European Conference on
Combinatorial Catalysis Research
and High-Throughput Technologies

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Co-Organisers:
IRCELYON-CNRS, 2, avenue Albert Einstein, 69626 Villeurbanne/F
CIRCC, University of Bari, Via Celso Ulpiani, 27, 70126 Bari/I
Programme / Contents

Sunday, 22 April 2007

16:00 Registration

18:00 M. Aresta, University of Bari/I,
C. Petrocelli, University of Bari/I
C. Mirodatos, IRCELYON-CNRS, Villeurbanne/F
Welcome and Opening

18:30 Evening Lecture
W.F. Maier, Saarland University, Saarbrücken/D
Combinatorial Materials Science - Promises, Problems and Successes 09

20:00 - 21:00 Welcome Reception

Monday, 23 April 2007

Data Management and Information Technologies
Chair: A. Corma, Valencia/E

08:30 Plenary Lecture
G. Rothenbeiy, University of Amsterdam/NL
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09:30 B. Schäfer, BSSN Software, Mainz/D; G.W. Kramer, NIST, Gaitersburg, MD/USA;
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10:00 L.A. Baumes, P. Serna, J.M. Serra, A. Corma, UPV-CSIC, Valencia/E
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10:30 M.P. Andersson, T. Bligaard, C.H. Christensen, J.K. Nørskov,
Technical University of Denmark, Lyngby/DK
Computational Screening for a Methanation Catalyst 13

11:00 Coffee Break and Exhibition

Case Studies: Heterogeneous Catalysis
Chair: S.I. Woo, Daejeon/ROK

11:30 M. Krämer, W.F. Maier, Saarland University, Saarbrücken/D
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12:00 A. Frey, A. Kustov, C. Christensen, Technical University of Denmark, Lyngby/DK; K. Larsen, J. Sehested, Haldor Topsee, Lyngby/DK; T. Bligaard, M. Andersson, J. Nørskov, Technical University of Denmark, Lyngby/DK
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12:30 P. Yaseneva, S. Pavlova, V. Sadykov, G. Alikina, A. Lykashevich, Boreskov Institute of Catalysis, Novosibirsk/RUS; S. Belochapkin, Materials & Surface Science Institute, Limerick/IRL; J. Ross, University of Limerick/IRL
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Exhibition and Postersession

Case Studies: Heterogeneous Catalysis
Chair: K. Stöwe, Saarbrücken/D

14:30 C. Fink, A. Hagemeyer, M. Schlichter, A.F. Volpe,
Symyx Technologies, Santa Clara, CA/USA
Aqueous Synthesis of High Surface Area Metal Oxides

15:00 A. Jentys, F.N. Naraschewski, P. Kumar, J.A. Lercher,
Technical University of Munich, Garching/D
Direct Oxidation Routes from Propane to Acrylic Acid

15:30 J.H. Lim, S.I. Woo, K.S. Oh, Korea Advanced Institute of
Science and Technology, Daejeon/ROK
Development of Mixed Metal Oxide Catalysts Using Combinatorial
Chemistry for Selective Oxidation of Propane to Acrylic Acid

16:00 Coffee Break and Exhibition

Hardware and Methodology Development
Chair: J. Pérez-Ramirez, Tarragona/E

16:30 T. Brinz, R. Emmerich, Robert Bosch GmbH, Waiblingen/D
Fully Automated Systems for the High-Throughput Development
of Materials and Formulations

17:00 T. Stegk, R. Janssen, G.A. Schneider, Hamburg University of Technology/D
High-Throughput Preparation and Analysis of Ceramic Material
Libraries Fabricated from Dry Ceramic Powders

17:30 P. Vandezande, L.E.M. Gevers, P.A. Jacobs, I.F.J. Vankelecom, University of
Leuven/B
High-Throughput Testing, Combinatorial Techniques and
Modelling: Powerful New Instruments for Membrane Optimization

18:00 Exhibition and Postersession

19:30 Evening Lecture
European Strategies for Promoting the HT Technologies:
The Flanders Materials Centre: Focus on Combinatorial Materials Research
Overview of the TOPCOMBI Integrated Project
C. Mirodatos, IRCELYON-CNRS, Villeurbanne/F
J. Paul, Flamac, Zwijnaarde/B

Tuesday, 24 April 2007

Case Studies: Heterogeneous Catalysis
Chair: M. Cohn, Des Plaines, IL/USA

08:30 Plenary Lecture
A. Corma, UPV-CSIC, Valencia/E
High-Throughput Experimentation in Successful Synthesis of
New Catalytic Materials and Catalytic Processes

09:30 J.-H. Park, S.J. Park, H.A. Ahn, I.-S. Nam, Pohang University
of Science and Technology/ROK; G.K. Yeo, J.K. Kil, Y.K. Youn, Hyundai
Motors Company & Kia Motors Corporation, Yongin-Si/ROK
A Fast and Quantitative Screening of Zeolite-Type Hydrocarbon
Trap Catalysts
10:00  W.F. Maier, N. Olong, Saarland University, Saarbrücken/D  
Combinatorial Discovery of New Mixed Metal Oxide Catalysts for Soot Oxidation  

10:30  E. Dejaegere, K. Mantri, G.V. Baron, J.F.M. Denayer, Vrije Universiteit Brussel/B  
A High-Throughput Experimentation and Modelling Approach in the Study of Adsorption Effects in Zeolite Catalyzed Alkylation and Acylation Reactions  

11:00  Coffee Break and Exhibition  

Data Management and Information Technologies  
Chair: D. Farrusseng, Villeurbanne/F  

11:30  S.C. Cruz, J.W. Thybaut, G.B. Marin, Ghent University/B;  
D. Farrusseng, IRCLEYON-CNRS, Villeurbanne/F; F. Gilardoni, Inforsense, London/UK  
Microkinetic Modeling in High-Throughput Workflows  

12:00  J. Sun, J.W. Joris, G.B. Marin, Ghent University/B  
Microkinetics of Methane Oxidative Coupling  

12:30  G. Morra, D. Farrusseng, C. Mirodatos, IRCLEYON-CNRS, Villeurbanne/F; E. Guillon, S. Morin, C. Bouchy, P. Duchene, IFP, Solaize/F  
A Screening Methodology for High-Throughput Kinetic Modelling  

13:00  Lunch Break  
Exhibition and Postersession  

Case Studies: Homogeneous and Polymerisation Catalysis  
Chair: G. Rothenberg, Amsterdam/NL  

14:30  M.O. Kristen, H. Schmitz, F. Fantinel, M. Fushimi, F. Gundert, Basell Polyolefine GmbH, Frankfurt am Main/D  
High Output Screening (HOPS) for Polylefin Catalysts - the Better Way of Fast Experimentation  

15:00  J. Almena, M. Schwarm, T. Riermeier, Degussa AG, Hanau/D  
High-Throughput Screening and Profiling of Homogeneous Catalysts  

15:30  B. Sandee, A.M. Van den Burg, J.M. Meeuwissen, J.N.H. Reek, University of Amsterdam/NL  
Prepare, Assemble and Screen Automation of Homogeneous Catalysis Research  

16:00  Coffee Break and Exhibition  

Case Studies: Heterogeneous Catalysis  
Chair: J. Margitfalvi, Budapest/H  

16:30  M. Klimczak, M. Lucas, P. Kern, Ch. Breuer, P.G. Claus, Technical University of Darmstadt/D  
Application of Monoliths as Highly Parallelised Micro Reactors for Environmental Catalysis
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High-Throughput Kinetics and Scale-up of Aldol Condensations over Activated Hydrotalcites

17:30 U. Ravon, A. Desmartin-Chomel, D. Farrussang, C. Mirodatos, IRCELYON-CNRS, Villeurbanne/F
High-Throughput Screening of Metal Open Frameworks for Gas Separation

18:00 J. Procelewska, J. Llamas Galilea, F. Clerc, F. Schüth, Max-Planck-Institute for Coal Research, Mülheim/D
Exploring of Chemoinformatics Strategies in the Development of a Knowledge-Based System for the Prediction of Solid Catalyst Performance

18:30 J. Beltran-Oviedo, I. Batyrshin, J.M. Dominguez, Instituto Mexicano del Petroleo, Mexico City/MEX
Modified Evolutionary Optimization Approach for Combinatorial Catalyst Development

19:00 M.C. Kerby, ExxonMobil Research & Engineering Co., Annandale, NJ/USA
Advanced Catalyst Technologies and High-Throughput Experimentation at ExxonMobil

19:30 Award of Poster Prizes
Presentations by Poster Prize Winners

20:00 Conference Dinner

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Industrial Case Studies and Success Stories
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M. Cohn, UOP LLC, Des Plaines, IL/USA
Combinatorial Chemistry: Creating Technology Step Changes

09:30 S.A. Schunk, S. Sundermann, hte Aktiengesellschaft, Heidelberg/D; H. Hibst, BASF Aktiengesellschaft, Ludwigshafen/D
Retrospective Hit-Deconvolution of Mixed Metal Oxides: Spotting Structure Property Relationships in Gas Phase Oxidation Catalysis Through High-Throughput Experimentation

Combining High-Throughput Experimentation and Test Reactions for Industrially Reliable Catalytic Processes

Development of High-Throughput Testing-Units for Hydroprocessing

11:00 Coffee Break and Exhibition
Case Studies: Heterogeneous Catalysis
Chair: A. Jentys, Garching/D

11:30 J. L. Margitfalvi, A. Tompos, M. Hegedűs, Chemical Research Center, Budapest/H
Combinatorial Approach to Design Highly Active and Selective Supported Gold Catalysts for PROX Application

12:00 M. Aresta, A. Dibenedetto, M. Distaso, C. Pastore, University of Bari/I; K. Mazur, Jagiellonian University, Krakow/PL
Selective Epoxidation of Propene Using Reticular Oxygen of Metal Oxides

12:30 P. Pescarmona, K.P.F. Janssen, P.A. Jacobs, University of Leuven/B
Novel Transition-Metal-Free Heterogeneous Epoxidation Catalysts Discovered by Means of High-Throughput Experimentation

13:00 W.F. Maier, Saarland University, Saarbrücken/D
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