

## INVITATION

Catalysis research has been accelerated by the application of combinatorial and high-throughput methods. The EuroCombiCat 2009 provides the European forum for presentation and intensive discussion of results obtained and methods used. An interesting programme with many contributions from academic and industrial experts will lead in detail through the progress made in the various fields of application. Furthermore, the equally important evolution on methodologies and their application will be debated in context, allowing for strong interaction and mutually beneficial discussions. The latest developments in commercial products and services will be presented in an exhibition of products and services suppliers.

Last minute posters can be submitted until **30 March 2009**.

### ► SCIENTIFIC COMMITTEE

Avelino Corma	Valencia/E (Chairman)
Claude Mirodatos	Lyon/F (Chairman)
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### ► ORGANISING COMMITTEE

Laurent Baumes	Valencia/E
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Monika Locherer	Frankfurt am Main/D

### ► SPONSORING

EuroCombiCat 2009 Conference invites interested sponsors. Please contact the conference office if you want to actively support this conference.

The EuroCombiCat-Conference 2009 is kindly supported by

6<sup>th</sup> European Framework Programme



of the European Commission DG Research



through the IP TOPCOMBI



## REGISTRATION

Conference ticket for		
Participants <sup>1)</sup>	Regular	Member <sup>2)</sup>
from industry	590 €	575 €
from academia	290 €	275 €
Students <sup>3)</sup>	150 €	135 €
Accompanying Person		100 €

1) According to § 13b UStG not subject to VAT; Reverse-Charge

2) Personal DECHEMA members and EFC/EFCE passport holders

3) Proof of status required

Please register with the attached registration form or online at [www.eurocombiat.org/2009](http://www.eurocombiat.org/2009). Deadline for entry in the list of participants is **30 March 2009**.

The participant's fee includes the list of participants, a book of abstracts, welcome reception, lunches, dinner, coffee breaks and the conference dinner. The fee for the accompanying person includes the welcome reception, dinner and the conference dinner.

### ► REMITTANCE OF FEES

Fees should be remitted on receipt of the invoice in favour of DECHEMA e.V., stating the invoice number, the name of the participant and the **keyword ECC09**, to one of the DECHEMA accounts as stated on the invoice. Payment by credit card is also possible.

### ► CANCELLATIONS AND REFUNDS

30 € for administrative costs will be charged for cancellations received by **31 March 2009**. Thereafter 80% of the registration fee will be invoiced; however the book of abstracts will be mailed. Only written cancellations will be accepted.

### ► INSURANCE

The organisers cannot accept responsibility for loss or damage to the private property of participants and accompanying persons which may occur either during or arising from the symposium. Participants should therefore take whatever steps they consider necessary regarding insurance.

The conference website will be continuously updated with relevant information. Please check it regularly for the latest developments.

[www.eurocombiat.org/2009](http://www.eurocombiat.org/2009)

### ► SOCIAL PROGRAMME

- Sight-seeing tour in Valencia, Sunday, 26 April 2009.
- Welcome reception after the evening lecture on Sunday, 26 April.
- Conference dinner on Tuesday, 28 April 2009.

## VENUE / ACCOMMODATION

A hotel reservation card is available at [www.eurocombiat.org](http://www.eurocombiat.org).

The Bayren Hotel, Gandia, is located right at the beach, 6 km from Gandia (which is between Alicante and Valencia). The closest international airport is Valencia at a distance of around 70 km. The nearest train station is about 6 km from the hotel. Gandia, a town with a population of around 77,000 is well known for its beautiful beaches and its interesting history, with the earliest settlements in this area date back to Palaeolithic times.



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### ► HOW TO REACH THE VENUE

To get to the conference venue take either the Aero Bus (20 minutes) or the Metro (lines 3 or 5) from the airport to the Estación del Norte (or Xativa), which is Valencia's central train station. From there, take the commuter train (Renfe) Line C1 to Gandia. It runs every half hour (on Sundays every hour). To get to Gandia takes about 58 minutes. From Gandia train station take a taxi or a bus (every 15 minutes) to the hotel (6 km).

A direct bus from Valencia airport to the conference hotel will be organised for the participants on Sunday, 26 April, leaving at ~17:00 h.

### ► CONFERENCE OFFICE

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Phone from April 23: +49 172 6188791 (mobile)

#### Office hours in Gandia:

Sunday	April 26	16:00 – 20:00 h
Monday	April 27	8:30 – 20:30 h
Tuesday	April 28	8:30 – 20:30 h
Wednesday	April 29	8:30 – 13:30 h

# EUROCOMBIAT 2009

## European Conference on Combinatorial Catalysis Research and High-Throughput Technologies



## PROGRAMME

April 26 – 29, 2009  
Hotel RH Bayren, Gandia, Spain

Organisers



[www.eurocombiat.org/2009](http://www.eurocombiat.org/2009)

## PROGRAMME

### Sunday, 26 April 2009

- 16:00 **Registration**  
 18:20 **Welcome and Opening: A. Corma, C. Mirodatos**  
 18:40 **EVENING LECTURE**  
 A. Corma, Universidad Politecnica de Valencia/E  
**Knowledge-based HT materials synthesis and testing for catalysts discovery**  
 20:00-22:00 **Welcome Reception**

### Monday, 27 April 2009

- Hardware and methodology development**  
*Chair: L. Baumes*  
 09:00 **PLENARY**  
 J. Norskov, Technical University of Denmark, Lyngby/DK  
**Computational screening for new catalysts**  
 10:00 **KEYNOTE**  
 G. Morra, D. Farrusseng, University of Lyon1/F; E. Guillon, S. Morin, C. Bouchy, IFP, Lyon/F; C. Mirodatos, University of Lyon1/F  
**Use of model reactions for QSAR studies and catalyst profiling in the frame of refinery applications**  
 10:40 Coffee  
 11:00 **KEYNOTE**  
 M. Holena, D. Linke, U. Rodemerck, Leibniz Institute for Catalysis, Berlin/D  
**The generator approach to evolutionary optimization of catalysts and its integration with surrogate modelling**  
 11:40 **HOT SLOT**  
 A. Nagy, R. Cowan, R. Brose, ILS-Integrated Lab Solutions GmbH, Berlin/D  
**Novel high-throughput systems for performing kinetic catalytic and adsorption studies on microporous materials**  
 12:00 **HOT SLOT**  
 A. Abou-Hamdan, Chemspeed Technologies AG, Augst/CH  
**High output polymer research, development and formulation**  
**Polymerisation catalysis**  
*Chair: A. Förster*  
 12:20 **PLENARY**  
 J. Paul, Flamac, Zwijnaarde/B  
**Use of high-throughput techniques for the development of thin functional coatings**  
 13:30 Lunch  
**Industrial case studies and success stories**  
*Chair: C. Mirodatos*  
 15:00 **KEYNOTE**  
 A. Chieffi, Procter & Gamble Ltd., Newcastle upon Tyne/UK  
**Industrial case study – P&G**  
 15:40 **KEYNOTE**

## PROGRAMME

- S.A. Schunk, N. Brehm, A. Sundermann, hte Aktiengesellschaft, Heidelberg/D, S. Altwasser, F. Rosowski, BASF SE, Ludwigshafen/D  
**Coherent synthesis and testing of dopant effects on the performance of oxidation catalysts: An integrated high throughput experimentation approach**  
 16:20 **KEYNOTE**  
 G. Diamond, Symyx Technologies Inc., Sunnyvale/USA  
**High-throughput catalyst discovery & development for industrial applications**  
 17:00 **Poster Session and Exhibition**  
**Heterogeneous catalysis**  
*Chair: J. M. Serra*  
 19:00 **KEYNOTE**  
 O. Trapp, Heidelberg University, Heidelberg/D  
**High-throughput screening of NHC-ligands in catalysis**  
 19:40 **KEYNOTE**  
 J. Jolly, B. Pavageau, Rhodia Laboratoire du futur (LOF), Pessac/F; J.-M. Tatibouët, Laboratoire de Catalyse en Chimie Organique (LACCO), Université de Poitiers/F  
**High throughput preparation and characterisation of heterogeneous catalysts**  
 21:00 **Dinner**

### Tuesday, 28 April 2009

- Heterogeneous catalysis**  
*Chair: J. Klein*  
 09:00 **KEYNOTE**  
 J. Serra, Universidad Politecnica de Valencia/E  
**Optimizing solid oxide fuel cell performances by combinatorial designs**  
 09:40 **KEYNOTE**  
 B.C. Gagea, P.P. Pescarmona, P. Van der Aa, P.A. Jacobs, J.A. Martens, K.U.Leuven, Heverlee/B  
**Ferromagnetic zeolite catalysts for liquid-phase high throughput experimentation**  
 10:20 **KEYNOTE**  
 F.N. Naraschewski, J.A. Lercher, A. Jentys, TU München/D  
**Quantitative description of the selective oxidation of propane to acrylic acid over MoVTeNb oxides**  
 11:00 Coffee  
**Heterogeneous catalysis**  
*Chair: M. Aresta*  
 11:20 **HOT SLOT**  
 S. Corthals, J. Van Noyen, P. Jacobs, B.F.Sels, K.U. Leuven, Heverlee/B  
**D-optimal designs in biogas catalysis**  
 11:40 **HOT SLOT**  
 H. Noei, Y. Wang, Ch. Wöll, M. Muhler, Ruhr-Universität Bochum/D  
**Infrared spectroscopic studies of chemical reactions on ZnO nanoparticles**

## PROGRAMME

- 12:00 **HOT SLOT**  
 J.L. Margitfalvi, Combitech-Nanotech Kft., Budapest/H; A. Tompos, Chemical Research Center, Budapest/H; L. Végyvári, Combitech-Nanotech Kft., Budapest/H  
**Optimization strategies for multi-component catalysts used in complex catalytic reactions**  
 12:20 **HOT SLOT**  
 M.A. Kolb, K. Stöwe, W.F. Maier, Saarland University/D  
**High-throughput development of mixed metal sulphide catalysts in the nano-scale regime**  
 12:40 **HOT SLOT**  
 A. Tompos, Institute of Nanochemistry and Catalysis, Budapest/H; J.L. Margitfalvi, Combitech-Nanotech Kft., Budapest/H; G.P. Szijjártó, Institute of Nanochemistry and Catalysis, Budapest/H; L. Végyvári, Combitech-Nanotech Kft., Budapest/H  
**High-throughput and combinatorial development of multi-component catalysts for ethanol steam reforming**  
 13:00 **HOT SLOT**  
 R. Domènech-Ferrer, G. Garcia, J. Rodriguez-Viejo, UAB Bellaterra/E  
**Infrared thermography as a combinatorial tool for the discovery of new materials for hydrogen storage**  
 13:30 Lunch  
**Heterogeneous catalysis**  
*Chair: K. Stöwe*  
 15:00 **HOT SLOT**  
 B. Meijerink, M. Brasz, M. Lok, Avantium Technologies/NL  
**Use of high-throughput experimentation in syngas based research**  
 15:20 **HOT SLOT**  
 A. Sorokin, E. Kudrik, IRCELYON, Villeurbanne/F  
**Phthalocyanine metal complexes: Versatile catalysts for selective oxidation and bleaching**  
**Homogeneous catalysis**  
*Chair: P. Bishop*  
 15:40 **KEYNOTE**  
 A. Maldonado, G. Rothenberg, University of Amsterdam/NL  
**Customizing predictive modeling and ligand design for industrial applications in homogeneous catalysis**  
 16:20 **HOT SLOT**  
 J. Christoffers, Oldenburg University/D  
**Cerium and bismuth catalysis hand in hand? Synthesis of an eight-membered-ring lactam-library**  
 16:40 **Poster session and exhibition**  
**Polymerisation catalysis**  
*Chair: J. Paul*  
 19:00 **PLENARY**  
 U. Schubert, Universität Jena/D  
**High-output experimentation in polymerization catalysis**  
 21:00 **Conference Dinner**

## PROGRAMME

### Wednesday, 29 April 2009

- Data management and information technologies**  
*Chair: D. Farrusseng*  
 09:00 **KEYNOTE**  
 J.W.A. Sachtler, UOP LLC, Des Plaines/USA  
**A statistical toolbox for high-throughput experimentation**  
 09:40 **KEYNOTE**  
 D. Nicolaidis, Accelrys Ltd., Cambridge/UK  
**Developing a platform and components for catalysis data management**  
 10:20 **KEYNOTE**  
 J.W. Thybaut, J. Sun, G.B. Marin, Ghent University/B; L. Olivier, A.C. Van Veen, C. Mirodatos, IRCELYON, Villeurbanne/F  
**Microkinetic analysis and optimisation of methane oxidative coupling**  
 11:00 Coffee  
**Data management and information technologies**  
*Chair: J. W. A. Sachtler*  
 11:20 **KEYNOTE**  
 A. Goulon, A. Faraj, IFP, Rueil-Malmaison/F; G. Pirngruber, M. Jacquin, F. Porcheron, P. Leflaive, IFP-Lyon, Vernaison/F; P. Martin, G.V. Baron, J.F.M. Denayer, Vrije Universiteit Brussel/B  
**Novel graph machines/QSAR approach for adsorption isotherms prediction**  
 12:00 **HOT SLOT**  
 F. Rudolphi, L.J. Goossen, TU Kaiserslautern/D  
**A free and platform-independent electronic laboratory notebook**  
 12:20 **HOT SLOT**  
 K. Metaxas, J.W. Thybaut, G.B. Marin, Ghent University/B; G. Morra, D. Farrusseng, C. Mirodatos, IRCELYON, Villeurbanne/F  
**Microkinetic model construction with significant parameter estimation**  
 12:40 **HOT SLOT**  
 V. Ostrovskii, Karpov Institute of Physical Chemistry, Moscow/RUS  
**Review of the molar heats of chemisorption of gases at metals: To what solution does the problem of homogeneity vs. heterogeneity of catalyzing surfaces lead to?**  
 13:00 **Closing remarks**  
 F. Ausfelder, A. Corma, C. Mirodatos  
 13:15 **End of conference**