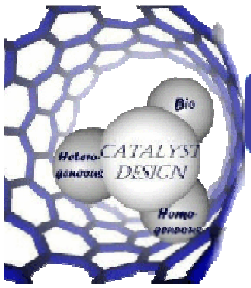


*IDECAT Conference on Catalysis*

**Concepts, complexity and diversity in catalysis**

**Porquerolles 12 - 17 May 2007**

# Programme

# SCHEDULE

| | **May, 12 (Saturday)** | **May, 13 (Sunday)** | **May, 14 (Monday)** | **May, 15 (Tuesday)** | **May, 16 (Wednesday)** | **May, 17 (Thursday)** |
|---|---|---|---|---|---|---|
| | | Breakfast | Breakfast | Breakfast | Breakfast | Breakfast |
| **9:00-9:45** | | Prof. B. Sels | Prof. A. Corma | Dr. A. Mc Connel | Prof. D.J. Cole-Hamilton | Departure |
| **9:45-10:30** | | Prof. F. Cavani. | Dr. R.B. Hall | Prof. G. Van Koten | Prof. B. Weckhuysen | |
| **10:30-11:00** | | Coffee Break | Coffee Break | Coffee Break | Coffee Break | |
| **11:00-11:45** | | Prof. M. Witko | Prof. J. Lercher | Prof. J. Evans | Dr. S. Shaikhutdinov | |
| **11:45-12:30** | | Dr. P. Sautet | 2 Oral communications | 2 Oral communications | 2 Oral communications | |
| **12:30-13:30** | | Lunch | Lunch | Lunch | Lunch | |
| **13:30-18:00** | Registration | Free time | Free time | Free time | Free time | |
| **18:00-18:45** | Registration | Prof. K. Domen | Prof. S. Bordiga | Dr. H. Olivier-Bourbigou | Dr. J. Nerlov | |
| **19:00-20:00** | Dinner | Dinner | Dinner | Dinner | Banquet | |
| **20:00:20:45** | Dr R. Schloegl | Prof. Hensen | Prof. R. Anwander | Prof. S. Sabo-Etienne | Prof. G. Centi | |
| **20:45-21:30** | Dr R. Farrauto | Poster session (group 1) | Dr. C. Copéret | Prof. K. Faber | Poster session (group 2) | |
| **21:30-23:00** | Reception* | Poster session (group 1) | Poster session (group 2) | Poster session (group 1) | Poster session (group 2) | |

* Poster should be posted during that time.

Total :
25 Lectures are 30 min long + 15 min of questions
6 Oral communications are 15 min long + 7 min of questions

Posters GROUP 1: odd numbers
Posters GROUP 2: even numbers

# Lectures and oral communications

**May, 12 (Saturday)**

*Chairperson: Jean-Marie Basset*

**20:00-20:45** **Schloegl Robert** Fritz-Haber-Institut der Max-Planck GERMANY
*Understanding heterogeneous catalysis of demanding processes: how essential is complexity ?*

**20:45-21:30** **Farrauto Robert** BASF Catalysts LLC. USA
*From the internal combustion engine to the fuel cell: moving towards the hydrogen economy*

**May, 13 (Sunday)**

*Chairperson: Elisabeth Bordes-Richard*

**09:00-09:45** **Sels Bert** KU Leuven, BELGIUM
*Fluorescence microscopic studies of the reactivity of heterogeneous*

**09:45-10:00** **Cavani Fabrizio** University of Bologna, ITALY
*Fluorescence microscopic studies of the reactivity of heterogeneous*

*Chairperson: Rutger van Santen*

**11:00-11:45** **Witko Malgorzata** University of Cracovy, POLAND
*Quantum chemistry as a tool to study catalytic active centers*

**11:45-12:30** **Sautet Philippe** ENS Lyon, FRANCE
*Alkane activation with Zr and W complexes grafted on gamma-alumina: synergy between support and complex reactivity from a quantum chemical approach*

*Chairperson: Robert Schloegl*

**18:00-18:45** **Domen Kazunari** The University of Tokyo JAPAN
*Design of photocatalysts for overall water splitting*

**20:00-20:45** **Hensen Emiel** TU Eindhoven, THE NETHERLAND
*Understanding alkane activation over Lewis acid sites in zeolites*

**May, 14 (Monday)**

*Chairperson: Gabriele Centi*

**09:00-09:45** **Corma Avelino** Instituto de Technologia Quimica, Valencia, SPAIN
*Molecular design of single and double site catalysts for one step and for cascade reactions*

**09:45-10:30** **Hall Richard** ExxonMobil Research and Eng. USA
*Influence of micropore cage dimension on MTO and olefin conversion*

*Chairperson: Carlo Lamberti*

**11:00-11:45** **Lercher Johannes A.** Technische Universität München GERMANY
*Alkane activation by solid acids*

**11:45-12:30** **2 oral communications (posters)**

*Chairperson:Ive Hermans*

**18:00-18:45** **Bordiga Silvia** University of Torino ITALY
*Combined use of spectroscopies and computational techniques to characterize molecularly defined species*

**20:00-20:45** **Anwander Reiner** University of Bergen, NORWAY
*Size/shape-selective reactions on periodic nanoporous silica*

**20:45-21:30** **Copéret Christophe** ESCPE Lyon FRANCE
*Molecular understanding of heterogeneous catalysts*

## May, 15 (Tuesday)

*Chairperson: Laurent Garel*

**09:00-09:45** **Mc Connell Ann** SASOL, Sasolburg, SOUTH AFRICA
*Recent progress towards the design and optimisation of highly selective ethylene oligomerisation catalysts*

**09:45-10:30** **Van Koten Gerard** Utrecht University, THE NETHERLANDS
*Making homogeneous catalysts (nano)filterable*

*Chairperson: Marcel Janssen*

**11:00-11:45** **Evans John** University of Southampton UNITED KINGDOM
*Rhodium: the chameleon catalyst*

**11:45-12:30** **2 oral communications (posters)**

*Chairperson: Paul Webb*

**18:00-18:45** **Hélène Olivier-Bourbigou** IFP FRANCE
*Ionic Liquids : Applications in catalysis*

**20:00-20:45** **Sabo Etienne Sylviane** LCC, Toulouse, FRANCE
*Concepts in catalysis: the sigma-CAM mechanism*

**20:45-21:30** **Faber Kurt** Karl Franzens Universität, Graz AUSTRIA
*Impossible reactions catalyzed by racemases, stereo-complementary dehydrogenases and sulfatases*

## May, 16 (Wednesday)

*Chairperson: Peter Haerter*

**09:00-09:45** **Cole-Hamilton David** University of St. Andrews UNITED KINGDOM
*New Homogeneous reactions and separation strategies*

**09:45-10:30** **Weckhuysen Bert** Utrecht University, THE NETHERLANDS
*Catalysts live and up close: probing catalytic solids with spectroscopy and microscopy*

*Chairperson: Sudhakar Chakka*

**11:00-11:45** **Shaikhutdinov Shamil** Fritz-Haber-Institut - MPG - Berlin GERMANY
*Model systems for heterogeneous catalysts at atomic resolution*

**11:45-12:30** **2 oral communications (posters)**

*Chairperson: John Evans*

**18:00-18:45** **Nerlov Jesper** Haldor Topsøe DENMARK
*Supported metal catalysts: From fundamental understanding to industrial application*

**20:00-20:45** **Centi Gabriele** Università di Messina, ITALY
*Nanostructured electrocatalysts*

# Posters titles

Posters GROUP 1: odd numbers  Posters GROUP 2: even numbers

1. **Abbenhuis Erik**
   *Hybrid Catalysis with Nanostructured POSS Metal derivatives*
2. **Ahr Mathieu**
   *Noels' and Grubbs' catalysts: two different systems, one unique active species*
3. **Albonetti Stefania**
   *Colloids as building blocks for nanosized supported catalysts*
4. **Baldé Cornelis**
   *Hydrogen storage in Nanostructured NaAlH4 deposited on Carbon Nanofibers*
5. **Bonnet Sylvestre**
   *Arene-pincer hybrids for catalysis: metal-to-metal interactions through simultaneous sigma- and pi-coordination.*
6. **Bordes-Richard Elisabeth**
   *Multicomponent oxides in selective oxidation of alkanes: Theoretical acidity vs. Selectivity*
7. **Botella Pablo**
   *Delaminated zeolitic materials for replacing mineral acid catalysts in industrial processes*
8. **Cavani Fabrizio**
   *A study on the nature of the surface active layer in Vanadyl Pyrophosphate, catalyst for the oxidation of n-butane to maleic anhydride*
9. **Clement Nicolas**
   *Industrially useful 100% atom efficient reactions: the Pd-catalysed telomerization and dimerization of butadiene. A theoretical and experimental mechanistic study*
10. **Cristol Sylvain**
    *Operando studies of alumina-supported oxomolybdates for methanol selective oxidation*
11. **Dal Santo Vladimiro**
    *Synergistic effect in arene hydrogenation over hybrid bimetallic sites Rh(I)-Pd(0)*
12. **Delbecq Françoise**
    *DFT study of a selective reaction: acrolein hydrogenation on Pt(111).*
13. **Estephane Jane**
    *Structure and reactivity of chromocene confined into nanovoids with a different polarity: from organometallic chemistry to catalysis*

**14. Fey Natalie**

*Maps of ligand space*

**15. Gambatesa Antonio**

*Selective Catalysts for Hydrogenolysis/Ring opening of Tetralin*

**16. Geske Michael**

*A View on the Mechanism of the Catalytic Partial Oxidation of Methane*

**17. Groppo Elena**

*Functionalization of nanoporous polystyrenes by means of an organometallic approach: new materials exploitable for catalytic applications*

**18. Groppo Elena**

*CH2Cl2 as a selective modifying agent to create a new family of highly reactive Cr polymerization sites*

**19. Groppo Elena**

*EXAFS study of the impregnation and reduction processes of Pd/C catalysts*

**20. Gruttadauria Michelangelo**

*Polystyrene supported L-proline: a recyclable organocatalyst for the asymmetric aldol reaction in the presence of water*

**21. Hejduk Pawel**

*Ammonia Activation at Low-indices V2O5 Surfaces in SCR Reaction – Cluster DFT Study*

**22. Hintermair Ulrich**

*Supported Ionic Liquid Phase Catalysis with Supercritical Flow*

**23. Jirglová Hana**

*Interactions of NH3 with Co ions in the zeolite framework studied by FTIR/UV-Vis spectroscopy*

**24. Kaucky Dalibor**

*Fe-zeolite catalysts doped with second noble metal for N2O decomposition.*

**25. Lallemand Michael**

*Development of new laboratory tools for the heterogeneous catalysis*

**26. Lamberti Carlo**

*Nanovoid-structured TiO2 encapsulating (I2)n molecules: a way to tune the photoactivity in the visible region*

**27. Leveneur Sébastien**

*Kinetic study and modelling of peroxypropionic acid synthesis from propionic acid and hydrogen peroxide using homogeneous catalysts*

**28. Liotta Leonarda**

*SO2 poisoning effect on the activity of Pd/Co3O4 and Pd/Co3O4-CeO2 catalysts for CH4 combustion*

**29. Llabrés i Xamena Francesc X.**

*Direct and reverse shape-selective catalysis by metal-organic*

*frameworks*

**30. Loffreda David**

*Theoretical Insight of Adsorption Thermodynamics and Soft Vibrations of Multifunctional Molecules on Metal Surfaces*

**31. Matas Guell Berta**

*Influence of the oxude support and oxygen addition on the steam reforming of acetic acid Pt based catalysts*

**32. MikkolaJyri-pekka**

*The effect of Lewis acid in supported ionic liquid catalysts (SILCA) applied in the hydrogenation of α,β-unsaturated aldehydes*

**33. Mitterpleininger Josef**

*A new efficient and environmentally sound synthesis of the catalyst Methyltrioxorhenium (MTO)*

**34. Moncho Salvador**

*The relative stability of 14-electron T-shaped palladium complexes from a computational point of view*

**35. Pale Patrick**

*Click Chemistry" in CuI-Zeolites*

**36. Rendón Nuria**

*Highly Active, Stable, and Selective Well-Defined Silica Supported Mo Imido Olefin Metathesis Catalysts*

**37. Rentzsch Christoph**

*Catalytic C-H Borylation of aromatic compounds mediated by different NHC-Iridium(I) Complexes*

**38. RivallanMickael**

*Structure and nuclearity of active sites in Fe-zeolites: comparison with iron sites in enzymes and homogeneous catalysts*

**39. Sazama Petr**

*Hydrogen function at decane-SCR-NOx over Ag/alumina*

**40. Shetty Sharankumar**

*CO induced reconstruction of Ru clusters*

**41. Stavitski Eli**

*Non-uniform catalytic behavior of zeolite crystals as revealed by in-situ optical micro-spectroscopy*

**42. Sterrer Martin**

*Controlling the properties of gold atoms and clusters on supported model catalysts by the oxide film thickness.*

**43. Su Dangsheng**

*Nanocarbons as Robust catalysts for Oxidative Dehydrogenation of Ethylbenzene to Styr*

**44. Ujaque Gregori**

*Functionalization of alkene catalyzed by gold complexes: solvent and*

*counterions are not mere spectators during reaction.*

**45. Varszegi Csaba**

*Selective adsorption of small olefins on zeolites*

**46. Veljanovski Draganco**

*Investigation of CpMoO2CH3 as an epoxidation catalyst, the next chapter in the MTO success story*

**47. Venezia Anna**

*Pd and PdAu on mesoporous silica for methane oxidation: effect of $SO_2$*