vece, S. Vartia, Argonne National Laboratory, IL and Yale University, New Haven, CT/USA
- **2D zeolites as practical and fundamental expansion of zeolites into new dimensions**
  - W.J. Roth, J. Celka, Institute of Physical Chemistry of the AS of the Czech Republic, Prague/CZ
- **Structural properties of acid and redox surface sites on [V,Al]-ITQ-6 bifunctional nanosheets**
  - M.K. de Piets, C.A. Franchini, M.A. Praga, Instituto Nacional Tecnologia, Rio de Janeiro/BR; H.O. Pastore, UNICAMP, Campinas/BR
- **First-principles design of highly active and selective CeO2 catalysts for phosgene-free synthesis of aromatic isocyanates**
  - S. Laursen, D. Combilla, M. Boronat, A. Corma, Universidad Politecnica Valencia-CSIC, Valencia/E
- **LUNCH BREAK (Lunch is available for self-payment at the congress venue)**

**Room Saal 1**

- Chairs: J. Sauer, Humboldt-Universität Berlin/D; N. Ritsch, TU München, Garching/D
- **PLENARY LECTURE**
  - Computational chemistry: a guide for understanding catalysts structure and function
  - P. Saudet, Ecole Normale Superieure de Lyon and CNRS/F

**Room 13 b**

- ** Novel routes to catalysis via nanotechnology**
  - Chairs: T. Tatsumi, Tokyo Institute of Technology, Yokohama/J; C. Louis, Université Pierre et Marie Curie, Ivy sur Seine/F
- **KEYNOTE LECTURE**
  - Surfactant-tailored hierarchical zeolites for high catalytic performance
  - R. Ryoo, Korea Advanced Institute of Science and Technology, Daejeon/ROK
## Lecture Program

**Monday, July 2, 2012**

### Room Saal 1

**09:00**

**OPENING**

Johannes A. Lercher, TU München/D  
Chairman of ICC 2012  
Walter Leitner, RWTH Aachen University/D  
Chairman of the German Catalysis Society  
Can Li, Dalian Institute of Chemical Physics/PRC  
Chairman of IACS

### Room 14 c

**17:50**

**Cross-disciplinary workshop photocatalysis**

Chair: J.-M. Herrmann, IRCELYON-CNRS, Villeurbanne/F  
Chairs: M.J. Bowker, Cardiff University, Wales/UK; V.N. Parmon, Boreskov Institute of Catalysis, Novosibirsk/RUS

**Thermodynamics and mechanism of photocatalytic CO₂ reduction in the gas and the liquid phase**

D. Uner, M.M. Oymak, Middle East Technical University, Ankara/TR; B. Ipek, Middle East Technical University, Ankara/TR and University of Delaware, Newark, DE/USA

**18:10**

**Slow photon photocatalytic enhancement in titania inverse opal photonic crystals**

V. Jovic, T. Söhnle, J.B. Melson, G.N. Waterhouse, The University of Auckland/NZ

**18:30**

**Enhanced photocatalytic activity of LaTiO₃N by Ca-modification**


**18:50**

**Understanding the high reducibility of gallium(III)-doped ceria**

M. Catarakis, F. Teisens, University P.M. Cune, Paris/F; M.J. Vecchietti, S. Collins, UNL CONICET, Santa Fe/AR; S. Bernal, University of Cadiz/E; A. Bonivardi, UNL CONICET, Santa Fe/AR

**19:10**

**Photocatalytically active hybrid thin films from ordered mesoporous TiO₂ by electrochemical deposition of co-catalysts in the pores**

M. Wark, Ruhr-Universität Bochum/D; I. Bannat, A.A. Ismail, D.W. Bahnemann, University Hannover/D

**21:30**

**Poster party**

### Room Saal 1

**09:30**

**PLENARY LECTURE**

Water splitting on heterogeneous photocatalysts

K. Domen, University of Tokyo/J

**11:00**

**COFFEE BREAK**

**Cross-disciplinary workshop photocatalysis**

Chair: K. Domen, The University of Tokyo/J; D. Uner, Middle East Technical University, Ankara/TR

**10:50**

**Historical recall of the last 50 years of photocatalysis**

J.-M. Herrmann, Université Lyon 1, Villeurbanne/F

**11:10**

**Photocatalytic hydrogen production: the role of metal centres**

M. Bowker, H. Bahruji, C. Morton, P. Davies, C. Brookes, Cardiff University/UK

**11:30**

**Photocatalytic hydrogen evolution from glycerol under visible light**

E. Kozlova, T. Lyubina, A. Vorontsov, V. Parmon, Borekov Institute of Catalysis, Novosibirsk/RUS

**11:50**

**KEYNOTE LECTURE**

The roles of cocatalyst and junctions in photocatalytic hydrogen production utilizing solar energy

C. Li, Dalian Institute of Chemical Physics/PRC

**12:30**

**LUNCH BREAK** (Lunch is available for self-payment at the congress venue)

### Room 14 c

**09:30**

**PLENARY LECTURE**

Computational chemistry: a guide for understanding catalysts structure and function

P. Sautet, Ecole Normale Supérieure of Lyon and CNRS/F

**11:00**

**COFFEE BREAK**

**Cross-disciplinary workshop photocatalysis**

Chair: H. Niemantsverdriet, Eindhoven University of Technology/NL; M. Wark, Ruhr Universität Bochum/D

**14:50**

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M. Wark, Ruhr-Universität Bochum/D; I. Bannat, A.A. Ismail, D.W. Bahnemann, University Hannover/D
Tuesday, July 3, 2012

**PLENARY LECTURE**
Engineering polyolefin solutions using advanced catalysis
C. Kresge, Dow Chemical Company, Midland, MI/USA

**COFFEE BREAK**

**Fine chemicals and pharmaceuticals (continued)**

**Chairs:** M. Iwamoto, Tokyo Institute of Technology, Yokohama/J; S. Jaenicke, National University of Singapore/SGP

**N-H activation by Rh via metal-ligand cooperation**
M. Feller, Y. Diskin-Posner, L.J.W. Shimon, E. Ben-Ari, D. Milstein, Weizmann Institute of Science, Rehovot/IL
10:20

**Mild and selective C-H oxidation catalysis with Cp*Ir complexes – mechanism & scope of application**
U. Hintermair, M. Zhou, R. Crabtree, Yale University, New Haven, CT/USA
10:40

**Role of subsurface hydrogen diffusion in hydrocarbon conversions on supported model catalysts**
S. Schauermann, W. Ludwig, A. Savara, H.-J. Freund, Fritz Haber Institute, Berlin/D
11:20

**Metathetical depolymerisation of solid state acrylonitrile-butadiene-rubber (NBR)**
G. Rempel, Q. Pan, J. Wu, Y. Liu, University of Waterloo/CDN
11:40

**LUNCH BREAK** (Lunch is available for self-payment at the congress venue)

**AWARD LECTURE INTERNATIONAL CATALYSIS AWARD**
Catalysts live and up close: heterogeneities in space and time
B.M. Weckhuysen, Utrecht University/NL
13:20

**Fine chemicals and pharmaceuticals**

**Chairs:** S. Perathoner, University of Messina/I; B. Lücke, Leibniz-Institut für Katalyse e.V., Rostock/D

**Immobilising homogeneous catalysts using water, ionic liquids or supercritical fluids**
14:20

**Poster session 1 – for even poster numbers**

**Transformation of aromatic molecules and heteroatom functionalization**

**Chairs:** E. Hensen, Eindhoven University of Technology/NL; Z. Sobaik, J. Heyrovsky Institute, Praha/CZ

**m-xylene isomerization over ZSM-5/MCM-41 composites with adjustable porosity**
J.J. Blaker, T. Odena, M.N. Altjat, King Fahd University of Petroleum and Minerals, Dhahran/SAR
17:20

**UZM-14 for improved performance in aromatic transalkylation**
E.P. Bildard, M.G. Gatter, R.W. Broach, D.S. Luyf, UOP - A Honeywell Company, Des Plaines, IL/USA
17:40

**Hydroalkylation of benzene with acetone over bifunctional solid catalysts**
O.V. Shul’kina, D.A. Ponomareva, I. Ivnova, Moscow State University/RUS
18:00

**Highly selective N-alkylation of amines with alcohols**
H.H. Liu, S. Jaenicke, National University of Singapore/SGP
18:20

**Enhanced selective hydrogenation of nitroarenes over Au supported on 8-MoO, C and 8-MoO, CAl,O,**
N. Perret, X. Wang, M.A. Keane, Heriot-Watt University, Edinburgh/UK; L. Detaino, C. Potvin, C. Louis, Université Pierre et Marie Curie - LPMC, Paris/F
18:40

**19:00**

At Süd-Chemie, we create original solutions that shape the way you see the future. Innovation is core to our business and has been our focus through our 150-year history. Our catalysts boost the performance and value of our customers’ operations, limiting their impact on the environment and ensuring that finite raw materials and energy are used efficiently.

Discover what the future holds for your business at www.sud-chemie.com
**Tuesday, July 3, 2012**

**Room Saal 1**

09:00  **PLENARY LECTURE**

Engineering polyolefin solutions using advanced catalysis

C. Kresge, Dow Chemical Company, Midland, MI/USA

10:00  **COFFEE BREAK**

**Mobile source emission**

Chairs: G. Bellussi, ENI S.p.A., San Donato Milanese/I; B.C. Gates, University of California, Davis, CA/USA

10:20  **KEYNOTE LECTURE**

Automotive emission control: a crowning achievement in heterogeneous catalysis

R. Farrauto, BASF and Columbia University, Iselin, NJ/USA

11:00  **Aging characteristics of Pd/Al₂O₃ automotive catalyst materials**

X. Chen, J.W. Schwank, University of Michigan, Ann Arbor, MI/USA; Y. Cheng, M. Jäger, R.W. McCabe, Ford Motor Company, Dearborn, MI/USA

11:20  The development of Short Time on Stream (STOS) SSITKA to identify true reaction intermediates in automotive catalysts

P. Burch, C. Hardacre, S. Chansai, Queen’s University Belfast/UK

11:40  Red-ox dynamics of Al₂O₃ and Ce₁₋ₓZrₓO₂ supported Pd studied by time-resolved modulation excitation hard X-ray diffraction


12:00  **LUNCH BREAK** (Lunch is available for self-payment at the congress venue)

**Room Saal 1**

13:20  **AWARD LECTURE INTERNATIONAL CATALYSIS AWARD**

Catalysts live and up close: heterogeneities in space and time

B.M. Weckhuysen, Utrecht University/NL

**Room Saal 1**

14:20  **Mobile source emission**

Chairs: O. Kröcher, Paul Scherrer Institute, Villigen/CH; F. Ribeiro, Purdue University, West Lafayette, IN/USA

14:40  Effect of cation nonstoichiometry on La₄MnO₁₂ perovskite for NO oxidation to NO₂

J. Chen, X. Wang, M. Shon, Tianjin University/PRC; G. Qi, W. Li, General Motors, Warren, MI/USA

18:00  Electrochemical-catalytic converter for NOx emission control of lean-burn gasoline and diesel engines

T. Huang, National Tsing Hua University, Hsinchu/TW

**Room 13 b**

17:20  NO-oxidation on Pt: reversible deactivation under reaction conditions


17:40  Cu-SSZ-13 catalysts for the selective catalytic reduction of NOx with NH₃: catalyst characterization and reaction mechanisms


18:40  – 19:00

Inhibition of Rh sintering on ZrO₂ compound with Al₂O₃ as a diffusion barrier


**Committed to catalysis**

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Tuesday, July 3, 2012
Room Saal 1

09:00
PLENARY LECTURE
Engineering polyolefin solutions using advanced catalysis
C. Kreike, Dow Chemical Company, Midland, MI/USA

10:00
COFFEE BREAK

Hydrotreating, hydrocracking and CC-coupling

Chairs: S.H. Moon, Seoul National University/ROK; R. Prins, ETH Zürich/CH

10:20
Sulfide catalysis without coordinatively unsaturated sites. Hydrogenation, cis-trans isomerization and H/D, scrambling over Mo5 and WS6
T. Drescher, Ruhr-Universität Bochum/D; Z. Huang, W. Bensch, L. Kiefer, Universität Kiel/D; W. Grünert, Ruhr-Universität Bochum/D

10:40
Synthesis of metal phosphides by hydrogenation plasma reduction and their performance in hydrodesulfurization
A. Wang, M. Qin, D. Piao, Y. Wang, J. Guan, X. Li, Y. Hu, Dalian University of Technology/PRC

11:00
New catalyst system for the conversion of oil residues

11:20
Deoxygenation mechanisms on Ni-promoted MoS2 bulk catalysts: a combined experimental and theoretical study
M. Ruinart de Brimont, C. Dupont, A. Daudin, IFPEN, Solaize/F; C. Geantet, IRCELYoN, Villeurbanne/F; P. Raybaud, IFPEN, Solaize/F

11:40
Selective methane coupling to ethane and hydrogen catalysed by grafted tantalum or tungsten hydride

12:00
LUNCH BREAK (Lunch is available for self-payment at the congress venue)

Room Saal 1

13:20
AWARD LECTURE INTERNATIONAL CATALYSIS AWARD
Catalysts live and up close: heterogeneities in space and time
B.M. Weckhuysen, Utrecht University/NL

Hydrotreating, hydrocracking and CC-coupling

Chairs: V.J. Parvez, University of Bucharest/RO; J. Schwark, University of Michigan, Ann Arbor, MI/USA

14:20
Ring opening of decalin over monofunctional WO3/Al2O3 or Ir/Al2O3 and bifunctional Ir/WO3/Al2O3 catalysts
R. Moraes, K. Thomas, S. Thomas, LCS, Caen/F; S. Van Dork, G. Grasso, Total Petrochemicals Research, Fkxy/B; J.P. Gilson, M. Houalla, LCS, Caen/F

14:40
Selective ring opening of naphthenes: from mechanistic studies with a model feed to the upgrading of a hydroprocessed gas oil
Y. Galemme, M. Ferrari, Eni Refining & Marketing Division, San Donato Milanese/I; S. Rabl, J. Wettkamp, University of Stuttgart/D

15:00
Poster session 1 – for even poster numbers

Tuesday, July 3, 2012
Room 14a

Hydrotreating, hydrocracking and CC-coupling


17:20
KEYNOTE LECTURE
Unique catalysis chemistry of nano-confined systems
X. Bao, Dalian Institute of Chemical Physics of the CAS/PRC

18:00
Synthesis and application of beta-KIT-6 composites in 4,6-DMDT hydodesulfurization
H. Wu, A. Duan, Z. Zhao, G. Jiang, J. Liu, China University of Petroleum, Beijing/PRC

18:20
Synthesis and hydrosulfurization properties of fullerene-like (Co, Ni)/Mo5 catalysts
G. Betchab, A. Nogueira, R. Zghaiou, E. Blancon, P. Alansoiev, CNRS/University Lyon I, Villeurbanne/F; D. Uzio, IFP Energies Nouvelles, Solaize/F

18:40
Unsupported NiMo5 sulfide catalysts for hydrosulfurization of dibenzothiophene by thermal decomposition of thiosalts
Y. H. G. Xiong, C. Liang, Dalian University of Technology/PRC, C.T. Williams, J. Lauterbach, University of South Carolina, Columbia, SC/USA

INDUSTRY-LEADING MINDS, OF COURSE.

Even with a wide range of proven catalysts like CENTERA® in our portfolio and nearly 300 cycles of commercial ULSD operations around the world, at CRITERION, we know the ultimate key to performance is our people. At Shell, we know that people are the heart of our Technology Platform and the key to not just surviving, but Thriving in the difficult refining industry. Rest assured, the next generation of refining technology is in good hands (and heads).
Tuesday, July 3, 2012

**Room Saal 1**

**PLENARY LECTURE**

Engineering polyolefin solutions using advanced catalysis  
C. Kreige, Dow Chemical Company, Midland, MI/USA

**COFFEE BREAK**

**Cross-disciplinary workshop industrial implementation**

Chairs: S. Alerasool, BASF SE, Ludwigshafen/D; J. Bricker, UOP Research Center – A Honeywell Company, Des Plaines, IL/USA

**INTRODUCTION**

Raw materials, energy & sustainability: fundamental and applied research  
J.N. Armor, GlobalCatalysis.com LLC, oilfield, PA/USA

Catalytic hydrodeoxygenation of biomass pyrolysis oil to transportation fuels  

Furfural – A promising platform for biofuels  
J.-P. Lange, E. van der Heide, J. van Bijnen, Shell Global Solutions Int., Amsterdam/NL; R. Price, Shell Global Solutions UK, Thornton/UK

Dry reforming of CH4 with CO2 at elevated pressures  

Catalytic conversion of methanol to olefins: some progresses on catalytic materials and reaction mechanism  
Z. Xie, SINOPEC Corp., Beijing/PRC; Z. Liu, C. Wang, Y. Wang, H. Yang, L. Ren, H. Liu, J. Teng, Shanghai Research Institute of Petrochemical Technology-SINOPEC/PRC

**LUNCH BREAK** (Lunch is available for self-payment at the congress venue)

**Room Saal 1**

Chairs: A. Corma, Universidad Politecnica de Valencia/E; M. Che, Université P. et M. Curie, Paris/F

**AWARD LECTURE INTERNATIONAL CATALYSIS AWARD**

Catalysts live and up close: heterogeneities in space and time  
B.M. Weckhuysen, Eindhoven University of Technology/NL

**Cross-disciplinary workshop industrial implementation**

Chairs: T. Tacke, Evonik Industries AG, Hanau/D; N.J. Schödel, Linde AG, Pullach/D

**Self-assembly of noble metal alloys for ultra low temperature oxidation catalysis**  
C.H. Kim, M. Balogh, S.H. Oh, W. Li, M. Verbrugge, General Motors Company, Warren, MI/USA; D.H. Kim, C.H.F. Peden, Pacific Northwest National Laboratory, Richland, WA/USA

Understanding automotive catalytic washcoats using imaging techniques  

**Poster session 1 – for even poster numbers**

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**Room 14 c**

**Cross-disciplinary workshop industrial implementation**


Development of an industrial catalyst for sustainable chlorine production  
A. Wolf, O.P.-K. Schlüter, L. Mecom, Sayer Technology Services, Leverkusen/D

Mechanistic study of hydrocarbon chain growth in the Fe-catalysed Fischer-Tropsch synthesis  
J.V. Fletcher, Sasol Technology R&D, Eindhoven/NL; N.S. Govender, Sasol Technology R&D, Sasolburg/ZA; M.H.J.M. de Croon, J.C. Schouten, Eindhoven University of Technology/NL

Operando FTIR investigations of Iridium catalysed hydroformylation  
B. Fink, D. Heiss, M. Pockers, D. Rosenthal, Evonik Industries AG, Marl/D; B. Hanmebauer, Evonik Industries AG, Hanau/D

Fundamental insights into a new generation of catalysts for the manufacture of acrylonitrile via propylene ammoxidation  
J. Bräunl, M. Toll, S. Motorna, INEOS Technologies, Naperville, IL/USA

Influence of Tp on the performance of a highly isoselective metallocene catalyst for propylene polymerisation  
K. Reischl, L. Pescorri, Borealis Polyolefine GmbH, Linz/A
### Lecture Program

**Wednesday, July 4, 2012**

#### Room Saal 1

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>09:00</td>
<td><strong>PLENARY LECTURE</strong> Models in heterogeneous catalysis: what has been learned?</td>
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<tr>
<td></td>
<td>H. Freund, Fritz-Haber-Institute, Berlin/D</td>
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<tr>
<td>10:00</td>
<td><strong>COFFEE BREAK</strong></td>
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**Green synthesis (to be continued on Friday)**

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<tr>
<th>Time</th>
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<tr>
<td>10:20</td>
<td>Phosphines become green: Pd-catalysed P-C coupling of molecules with carboxylic acids in water</td>
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<tr>
<td></td>
<td>M. Ranocchiari, S. Rummelt, J.A. van Bokhoven, Paul Scherrer Institut, villigen PSI/CH</td>
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<tr>
<td>10:40</td>
<td>Performance of W-Nb-O/ZrO2 for the gas phase dehydrogenation of glycerol to acrolein</td>
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<td>M. Massa, A. Andersson, Lund University/S</td>
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<tr>
<td>11:00</td>
<td>Heterogeneous catalysts for intermolecular amination reactions</td>
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<td></td>
<td>A. Posters, P. Valverdes, D. De Vos, K.U. Louven, Heverlee/B</td>
</tr>
<tr>
<td>11:20</td>
<td>Nanostructured Ni-based catalysts for hydrogenolysis of polyalcohols</td>
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<td></td>
<td>T. Sokic, T. Schmidt, M. Hronec, Slovak University of Technology, Bratislava/SK</td>
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<tr>
<td>11:40</td>
<td>Making the best of the unique properties of water – a special solvent for cross-coupling reactions</td>
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<td>J. Eppinger, D. Janik, P. Walter, S. Laur, A. Zernick, J. Ramasamy, King Abdullah University of Science and Technology, KAUST, Thuwal/SAR</td>
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<tr>
<td>12:00</td>
<td><strong>LUNCH BREAK</strong> (Lunch is available for self-payment at the congress venue)</td>
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#### Room 13 a

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>13:20</td>
<td>Catalytic chemicals production using supported metal catalysts with water and carbon dioxide</td>
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<tr>
<td></td>
<td>M. Shirai, A. Yamaguchi, O. Sato, N. Hiyoshi, National Institute of Advanced Industrial Science and Technology (AIST), Sendai/J</td>
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<tr>
<td>13:40</td>
<td>Ru-catalyzed hydroamination of terminal alkynes – reaction development, mechanism and applications</td>
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<td>L. Gooßen, M. Arndt, A. Fromm, K.S.M. Salh, A. Buba, F. Menges, G. Niedner-Schatteburg, TU Kaiserslautern/D</td>
</tr>
<tr>
<td>14:00</td>
<td>Sulfonated hybrid solid material as catalyst for multi-component reactions (MCR)</td>
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<td>S. Santiago, J. Viveros, Autonomous Metropolitan University, Iztapalapa, Mexico, D.F./MEX</td>
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<tr>
<td>14:20</td>
<td>Nanoscopic magnesium fluorides - tunable catalysts for fine chemicals synthesis and biomass capitalisation</td>
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<td>S. Coman, A. Negoi, A. Nae, V. I. Panavuscu, University of Bucharest/RO; S. Wuttke, University of Munich/DE; E. Kemnitz, Humboldt-Universität zu Berlin/D</td>
</tr>
<tr>
<td>14:40</td>
<td>Silica supported alkaline earths for aldol condensation: optimum acid and base bifunctionality</td>
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<td>W. Shen, G. Tompsett, R. Xing, G. Huber, W. Curtis Conner J., University of Massachusetts, Amherst, MA/USA</td>
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<tr>
<td>15:00</td>
<td><strong>Poster session 2</strong> – for odd poster numbers</td>
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**Olefins and production and conversion**

<table>
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<tr>
<td>17:20</td>
<td>Sodium plus sulfur promoted supported iron catalysts for the selective production of lower olefins from synthesis gas</td>
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<td>H.M. Torres Galvis, J.H. Bitter, K.P. de Jong, Utrecht University/NL</td>
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<tr>
<td>17:40</td>
<td>Alumina catalyzed oxidative dehydrogenation of ethylbenzene. Creating selective sites by thermal treatments</td>
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<td>V. Zverina, H.J. Heeres, I. Molian Cabrera, University of Groningen/NL; G. Niederlof, F. Kapteijn, TU Delft/NL</td>
</tr>
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Wednesday, July 4, 2012

Room Saal 1

09:00 PLENARY LECTURE
Models in heterogeneous catalysis: what has been learned?
H. Freund, Fritz-Haber-Institute, Berlin/D

10:00 COFFEE BREAK

Advances in computational catalysis

Room 13 b

10:20 KEYNOTE LECTURE
Selective oxidation by solid oxides - mechanisms and catalysts
J. Sauer, Humboldt-Universität zu Berlin/D

11:00 Efficient coupling between microkinetic modeling and CFD: towards a fully first-principles catalytic reaction engineering
M. Maestri, A. Cuoci, Politecnico di Milano/I

11:20 The role of the metal-cation ensemble as the active sites in catalytic reaction
W.X. Li, Dalian Institute of Chemical Physics/PRC

11:40 Designing catalysts based on their electronic structure fingerprints: predictive structure-performance models for metal alloy catalysts
H. Xin, University of Michigan, Ann Arbor, MI/USA; E. Nikolla, Wayne State University, Detroit, IL/USA; S. Linic, University of Michigan, Ann Arbor, MI/USA

12:00 LUNCH BREAK (Lunch is available for self-payment at the congress venue)

Room 13 b

13:20 Morphology of sub-nanometer platinum particles supported on γ-Al2O3: effects of support chlorination and H2 atmosphere
C. Mager-Maury, C. Chizallet, IFP Energies nouvelles, Solaize/F; P. Sautet, ENS Lyon/F; P. Raybaud, IFP Energies nouvelles, Solaize/F

13:40 Reaction path analysis of propene selective oxidation over V2O5 and V2O5/TiO2
K. Alexopoulos, M.-F. Reyniers, G.B. Marin, Ghent University/B

14:00 Mechanistic and microkinetic studies of N2O decomposition over alkaline earth nanooxides – tuning the elementary steps by basicity variation
F. Zasada, W. Piskorz, P. Steinmackowski, A. Klotz, W. Sojka, Jagiellonian University, Krakow/PL

14:20 A comparison in activity between transition-metal oxides and transition metals
A. Vejvodic, Stanford University, CA/USA; F. Albild-Pedersen, F. Studt, T. Bigsaard, SLAC National Accelerator Laboratory, Menlo Park, CA/USA; J.K. Norskov, Stanford University, CA/USA

14:40 Towards a first-principles electronic structure based understanding of reactor response in heterogeneous catalysis
S. Maters, K. Reuter, TU München, Garching/D

15:00 Poster session 2 – for odd poster numbers

Wednesday, July 4, 2012

Room 13 b

17:20 CO2 reforming of CH4 to produce synthesis gas over modified and un-modified Ni/Al2O3 catalysts
S. Sengupta, G. Deo, Indian Institute of Technology Kanpur/IND

17:40 CO2 hydrogenation over Ru electropromoted catalysts
D. Thevetis, S. Soudrie, A. Katsaounis, C. G. Vayenas, University of Patras/GR

18:00 Understanding the reaction mechanism and the role of Rh nanoparticles in the CO2 hydrogenation to methane at low temperature
A. Karetsou, C. Svalos, F. Ruiz, Université Catholique de Louvain/B

18:20 Carbon nanotubes intercrossed Cu/Zn based catalyst for CO2 hydrogenation to methanol/dimethyl ether
O. Zheng, Y.Z. Zuo, X. An, M.H. Han, J.F. Wang, Y. Jin, F. Wei, Tsinghua University, Beijing/PRC

18:40 Catalytic conversion of CO2 and ethylene to acrylic acid
S.Y.T. Lee, M. Cokoja, F.E. Kühn, M. Drees, TU München, Garching/D

19:00 Bavarian Evening at the Paulaner am Nockherberg (Ticket necessary)
### Lecture Program

**Wednesday, July 4, 2012**

**Room Saal 1**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00</td>
<td><strong>PLENARY LECTURE</strong></td>
<td>Models in heterogeneous catalysis: what has been learned?</td>
</tr>
<tr>
<td></td>
<td></td>
<td>H. Freund, Fritz-Haber-Institute, Berlin/D</td>
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<tr>
<td>10:00</td>
<td><strong>COFFEE BREAK</strong></td>
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</table>

**Synthesis gas generation and conversion**

**Chairs:** M. Claeys, University of Cape Town/ZA; M. Flytzani-Stephanopoulos, Tufts University, Medford, MA/USA

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>10:40</td>
<td>Catalytic transformation of biofuels into synthesis gas and hydrogen over monolithic catalysts</td>
<td>H. Moezzenbeg, V. Sadykov, V. Peliproko, Boreskoff Institute of Catalysis, Novosibirsk/RUS; A.C. Roger, University of Strasbourg/F; J.P.H. Ross, University of Limetick/RB</td>
</tr>
<tr>
<td>11:00</td>
<td>Investigation of cobalt coordination environment and support morphology effects under reaction conditions in ethanol steam reforming</td>
<td>I. Ilgaz Soykal, B. Bayram, U.S. ozkan, The ohio State University, Columbus, OH/USA</td>
</tr>
<tr>
<td>11:20</td>
<td>New approach for kinetic modeling of Fisher-Tropsch on cobalt based catalysts</td>
<td>M. Holmen, Norwegian University of Science and Technology, Trondheim/N</td>
</tr>
<tr>
<td>11:40</td>
<td>An in situ XRD reaction cell for the characterisation of a Co/γ-Al2O3 catalyst under Fischer-Tropsch synthesis conditions</td>
<td>B. Clapham, T. Fettig, N. Fischer, M. Claeys, University of Cape Town, Rondelbosch/ZA</td>
</tr>
<tr>
<td>12:00</td>
<td><strong>LUNCH BREAK</strong> (Lunch is available for self-payment at the congress venue)**</td>
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**Room 14 a**

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Authors</th>
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</thead>
<tbody>
<tr>
<td>17:40</td>
<td>Dynamic structure and catalytic performance of Pd/ZnO and Pd/Ga2O3 methanol reforming catalysts: an in situ study</td>
<td>K. Foettigner, A. Haghoffer, Vienna University of Technology/A; M. Nachtigal, Paul-Scherrer-Institute, Witten/CH; J.A. van Bokhoven, ETH Zurich and Paul-Scherrer-Institute, Witten/CH; G. Rupprecht, Vienna University of Technology/A</td>
</tr>
<tr>
<td>18:00</td>
<td>Catalytic consequences of oxygen chemical potential during alkane oxidation on group VIII metal clusters</td>
<td>Y.H. Choe, University of California at Berkeley, CA/USA; C. Buda, University of Virginia, Charlottesville, VA/USA; M. Garcia-Diezquez, University of California at Berkeley, CA/USA; M. Neurock, University of Virginia, Charlottesville, CA/USA; E. Iglesia, University of California at Berkeley, CA/USA</td>
</tr>
<tr>
<td>18:20</td>
<td>How to prepare a good methanol synthesis catalyst: structure-performance-relationships of Cu/ZnO/Al2O3</td>
<td>M. Behrens, R. Schlogl, Fritz-Haber-Institute, Berlin/D</td>
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<tr>
<td>19:00</td>
<td>Bavarian Evening at the Paulaner am Nockherberg (Ticket necessary)</td>
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</tbody>
</table>
Wednesday, July 4, 2012

Room Saal 1

09:00
PLENARY LECTURE
Models in heterogeneous catalysis: what has been learned?
H. Freund, Fritz-Haber-Institute, Berlin/D

10:00
COFFEE BREAK
Room 14 c

Cross-disciplinary workshop organo-metallic catalysis

Chairs: M. Beller, Leibniz-Institut für Katalyse e.V., Rostock/D; C. Coperet, ETH Zürich/CH

10:20
INVITED LECTURE
Hydrogen transfer processes and sp³C-H functionalization
M. Achard, B. Sundararaju, Z. Sahli, C. Bruneau, University of Rennes/F

10:40
INVITED LECTURE
Organometallic nanoparticles: large organometallic complexes or more?
B. Chaudret, CNR Toulouse/F

11:00
The rise of the zinc age in homogeneous catalysis?
S. Enthaler, TU Berlin/D

12:00
LUNCH BREAK (Lunch is available for self-payment at the congress venue)
Chairs: F.E. Kühn, Technische Universität München, Garching/D; R. Kumar, TATA Chemicals Ltd., Pune Mulshi/IND

13:20
INVITED LECTURE
Oxidative coupling, chemistry between two „nucleophiles“
A. Lei, Wuhan University/PRC

14:00
INVITED LECTURE
Organometallic chemistry and catalysis with water soluble phosphines: the enlightening story of PTA
M. Peruzzini, CNR Florence/I

14:40
Iron-catalyzed reactions: the many roles of olefins
A. Jacoby von Wangelin, University of Regensburg/D

15:00
Poster session 2 – for odd poster numbers
Chairs: B. Chaudret, CNRS, Toulouse/F; C. Bruneau, CNRS Université de Rennes/F

17:20
INVITED LECTURE
Homogeneous catalysis applied to the production of pharmaceutical products
L. Lefort, DSM Innovative Synthesis B.V., Geleen/NL

18:00
INVITED LECTURE
Catalytic carbon dioxide – formic acid systems for hydrogen storage and delivery
G. Laurenczy, EPFL Lausanne/CH

18:40
Catalysis with oleochemicals
M.A.R. Meier, Karlsruhe Institute of Technology KIT/D

19:00
Bavarian Evening at the Paulaner am Nockherberg (Ticket necessary)
Thursday, July 5, 2012

Room Saal 1

09:00
PLENARY LECTURE
Progress towards understanding the relationships between catalyst composition and structure and catalyst activity and selectivity
A. Bell, University of California, Berkeley, CA/USA

10:00
COFFEE BREAK

Platform and specialty chemicals from renewables

Chairs: N. Essayem, Université de Lyon 1, Villeurbanne/F; A.K. Datye, University of New Mexico, Albuquerque/USA

10:20
Molecular aspects of acid-catalyzed sugar conversion
E.A. Pidko, G. Yang, E.J.M. Hensen, Eindhoven University of Technology/NL

10:40
Acid-catalysed direct formation of sec-butyl levulinate from the reaction of cellulose with 2-butene in super-critical conditions
S. Sapaly, M. Eternot, F. Rataboul, N. Essayem, CNRS-IRCELYoN, villeurbanne/F

11:00
Polyoxometalate-supported Ru nanoparticles as efficient catalysts for conversions of cellulose and inulin to hexitols in H₂O
W.P. Deng, M. Liu, Z.C. Tang, Y.L. Wang, Q.H. Zhang, Y. Wang, University of Xiamen/PRC

11:20
Hydrolytic hydrogenation of hemicellulose
D. Murzin, B. Kusema, N. Kumar, P. Mäki-Arvela, T. Salmi, Åbo Akademi University, Turku/FIN; L. Faba, E. Diaz, S. Ondez, University of Oviedo/E

11:40
Conversion of lignocellulose into platform chemicals by carbon and supported metal catalysts
A. Fukuoka, Hokkaido University, Sapporo/J

12:00
LUNCH BREAK (Lunch is available for self-payment at the congress venue)

Room Saal 1

Chairs: A.T. Bell, University of California, Berkeley, CA/USA; C. Li, Dalian Institute of Chemical Physics/PRC

13:20
AWARD LECTURE HEINZ HEINEMANN AWARD
Catalysis using gold nanoparticles
G. Hutchings, University of Cardiff/UK

Platform and specialty chemicals from renewables

Chairs: C.L. Marshall, Argonne National Laboratory, IL/USA; T. Oyama, The University of Tokyo/J

14:20
Hydrogenolysis of sorbitol over supported metal catalysts
M. Banu, B. Viswanathan, S. Boseker, Indian Institute of Technology, Chennai/IND; P. Venkatalingam, Bharathidasan University, Trichirapalli/IND

14:40
Titania as a water-tolerant Lewis acid catalyst for the selective conversion of glucose into 5-hydroxymethylfurfural
M. Hara, K. Nakajima, M. Kitano, Tokyo Institute of Technology, Yokohama/J; S. Hayashi, AIST, Tsukuba/J

15:00
COFFEE BREAK

15:20
KEYNOTE LECTURE
The critical role of OH in the selective oxidation or hydrogenolysis of biomass-derived molecules over supported metal catalysts
R. Davis, University of Virginia, Charlottesville, Virginia/USA

Chairs: W. Conner, University of Massachusetts, Amherst, MA/USA; T. Zhang, Dalian Institute of Chemical Physics, Dalian/PRC

16:00
Biomass to chemicals over tailored hierarchical zeolite catalysts
P. Dapos, G. Verboekend, G. Vle, C. Monelli, J. Perez-Ramirez, ETH Zurich/CH

16:20
Catalytic valorisation of isosorbide as versatile renewable platform chemical
M. Rose, R. Pakivovits, RWTH Aachen University/D

16:40
Synthesis of chemicals from renewable feedstocks catalysed by polyoxometalates
I. Kuzhelevnikov, University of Liverpool/UK

17:00
COFFEE BREAK

Room 13 a

Plenary and speciality chemicals from renewables

Chairs: F. Jentoft, University of Oklahoma, Norman, OK/USA; X. Li, Qingdao Institute of Bioenergy and Bioprocess Technology of the CAS/PRC

17:20
Selective oxidation of glycerol catalyzed by gold supported on different carbon materials
E.G. Rodrigues, M.F.R. Pereira, Porto University/P; X. Chen, J.J. Delgado, Cadiz University, Puerto Real/E; S.A.C. Carabineiro, J.L. Figueiredo, J.J.M. Orfo, Porto University/P

17:40
Selective hydrogenolysis of glycerol to propene
C. Moia, V. Gonzalves, Federal University of Rio de Janeiro/BR; R. Gambetta, Embrapa Agroenergia, Brasilia/BR; J. Fadigas, Braskem, Sao Paulo/BR

18:00
Catalytic and DFT study of the MgO active site participating in glycerolysis reactions towards monoglycerides
C.A. Ferretti, C.R. Apesteguia, J.J. Gil Cosme, INCAFE, Santa Fe/RA; S. Fuente, R. Ferullo, N. Castellani, Dept. Physics, Baha Blanca/RA

18:20
Hydrogenolysis of glycerol into 1,3-propanediol over iridium-rhenium catalyst
Y. Nakagawa, Y. Amada, K. Tomishige, Tohoku University, Sendai/J

18:40
W-V-O bronzes, catalysts for the oxidative dehydration of glycerol into acrylic acid
F. Cavani, S. Guidetti, G. Trivisani, University of Bologna/IT; M.D. Sonino, P. Concepcion, J.M. Lopez Nieto, Politecnico University of Valencia/E

19:00
Selective hydrogenolysis of glycerol to propene
C.A. Ferretti, C.R. Apesteguia, J.J. Gil Cosme, INCAFE, Santa Fe/RA; S. Fuente, R. Ferullo, N. Castellani, Dept. Physics, Baha Blanca/RA

20:00
Congress Dinner at the Residenz Munich (Ticket necessary) or
20:30
Students Party at the Club P1 (Ticket necessary)
Thursday, July 5, 2012

**PLENARY LECTURE**

Progress towards understanding the relationships between catalyst composition and structure and catalyst activity and selectivity
A. Bell, University of California, Berkeley, CA/USA

10:00 COFFEE BREAK

**Catalysis in CO₂ capture, sequestration and utilization (continued)**

Chairs: X.E. Verykios, University of Patras/GR; B. Reeger, Technische Universität München, Garching/D

10:20 A diagonal approach to chemical recycling of carbon dioxide: new catalytic transformations for the reductive functionalization of CO₂

10:40 Fixation of carbon dioxide into useful products over Cu/ZnO based catalysts
K.M.K. Yu, S.C.E. Tsang, Oxford University/UK

11:00 Direct synthesis of dimethyl and diethyl carbonate from alcohols and carbon dioxide over bimetallic Cu-Ni catalysts supported on ZrO₂
O.F. Arellano, A.F. Orrego, L.F. Bazan, A.L. Vila, University of Antioquia, Medellin/CO

11:20 Fe-catalyzed synthesis of penta- and hexacyclic organic carbonates
C.J. Whiteoak, Institute of Chemical Research of Catalonia (ICIQ), Tarragona/E; O.F. Arbelaez, A.F. Orrego, L.F. Bustamante, A.L. Vila, University of Antioquia, Medellin/CO

11:40 CO₂ capture and conversion from natural gas, coal, and biomasses: reaction pathways and mechanism
W. Ahn, Inha University, Incheon/RoK

12:00 LUNCH BREAK (lunch is available for self-purchase at the congress venue)

Chairs: F. Seitz, BASF SE, Ludwigshafen/D; F. Schüth, Max-Planck-Institut für Kohlenforschung, Mülheim/D

09:00 PLENARY LECTURE

**Cleaning exhaust streams**

Chairs: R. Burch, Queen’s University of Belfast, Northern Ireland/UK; W. Grünert, Ruhr-Universität Bochum/D

14:20 Oxidation of fuel cell anode gas using base metal catalysts
C. Retnamurthy, J.P. Wagner, G. Cullen, Süd-Chemie Inc., Louisville, KY/USA; G. Antang, Süd-Chemie AG, Heulödt/D

14:40 Oxygen mobility and catalytic activity in oxidation reactions of nanocrystalline high surface area hexaaluminates
S. Lasserre, Université Laval, Québec/CDN; D. Duprez, S. Royer, Université de Poitiers/F; H. Almandari, Université Laval, Québec/CDN

15:00 COFFEE BREAK

15:20 Design of alumina-supported nanosized cesia-lanthana solid solutions for CO oxidation
P. Sudarsanan, K. Lakshmi, B.M. Reddy, Indian Institute of Chemical Technology (IIT), Hyderabad/IND; M. Mühler, W. Grünert, Ruhr-Universität Bochum/D

15:40 Room temperature oxidation of carbon monoxide on Pt/CoO₂-ZrO₂-Bi₂O₃ catalysts
T. Masui, H. Imadou, K. Yasuda, N. Imanaka, Osaka University/J

16:00 Resolving the pathways of selective NO reduction by propene over the Co-BEA zeolite by operando IR, EPR and DFT investigations
P. Pietrzyk, K. Gora-Marek, Jagiellonian University, Krakow/PL; Ch. Djuradin, P. Granger, University of Life/F; Z. Sodik, Jagiellonian University, Krakow/PL

16:20 Density functional theory investigation into alkane, alkene and aromatic oxidation on platinum
N. Kaiser, J. Hyy, B. Shan, G. Yuan, W. Wang, Xiao Hao, Nanostellar Inc., Redwood City, CA/USA; K. Cho, University of Texas at Dallas, Richardson, TX/USA

16:40 Toluene adsorption and oxidation on ZrO₂-biomass gasification gas clean-up catalysts: characterization by DRIFTS
T. Vinkó, I. Kauppi, J. Piotrowski, O. Krause, Aalto University/FIN

17:00 COFFEE BREAK

17:20 KEYNOTE LECTURE

Size effects in combustion of hydrocarbons and CO over supported metal catalysts for abatement of car exhausts
V. Bublikhnya, Burevskiy Institute of Catalysis, Novosibirsk/RU; A. Slakheev, Zelinsky Institute of Organic Chemistry, Moscow/RU

18:00 A mechanistic study of mercury oxidation over SCR catalysts

18:20 Novel Pt-Co/Al₂O₃ catalyst for the selective catalytic reduction of NOx by H₂ in the presence of oxygen
Z.M. Lu, C.H. Ni, Beijing University of Chemical Technology/PRC; L.L. Ma, Institute of High Energy Physics of the CAS, Beijing/PRC

18:40 Efficient removal of emerging contaminants from wastewaters by means of catalytic wet air oxidation
M. Bistain, T. Tisler, A. Pintar, National Institute of Chemistry, Ljubljana/SLO

19:00 Congress Dinner at the Residenz Munich (Ticket necessary)

01:00 Students Party at the Club P1 (Ticket necessary)

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Subject to change
Thursday, July 5, 2012

Room Saal 1

09:00 PLENARY LECTURE
Progress towards understanding the relationships between catalyst composition and structure and catalyst activity and selectivity
A. Bell, University of California, Berkeley, CA/USA

10:00 COFFEE BREAK

Cross-disciplinary workshop organocatalysis / biocatalysis

Chairs: A. Jacobi von Wangenheim, Universität Regensburg/D; U. Kragl, Universität Rostock/D

10:20 INVITED LECTURE
A quantitative approach to nucleophilic organocatalysis
S. Lakhdar, B. Maji, A.R. Ofial, H. Mayr, Universität München/D

11:00 Microporous polymer networks as highly selective heterogeneous asymmetric organocatalysts
J. Schmidt, D.S. Kundu, C. Bleschke, S. Blechert, A. Thomas, TU Berlin/D

11:20 A new strategy in asymmetric catalytic reaction: emulsion catalysis
Q. Gao, Y. Li, C. Li, Dalian Institute of Chemical Physics/PRC

11:40 Organochiral Vis-light photocatalysis with porphyrin PMO materials
S.-E. Park, E.-Y. Jeong, Inha University, Incheon/ROK

12:00 LUNCH BREAK (Lunch is available for self-payment at the congress venue)

Room Saal 1

13:20 AWARD LECTURE HEINZ HEINEMANN AWARD
Catalysis using gold nanoparticles
G. Hutchings, University of Cardiff/UK

Cross-disciplinary workshop organocatalysis / biocatalysis

Chairs: A. Jacobi von Wangenheim, Universität Regensburg/D; U. Kragl, Universität Rostock/D

14:20 KEYNOTE LECTURE
Directed evolution of selective enzymes: a prolific source of catalysts for organic chemistry and biotechnology
M.T. Reetz, Universität Marburg/D

15:00 COFFEE BREAK

15:20 Synergetic effects in energy-efficient organocatalysed formation of organic carbonates
C.J. Whiteoak, A.W. Kleij, Institute of Chemical Research of Catalonia (ICIQ), Tarragona/ES

15:40 Bifunctional phosphonium salt catalyzed addition of carbon dioxide to epoxides
T. Werner, H. Blüttner, Leibniz-Institute for Catalysis, Rostock/D

16:00 Covalent triazine frameworks as metal-free heterogeneous catalysts for the activation and conversion of CO₂
J. Roesser, K. Kalaisam, A. Thomas, TU Berlin/D

16:20 INVITED LECTURE
About the asymmetric functionalisation of carbonyls after the advent of cinchona-based primary amine catalysis
P. Meichsner, Institute of Chemical Research of Catalonia (ICIQ), Tarragona/ES

17:00 COFFEE BREAK

Thursday, July 5, 2012

Room 14 c

Cross-disciplinary workshop organocatalysis / biocatalysis

Chairs: A. Jacobi von Wangenheim, Universität Regensburg/D; U. Kragl, Universität Rostock/D

17:20 Paramagnetic epoxy-functionalised mesostructured cellular foams for immobilisation of penicillin G acylase
L. Yang, Z.Y. Gao, Y.L. Guo, W.C. Zhan, G.Z. Lu, East China University of Science and Technology, Shanghai/PRC

17:40 Application and scope of fully organic photoredox catalysis in single electron transfer reactions
B. López-Sánchez, K. Zeitler, Regensburg University/D

18:00 Design approach and new insights in support-catalyst interactions in single-site heterogeneous organocatalysts
D. Xuereb, F. Raja, University of Southampton/UK

20:00 Congress Dinner at the Residenz Munich (Ticket necessary)

or

20:30 Students Party at the Club P1 (Ticket necessary)
Friday, July 6, 2012

Room Saal 1

09:00
PLENARY LECTURE
Design and study of molecular catalysts for small molecule activation and conversion
R. Petiana, The Scripps Research Institute, Jupiter, FL/USA

10:00
COFFEE BREAK

Room 14 c

Green synthesis (continued)

Chairs: V.I. Parvulescu, University of Bucharest/RO; J. Armor, GlobalCatalysis.com LLC., Oxford, PA/USA

10:20
KEYNOTE LECTURE
What’s really happening inside a catalyst pore?
L.F. Gladden, University of Cambridge/UK

11:00
Metal incorporated mesoporous silicas as heterogeneous catalysts for olefin epoxidation
A. Ramanathan, M. Ghanta, B. Subramaniam, University of Kansas, Lawrence, KS/USA

11:20
Catalytic epoxidation of organic compounds over peroxophosphotungstate entrapped in mesoporous SBA-15
E. Poil, F. Jerome, J.-M. Calozes, Y. Poulhoux, Poitiers University/F

11:40
Efficiently asymmetric epoxidation of olefins with chiral bioinspired catalysts

12:00
LUNCH BREAK (Lunch is available for self-payment at the congress venue)

Chairs: W. Lethner, RWTH Aachen/D; R. Feurmann, Technical University of Denmark, Kgs. Lyngby/DK

13:20
AuPd and AuPt supported nanocrystals for poloy oxidation
P. Mertics, Cardiff Catalysis Institute/UK; G.L. Brett, T. Koltunova, Y. Ryabentkova, University of Cardiff/UK

13:40
Driving selective oxidation of aromatic alcohols with sunlight using photocatalysts of gold and palladium alloy nanoparticles
S. Sarina, E. Jaalinen, H.Y. Zhu, Queensland University of Technology, Brisbane/AUS

14:00
Laccase immobilization on metal oxides for enzyme-catalysed oxidations
R. Mateus Bianco, F. Naveau, M.E. Gaigneaux, E. Enaud, Université catholique de Louvain, Louvain la Neuve/B

14:20
Controlled gas phase hydrogenation of m-dinitrobenzene: a comparison of the catalytic action of carbon supported gold and silver
F. Cárdenas-Lizana, L. Kivi-Minskier, École Polytechnique Fédérale de Lausanne/CH; S. Gómez-Quero, University of Cambridge/UK

14:40
Methanlated cyclodextrin-stabilized Ruthenium(0) nanoparticles as active scaffolds for catalytic hydrogenation
B. Lieger, R. Herbois, S. Noel, University of Artois, Lens/F; A. Roucoux, ENS Cîte de Rennes/F; E. Montlier, A. Ponchel, University of Artois, Lens/F

15:00
COFFEE BREAK

Chairs: B. Subramaniam, The University of Kansas, Lawrence, KS/USA; V. Teixeira da Silva, Federal University of Rio de Janeiro/BR

15:20
Synthesis of sulfonated diphosphines-stabilized ruthenium nanoparticles: efficient nanocatalysts in hydrogenation reactions in biphasic media
M. Guerreiro Hernandez, K. Phlivip, K. Fajerweg, Centre National de la Recherche Scientifique, Toulouse/F; E. Montlier, H. Bricout, Université d’Artois, Lens/F; A. Roucoux, A. Nowicki, ENS Cîte de Rennes/F

15:40
Hydroxyapatite hosting niobium: a new class of amphoteric catalysts for carbohydrate transformation reactions
P. Carniti, A. Gervasini, M. Marzo, University of Milan/I

16:00
Closing ceremony

Room Saal 1

ICC 2012 – POSTER SYMPOSIA

At the 15th International Congress on Catalysis (ICC 2012) we explore a new form of communication for more specialized topics.

Approximately 10 contributions selected as posters have been grouped to a thematic cluster in which participants interested in the topic can exchange and can share this with other participants. Selected posters are marked with the number of the poster symposia, e.g. PS.07 in the separate brochure “Poster Program”.

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<tr>
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<th>Symposia name</th>
<th>Day</th>
<th>Time</th>
<th>Room</th>
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<tbody>
<tr>
<td>PS.01</td>
<td>Structure activity relations in FT processes</td>
<td>Monday, July 2</td>
<td>10:50 – 12:30</td>
<td>11a</td>
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<tr>
<td></td>
<td>A. Van Steen, University of Cape Town/ZA;</td>
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<td>A. Holmen, Norwegian Institute of Technology, Trondheim/N</td>
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<tr>
<td>PS.02</td>
<td>Oxidative de-hydrogenation</td>
<td>Monday, July 2</td>
<td>10:50 – 12:30</td>
<td>11b</td>
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<td>A. Lemonidou, Aristotle University of Thessaloniki/GRC;</td>
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<td>V. Cortes Corberan, C.S.I.C., Madrid/E</td>
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<tr>
<td>PS.03</td>
<td>Friedel crafts and alkane alkylation</td>
<td>Monday, July 2</td>
<td>10:50 – 12:30</td>
<td>12a</td>
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<tr>
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<td>S.E. Park, Inha University, Inchon/KR;</td>
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<td>G. Mj, University of Twente, Enschede/NL;</td>
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<td>PS.04</td>
<td>Epoxidation with Ti silicates</td>
<td>Monday, July 2</td>
<td>10:50 – 12:30</td>
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<td>F. Bonino, University of Turin/I;</td>
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<td>F.S. Xiao, Zhengjiang University, Hangzhou/PRC</td>
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<td>PS.05</td>
<td>Hydrotreating catalysts: new solutions to old challenges</td>
<td>Monday, July 2</td>
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<td>K. Smith, University of British Columbia, Vancouver/CA;</td>
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<td>A. Kuperman, Chevron Energy Research and Technology Company, Richmond, CA/USA</td>
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<td>Methanol and direct DME synthesis</td>
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<td>M. Behrens, Fritz-Haber-Institut der MPG, Berlin/D;</td>
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<td>D. Jackson, University of Glasgow/UK</td>
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<td>PS.07</td>
<td>Selective alcohol oxidation</td>
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<td>I. Hermans, ETH Zurich/CH;</td>
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<td>Y. Wang, Pacific Northwest National Laboratory, Richland, WA/USA</td>
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<td>PS.08</td>
<td>Novel aspects of NOx reduction (with NH3)</td>
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<td>E. Tronconi, Politecnico di Milano/I</td>
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<td>PS.09</td>
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<td>F. Ribero, Purdue University, West Lafayette, IN/USA</td>
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<td>PS.10</td>
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<td>M. Stockenhuber, University of Newcastle, Callaghan/AUS</td>
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<td>PS.11</td>
<td>Versatile TiO2-based photocatalysts</td>
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<td>PS.12</td>
<td>Towards understanding sulfide catalysts</td>
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<td>PS.13</td>
<td>Manipulating product distribution in FT processes</td>
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<td>PS.15</td>
<td>Imaging/local probes for catalyst characterization</td>
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<td>PS.16</td>
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<td>Catalyst immobilization and flow systems</td>
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<td>Mechanistic aspects of the water-gas shift reaction</td>
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<td>PS.19</td>
<td>CC-coupling/cleavage</td>
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<td>Catalysis in fuel cells</td>
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<td>Chairs: C. Pak, Samsung Advanced Institute of Technology, Yongin/KR; K. Eguchi, Kyoto University/J</td>
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<td>PS.21</td>
<td>Physicochemical effects influencing cracking</td>
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<td>PS.22</td>
<td>Metathesis reactions</td>
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<td>PS.23</td>
<td>Chemoselsective hydrogeneration</td>
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<td>PS.24</td>
<td>Degradation of pollutants through photocatalysis</td>
<td>Wednesday, July 4</td>
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<td>Chairs: V. Keller, University of Strasbourg/F; P. Sermon, Brunel University, Uxbridge/UK</td>
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<td>PS.25</td>
<td>Hydrocracking and hydroisomerization</td>
<td>Wednesday, July 4</td>
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<td>Chairs: A. Borgna, Institute of Chemical and Engineering Sciences, Singapore/SGP; Z. Sobalík, J. Heyrovsky Institute of Physical Chemistry of ASCR, Prague/CZ</td>
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<td>PS.26</td>
<td>Hydroformylation and other reactions involving CO addition</td>
<td>Wednesday, July 4</td>
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<td>PS.27</td>
<td>Enantioselective catalysis</td>
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<td>PS.28</td>
<td>Novel photocatalysts for hydrogen generation</td>
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<td>PS.29</td>
<td>Ruthenium Dioxide, a versatile oxidation catalyst in heterogeneous and electro-catalysis</td>
<td>Wednesday, July 4</td>
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<td>PS.30</td>
<td>Chemistry of alcohols</td>
<td>Wednesday, July 4</td>
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<td>Chairs: R. Davis, University of Virginia, Charlottesville, VA/USA; C. Sievers, Georgia Institute of Technology, Atlanta, GA/USA</td>
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## POSTER SYMPOSIA

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<td>PS.31</td>
<td>Synchrotron methods for catalyst characterization</td>
<td>S. Bare, UOP LLC a Honeywell Company, Des Plaines, IL/USA;</td>
<td>Wednesday, July 4</td>
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<td>B.M. Weckhuysen, University Utrecht/NL</td>
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<td>PS.32</td>
<td>Tailored Au and Au alloy particles</td>
<td>C. Louis, Université Pierre et Marie Curie – UPMC, Paris/F</td>
<td>Wednesday, July 4</td>
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<td>PS.33</td>
<td>Metal organic frameworks</td>
<td>M. Hartmann, Universität Erlangen-Nürnberg/D;</td>
<td>Thursday, July 5</td>
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<td>D. Farrusseng, IRCELYON-CNRS, Villeurbanne/F</td>
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<td>PS.34</td>
<td>Conversion of triglyceride and fatty acids to fuels</td>
<td>V. Teixeira da Silva, Federal University of Rio de Janeiro/BR;</td>
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<td>D.E. Resasco, University of Oklahoma, Norman, OK/USA</td>
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<td>PS.35</td>
<td>First principles based modeling</td>
<td>K. Reuter, TU München/D;</td>
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<td>PS.36</td>
<td>Advanced characterization using NMR</td>
<td>J. Dedecel, Jaroslav Heyrovsky Institute of Physical Chemistry,</td>
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<td>Prague/CZ;</td>
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<td>L.F. Gladden, University of Cambridge/UK</td>
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<td>PS.37</td>
<td>Conversion of lignocellulosic biomass to fuels and chemicals</td>
<td>H. Liu, Peking University/PRC;</td>
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<td>F. Jentoft, University of Oklahoma, Norman, OK/USA</td>
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<td>PS.38</td>
<td>Lignin depolymerization and conversion of lignin model</td>
<td>R. Pakovits, RWTH Aachen/D;</td>
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<td>compounds</td>
<td>D. Mazan, Åbo Akademi University, Turku/_FIN</td>
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<td>PS.39</td>
<td>Selective hydrogenation of CO₂</td>
<td>M. Landsau, Ben-Gurion University of the Negev, Beer-Sheva/IL;</td>
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<td>K. Köhler, TU München, Garching/D</td>
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<td>PS.40</td>
<td>In situ methods for characterizing catalyst and reactions</td>
<td>E.E. Wolf, University of Notre Dame, IN/USA;</td>
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<td>C. Peden, Pacific Northwest National Laboratory, Richland, WA/USA</td>
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<td>PS.41</td>
<td>Steam reforming of alcohols</td>
<td>C. Chin, University of Toronto/CDN;</td>
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<td>PS.42</td>
<td>Synthesis of organic carbonates</td>
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<td>PS.43</td>
<td>Advances in electron-microscopy</td>
<td>I. Arslan, Pacific Northwest National Laboratory, Richland, WA/USA;</td>
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<td>A. Datye, University of New Mexico, Albuquerque, NM/USA</td>
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<td>PS.44</td>
<td>Selective methane oxidation</td>
<td>H.H. Kung, Northwestern University, Evanston, IL/USA;</td>
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## POSTER PROGRAM

(see separate brochure)

Total is proud to sponsor the Poster Sessions at the 15th ICC in Munich, bringing together prominent researchers from the industry and the university communities to focus on the current developments and challenges in catalysis.

### POSTER SESSIONS

The opportunities for poster authors to present their posters and to discuss with colleagues are:

- **Poster Session on Tuesday**, July 3, 2012, for posters with even numbers from 3 p.m. till 5:20 p.m.
- **Poster Session on Wednesday**, July 4, 2012, for posters with odd numbers from 3 p.m. till 5:20 p.m.
**Wednesday, July 4, 2012**

**Bavarian evening** at the Paulaner am Nockherberg

15 € – drinks and buffet included.

Enjoy an typical Bavarian evening with your colleagues in a traditional Bavarian brewery. A bus shuttle service will be provided.

Departure time from the congress center to the brewery 7 p.m.;
Departure time from the brewery to the main railway station from 10 p.m. to 11 p.m. every 15 min.

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**Thursday, July 5, 2012**

**Congress Dinner** at the Residenz Munich

75 € – drinks and menu included.

The Munich Residenz served as the seat of government and residence of the Bavarian dukes, electors and kings from 1508 to 1918, and began in 1385 as a castle. The architecture, interior decoration and works of art collected in the Residenz range in time from the Renaissance, via the early Baroque and Rococo periods to the neoclassical era.

The Munich Residenz is located in the city center and can easily be reached by public transport. U-tram station U3-U6 Odeonsplatz nearby the Residenz.

Entrance from Hofgarten or Residenzstrasse into the Kaiserhof (Emperor’s Court), to the Kaisersaal (Emperor’s Hall) and the adjoining Vierschimmelsaal (Four Greys Room) on the first floor.

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**Thursday, July 5, 2012**

**Students Party** at the Club P1

10 € – drinks included.

Munich’s most legendary and most traditional night club welcomes you.

„P-one“ - as an abbreviation for „Prinzregentenstraße 1“, nearby U-station Odeonsplatz