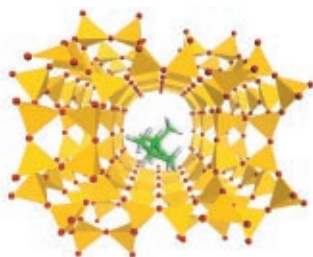


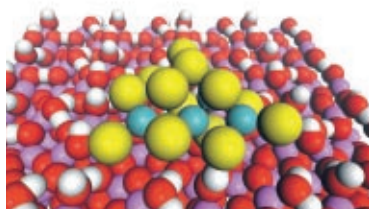
Research Advances in Rational Design of Catalysts and Sorbents

14 - 16 December 2005, IFP-Lyon, France

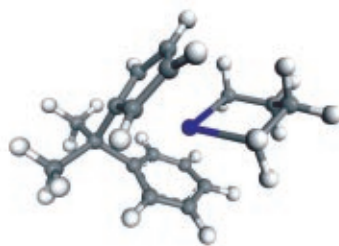
Second Announcement and Registration Form



Adsorption of dimethyl-hexane
in TON-zeolite



γ -alumina supported MoS₂ catalyst



Ti-complex catalyst
of ethylene oligomerization

Under the auspices of the French Academy of Sciences
Sous les auspices de l'Académie des sciences



Sustainable development aims at making our energy use more efficient while preventing global and local atmospheric pollution. This aim and economic incentives call for process intensification, with special emphasis on the development of improved catalysts and sorbents. The petrochemical, refining, and automotive industries and their suppliers are strong players in these developments.

Researchers in materials science and organometallic chemistry are therefore working with chemical engineers to explore innovative approaches and to find new concepts to help in designing catalysts and sorbents.

Recent advances in molecular modeling techniques, based both on first principles (Density Functional Theory, DFT) and on classical Monte Carlo simulation approaches, offer new ways of investigating and understanding even systems as complex as homogeneous catalysts, supported heterogeneous catalysts, and molecular sieves at high pressures.

These modern simulation techniques have been “knocking at experimental labs’ doors” for almost a decade. Dialogue has been established between experimentalists and “modelers”, leading to a worthwhile updating of concepts such as confinement in sorbents, periodic trends, effects of promoters or supports in heterogeneous catalysis, and effects of ligands in homogeneous catalysis. Another important development is the recent success, in both homogeneous and heterogeneous catalysis, of predictive kinetic models based on computational descriptions of reaction pathways.

At the same time, the emergence of high throughput experimentation (HTE) techniques has also modified the traditional experimental approaches. An increased need for theoretical tools to provide guidelines, and knowledge-based chemical descriptors, is foreseen. Indeed, it is a major challenge not only to organize in a useful way the vast amount of data generated by HTE, in order to optimize the information fed back into the loops, but also to rationally restrain the search space.

The objective of this IFP international conference is accordingly to highlight and discuss the recent achievements of combined experimental and molecular modeling approaches in research on catalysts and sorbents. We anticipate that the presentations at this workshop will contribute to the growing awareness of the scientific community of the key issue of rational design of these materials.

This international conference will be held at IFP, 69390 Vernaison (France), from Wednesday 14 to Friday 16 December 2005.

Scientific Committee

- Pr. Michel Che (University of Paris VI, France)
- Pr. Robert Crabtree (Yale University, USA)
- Dr. Jean-Luc Dubois (Arkema, France)
- Pr. Alain Fuchs (University of Paris-Sud, France)
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- Pr. Philippe Sautet (ENS-Lyon, France)
- Dr. Hervé Toulhoat (IFP, France)

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- Philippe Ungerer
- Denis Uzio

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For more information on this international conference and other events organized by IFP, we encourage you to connect to <http://events.ifp.fr>

Information about the program

Scientific Sessions

The sessions will be introduced by a keynote and illustrated by oral presentations and posters. Posters are an integral part of the conference.

The program will consist in 4 sessions:

- Active sites, mechanisms and kinetics
- Chemical trends and the discovery of new catalysts
- Support effects in catalysis
- Adsorption and confinement

Oral presentations: the conference will include 27 oral presentations

- 40 minutes for keynote speakers, including 10 minutes discussion
- 20 minutes for the other speakers, including 5 minutes discussion

Poster sessions: 62 posters will be displayed simultaneously during the whole conference.

A **round table** is organised to draw the future challenges for the accelerated design of catalysts, chemicals and other materials.

A **visit** of IFP labs is proposed.

Conference Proceedings

Abstracts from the oral and poster presentations will be included in a volume given out on site to all registered participants.

A selection of the oral presentations will be published after the conference in a special issue of Oil & Gas Science and Technology - La Revue de l'IFP.

One copy will be offered to each registered participant.

For additional orders, please contact Editions Technip, 27 rue Ginoux, 75015 Paris, France.

Tel.: +33 (0)1 45 78 33 80, Fax: +33 (0)1 45 75 37 11,

Web site: <http://www.editionstechnip.com>

Official Language

English will be the official language.

Simultaneous interpretation will not be provided.

Program

Wednesday 14 December

8.30 - 9.15 Registration

9.15 - 9.30 Welcome address and introduction
J. Lecourtier, Scientific Director (IFP, France)

Session I: Active sites, mechanisms and kinetics

9.30 - 10.10 **Keynote address:** Rational design of heterogeneous catalysts via surface organometallic catalysis: known and new reactions
Pr. J.-M. Basset (CPE-Lyon, LCOMS, France, Member of the French Academy of Sciences)

10.10 - 10.50 **Keynote address:** first-principles statistical mechanics for heterogeneous catalysis
Dr. K. Reuter (Fritz-Haber-Institut, Berlin, Germany)

10.50 - 11.20 *Break*

11.20 - 11.40 **Monomolecular cracking of alkanes over acidic zeolites**
T. Bučko, J. Angyán, L. Benco, J. Hafner (CMS-Univ. Wien, Austria)

11.40 - 12.00 **Hydroxyl groups and basic reactivity on MgO: a theoretical and experimental study**
C. Chizallet¹, G. Costentin¹, H. Lauron-Pemot¹, F. Delbecq², P. Sautet², M. Che¹ (¹LRS-UPMC, Paris, France; ²ENS-Lyon, France)

12.00 - 12.20 **Ethene epoxidation selectivity inhibited by twisted oxametallacycle: a DFT study on Ag surface-oxide**
M.L. Bocquet, D. Loffreda (ENS-Lyon, France)

12.20 - 12.40 **Fischer-Tropsch synthesis: development of a microkinetic model for metal catalysis**
G. Lozano Blanco¹, J.W. Thybaut¹, K. Surla², P. Galtier², G.B. Marin¹ (¹LPT-Univ. of Ghent, Belgium; ²IFP, France)

12.40 - 13.00 **DRIFTS-MS-SSITKA study of reaction intermediates and spectators during the water-gas-shift reaction over Pt/Ceria**
F. Meunier, D. Reid, S. Shekhtman, A. Goguuet, D. Tibiletti, J. Breen, C. Harcacre, R. Burch (CenTACat, Queens Univ. Belfast, UK)

13.00 - 14.30 *Lunch*

Wednesday 14 December

Session 2: Chemical trends and the discovery of new catalysts

- 14.30 - 15.10 **Keynote address:** Heterogeneous catalysis from first-principles
Pr. J.K. Nørskov (CAMP, NanoDTU, Technical Univ. of Denmark)
- 15.10 - 15.50 **Keynote address:** Periodic trends in transition metal sulfide catalysis: intuition and theory
Dr. R.R. Chianelli (MRTI, Univ. of Texas, El Paso, USA)
- 15.50 - 16.10 **Dual effect of H₂S on volcano curves in hydrotreating sulfide catalysts**
N. Guemalec¹, C. Geantet¹, P. Raybaud², T. Cseri², M. Vrinat¹
(¹IRC-CNRS, France; ²IFP, France)
- 16.10 - 16.30 **Large-scale, first-principles screening of alloys for heterogeneous catalysis**
J. Greeley, K.W. Jacobsen and J.K. Nørskov (Technical Univ. of Denmark)
- 16.30 - 16.50 **Design of new heterogeneous chiral catalysts based on surface confinements effects**
J.M. Fraile, J.I. García, J.A. Mayoral, E. Pires, I. Villalba
(ICMA, CSIC-Univ. de Zaragoza, Spain)
- 16.50 - 17.00 *Break*
- 17.00 - 18.15 *Poster session*
- 18.15 - 19.30 **Round table: Molecular modeling and High-Throughput Experimentation (HTE) versus the challenges of catalysts, chemicals and other materials design**
- Participants:**
- | | |
|--------------------|---------------------------------|
| Pr. G.V. Baron | (Vrije Univ. Brussels, Belgium) |
| Dr. R.R. Chianelli | (Univ. of Texas, El Paso, USA) |
| Dr. D. Farrusseng | (IRC-CNRS, Lyon, France) |
| Dr. S. Morin | (IFP, France) |
| Pr. J.K. Nørskov | (Technical Univ. of Denmark) |
| Dr. C. Wolverton | (Ford Motor Company, USA) |
- 19.30 *Cocktail*
- 21.00 *Bus departure*

Thursday 15 December

8.30 - 9.15 Registration

Session 3: Support effects in catalysis

9.15 - 9.55 **Keynote address:** The use of density functional calculations in the automotive industry: catalyst supports and hydrogen storage materials
Dr. C. Wolverton (Ford Motor Company, USA)

9.55 - 10.35 **Keynote address:** Support materials and characterization tools for nanostructured catalysts
Pr. K.P. de Jong (Utrecht Univ., The Netherlands)

10.35 - 11.00 *Break*

11.00 - 11.20 **Arrays of metal clusters grown on nanostructured alumina surfaces: toward ideal supported model catalysts**
C.R. Henry, G. Hamm, J.-C. Dupin (CRMCN-CNRS, Marseille, France);
C. Becker (IPTC, Univ. of Bonn, Germany)

11.20 - 11.40 **Modeling and understanding the support effect on the surface properties and functions of oxide catalysts: the example of vanadia**
V. Ganduglia-Pirovano, T.K. Todorova, V. Brázdová, J. Sauer
(Humboldt-Univ. zu Berlin, Germany)

11.40 - 12.00 **Adsorption of a palladium atom on γ -Al₂O₃ surfaces: a DFT study**
M. Corral Valero^{1,2}, P. Raybaud², P. Sautet¹
(¹ENS-Lyon, France; ²IFP, France)

12.00 - 12.20 **Modeling active sites of metals supported on metal oxides**
S. French (Johnson Matthey, UK), A.A. Sokol, R. Catlow (Royal Institution, UK)

12.20 - 12.40 **Influence of support and reaction conditions on catalyst reduction state and on oxidative dehydrogenation of propane over VO_x/Ti-SiO_x**
O. Ovsitser, M. Cherian, E. Kondratenko, M. Baerns, U. Dingerdissen
(Institute for Applied Chemistry Berlin-Adlershof, Germany)

12.40 - 13.00 **³⁵S tracer study of the effect of support on the nature of active sites of Co(Ni)Mo sulphide catalysts supported on Al₂O₃ and activated carbon and modified by P and F additives**
V.M. Kogan, N.N. Rozhdestvenskaya
(N.D. Zelinsky Institute of Organic Chemistry, Moscow, Russia)

13.00 - 14.30 *Lunch*

Thursday 15 December

Session 4: Adsorption and confinement

- 14.30 - 15.10 **Keynote address:** Adsorption and reactions in confined spaces
Pr. J.F.M. Denayer, Pr. G.V. Baron (Vrije Univ. Brussels, Belgium)
- 15.10 - 15.50 **Keynote address:** Understanding shape selectivity in zeolite
Pr. B. Smit (Univ. of Amsterdam, The Netherlands; CECAM, France)
- 15.50 - 16.10 **Development and application of molecular simulation methods for the screening of industrial zeolite adsorbents**
A. H. Fuchs¹, A. Boutin¹, J.-M. Teuler¹, A. Di Lella¹, A. Wender², B. Tavitian², P. Ungerer¹⁻² (¹ LCP, Univ. de Paris Sud XI, CNRS; ² IFP, France)
- 16.10 - 16.30 **Energetic and entropic contributions controlling the sorption of benzene in zeolites**
A. Jentys, R.R Mukti, J.A. Lercher (TU München, Germany)
- 16.30 - 16.50 *Break*
- 16.50 - 17.10 **Protonated hydrocarbons in zeolites: carbenium ions or alkoxides?**
J. Sauer, C. Tuma (Humboldt-Univ. zu Berlin, Germany)
- 17.10 - 17.30 **Kinetics of water sorption on “CaCl₂ confined to silica (alumina)”:**
macro- versus mesopore diffusion
I. Glaznev, I. Koptuyug, Y. Aristov
(Boriskov Institute of Catalysis, ITC, Novosibirsk, Russia)
- 17.30 - 17.50 **Coadsorption of ethylmercaptan and toluene or heptane on the zeolite NaX**
F. Benoit¹, G. Weber¹, J.-P. Bellat¹, P. Mougin², M. Thomas¹
(¹ LRRS, Univ. de Bourgogne; ² IFP, France)
- 17.50 - 18.00 *Closing address*
- 18.00 *Bus departure*

Friday 16 December

Visits of IFP labs are proposed on Friday 16 December, morning.

As the number of participants is limited, please register with the form here enclosed.

Registered participants will be informed of the visit schedule by e-mail.

Posters

Posters of session I

- 1. How catalytic reactions may occur?**
F. Garin (LMSPC, Univ. Louis Pasteur, Strasbourg, France)
- 2. Brønsted acid sites in EU-I zeolite: DFT, infrared and NMR studies**
T. Armaroli, A.A. Quoineaud, T. Demuth, S. Lacombe, P. Raybaud (IFP, France)
- 3. Stability and reactivity of lewis sites in zeolites**
L. Benco, T. Bucko, J. Hafner (Univ. of Wien, Austria); H. Toulhoat (IFP, France)
- 4. Quantum chemical approach for the modeling of active sites in TMI-zeolites**
D. Berthomieu, N. Jardillier, A. Goursot, G. Delahay, B. Coq (ENSCM, Montpellier, France)
- 5. Nature of active sites in Fe-zeolites and their role in the catalytic abatement of NO_x and N₂O**
A. Brückner, K. Santhosh (ACA, Germany); M. Schwidder, W. Grünert (Rhur-Univ. Bochum, Germany); N. Debbagh, J. Perez-ramirez (ICIQ, Tarragona, Spain)
- 6. Nature and structure of active sites for acid-catalyzed reaction on cationic zeolites in presence of H₂S**
V. Blasin-Aubé, M. Gaillard, V. Montouillout, L. Oliviero, A. Vimont, C. Fernandez, F. Maugé (LCS-CNRS, Caen, France)
- 7. A combined dispersive-EXAFS and theoretical study of the location of Ni²⁺ in faujasite**
P. Massiani, D. Costa, J.F. Groust (LRS-UPMC, Paris, France)
- 8. Effect of crystal size on the spectroscopic and acidity properties of H-ZSM-5 zeolite**
T. Armaroli, L. Simon (IFP, France); T. Montanari, M. Bevilacqua, G. Busca (Genova Univ., Italy); V. Valtchev, J. Patarin (LMPC Mulhouse, France)
- 9. Influence of zeolite nature and active sites in hydroisomerization of hydrocarbons of gasoline**
A.V. Abramova, A.A. Panin, G.A. Kliger (Academy of Sciences, Russia)
- 10. Preferred adsorption sites for Pd²⁺ ions within the mordenite structure with double Al/Si substitution. Periodic DFT calculations.**
R. Grybos, L. Benco, J. Hafner (Univ. of Wien, Austria)
- 11. Mechanistic studies of the methanol-to-hydrocarbons reaction (MTH)**
S. Velle, M. Bjørngen, B. Arstad, U. Olsbye, K.P. Lillerud, S. Kolboe (Univ. of Oslo, Norway)
- 12. Activation of n-butane isomerization on sulphated zirconia by DFT calculations**
A. Hofmann, J. Sauer (Humboldt-Univ. zu Berlin, Germany)

Posters of session I

13. **Mechanisms of the oxidative dehydrogenation of propane by supported vanadium oxide**
X. Rozanska, J. Sauer (Humboldt-Univ. zu Berlin, Germany)
14. **Adsorption of S on (001), (110) and (111) surfaces of CeO₂ - performances of various hamiltonians**
P. Baranek (EDF R&D-MMC, France); L. Gautier, M. Marrony (European Institute of Energy Research, Germany)
15. **Activity of Zn-V-O catalysts in the reaction of conversion of ethanol into the acetone**
N. Baghirova, V. Baghiyev, A. Guliyev (Institute of Petrochemical Processes, Azerbaijan)
16. **Ru-Ce catalysts based on porous graphite-like carbon sibunit for catalytic wet air oxidation**
N. Dobrynkin, M. Batygina, O. Pestunova, V. Parmon (Boreskov Institute of Catalysis, Novosibirsk, Russia); M. Besson, P. Gallezot (IRC, France)
17. **Obtaining of acetone from isopropyl alcohol over industrial Ni/Cr₂O₃ catalyst**
S. Mammadkhanova, K. Adjamov (Azerbaijan State Oil Academy, Azerbaijan)
18. **Vanadia-titania aerogel catalysts for the selective oxidation of hydrogen sulfide - containing excess water and ammonia**
D.W. Park, M. Kim (Pusan National Univ., Korea)
19. **Identification of adsorbed reactants by theoretical simulations of HREELS spectra**
F. Delbecq, D. Loffreda, F. Vigne, P. Sautet (ENS Lyon, France)
20. **Why copper is intrinsically more selective than silver in alkene epoxidation: ethylene oxidation on Cu(111) versus Ag(111)**
D. Torres Rangel (Univ. de Barcelona, Spain)
21. **A DFT study of CO and O adsorption and vibrations on platinum-tin surfaces**
C. Dupont, D. Loffreda, Y. Jugnet, F. Delbecq (ENS Lyon, France)
22. **Methane activation on flat and defective Ni(111) surface**
M.F. Haroun, P.S. Moussounda, P. Legare (Univ. Louis Pasteur, Strasbourg, France)
23. **Competitive routes for a chemo-regioselective reaction on a metal surface from an atomistic theoretical approach**
D. Loffreda, F. Delbecq, F. Vigne, P. Sautet (ENS Lyon, France)
24. **Theoretical calculations of electrochemical ammonia synthesis under ambient pressure and temperature**
T. Bligaard¹, E. Skulason², H. Jonsson², J.K. Nørskov¹
(¹Technical Univ. of Denmark; ²Univ. of Iceland)

Posters of session I

25. **The simplest model of adsorption on stepped surface: transfer matrix approach**
A.V. Myshlyavtsev, M.D. Myshlyavtseva (Omsk State Technical Univ., Russia)
26. **Surface organo-metallic chemistry on metals, characterization and application in catalysis**
J.-P. Candy, J.-M. Basset (CNRS-CPE Lyon, France)
27. **Alkane Metathesis on silica supported tantalum hydride: a DFT study**
S. Schinzel, H. Chermette (Univ. Claude Bernard Lyon I, France);
C. Copéret, J.-M. Basset (CNRS, CPE Lyon, France)
28. **Application of isotope methods for determination of mechanisms of heterogeneous selective oxidation mediated by iron phthalocyanines**
A. Sorokin (IRC-CNRS, France)
29. **Pt-(0)-alkene complexes: a tool for exploration of surface phenomena in heterogeneously catalyzed hydrogenations**
P. Kacer¹, D. Karhanek¹, H. Siklova¹, M. Kuzma², L. Cerveny¹
(¹ ICT Prague; ² Institute of Microbiology Academy of Sciences, Prague, Czech Republic)
30. **A DFT study on trimerisation of ethylene to 1-hexene using cationic titanium complexes: the influence of (hemi)-labile ligands**
T. De Bruin, L. Magna, P. Raybaud, H. Toulhoat (IFP, France)
31. **Hydrotalcite-like compounds as catalysts in the oxidation of olefins**
S. Ruwaida (Univ. of KwaZulu-Natal, South Africa)
32. **In situ radioisotopic study into the active sites of sulphide hydrotreating catalysts function**
V. Kogan (N.D. Zelinsky Institute of Organic Chemistry, Russia)
33. **Catalytic behaviors of β - $M_{0.78}O_2$ as hydrodesulfurization catalyst**
S.W. Gong, H.K. Chen, W. Li, B.Q. Li (Chinese Academy of Sciences, China)
34. **Effect of promoter on sulfidation of hydrotreating catalysts: measurements of solid mass under pressure conditions**
T. Homma, M. Echard, J. Leglise (LCS-ENSI Caen, France)
35. **Hydroconversion of a vacuum residue with Ni-Mo metallic nanoparticles**
J. Córdova¹, C. Bolívar¹, P. Rodríguez¹, G. Gonzalez², A. Sagarzazu², C.E. Scott¹
(¹ Univ. Central de Venezuela; ² Instituto Venezolano de Investigaciones Científicas, Venezuela)
36. **Oscillation theory peculiarities and practical importance**
L.B. Datsevich, A. Jess, T. Oehmichen (Univ. of Bayreuth, Germany)

Posters of session 2

1. Combining solid state physics concepts and x-ray absorption spectroscopy to understand heterogeneous catalysis
D. Bazin (Univ. Paris XI, France)
2. Radioisotopic monitoring of active sites for design of new hydrotreating catalysts
V. Kogan, N.A. Popov (N.D. Zelinsky Institute of Organic Chemistry, Russia)
3. New approach for the understanding of hydrodesulfurization mechanism over unsupported transition metal sulfides
M. Arias, D. Laurenti, M. Vrinat, M. Lacroix (IRC-CNRS, France)
4. H₂ activation by transition metal center on carbon surfaces (nanotube and graphite): trends and rationalization
G. Frapper, H. Valencia (LACCO-Univ. de Poitiers, France)
5. Oxygen-free conversion of methane over catalysts prepared by metavapor method
V.M. Akhmedov, M.A. Dosari, S.H. Al-Khowaiter (PPRI, Saudi Arabia)
6. Selective production of hydrogen for pem fuel cells via oxidative steam reforming of methanol using cerium promoted copper-alumina catalysts
S. Patel, K.K. Pant (Indian Institute of Technology, New Delhi, India)

Posters of session 3

- 1. Nanomaterials: new, active and highly selective catalyst for green chemistry**
J. Barrault (LACCO-ESIP, CNRS, France)
- 2. DFT study of the interaction of MoS₂ with γ -alumina and anatase TiO₂**
D. Costa^{1,2}, C. Arrouvel^{1,2}, M. Bresse², H. Toulhoat¹, P. Raybaud¹
(¹ IFP, France; ² LRS-UPMC, France)
- 3. Theoretical study of ruthenium support effect in adsorption properties of metallic and bimetallic monolayers**
S. González, C. Sousa, F. Illas (Univ. de Barcelona, Spain)
- 4. Interaction of cobalt particles with dehydroxylated alumina**
M.N. Mikhailov, G.M. Zhidomirov, A.Y. Krylova (Yukos R&D Centre, Russia)
- 5. CO and Lewis bases adsorption on MgCl₂ surfaces: precise IR spectra simulation, comparison with experiment**
D. Trubitsyn, A. Potapov (Russia)
- 6. Effect of pore length of Pt/KL zeolite catalyst on n-octane aromatization**
S. Trakamroek, S. Jongpatiwut, T. Rirksomboon, S. Osuwan (Chulalongkorn Univ., Bangkok, Thailand), D.D. Resasco (Univ. of Oklahoma, Norman, USA)
- 7. CO₂ formation reactions under Fischer-Tropsch synthesis conditions**
A. Krylova, L. Sineva, D. Tarakanov (Yukos R&D Centre, Russia)
- 8. Characteristics of vanadia on the surface of V₂O₅/sulfated Ti-PILC catalyst for the reduction of NO by ammonia**
L. Khalfallah Boudali, A. Ghorbel (Faculté des Sciences de Tunis, Tunisia); P. Grange (Univ. Catholique de Louvain, Belgium)
- 9. Related influences of precursors salts and supports on iron-molybdenum sulfides catalysts**
A. Rives¹, J. Altafulla², R. Hubaut¹, C.E. Scott²
(¹ UST de Lille, France; ² Univ. Central de Venezuela, Caracas, Venezuela)
- 10. One-step nonhydrolytic sol-gel synthesis of epoxidation catalysts**
P.H. Mutin, V. Lafont, A. Vioux (Univ. Montpellier II, France)

Posters of session 4

- 1. Molecular simulation of adsorption of alkanes in faujasite**
A. Wender¹⁻², A. Boutin², B. Tavitian¹, A.C. Dubreuil¹⁻², A.H. Fuchs²
(¹ IFP, France; ² LCP-CNRS, Univ. de Paris Sud XI, France)
- 2. Theoretical determination of aluminium distribution in aluminosilicates**
E. García-Pérez¹; D. Dubbeldam²⁻³, B. Smit²⁻³, S. Calero¹
(¹ Univ. Pablo de Olavide, Spain; ² Univ. of Amsterdam, The Netherlands; ³ CECAM-Lyon, France)
- 3. Adsorption of water in zeolites, as studied by molecular simulations**
A. Di Lella¹⁻², A. Boutin¹, P. Ungerer¹⁻², A.H. Fuchs¹
(¹ LCP-CNRS, Univ. de Paris Sud XI, France; ² IFP, France)
- 4. Grand canonical Monte Carlo simulations of sorption equilibria in different types of zeolite for various pollutants**
P. Cosoli, Fermeglia, Ferrone, Paneni, Pricl (Univ. Trieste, Italy)
- 5. Exploring the limits of classical molecular simulations: a classical force field for linear alkanes in protonized aluminosilicates**
S. Calero, M.D. Lobato, E. García-Pérez, J.A. Mejias, S. Lago (Univ. Pablo de Olavide, Sevilla, Spain); T.L.M. Maesen (Chevron Texaco, USA); B. Smit, D. Dubbeldam (Univ. of Amsterdam, The Netherlands; CECAM, Lyon, France)
- 6. Kinetic Monte Carlo study of binary diffusion in MFI-type zeolite**
N. Laloué, C. Laroche (IFP, France)
- 7. Structural effect on the adsorption of C₆ paraffins in a zeolite ZSM-5**
J.P. Bellat, E. Lemaire, G. Weber, I. Bezverkhy, Q. Berges, J.M. Simon (Univ. de Bourgogne, Dijon, France); A.C. Dubreuil (IFP, France)
- 8. Use of 12-mercaptododecylphosphonate modified titania as sorbent for mercury removal**
G. Guerrero, P.H. Mutin (Univ. de Montpellier II, France)
- 9. Iron-based adsorbents for desulfurization of fuels**
A. Hasblady, M.J. Pérez Zurita, **C. Scott** (Univ. Central de Venezuela, Caracas, Venezuela)
- 10. Composites “salt inside porous matrix”: design of phase composition and sorption properties**
G. Larisa, T. Mikhail, A. Yurii (Boreskov Institute of Catalysis, Russia)

General Information

Venue and date

The conference will be held at IFP-LYON, 69390 Vernaison, France
Tel.: +33 (0)4 78 02 20 20 - Fax: +33 (0)4 78 02 20 15

The organizer

IFP is a scientific research and industrial development, training, and information services center active in the fields of oil & natural gas, their use, in particular by vehicles, and new energy and environmental technologies (production of fuels from biomass, biofuels, hydrogen, the capture and storage of CO₂, etc.).

In an international energy context marked by a number of major challenges – the need to respond to a relentless growth in energy demand, and thus, notably to renew oil reserves, expand the energy mix and combat climate change - IFP innovates, developing and transferring the technologies needed to produce, transform, and use energy to meet the growing needs of the transport and petrochemicals sectors in a way that can be sustained for the rest of the 21st century.

For more information: <http://www.ifp.fr>

Visa

You may need a visa to enter France from any countries outside the European Union. Please contact the French embassy or consulate in your country, or your travel agency to check whether or not you will need a visa.

Registration

Conference fees (VAT incl.)

Before 4 November 2005:

- 420 € for academics or public institute affiliates
- 600 € for industry affiliates

After 4 November 2005:

- 540 € for academics or public institute affiliates
- 720 € for industry affiliates

Special rate for students: 150 €

new!

Reduced conference fees will be allowed to students in order to facilitate their participation to this conference upon presentation of the student card copy and a letter of approbation from the laboratory manager.

The conference fees cover attendance at the conference, the conference proceedings, lunches, Breaks, shuttle service and cocktail on 14 December. They do not cover accommodation and dinners.

To register, please complete the enclosed registration form and send it, with your payment, to the administrative secretariat CPH.

To be accepted, the registration form must be accompanied by the corresponding payment.

As attendance is limited, we will proceed on a "first come, first served" basis.

Upon receipt of the registration form and the relevant payment, the administrative secretariat CPH will send each participant a letter of acknowledgment.

Payment

All fees are payable in Euros only:

- by check made out to CPH Conseil Participation Holding
- by wire transfer to the bank:

Agence Entreprise Tain L'Hermitage, 1 Place du Taurobole, BP 1 - 26600 Tain L'Hermitage

Account owner: CPH Conseil Participation Holding, Grangeon, 07290 Satillieu

Account n° 10096 18521 00017615101 63

IBAN: FR76 1009 6785 2100 0176 1510 163 - BIC: CMCIFR2L

- by credit card

Accommodation

Accommodation is not included in the conference registration fees.

Block booking at preferential rate has been made for 3 nights (Tuesday 13, Wednesday 14 and Thursday 15 December 2005), but the deadlines for booking are the responsibility of each hotel. After these dates, room availability is not guaranteed.

The hotels are located in the area of Lyon-Perrache station.

Booking accommodation and payment to the hotels are the responsibility of each participant.

You must contact the hotel directly to confirm your booking and give a credit card number. The reference “**IFP Conference**” has to be given to the hotel when booking.

As there are other congresses in Lyon at this period of the year we encourage you to make your reservation as soon as possible.

Hotel name	Address	Rate per night	Deadline
Ibis Centre Perrache ***	28, cours Verdun 69002 Lyon Tel.: +33 4 78 37 56 55 Fax: +33 4 78 37 02 58	Single room: 84 € Breakfast included	31-oct-05
Axotel **	12, rue Marc-Antoine Petit 69002 Lyon Tel.: +33 4 72 77 70 70 Fax: +33 4 72 40 00 65	Single room: 80 € Breakfast included	21-oct-05
Kyriad Perrache **	24, quai Perrache 69002 Lyon Tel.: +33 4 78 37 16 64 Fax: +33 4 78 37 67 98	Single room: 65 € Breakfast included	21-oct-05
Berlioz Hotel **	12 cours Charlemagne 69002 Lyon Tel.: +33 4 78 42 30 31 Fax: +33 4 72 40 97 58	Single room: 56 € Breakfast included	21-oct-05

Access to IFP

By road

From Lyon to Solaize: take the A7 highway (towards Vienne-Marseille) to the SOLAIZE exit, then proceed towards VERNAISON

From Lyon-Saint Exupéry Airport: take the A43 highway towards Lyon, then the ring road towards Marseille, then the A7 highway

By train

Get off at the SNCF Lyon-Perrache or Lyon-La-Part-Dieu station, then take a taxi

Shuttle

A **free shuttle service** will be organised between the Ibis hotel, 28 cours de Verdun - 69002 Lyon (near Lyon-Perrache station) and IFP as follows:

On 14 December: departure at 8.00 am from the Ibis hotel to IFP

On 15 December: departure at 8.15 am from the Ibis hotel to IFP

at the end of both days: departure from IFP to the hotels

On 16 December: departure in the morning from the Ibis hotel to IFP

The exact time of departure will be communicated to the participants to the labs visits.

Please register with the form here enclosed if you wish to use this service.





www.ifp.fr

IFP - Information

IFP

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