

LECTURE PROGRAMME

Wednesday, October 8, 2008

- 8:20 **Opening**
- 8:30 **PLENARY LECTURE**
Hybrid porous solids: past, present, future
 G. Férey, University of Versailles/F
Chair: R.E. Morris, University of St. Andrews/UK
- 9:15 **High-throughput methods for the investigation of amino-functionalized compounds based on MIL-53, MIL-88, and MIL-101**
 N. Stock, S. Bauer, T. Ahnfeldt, University of Kiel/D;
 P. Horcajada, C. Serre, T. Devic, T. Loiseau, G. Férey, University of Versailles/F; J. Senker, University of Bayreuth/D
- 9:40 **Step-by-step route for the synthesis and controlled growth of metal-organic frameworks on functionalized organic surfaces**
 O. Shekhan, H. Wang, D. Zacher, H. Parala, R.A. Fischer, C. Wöll, University of Bochum/D
- 10:05 **Oriented growth of different metal-organic framework structures on self-assembled monolayers**
 C. Scherb, T. Bein, University of Munich/D
- 10:30 **Coffee break with exhibition and poster presentation**
- 11:00 **Hybridization of heterometal porous coordination polymer crystals, a single crystal film epitaxial growth on a single crystal substrate**
 S. Furukawa, Japan Science and Technology Agency, Kyoto/J; K. Hirai, Kyoto University/J; R. Haruki, O. Sakata, Japan Synchrotron Research Institute, Hyogo/J; S. Kitagawa, Kyoto University/J
- 11:25 **High-dimensional metal-organic frameworks based on organic free radicals showing magnetic properties**
 N. Roques, A. Dacu, Institut de Ciència de Materials de Barcelona, Cerdanyola/E; D. Maspoch, I. Imaz, Institut Català de Nanotecnologia, Cerdanyola/E; J.-P. Sutter, Université Paul Sabatier, Toulouse/F; C. Rovira, J. Veciana, Institut de Ciència de Materials de Barcelona, Cerdanyola/E
- 11:50 **Manufacture of dense coatings of Cu₃(BTC)₂ on porous α -alumina**
 J. Gascon, S. Aguado, F. Kapteijn, Delft University of Technology/NL

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- 12:15 **Novel copper and zinc metal-organic frameworks built from 4,4'-azopyridine and 1,4-BDC or 1,3,5-BTC with (4,4)-grid-like topologies**
 V. Zelenak, Z. Vargova, M. Almasi, M. Burcak, P.J. Safarik University, Kosice/SK; I. Cisarova, Charles University, Prague/CZ
- 12:40 Lunch break
Chair: S. Kaskel, TU Dresden/D
- 14:10 **KEYNOTE LECTURE**
The state of the art for in-situ MOF problematics, methodology and results
 F. Taulelle, University of Versailles/F
- 14:55 **Coffee break with exhibition and poster presentation**
- 15:25 **Supermolecular building blocks approach to construct open metal-organic frameworks: design strategies and sorption properties**
 M. Eddaoudi, University of South Florida, Tampa, FL/USA; R. Staudt, Institute of Non-Classical Chemistry, Leipzig/D; J. Möllmer, M. Thommes, Quantachrome Instruments, Boynton Beach, FL/USA
- 15:50 **Isobutane/isobutene separation over Cu₃(BTC)₂**
 M. Hartmann, S. Kunz, D. Himsl, O. Tangermann, University of Augsburg/D; A. Wagener, S. Ernst, TU Kaiserslautern/D
- 16:15 **Selective adsorption and separation of aromatics with the metal-organic frameworks MIL-47 and MIL-53**
 L. Alaerts, M. Maes, P.A. Jacobs, Katholieke Universiteit Leuven/B; J.F.M. Denayer, Vrije Universiteit Brussel/B; C.E.A. Kirschhock, D.E. De Vos, Katholieke Universiteit Leuven/B
- 16:40 **KEYNOTE LECTURE**
Metal-organic frameworks for hydrogen storage
 M. Hirscher, MPI for Metals Research, Stuttgart/D
- 17:25 **Poster party**
- 19:30

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Chair: D. De Vos, University of Leuven/B

- 8:30 **KEYNOTE LECTURE**
Molecular modeling of adsorption and diffusion on metal-organic frameworks
 R. Snurr, Northwestern University, Evanston, IL/USA
- 9:15 **Computational study of hydrogen adsorption in MOF-5**
K. Sillar, A. Hofmann, J. Sauer, Humboldt-Universität zu Berlin/D
- 9:40 **Diffusion of H₂, CH₄ and CO₂ in metal-organic framework materials: molecular dynamics compared to quasi-elastic neutron scattering**
 F. Salles, University of Montpellier 2/F; H. Jobic, University of Lyon/F; N. Rosenbach, University of Montpellier 2/F; S. Bourrelly, P. Llewellyn, University of Provence, Marseille/F; T. Devic, C. Serre, G. Férey, University of Versailles/F; G. Maurin, University of Montpellier 2/F
- 10:05 **Hydrogen storage in 3-D COFs. A multi-scale theoretical investigation**
 E. Klontzas, E. Tylanakis, G.E. Froudakis, University of Crete, Heraklion/GR
- 10:30 **Coffee break with exhibition and poster presentation**
- 11:00 **Role of exposed metal sites in the hydrogen storage in metal-organic frameworks**
J.G. Vitillo, L. Regli, S. Chavan, G. Ricchiardi, G. Spoto, Università di Torino/I; P.D.C. Dietzel, SINTEF, Oslo/N; S. Bordiga, A. Zecchina, Università di Torino/I
- 11:25 **Hydrogen storage in metal-organic frameworks**
A. Dailly, General Motors Corporation, Warren, MI/USA; E. Poirier, Purdue University, West Lafayette, IN/USA; G.C. Garabedian, General Motors Corporation, Warren, MI/USA
- 11:50 **Metal-organic framework materials: porosity and storage**
X. Lin, S. Yang, N. Champness, P. Hubberstey, M. Schröder, University of Nottingham/UK
- 12:15 **Unprecedented insight into MOF transport properties by monitoring transient concentration profiles**
D. Tzoulaki, L. Heinke, J. Kärger, University of Leipzig/D; H. Lim, J. Li, Rutgers University, Piscataway, NJ/USA
- 12:40 Lunch break

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Chair: M. Hartmann, University of Augsburg/D

- 14:10 **KEYNOTE LECTURE**
Metal-organic frameworks for gas storage in medical applications
 R.E. Morris, University of St. Andrews/UK
- 14:55 **Solid state and material engineering approaches for highly shape selective alkylations**
 U. Ravon, M.E. Domine, C. Gaudillere, M. Savonnet, D. Farrusseng, CNRS, Lyon/F
- 15:20 **Utilization of coordinatively unsaturated metal sites for liquid-phase catalysis in nanoporous metal carboxylates**
 Y.K. Hwang, D.-Y. Hong, Y.-K. Seo, Korea Research Institute of Chemical Technology (KRICT), Daejeon/ROK; S.H. Jung, Kyungpook National University, Daegu/ROK; C. Serre, G. Férey, University of Versailles/F; J.-S. Chang, Korea Research Institute of Chemical Technology (KRICT), Daejeon/ROK
- 15:45 **Coffee break with exhibition and poster presentation**
- 16:15 **Combining different metal-organic frameworks for the selective oxidation of cycloalkanes**
F.X. Llabrés i Xamena, O. Casanova, R. Galiasso, H. Garcia, A. Corma, TU Valencia/E
- 16:40 **Catalytic oxidation by cobalt(II)-containing metal-organic frameworks**
 D. Volkmer, Ulm University/D
- 17:05 **Novel hydrogenation catalysts based on Pd supported on MOF-5**
S. Opelt, E. Dietzsch, Chemnitz University of Technology/D; S. Kaskel, TU Dresden/D; E. Klemm, Chemnitz University of Technology/D
- 17:30 **End of the 2nd conference day**
- 18:30 **Shuttle bus to the conference dinner, departure at Kongresshalle Augsburg**
- 19:00 **Conference dinner at Bahnpark Augsburg**
- 23:30

LECTURE PROGRAMME

Friday, October 10, 2008

Chair: R.A. Fischer, University of Bochum/D

- 9:00 **KEYNOTE LECTURE**
Chemistry and application of soft porous crystals
 S. Kitagawa, Kyoto University/J
- 9:45 **Asymmetric ring opening reaction of epoxide with amine in the chiral open space of a novel chiral porous metal-organic framework**
K. Tanaka, S. Oda, Kansai University, Osaka/J; M. Shiro, Rigaku X-ray Laboratory, Tokyo/J
- 10:10 **Photochemistry inside metal-organic frameworks functionalised by organometallic compounds**
S.M. Chavan, E. Groppo, F. Bonino, University of Turin/I; K.P. Lillerud, University of Oslo/N; C. Larabi, CNRS/CPE, Lyon/F; S. Bordiga, University of Turin/I
- 10:35 **Coffee break with exhibition and poster presentation**
- 11:05 **Rotational dynamics of molecular dipoles on a MOF-5 crystal lattice**
 E.B. Winston, J.C. Price, J. Michl, J. Vacek, J. Chocholoušová, P.J. Lowell, University of Colorado, Boulder, CO/USA
- 11:30 **Calculation of static and dynamic properties of metal-organic frameworks and COFs using force fields parameterized systematically from first principles**
R. Schmid, S. Amirjalayer, M. Tafipolsky, University of Bochum/D
- 11:55 **Structure and proton conductivity of the oxalate-bridged honeycomb shaped coordination polymer with hydrogen bond network**
M. Sadakiyo, T. Yamada, H. Okawa, H. Kitagawa, Kyushu University, Fukuoka/J
- 12:20 Lunch break

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Chair: G. Férey, University of Versailles/F

- 14:00 **Proton conducting metal-organic frameworks**
G. Shimizu, J.A. Hurd, R. Vaidhyanathan, J.M. Taylor, V. Thangadurai, University of Calgary/CDN
- 14:25 **Metal-organic frameworks as new materials for drug delivery**
P. Horcajada Cortes, C. Serre, University of Versailles/F; G. Maurin, N.A. Ramsahye, University of Montpellier 2/F; F. Balas, M. Vallet-Regi, University Complutense of Madrid/E; M. Sebban, F. Taullele, G. Férey, University of Versailles/F
- 14:50 **Toward metal-organic frameworks in industrial processes: carbon dioxide capture**
R. Willis, A. Benin, S. Faheem, J. Low, G. Venimadhaven, UOP LLC, a Honeywell Company, Des Plaines, IL/USA; R. Snurr, O. Yazaydin, Northwestern University, Evanston, IL/USA; A. Matzger, A. Wong-Foy, K. Koh, University of Michigan, Ann Arbor, MI/USA; D. LeVan, J. Liu, Vanderbilt University, Nashville, TN/USA; S. Brandani, University of Edinburgh/UK
- 15:15 **KEYNOTE LECTURE**
Metal-organic frameworks – perspective applications in chemical industry
 U. Müller, BASF SE, Ludwigshafen/D
- 16:00 **Poster award / Closing remarks**
- 16:10 **End of conference**