

VENUE

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COPS CONFERENCE OFFICE FROM 5 – 8 JUNE 2011

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OFFICE HOURS

Sunday, 5 June 2011	16:00 – 20:00
Monday, 6 June 2011	8:00 – 19:00
Tuesday, 7 June 2011	8:30 – 17:30
Wednesday, 8 June 2011	8:30 – 16:30

LECTURE PROGRAMME

Sunday, 5 June 2011

- 16:00 **Registration at the MARITIM conference centre**
18:00 **Welcome reception at the conference centre (to 20:00)**

Monday, 6 June 2011

- 9:00 **Opening of the Conference**
S. Kaskel, TU Dresden/D
- Chair: P.L. Llewellyn, Université Aix-Marseille, Marseille/F*
- 9:20 **PLENARY LECTURE**
Peering into physisorption mechanisms by small-angle scattering methods
B. Smarsly, TU Gießen/D

Oral Session 1

- 10:10 **Adsorption on CMK-5 monitored by in situ XRD**
W. Schmidt, MPI für Kohlenforschung, Mülheim/D; H. Amenitsch, Austrian Academy of Sciences, Graz/A; A.H. Lu, Dalian University of Technology/PRC; J. Nitz, MPI für Kohlenforschung, Mülheim/D
- 10:30 **Revealing reactivity and porosity in fluid catalytic cracking – particles by confocal fluorescence microscopy**
J. Ruiz-Martínez, I.L.C. Buurmans, B.M. Weckhuysen, Utrecht University/NL
- 10:50 **New insights into MOFs: exploring the fundamentals of mass transfer by microscopic techniques**
C. Chmelik, Universität Leipzig/D
- 11:10 **Coffee Break**
- Chair: F. Rodriguez-Reinoso, Universidad de Alicante/E*
- 11:40 **A novel method to determine accessible volume, geometrical area and accessible pore size distribution (APSD) of carbonaceous materials**
D.D. Do, L. Herrera, C. Fan, V. Nguyen, D. Nicholson, University of Queensland, Brisbane/AUS
- 12:00 **Pre-combustion CO₂ capture by pressure swing adsorption**
N. Casas, J. Schell, M. Mazzotti, ETH Zurich/CH
- 12:20 **Nanoscale carbon cage-encapsulated metal-organic framework**
Y. Fujishima, Chiba University/J; A. Kondo, Tokyo University of Agriculture and Technology, Koganei/J; H. Kajiro, Nippon Steel Corporation, Futtsu/J; T. Ohba, Chiba University/J; K. Kaneko, Shinshu University, Nagano/J; H. Kanoh, Chiba University/J
- 12:40 **Mesoporous carbon gels for electrochemical applications**
M. Haro, Instituto Nacional del Carbón (CSIC), Oviedo/E; G. Rasines, C. Macías, Nanoquímica S.L., Córdoba/E; J.B. Parra, C.O. Ania, Instituto Nacional del Carbón (CSIC), Oviedo/E
- 13:00 **Lunch**

Monday, 6 June 2011

Oral Session 2

Chair: T. Düren, The University of Edinburgh/UK

14:30 **Status report of the new IUPAC taskgroup on physisorption of gases, with special reference to the evaluation of surface area and pore size distribution**

M. Thommes, Quantachrome Instruments, Boynton Beach, FL/USA; K. Kaneko, Shinshu University, Nagano/J; A.V. Neimark, Rutgers University, Piscataway, NJ/USA; J. Olivier, Micromeritics, Atlanta, GA/USA; F. Rodríguez-Reinoso, Universidad de Alicante/E; J. Rouquerol, CNRS - Université de Provence, Marseille/F; K.S.W. Sing, Devonshire/UK

14:50 **Mixed ligand MOFs: from avoided interpenetration to increased porosity**

N. Klein, I. Senkovska, I. Baburin, S. Kaskel, TU Dresden/D

15:10 **Evaluation of H₂O effect on CO₂ adsorption on MOFs: case of UiO-66 and Cu-BTC**

E. Soubeyrand-Lenoir, C. Vagner, Université Aix-Marseille/F; F. Ragon, C. Serre, Université de Versailles/F; J.S. Chang, Korean Research Institute of Chemical Technology, Daejeon/ROK; P.L. Llewellyn, Université Aix-Marseille/F

15:30 **Structural stability of metal-organic frameworks under humid conditions**

P.M. Schoenecker, C.G. Carson, K.S. Walton, Georgia Institute of Technology, Atlanta, GA/USA

15:50 **Coffee Break**

Chair: B. Smarsly, TU Gießen/D

16:20 **Molecular sieve carbons for CO₂ capture**

J.D. Carruthers, M.A. Petruska, E.A. Sturm, S. Wilson, ATMI Inc., Danbury, CT/USA

16:40 **Development of a method to efficiently screen adsorbents for gas separation applications involving methane, nitrogen, and carbon dioxide**

N.K. Jensen, E.F. May, G.C.Y. Watson, T.E. Rufford, D.K. Zhang, The University of Western Australia, Crawley/AUS; K.I. Chan, Chevron Energy Technology Company, Houston, TX/USA

17:00 **From small pores to large adsorbers**

A. Siegel, T. Eckardt, BASF Catalysts Germany GmbH, Nienburg/D

17:20 **Poster Session A with beer and pretzels**

19:00 **End of conference day**

LECTURE PROGRAMME

Tuesday, 7 June 2011

Chair: J. Rouquerol, CNRS – Université de Provence, Marseille/F

9:00 **PLENARY LECTURE**

Dynamics of capillary condensation and evaporation in mesoporous materials

P.A. Monson, University of Massachusetts, Amherst, MA/USA

Oral Session 3

9:50 **Historical aspects of capillarity and capillary condensation**

K. Sing, Brunel University, Uxbridge, Uxbridge/UK; R. Williams, Open University, Milton Keynes/UK

10:10 **Molecular simulation of enhanced CO₂ solubility in hybrid MCM-41**

N.L. Ho, F. Porcheron, IFP Energies nouvelles, Solaize/F; R.J.-M. Pellenq, Centre Interdisciplinaire des Nanosciences de Marseille/F & Massachusetts Institute of Technology, Cambridge, MA/USA; J. Perez Pellitero, IFP Energies nouvelles, Solaize/F

10:30 **Mesoporous organosilicas with large cage-like pores: synthesis, characterisation and application for immobilisation of enzymes**

Z. Zhou, S. Kullmann, M. Hartmann, R.N. Klupp Taylor, H. Bao, Universität Erlangen-Nürnberg, Erlangen/D

10:50 **Coffee Break**

Chair: S. Kaskel, TU Dresden/D

11:20 **Multi-step adsorption of flexible porous coordination polymers investigated by coincident measurement of adsorption and X-ray powder diffraction**

K. Nakai, BEL Japan, Inc, Osaka/J; R. Matsuda, Japan Science and Technology Agency, Kyoto/J and Kyoto University/J; S. Bureekaew, J. Seo, H. Sato, Japan Science and Technology Agency, Kyoto/J; S. Kitagawa, Japan Science and Technology Agency, Kyoto/J and Kyoto University/J

11:40 **Structural transitions in MOF: view from outside and inside**

A.V. Neimark, Chimie ParisTech/F and Rutgers University, Piscataway, NJ/USA; F.-X. Coudert, Chimie ParisTech/F and CNRS, Paris/F; C. Triguero, Chimie ParisTech/F; A. Boutin, ENS, Paris/F; A.H. Fuchs, Chimie ParisTech/F and CNRS, Paris/F; I. Beurroies, R. Denoyel, Université de Provence, Marseille/F

12:00 **Dynamic model of breathing transitions in MOF's**

C. Triguero, Chimie ParisTech, Paris/F; F.-X. Coudert, Chimie ParisTech and CNRS, Paris/F; A. Boutin, ENS, Paris/F; A.H. Fuchs, Chimie ParisTech and CNRS, Paris/F; A.V. Neimark, Rutgers University, Piscataway, NJ/USA

12:20 **Detailed and extended free-energy analysis of adsorption-induced lattice transition of MOFs with flexible structures**

M. Miyahara, R. Numaguchi, H. Sugiyama, S. Watanabe, H. Tanaka, Kyoto University/J

12:40 **On suitability of metal organic frameworks for separation of chiral biomolecules**

R. Bueno-Pérez, A. Martín-Calvo, P.J. Merkling, S. Calero, Universidad Pablo de Olavide, Sevilla/E

13:00 **Lunch followed by Poster Session B with coffee and biscuits**

Tuesday, 7 June 2011

Oral Session 4

Chair: K. Sing, Brunel University, Lustleigh, Newton Abbot/UK

15:00 **Methods presently available for the characterisation of macroporous solids: an overview**
J. Rouquerol, CNRS - Université de Provence, Marseille/F; G. Baron, Vrije Universiteit Brussel/B;
 R. Denoyel, Université de Provence, Marseille/F; H. Giesche, Alfred University, NY/USA;
 J. Groen, Delft Solid Solutions B.V./NL; P. Klobes, BAM – Federal Institute for Materials
 Research and Testing, Berlin/D; P. Levitz, Ecole Polytechnique, Palaiseau/F; A.V. Neimark,
 Rutgers University, Piscataway, NJ/USA; S. Rigby, Bath University/UK; R. Skudas, University
 of Mainz/D; K. Sing, Brunel University, Lustleigh, Newton Abbot/UK; M. Thommes,
 Quantachrome Instruments, Boynton Beach, FL/USA; K. Unger, University of Mainz/D

15:20 **A novel method for pore size and porosity analysis of meso- and macroporous solids using electroacoustics**
A. Dukhin, Dispersion Technology Inc., Bedford Hills, NY/USA; M. Thommes, Quantachrome
 Instruments, Boynton Beach, FL/USA; P. Goetz, Dispersion Technology Inc., Bedford Hills,
 NY/USA

15:40 **Generating validated 3D models of various ceramics with heterogeneous microstructure**
K. Schmidt, S. Ripperger, TU Kaiserslautern/D

16:00 **Coffee Break**

Chair: P.A. Monson, University of Massachusetts, Amherst, MA/USA

16:30 **Molecular modelling of nanoporous carbons: understanding adsorption and characterisation**
J.C. Palmer, North Carolina State University, Raleigh, NC/USA; J.K. Brennan, US Army
 Research Laboratory, Aberdeen, MD/USA; K.E. Gubbins, North Carolina State University,
 Raleigh, NC/USA

16:50 **Putting the chemistry into virtual porous carbons**
 A.A. Forghani, C. Hu, M.J. Biggs, P. Kwong, The University of Adelaide/AUS; P. Pendleton,
 University of South Australia, Adelaide/AUS; F. Rodriguez-Reinoso, Universidad de
 Alicante/E; K. Kaneko, Shinshu University, Nagano/J

17:10 **The structure determination of adsorbed phases in the carbon micropore by ND, XRD and RMC simulation**
T. Iiyama, F. Fujisaki, R. Futamura, A. Hamasaki, S. Ozeki, Shinshu University, Matsumoto/J;
 A. Hoshikawa, T. Ishigaki, Ibaraki University, Tokai/J

17:30 **End of conference day**

19:00 **Departure to Schloss Wackerbarth: Conference Dinner**

LECTURE PROGRAMME

Wednesday, 8 June 2011

Chair: *K. Kaneko, Shinshu University, Nagano/J*

9:00 **PLENARY LECTURE**

Porous organic polymers and molecules

A. Cooper, University of Liverpool/UK

Oral Session 5

9:50 **Guest-induced gate opening in zeolite imidazolate frameworks**

S. Aguado, D. Farrusseng, M. Pera-Titus, G. Bergeret, Université de Lyon, Villeurbanne/F; V. Moizan, N. Bats, IFP Energies nouvelles, Solaize/F; C. Nieto-Draghi, IFP Energies nouvelles, Rueil-Malmaison/F

10:10 **Characterising unexpected flexibility of ZIF-8 through experiments and simulations: swing effect of imidazolate rings on SOD topology**

D. Fairen-Jimenez, S.A. Moggach, The University of Edinburgh/UK; M.T. Wharmby, University of St. Andrews/UK; N.A. Seaton, University of Surrey, Guildford/UK; T. Düren, The University of Edinburgh/UK

10:30 **Reactive adsorption of acidic gases on MOF/graphite oxide composites**

C. Petit, B. Levasseur, B. Mendoza, T.J. Bandosz, The City College of New York, NY/USA

10:50 **Coffee Break**

Chair: *M. Thommes, Quantachrome, Boynton Beach, FL/USA*

11:20 **Effect of surface functionalities in the removal of NH₃ using activated carbon**

M. Gonçalves, L. Sanchez-García, J. Silvestre-Albero, A. Sepúlveda-Escribano, F. Rodríguez-Reinoso, Universidade de Alicante/E

11:40 **Characterisation of activated carbon at the sub-nm scale via adsorption (H₂, N₂, CH₄, isosteric heats), TEM, FT-IR, neutron (IINS) and x-ray (SAXS/USAXS); and application towards optimization of H₂ storage**

C. Wexler, P. Pfeifer, M. Kraus, M. Beckner, J. Romanos, D. Stalla, T. Rash, H. Taub, P. Yu, R. Olsen, University of Missouri, Columbia, MO/USA; J. Ilavsky, Argonne National Laboratory, IL/USA

12:00 **Length change upon micropores and multilayer adsorption**

C. Balzer, G. Reichenauer, S. Braxmeier, L. Weigold, Bavarian Center for Applied Energy Research, Würzburg/D

12:20 **Structural characterisation of soft-matter assemblies embedded in ordered mesoporous silica**

G.H. Findenegg, T. Shin, M. Xue, TU Berlin/D; D. Mütter, MPI of Colloids and Interfaces, Potsdam/D; O. Paris, University of Leoben/A

12:40 **Temperature dependent immobilisation of CH₄ and N₂ in narrow pore zeolites for energy storage processes**

F. Dreisbach, Rubotherm GmbH, Bochum/D; T. Fieback, Ruhr-University Bochum/D

13:00 **Lunch**

Wednesday, 8 June 2011

Oral Session 6

Chair: M. Hartmann, Universität Erlangen-Nürnberg, Erlangen/D

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- 14:30 **Picometer-resoluted characterisation of nanoporous carbons with quantum fluids**
 T. Tamura, T. Ohba, Chiba University/J; T. Fujimori, S. Niimura, T. Itoh, Shinshu University, Nagano/J; H. Kagita, D. Noguchi, H. Kanoh, Chiba University/J; H. Tanaka, Kyoto University/J; K. Kaneko, Chiba University/J and Shinshu University, Nagano/J
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- 14:50 **Different formation and reactivity of the same active O[•] species in VO_x/MCM-41 and FeO_x/ZSM-5 evidenced by in situ-EPR and UV-vis spectroscopy**
 A. Brückner, E. Kondratenko, Leibniz-Institut für Katalyse, Rostock/D; W. Grünert, Ruhr University Bochum/D
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- 15:10 **NMR studies of co-adsorption and liquid porosimetry in mesoporous catalysts coked under supercritical conditions**
 S. Rigby, University of Nottingham/UK; N. Gopinathan, J. Lowe, M. Greaves, University of Bath/UK
-
- 15:30 **Characterisation of mesoporous materials by high-resolution SEM**
 A. Endo, N. Ikawa, M. Yamada, National Institute of Advanced Industrial Science and Technology, Tsukuba/J; A. Miyaki, Hitachi High-Technologies Corporation/J
-
- 15:50 **Novel hollow particulates of metals and semiconductors**
 A.A. Zinchenko, S. Pu, Nagoya University, Nagoya/J; S. Murata, Nagoya University, Nagoya/J
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- 16:10 **Closing Session**
 S. Kaskel, TU Dresden/D
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- 16:20 **End of the conference**

GENERAL INFORMATION

TOURIST INFORMATION

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