



**EURESCO
Conferences**

A Programme of the European Science Foundation

Zeolite Molecular Sieves

EuroConference on Guest-Functionalised Molecular Sieve Systems

Supported by the European Commission, Research DG, Human Potential Programme, High-Level Scientific Conferences
(Contract No: HPCF-CT- 2001-00035)

Hattingen (near Essen), Germany, 20-25 March 2004

Chair: **Frank Marlow (D, MPI für Kohlenforschung, Mülheim a.d. Ruhr, D)**
Vice-Chair: **Mika Lindén (SF, Åbo Akademi University, SF)**

Speakers will provisionally include

George S. Attard (Southampton, UK)	Hugh W. Hillhouse (West Lafayette, US)	Günter Schulz-Ekloff (Bremen, D)
Thomas Bein (Munich, D)	Nicola Hüsing (Wien, A)	Stephan A. Schunk (Heidelberg, D)
Christoph Bräuchle (Munich, D)	J.C. Jansen (Delft, NL)	Osamu Terasaki (Stockholm., S)
Jürgen Caro (Hannover, D)	Franco G. Laeri (Darmstadt, D)	Fanny Tihay (Rueil-Malmaison, F)
Michael Fröba (Gießen, D)	Ulrich Müller (Ludwigshafen, D)	Bert Weckhuysen (Utrecht, NL)
Hermenegildo Garcia (Valencia, E)	Jean-Louis Paillaud (Mulhouse, F)	Dieter Wöhrle (Bremen., D)
Hermann Gies (Bochum, D)	Clément Sanchez (Paris, F)	Paul Wright (St. Andrews, UK)

Scope of the conference

This conference – the second of the series – will deal with the synthesis, characterization, properties and applications of guest-functionalized crystalline or organized porous solids (zeolites, mesoporous solids, macroporous solids). The aim is an assessment of the relationship between methods of preparation, characterization of the composites and properties of the materials. It should open the way to progress in the synthesis of novel materials and the tailoring of their properties. The development of new applications concepts is also expected. Sessions will focus on: • Modification • Characterization • Novel Functions.

The scientific programme will include about 13 invited lectures, 8 sessions of short oral presentations of selected posters given by young researchers, 8 discussion sessions, 4 poster sessions and 2 round-table discussions chaired by industrial researchers. Oral presentations of posters by young researchers (10 minutes including discussion) will be selected from the abstracts (two pages maximum – line spacing: 1.5 – size: 12 pt). The number of oral presentations will not exceed 40. There will be no Proceedings and no Book of Abstracts.

The conference is open to researchers world-wide, whether from industry or academia. Participation will be limited to 100. The emphasis will be on discussion about new developments. The conference fee covers registration, full board and lodging. Grants will be available, in particular for nationals under 35 from EU or Associated States.

Deadline for applications EXTENDED to: 5 January 2004

Scientific Programme and on-line Application at: <http://www.esf.org/euresco/04/pc04180>

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Organising Committee: Michael Fröba; Hermann Gies; Jörg Kärger; Denan Konjhodžić; Mika Lindén;
Frank Marlow; Ulrich Müller; Wolfgang Schmidt & Ferdi Schüth

Advisory Board: Peter Behrens; Laurent Bonnevot; Jürgen Caro, Francesco DiRenzo & Joël Patarin

Organised in association with the
Federation of European Zeolite Associations (FEZA)

Final Programme

On line at: <http://www.esf.org/euresco/04/pc04180>

Saturday 20 March

Late afternoon / early evening	Registration at the hotel reception and ESF desk
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19.00	Supper
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20.30	Get-together-drinks
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Sunday 21 March

08.15	Conference Opening
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08.30	Hermenegildo Garcia (E, Inst. de Tecnologia de Quimica, Valencia, E) <i>Synthesis of periodic mesoporous organosilicas</i>
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09.30	Clément Sanchez (F, Université Paris VI Pierre & Marie Curie, F) <i>Designed construction of nanostructured hybrid materials</i>
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10.30	Coffee break
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11.00	Presentation of selected posters
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12.00	Discussion session Discussion leaders: Michael Fröba (D, Justus-Liebig-University Gießen, D) & Fanny Tihay (F, Institut Français du Pétrole, Rueil-Malmaison, F)
12.30	Lunch
15.30	Dieter Wöhrle (D, Bremen University, D) <i>Methods for the monomolecular encapsulation of organic dyes in microporous and mesoporous molecular sieves</i>
16.30	Presentation of selected posters
17.00	Discussion session Discussion leaders: Michael Fröba (D, Justus-Liebig-University Gießen, D) & Fanny Tihay (F, Institut Français du Pétrole, Rueil-Malmaison, F)
17.30	Coffee break
18.00	Poster session
19.30	Dinner
20.30	Round-table discussion Discussion leaders: Ulrich Müller (D, BASF AG, D) & Stephan A. Schunk (D, HTE AG, Heidelberg, D)

Monday 22 March

08.30	Bert Weckhuysen (B, Utrecht University, NL) <i>Optical characterization techniques</i>
09.30	Jean-Louis Paillaud (F, Ecole Nationale Supérieure de Chimie, Mulhouse, F) <i>Characterisation of electrical and magnetic properties*</i>
10.30	Coffee break
11.00	Presentation of selected posters
12.00	Discussion session Discussion leaders: Hermann Gies (D, Ruhr Universität Bochum, D) & Jacobus C. Jansen (NL, TU Delft, NL)
12.30	Lunch
15.30	Osamu Terasaki (J, Stockholm University, S) <i>Characterisation of guest-functionalized porous systems by X-ray diffraction and electron microscopy</i>
16.30	Presentation of selected posters
17.00	Discussion session Discussion leaders: Hermann Gies (D, Ruhr Universität Bochum, D) & Jacobus C. Jansen (NL, TU Delft, NL)
17.30	Coffee break
18.00	Poster session
19.30	Dinner

Tuesday 23 March

08.30	Jacobus C. Jansen (NL, TU Delft, NL) <i>Novel complex catalysts*</i>
09.30	Paul Wright (UK, St. Andrews University, UK) <i>Organised biocatalysts*</i>
10.30	Coffee break
11.00	Presentation of selected posters
12.00	Discussion session Discussion leaders: George S. Attard (MT, Southampton University, UK) & Nicola Hüsing (D, TU Wien, A)
12.30	Lunch
Afternoon	Free time - excursion
19.00	Dinner
20.00	Round-table discussion Discussion leaders: Stephan A. Schunk (D, HTE AG, Heidelberg, D), Thomas Bein (D, Munich University, D), Christoph Bräuchle (D, Munich University, D) & Frank Marlow (D, MPI für Kohlenforschung, Mülheim/Ruhr, D)

Wednesday 24 March

08.30	Christoph Bräuchle (D, Munich University, D) <i>Dynamics of single molecules in molecular sieves</i>
09.30	Franco G. Laeri (CH, TU Darmstadt, D) <i>Properties of nanoporous host-guest materials for laser applications</i>
10.30	Coffee break
11.00	Presentation of selected posters
11.30	Discussion session Discussion leaders: Hugh W. Hillhouse (US, Purdue Univ., US) & Günter Schulz-Ekloff (D, Bremen University, D)
12.30	Lunch
15.30	Thomas Bein (D, Munich University, D) <i>Functional Porous Nanostructures</i>
16.30	Presentation of selected posters
17.00	Discussion session Discussion leaders: Hugh W. Hillhouse (US, Purdue Univ., US) & Günter Schulz-Ekloff (D, Bremen University, D)
17.30	Coffee break
18.00	Poster session
19.30	Special discussion about the future of this conference series Discussion leaders: Frank Marlow (D, MPI für Kohlenforschung, Mülheim/Ruhr, D) & Mika Lindén (SF, Åbo Akademi University, SF)

20.30

Conference Dinner

Thursday 25 March

08.30

Jürgen Caro (D, Hannover University, D)
Smart membranes in separation and catalysis

09.30

Presentation of selected posters

10.30

Coffee break and poster session

11.30

Discussion session and summaries of round-table discussions
Discussion leaders: **George S. Attard** (MT, Southampton University, UK) &
Nicola Hüsing (D, TU Wien, A)

12.45

Lunch and departure

* Tentative titles

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Nr.	Surname	Name	Poster title	Oral presentation
1	Andersson	Jenny	One-pot synthesis of highly crystalline hydroxyapatite coated by mesoporous silicate	Thursday, 25 March - 09.30
2	Atienzar Corvillo	Pedro	Synthesis of Chiral Periodic Mesoporous organosilica containing Binaphthyl units in the walls and enantioselective enhancement of its fluorescence	Wednesday, 24 March - 11.00
3	Bonino	Francesca Carla	Dimethyl Carbonate activation by alkaline cations exchanged zeolites: a FTIR and Raman study	Tuesday, 23 March - 11.00
4	Brodie-Linder	Nancy	Some factors which influence pore size and surface modification in SBA-15 materials	
5	Busco	Claudia	Characterization of Lewis and Brønsted acidic centres confined in zeolite nano-cavities. A microcalorimetric and computer modeling study	Monday, 22 March - 11.00
6	Castañeda Sánchez	Rafael	Selecting a given zeolite among several competing structures by synthesis design	Sunday, 21 March - 11.00
7	Chmelik	Christian	Application of Interference and IR Microscopy for Studies of Intracrystalline Molecular Transport in Ferrierite Crystals	Monday, 22 March - 11.00
8	Damin	Alessandro	M+(dimethyl carbonate) adducts in M+ (M+ = Li+, Na+, K+, Rb+, Cs+) exchanged zeolites: a computational study of the perturbation induced by the cations on the geometrical and vibrational features of dimethyl carbonate	
9	Davidson	Anne	Crystallization of pyrolusite MnO ₂ nanowires in the pores of SBA-15: in situ observation using synchrotron radiation	Monday, 22 March - 16.30
10	Diaz-Ventura	Leire	Characterisation of the Surface of Silica Gel by Flow Microcalorimetry and Inverse Gas Chromatography	
11	Domine	Marcelo Eduardo	New Approaches towards the Heterogeneization of Amine Adducts of Methyltrioxorhenium (VII)	
12	Donzel	Nicolas	Preparation and functionalisation of large pore periodic organosilicas	
13	Doussineau	Tristan	Bio-Functionalization of Microporous Nanoparticles	Wednesday, 24 March - 11.00
14	Ferreira	Paula	ORDERED BENZENE-SILICA HYBRIDS WITH MOLECULAR-SCALE PERIODICITY IN THE WALLS AND DIFFERENT MESOPORE SIZES	Sunday, 21 March - 16.30
15	Fiorilli	Sonia	Cyclic voltammetry of guest molecules in Na-X zeolites	Wednesday, 24 March - 16.30
16	Förster	Ute Katrin	Bleach and recovery kinetics of the fluorescence of organic dyes in molecular sieves crystals	Wednesday, 24 March - 11.00
17	Frydrych	Emilia	Encapsulation of organic molecules during the spontaneous crystallization of zincophosphate sodalite	
18	Garcia-Bennett	Alfonso	Structural Investigations of AMS-n mesoporous materials by Electron Microscopy	Monday, 22 March - 16.30
19	Glazneva	Tatyana	Diffusion and dehydration of i-C ₃ H ₇ OH on zeolite HAI-ZSM-5. In situ FTIR kinetic study	

20	Hillhouse	Hugh	Ion Transport and Electrochemical Growth of Nanowires in Nanoporous Materials	Monday, 22 March - 16.30
21	Hodgkins	Robert Peter	Towards the use of Nanoporous Solids as Catalytic Supports	Tuesday, 23 March - 11.00
22	Jankowska	Aldona	Various colors of the ultramarine analogs prepared from zeolite A	Sunday, 21 March - 16.30
23	Justyna	Pawlesa	Generation of the aromatic radicals inside the zeolite cavities	
24	Kleitz	Freddy	Polymerization in Mesoporous Silica: Synthesis of Functional Polymer-Inorganic Composite Materials with Well-Defined Nanopores	Sunday, 21 March - 11.00
25	Klisakova	Jana	Catalysts for acylations of Benzene and Toluene with Isobutyric acid derivates	
26	Koller	Hubert	Anomalous Porosity in a Self-Assembled Silica Drug Delivery System Detected by Positron Annihilation Lifetime Spectroscopy	Monday, 22 March - 11.00
27	Konjhodzic	Denan	Characterization and Structure Determination of Mesoporous Silica Films for Optical Applications	
28	Li	Hongliang	A new capillary-assistant method for the preparation of opal-like photonic crystals	
29	Louis	Benoît	Synthesis of ZSM-5 coatings on metals and glass-fibres: an effective structured catalyst for the partial oxidation of benzene by N ₂ O	Wednesday, 24 March - 16.30
30	Macario	Anastasia	Synthesis of microporous and mesoporous materials containing Zn, Cu or Fe: Factors Influencing Morphology and Crystal Size	
31	Majda	Dorota	Determination of enthalpy and entropy of adsorption of linear alkanes on selected zeolites by means of equilibrium controlled temperature programmed desorption	
32	Mallada	Reyes	Modification of MCM-48 membranes by means of zeolitization and silylation	Thursday, 25 March - 09.30
33	Mihaylov	Mihail	Selective Catalytic Reduction of NO _x with Hydrocarbons over Ni-ZSM-5 and NiY: FTIR Mechanistic Studies	
34	Moloy	Eric C.	Molecular Simulations of Hydrated Na ₆ [Si ₆ Al ₆ O ₂₄]•(H ₂ O) _n Sodalite	
35	Nechita	Mircea-Teodor	A novel route to zeolite functionalization with Fe(III) oxalates	Monday, 22 March - 11.00
36	Nowak	Izabela	Synthesis and characterization of liquid phase oxidation catalysts – hexagonally arranged niobium-containing molecular sieves	Tuesday, 23 March - 11.00
37	Okubo	Tatsuya	Comprehensive insight into phase transformation of mesoporous silica	
38	Onida	Barbara	Reichardt's dye entrapped in SBA-3 mesophase: a potential NH ₃ optical sensor	Wednesday, 24 March - 11.00
39	Parmentier	Julien	SiO ₂ , SiO ₂ /C, SiC and C Porous Macroscopic Spheres	Sunday, 21 March - 16.30

40	Penkova	Anna	FTIR Spectroscopic Study of CO and NO Adsorption on Cr-ZSM-5	
41	Perera	Ibon	MPIGC Of Silicas And Calcined Silicas	
42	Porcher	Florence-Francoise	Composite-based materials for optical applications : structure, interactions and properties	
43	Predoeva	Albena	Catalytic and basicity behavior of X zeolite modified with monoalkaline earth and bialkaline earth oxides	
44	Prokesova	Pavla	STUDY OF FORMATION OF MICRO/MESOPOROUS COMPOSITES FROM ZEOLITE BETA SEEDS AND MESOPOROUS PRECURSOR SOLUTIONS	
45	Rosenholm	Jessica	Mesoporous Biodegradable Silica Materials as Carriers for Controlled Drug Release	Wednesday, 24 March - 11.00
46	Salih	Dervishe	The computational modelling of the synthetic zeolites Na-JBW and Li-ABW to investigate their crystal structures and growth mechanisms	
47	Sendor	Dorota	Noble Gas Diffusion in the Pores of Cetineite Single Crystals	
48	Sewell	Gavin	Photoinduced Energy Transfer in Ruthenium Polypyridyl Doped Zeolite Y	
49	Sillar	Kaido	ONIOM study of the acid sites in the zeolite ZSM-5	
50	Simon-Masseron	Angélique	p-FLUOROACETOPHENONE ADSORPTION IN PURELY SILICEOUS MFI STRUCTURE TYPE	Sunday, 21 March - 11.00
51	Smaihi	Monique	Bio-Fonctionnalization of Microporous Nanoparticles	
52	Sobczak	Izabela	Cu and Pt supported on MCM-41 mesoporous molecular sieves as active species in DeNOx processes	
53	To	Judy	A computational study of the catalytic sites in titanium molecular sieves and related materials	
54	Tosheva	Lubomira	Mesoporous Silica-Manganese Composite Beads Prepared by Resin Templating	Tuesday, 23 March - 11.00
55	Turnes Palomino	Gemma	Gallium-substituted MCM-41 and MCM-48 mesoporous silicas: NMR and FTIR characterization	
56	Ufer	Boris	Swelling the MCM-22 precursor with Azobenzene-bearing Surfactants	
57	Walspurger	Stephane	Quantitative Brönsted acid sites determination on zeolites: a new approach towards the chemical composition of zeolites	
58	Yang	Chia-Min	Template Preparation of Graphitic Mesoporous Carbon	Sunday, 21 March - 11.00
59	Zhang	Paul	Encapsulation of Microperoxidases on Nanoporous Support Materials	









