

POSTER PROGRAMME

Posters must be placed on the assigned boards by Monday, September 6, 2010, 11:00 at the latest.

Authors are requested to be present at their posters during the **poster party** on Tuesday, September 7, 2010 from 17:30 until 20:00.

Posters will also be viewed and discussed during the coffee and lunch breaks.

Topic 1: New syntheses and structures

- P 001 **In situ imidazolate-4-amide-5-imidate ligand synthesis leading to new microporous zinc-organic frameworks**
F. Debatin, K. Behrens, University of Potsdam/D; A. Thomas, TU Berlin/D; A. Kelling, University of Potsdam/D; N. Hedin, University of Stockholm/S; S. Kaskel, Dresden University of Technology/D; A. Friedrich, H.-J. Holdt, University of Potsdam/D
- P 002 **High activities of iron-FSM-16 mesoporous materials synthesized by a microwave-hydrothermal process in Friedel-Crafts alkylations**
K. Bachari, A. Touileb, CRAPC, Algiers/DZ; N. Tahir, A. Saadi, D. Halliche, O. Cherifi, USTHB, Algiers/DZ
- P 003 **The hydrogels on the base of polyacrylonitrile fiber wastes and polyvalent metals**
A. Asamatdinov, Nukus State Pedagogical Institute, Nukus/UZB
- P 004 **Design of V- and Cr-MOFs for catalytic applications**
B. Jäger, B. Ondruschka, P. Scholz, University of Jena/D
- P 005 **Molecular modelling of chemical functionalization of zeolitic imidazolate frameworks**
H. Amrouche, IFP, Rueil-Malmaison/F; F.R. Siperstein, University of Manchester/UK; C. Nieto-Drahi, IFP, Rueil-Malmaison/F; J. Perez-Pellitero, IFP, Lyon/F
- P 006 **„The Simpler the Better“: synthetic strategies for coordination polymers (MOF's) from monotopic/ditopic ligands**
Z. Majeed, S. Nayak, K.C. Mondal, G.E. Kostakis, Y. Lan, C.E. Anson, A.K. Powell, KIT – Karlsruhe Institute of Technology/D
- P 007 **A chiral Co(II) MOF containing a thiazolidine-based spacer**
A. Rossin, B. Di Credico, G. Giambastiani, M. Peruzzini, G. Reginato, ICCOM-CNR, Sesto Fiorentino/I

POSTER PROGRAMME

- P 008 **On the way to new metal-organic framework compounds using fluorinated dicarboxylates as bridging ligands**
C. Seidel, U. Ruschewitz, University of Cologne/D
- P 010 **Spin crossover phenomena in new 2D Hofmann-like microporous metal-organic frameworks produced as nanocrystals and nanoparticles**
A.B. Gaspar, J.A. Real, University of Valencia/E; M.C. Muñoz, Polytechnic University of Valencia/E; V. Martínez, I. Boldog, F.J. Muñoz-Lara, University of Valencia/E
- P 011 **ZIF-8 nanocrystal nucleation and growth: a time-resolved *In-Situ* synchrotron SAXS/WAXS study**
J. Cravillon, C. Schröder, University of Hanover/D; R. Nayuk, K. Huber, University of Paderborn/D; J. Gummel, T. Narayanan, European Synchrotron Radiation Facility, Grenoble/F; M. Wiebcke, University of Hanover/D
- P 012 **Zeolitic imidazolate framework nanocrystal aggregates with hierarchical porosity and high thermal stability**
J. Cravillon, F. Brieler, A. Feldhoff, M. Wiebcke, University of Hanover/D
- P 013 **Porous interpenetrated zirconium-organic frameworks (PIZOFs) containing a variety of functionalized long linkers**
A. Schaate, J. Lippke, University of Hanover/D; P. Roy, University of Bielefeld/D; F. Waltz, University of Hanover/D; A. Godt, University of Bielefeld/D; P. Behrens, University of Hanover/D
- P 014 **A new family of porous MOFs with an unprecedented Al-containing brick: [Al₂(OCH₃)₄O₂C-X-CO₂] (X = aryl)**
H. Reinsch, M. Feyand, T. Ahnfeldt, N. Stock, Universität zu Kiel/D
- P 015 **Post-synthetic chemical modification of Cr-MIL-101**
S. Bernt, N. Stock, Universität zu Kiel/D; C. Serre, V. Guillerm, Université de Versailles/F
- P 016 **In-situ EDXRD investigation of the formation of isorecticular CAU-1 compounds**
T. Ahnfeldt, N. Stock, University zu Kiel/D
- P 018 **A new series of isorecticular MOFs with non-linear linkers for hydrogen storage applications**
S.E. Wenzel, M. Fischer, F. Hoffmann, M. Fröba, University of Hamburg/D

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- P 019 **Rational design of organic building blocks to achieve control over catenation in metal-organic frameworks**
O. Farha, Northwestern University, Evanston, IL/USA
- P 020 **On the reticular construction concept of 2D covalent organic frameworks**
B. Lukose, A. Kuc, Jacobs University Bremen/D;
J. Frenzel, Ruhr-Universität, Bochum/D; T. Heine,
Jacobs University Bremen/D
- P 021 **Metal-organic framework materials – synthesis steps in a production scale**
N. Trukhan, U. Mueller, BASF SE, Ludwigshafen/D
- P 022 **Synthesis and properties of different ligandes coordination compounds**
K. Salieva, B. Borkoev, Kyrgyzstan-Turkey Manas University, Bishkek/KIR
- P 023 **Using hydrothermal and electro-hydrothermal synthesis for preparation of new MOFs based on redox-active ligands**
T. Nguyen, T. Devic, A.-M. Gonçalves, G. Férey, Université de Versailles/F; R. Demir-Cakan, M. Morcrette, J.-M. Tarascon, Université de Picardie Jules Verne, Amiens/F; T. Ahnfeldt, N. Stock, Universität zu Kiel/D; P. Auban-Senzier, C. Pasquier, Université Paris Sud, Orsay/F; Y. Filinchuk, ERSF, Grenoble/F
- P 024 **Mixed-ligand metal-organic frameworks**
A.D. Burrows, L.C. Fisher, S.P. Rigby, University of Bath/UK
- P 025 **Solid-state interconversion of coordination networks via conformational change of a semi-rigid linker**
A.D. Burrows, M.F. Mahon, P.R. Raithby, C. Richardson, A.J. Stevenson, University of Bath/UK
- P 026 **Synthesis optimization and structure elucidation of CAU-1 by NMR crystallography**
D. Gunzelmann, University of Bayreuth/D; T. Ahnfeldt, N. Stock, Universität zu Kiel/D; J. Senker, University of Bayreuth/D
- P 027 **Elaboration of photoactive crystalline highly porous titanium (IV) dicarboxylate**
L. Rozes, L. D'Arras, Université Pierre et Marie Curie, Paris/F; A. Nguyen, Université de Versailles/F;
C. Sassoie, Université Pierre et Marie Curie, Paris/F;
T. Devic, C. Serre, G. Férey, Université de Versailles/F;
C. Sanchez, Université Pierre et Marie Curie, Paris/F

POSTER PROGRAMME

- P 028 **Size controlled formation of porous coordination polymer nanocrystals by coordination modulation**
S. Diring, S. Furukawa, S. Kitagawa, Japan Science and Technology Agency, Kyoto/J
- P 029 **Systematic investigations of the Zn(dpa)(4,4'-bpy) system by high throughput techniques**
J. Cavka, SINTEF, Oslo/N; H. Fjellvåg, University of Oslo/N; P.D.C. Dietzel, SINTEF, Oslo/N
- P 030 **Novel environmentally-friendly syntheses of aluminum-based porous coordination polymers**
J. Reboul, S. Furukawa, S. Kitagawa, Japan Science and Technology Agency, Kyoto/J
- P 031 **One-dimensional infinite coordination polymers from cyclam-coordinated building blocks and dicarboxylate linkers**
G. Platz, R. Munnkhoff, P. Behrens, University of Hanover/D
- P 032 **Synthesis of functional linkers and postsynthetic modification of Zr-MOFs**
P. Roy, A. Godt, University of Bielefeld/D; A. Schaate, P. Behrens, University of Hanover/D
- P 033 **Phase transition from open to dense structures by thermal treatment of MOFs**
J.-C. Rybak, K. Müller-Buschbaum, University of Würzburg/D
- P 034 **Metal-organic framework (MOF) aerogels with high micro- and macroporosity**
M. R. Lohe, M. Rose, I. Senkovska, S. Kaskel, Dresden University of Technology/D
- P 035 **Layered lanthanide-organic frameworks: structural studies by synchrotron powder X-ray diffraction**
L. Cunha Silva, University of Porto/P; J. Rocha, F.A. Almeida Paz, University of Aveiro/P
- P 036 **DUT-6 – a mesoporous MOF based on BTB and 2,6-NDC**
N. Klein, I. Senkovska, K. Gedrich, U. Stoeck, A. Henschel, Dresden University of Technology/D; U. Mueller, Helmholtz-Centre Berlin for Materials and Energy/D; S. Kaskel, Dresden University of Technology/D

POSTER PROGRAMME

- P 037 **Microwave synthesis of MOFs under atmospheric pressure**
G. Blanita, O. Ardelean, D. Lupu, D. Lazar, G. Borodi, A. Biris, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca/RO; M. Vlassa, Babes-Bolyai University, Cluj-Napoca/RO; E. Surducan, I. Coldea, I. Misan, V. Surducan, G. Popeneciu, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca/RO
- P 038 **Synthesis of three novel metal-organic frameworks with the IRMOF-9 topology**
T. Philippi, S. Foit, W. Thiel, E. Keceli, S. Ernst, University of Kaiserslautern/D
- P 039 **New highly porous and rigid iron(III) polycarboxylates**
H. Chevreau, C. Serre, M. Dan-Hardi, T. Devic, P. Horcajada, Institut Lavoisier, Université de Versailles/F; G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; G. Férey, Institut Lavoisier, Université de Versailles/F; D. Popov, C. Riekel, ESRF, Grenoble/F
- P 040 **Metal-organic chains incorporating phenyl-carbaborane anions**
L. Cunha-Silva, University of Porto/P; R. Ahmad, M. J. Carr, A. Franken, J. D. Kennedy, M.J. Hardie, University of Leeds/UK
- P 041 **New porous catalytic active element organic frameworks based on Sn, Sb, and Bi**
J. Fritsch, M. Rose, S. Kaskel, Dresden University of Technology/D
- P 042 **New porous metal organic frameworks with porphyrinic linkers**
A. Fateeva, T. Devic, S. Miller, C. Serre, G. Férey, Institut Lavoisier, Université de Versailles/F; R. Demir-Cakan, M. Morcrette, J.M. Tarascon, LRCS, Amiens/F; S. Devautour-Vinot, G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; P. Llewellyn, CNRS – Aix-Marseille University/F; S. Wutke, A. Vimont, LCS, Caen/F
- P 043 **Heteronuclear coordination polymers for application in catalysis**
F. Kettner, H. Krautscheid, University of Leipzig/D
- P 044 **Heteronuclear MOFs – cobalt containing zinc and cadmium coordination polymers**
D. Lässig, J. Lincke, J. Griebel, R. Kirmse, H. Krautscheid, University of Leipzig/D

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- P 045 **MOFs using calix[4]arene carboxylate linkers**
V. Pop, A. Burrows, M. Mahon, A. Stevenson, University of Bath/UK; S. Bew, S. Thurston, University of East Anglia, Norwich/UK
- P 046 **A new chiral and flexible MOF with a bifunctional spiro linker**
K. Gedrich, I. Senkovska, Dresden University of Technology/D; I.A. Baburin, Max Planck Institute for Chemical Physics of Solids, Dresden/D; O. Trapp, University of Heidelberg/D; S. Kaskel, Dresden University of Technology/D
- P 047 **New chiral MOFs based on substituted BTB linkers**
A. Notzon, University of Münster/D; K. Gedrich, Dresden University of Technology/D; M. Heitbaum, University of Münster/D; I. Senkovska, Dresden University of Technology/D; F. Glorius, University of Münster/D; S. Kaskel, Dresden University of Technology/D
- P 048 **Pore modification of covalent organic frameworks**
M. Dogru, A. Sonnauer, A. Gavryshin, P. Knochel, T. Bein, University of Munich/D
- P 049 **Insights into the structure of MOFs evidenced from solid-state NMR studies**
A. Kuttathayil, B. Marko, L. Daniel, L. Joerg, K. Harald, University of Leipzig/D
- P 050 **Ionothermal route to two-dimensional, layered polymer-frameworks based on heptazine and triazine linkers**
M. Bojdys, S. Wohlgemuth, Max Planck Institute of Colloids and Interfaces, Potsdam/D; A. Thomas, TU Berlin/D; M. Antonietti, Max Planck Institute of Colloids and Interfaces, Potsdam/D
- P 051 **Novel gallium based metal-organic frameworks: green synthesis with easy recycling process**
T. Lescouet, M. Savonnet, A. Camarata, D. Farrusseng, IRCE Lyon - CNRS, Villeurbanne/F
- P 052 **Synthesis of novel amine functionalized MOF based on copper carboxylate units for CO₂ adsorption**
R. Sanz Martín, F. Martínez Castillejo, D. Briones Gil, Universidad Rey Juan Carlos University, Móstoles/E
- P 053 **Alternative syntheses of IRMOFs and its main and transition metal homologues**
F. Mertens, S. Hausdorf, TU Bergakademie Freiberg/D

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- P 054 **Synthesis and characterization of the iron(II) member of the isostructural $M_2(\text{dhtp})$ series containing coordinatively unsaturated metal cations**
M. Maerz, University of Oslo/N; P.D.C Dietzel, SINTEF Materials and Chemistry, Oslo/N; R.E. Johnson, H. Fjellvåg, University of Oslo/N
- P 055 **Synthesis and crystal structure of In-based pyromellitate (Mil-117)**
M. Mazaj, National Institute of Chemistry, Ljubljana/SLO; C. Volkringer, G. Férey, T. Loiseau, Institut Lavoisier, Université de Versailles/F
- P 056 **Incipient wetness synthesis route for zirconium MOFs: The formation of UiO-66 followed by in situ XRD, EXAFS and Raman**
M. Nilsen, University of Oslo/N; E. Groppo, F. Bonino, C. Lamberti, S. Bordiga, University of Torino/I; U. Olsbye, K.P. Lillerud, University of Oslo/N
- P 057 **Synthesis of nanoparticles of porous iron carboxylates MOFs for biomedical applications**
D. Heurtaux, Université de Versailles/F; T. Chalati, Université Paris, Chatenay Malabry/F; P. Horcajada, C. Serre, Université de Versailles/F; R. Gref, Université de Paris, Chatenay Malabry/F; B. Gillet, C. Sebrie, Université de Paris, Gif-sur-Yvette/F; J.S. Chang, KRICT, Daejeon/ROK; G. Férey, Université de Versailles/F; P. Couvreur, Université de Paris, Chatenay Malabry/F
- P 058 **The Influence of base and imidazole ratio on the structure of imidazole-containing metal-carboxylate frameworks**
C.G. Perkins, J. Bacsa, M.J. Rosseinsky, University of Liverpool/UK
- P 059 **Computational assisted structure determination of flexible MOFs**
F. Salles, G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; T. Devic, C. Serre, P. Horcajada, G. Férey, Université de Versailles/F; H.J. Choi, J. Long, University of California, Berkeley, CA/USA; P. Llewellyn, CNRS – Aix-Marseille University/F
- P 060 **Synthesis and applications of new chiral metal-organic frameworks (MOFs)**
M. Padmanaban, University of Münster/D; K. Gedrich, P. Müller, I. Senkovska, Dresden University of Technology/D; F. Glorius, University of Münster/D; S. Kaskel, Dresden University of Technology/D

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- P 061 **Microwave synthesis of copper carboxylate and its sorption properties**
Y.K. Hwang, I.T. Jang, Y.K. Seo, J.W. Yoon, D.W. Hwang, U.H. Lee, J.S. Chang, Korea Research Institute of Chemical Technology, Daejeon/ROK
- P 062 **New porous zirconium metal organic frameworks**
V. Guillerm, T. Devic, G. Férey, C. Serre, Institut Lavoisier, Université de Versailles/F; S. Gross, A. Vittadini, Università degli Studi di Padova/I
- P 063 **Design and synthesis of coordination polymers based on tri-, tetra- and hexanuclear carboxylate clusters**
S. Baca, O. Botezat, G. Dulcevscaia, Yu. Simonov, V. Kravtsov, I. Filippova, Academy of Sciences of Moldova, Chisinau/MD; I. Malaestean, M. Speldrich, P. Kogerler, RWTH Aachen University/D; T. Keene, University of Sydney/AUS; S. Decurtins, University of Bern/CH
- P 064 **Synthesis and adsorption properties of the first permanently porous lanthanide bisphosphonate framework materials**
M.T. Wharmby, P.A. Wright, University of St Andrews/UK; S.R. Miller, Institut Lavoisier, Université de Versailles/F; D. Fairen, T. Duren, University of Edinburgh/UK; N. Stock, Universität zu Kiel/D
- P 065 **New CPs based on the trinuclear triangular SBU $[\text{Cu}_3(\mu_3\text{-OH})(\mu\text{-pz})_3]^{2+}$ connected through 4,4'-Bipyridine. Influence of the coordinated anions and reaction conditions**
C. Di Nicola, C. Pettinari, University of Camerino/I; F. Garau, L. Pandolfo, University of Padova/I; M. Monari, University of Bologna/I; M.F.C. Guedes da Silva, A.J.L. Pombeiro, Instituto Superior Técnico, Lisbon/P
- P 066 **New 1-D, 2-D and 3-D CPs from reactions of pyrazole with copper(II) bicarboxylates**
F. Garau, University of Padova/I; M. Monari, University of Bologna/I; L. Pandolfo, University of Padova/I; C. Pettinari, University of Camerino/I
- P 067 **High throughput production of MOF nanoparticles by NETmix® technology**
V. Silva, Universidade do Porto/P; P. Horcajada, Université de Versailles/F; D. Constantino, P. Gomes, Universidade do Porto/P; T. Devic, Université de Versailles/F; M. Dias, J.C. Lopes, Universidade do Porto/P; C. Serre, Université de Versailles/F; A.E. Rodrigues, Universidade do Porto/P

POSTER PROGRAMME

- P 068 **Mechanochemical synthesis of MOFs - a fast and facile approach towards quantitative yields and high specific surface areas**
M. Klimakow, P. Klobes, A. Thünemann, BAM Federal Institute for Materials Research and Testing, Berlin/D; K. Rademann, Humboldt University of Berlin/D; F. Emmerling, BAM Federal Institute for Materials Research and Testing, Berlin/D
- P 069 **Adsorption in flexible functionalized iron terephthalate MIL-53 (Fe)**
S. Bourrelly, D. Phanon, P. Llewellyn, CNRS – Aix-Marseille University/F; G. Maurin, F. Salles, CNRS-Institut Charles Gerhardt Université Montpellier2/F; T. Devic, P. Horcajada, C. Serre, G. Férey, Université de Versailles/F
- P 070 **Microwave synthesis of porous metal carboxylates**
 Y.K. Hwang, Y.K. Seo, J.S. Lee, J.S. Chang, Korea Research Institute of Chemical Technology, Daejeon/ROK; P. Horcajada, C. Serre, G. Férey, Université de Versailles/F
- P 071 **Preferential gas sorption in a reducible iron trimesate MIL-100 (FE) with coordinatively unsaturated sites**
 J.W. Yoon, Y.K. Hwang, J.S. Chang, Korea Research Institute of Chemical Technology, Daejeon/ROK; C. Serre, P. Horcajada, G. Férey, Université de Versailles/F; A. Vimont, M. Daturi, ENSICAEN, Caen/F; P. Llewellyn, CNRS – Aix-Marseille University/F
- P 072 **Stable encapsulation of polyoxometalates within the mesoporous metal-organic framework MIL-100(Fe).**
C. Roch-Marchal, R. Canioni, P. Horcajada, C. Serre, M. Dan-Hardi, J.-M. Grenéche, F. Levebvre, F. Sécheresse, CNRS, Marseille/F

Topic 2: Gas and liquid adsorption

- P 073 **Metal-organic framework MIL-101 for adsorption and effect of terminal water molecules: a computational study**
Y. Chen, R. Babarao, J.W. Jiang, National University of Singapore/SGP
- P 074 **Experimental and theoretical study on hydrogen interaction with unsaturated metal-organic frameworks**
N. Nijem, J.F. Veyan, University of Texas at Dallas, Richardson, TX/USA; L. Kong, K. Li, Rutgers University, Piscataway, NJ/USA; Y.J. Chabal, University of Texas at Dallas, Richardson, TX/USA; D.C. Langreth, J. Li, Rutgers University, Piscataway, NJ/USA

POSTER PROGRAMME

- P 075 **Modelling the interaction of hydrogen with unsaturated metal sites in MOFs: a combined DFT and molecular mechanics approach**
M. Fischer, F. Hoffmann, M. Fröba, University of Hamburg/D; B. Kuchta, University of Marseille/F; L. Firlje, University of Montpellier 2/F
- P 076 **Designing novel 3-D COFs with enhanced hydrogen storage capacity**
G. Froudakis, E. Tylianakis, University of Crete, Heraklion/GR
- P 077 **Enhancement of hydrogen adsorption in MOFs by the incorporation of the sulfonate group and Li cations. A multiscale computational study.**
E. Klontzas, E. Tylianakis, A. Mavrandonakis, E. Froudakis, University of Crete, Heraklion/GR
- P 078 **Linker design in metal-organic frameworks for enhanced H₂ storage**
R.B. Getman, R.Q. Snurr, Northwestern University, Evanston, IL/USA
- P 079 **Molecular Simulation Studies of Liquid Adsorption in Metal-Organic Frameworks**
P.Z. Moghadam, T. Düren, University of Edinburgh/UK
- P 080 **Experimental adsorption equilibria of biogas components, alkanes and alkenes C1 - C4 on metal-organic frameworks**
A. Lyubchik, I.A.A.C. Esteves, J.P.B. Mota, Universidade Nova de Lisboa, Caparica/P
- P 081 **Materials for carbon dioxide adsorption-based separation in the region of low equilibrium pressures**
A. Zukal, J. Mayerova, J. Heyrovsky Institute, Prague/CZ
- P 082 **From microscopic insights of hydrogen adsorption in MOFs to macroscopic estimations of uptakes**
 D.A. Gomez, G. Sastre, Universidad Politecnica de Valencia/E
- P 083 **Molecular sieve MOF membrane with hydrogen permselectivity: ZIF-22 in LTA topology prepared using 3-aminopropyltriethoxysilane as covalent**
A. Huang, H. Bux, F. Steinbach, J. Caro, University of Hanover/D
- P 084 **New metal-organic framework materials for hydrogen storage applications**
D. Frahm, M. Fröba, University of Hamburg/D

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- P 085 **Isosteric heat of hydrogen adsorption in lithium-alkoxide-modified metal-organic frameworks**
M. Hartmann, D. Himsel, University of Erlangen-Nuremberg/D
- P 086 **New interpenetrated copper coordination polymer frameworks having porous properties**
P. Kanoo, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore/IND; R. Matsuda, Kyoto University/J; M. Higuchi, S. Kitagawa, Kyoto University/J; T.K. Maji, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore/IND
- P 087 **Binary adsorption of CO₂ and CH₄ on HKUST-1**
J. Möllmer, A. Möller, Institut für Nichtklassische Chemie e.V., Leipzig/D; R. Gläser, University of Leipzig/D; R. Staudt, Institut für Nichtklassische Chemie e.V., Leipzig/D
- P 088 **Interpretation of high-pressure adsorption phenomena on HKUST-1**
J. Möllmer, A. Möller, Institut für Nichtklassische Chemie e.V., Leipzig/D; F. Dreisbach, Rubotherm GmbH, Bochum/D; R. Gläser, University of Leipzig/D; R. Staudt, Institut für Nichtklassische Chemie e.V., Leipzig/D
- P 089 **Methane storage mechanism in the metal-organic framework Cu₃(btc)₂: an in situ neutron diffraction study**
J. Getzschmann, I. Senkovska, Dresden University of Technology/D; D. Wallacher, M. Tovar, Helmholtz Centre Berlin for Materials and Energy/D; S. Kaskel, Dresden University of Technology/D
- P 090 **A crystal container with size selectivity for alkane isomers based on a hybridized porous coordination polymer**
K. Hirai, Kyoto University/J; S. Furukawa, Japan Science and Technology Agency/J; O. Sakata, JASRI, Hyogo/J; S. Kitagawa, Kyoto University/J
- P 091 **Tuning the organic linker of MOF-5 for hydrogen storage**
J. Yang, A. Grzech, F.M. Mulder, T.J. Dingemans, Delft University of Technology/NL
- P 092 **Simulations and experiments in zeolitic imidazolate frameworks**
J. Perez, IFP, Solaize/F; H. Amrouche, C. Nieto-Draghi, IFP, Rueil-Malmaison/F; F.R. Siperstein, University of Manchester/UK; D. Peralta, A.A. Quoineaud, D. Bazer-Bachi, G. Pirngruber, K. Barthelet, N. Bats, IFP, Solaize/F

POSTER PROGRAMME

- P 093 **Purification of chiral compounds on modified MIL 101**
A. Severino, G. De Weireld, University of Mons/B; H. Chevreau, M. Matjaz, T. Devic, C. Serre, Université de Versailles/F
- P 094 **A versatile high throughput adsorption screening instrument**
P. Wollmann, S. Kaskel, Dresden University of Technology/D; M. Leistner, W. Grähler, Fraunhofer IWS, Dresden/D; F. Dreisbach, Rubotherm GmbH, Bochum/D
- P 095 **Nitrogen-Oxygen separation using cation containing MOFs**
N. Heymans, G. De Weireld, University of Mons/B; T. Devic, A. Fateeva, J. Eubank, C. Serre, Institut Lavoisier, Université de Versailles/F; G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F
- P 096 **Framework flexibility of hybrid MIL-53(Al) material studied by ¹²⁹Xe NMR**
M. Springuel, A. Nossou, F. Guenneau, A. Gédéon, Université Pierre et Marie Curie, Paris/F; C. Volkringer, T. Loiseau, G. Férey, Institut Lavoisier, Université de Versailles/F
- P 097 **Integrated adsorbent application modeling synthesis gas purification PSA unit**
S. Vaesen, N. Heymans, G. De Weireld, University of Mons/B; V. Guillermin, T. Devic, C. Serre, Institut Lavoisier, Université de Versailles/F
- P 098 **Hydrogen storage in nanoporous materials: MOFs and COFs**
L. Zhechkov, B. Broda, M. Wahiduzzaman, A. Kuc, B. Lukose, T. Heine, Jacobs University Bremen/D
- P 099 **Molecular modelling of olefin/paraffin adsorption in a metal-organic framework with open metal sites**
M. Jorge, Universidade do Porto/P; J.R.B. Gomes, Universidade de Aveiro/P; A.E. Rodrigues, Universidade do Porto/P
- P 100 **The characterisation of porous hydrogen storage materials: activated carbons, zeolites, MOFs and PIMs**
S. Tedds, A. Walton, D. Book, University of Birmingham/UK

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- P 101 **Hydrogen storage in metal-organic frameworks**
B. Streppel, I. Krkljus, J. Teufel, M. Hirscher, Max-Planck-Institute for Metals Research, Stuttgart/D; B. Assfour, G. Seifert, Dresden University of Technology/D; L. Zhechkov, T. Heine, Jacobs University Bremen/D
- P 102 **Metal-organic frameworks for hydrocarbon separation**
D. Peralta, K. Barthelet, G. Pirngruber, IFP Lyon/F; G. Chaplais, A. Simon-Masseron, IS2M, Mulhouse/F
- P 103 **High and selective CO₂ uptake over CH₄ in sulfone functionalized metal-organic frameworks**
E. Neofotistou, E. Baka, I. Papadaki, University of Crete, Heraklion/GR; C. Malliakas, Northwestern University, Evanston, IL/USA; P.N. Trikalitis, University of Crete, Heraklion/GR
- P 104 **Carbon dioxide capture using MOFs : a comparison**
J. Kim, D.-A. Yang, S.-H. Kim, W.-S. Ahn, Inha University, Incheon/ROK
- P 105 **Gas separation properties of interdigitated porous frameworks**
Y. Inubushi, Kuraray Co., Ltd, Kurashiki, Okayama/J; S. Horike, S. Kitagawa, Kyoto University/J
- P 106 **Structural stability of metal-organic frameworks under humid conditions**
K. Walton, P.M. Schoenecker, C. Carson, Georgia Institute of Technology, Atlanta, GA/USA
- P 107 **Assessment of MOF performance for gas separation: FTIR based breakthrough testing**
M. Leistner, W. Graehlert, Fraunhofer IWS Dresden/D; S. Kaskel, Dresden University of Technology/D
- P 108 **Triggering sorption selectivity in metal-organic frameworks by functionalization with donor groups**
S. Henke, R. Schmid, R.A. Fischer, Ruhr-Universität Bochum/D
- P 109 **A porous coordination polymer hybrid with quartz oscillator**
H. Uehara, S. Furukawa, M. Nakahama, S. Diring, S. Kitagawa, Japan Science and Technology Agency, Kyoto/J
- P 110 **Characterization of gas adsorption in MOFs by thermal desorption spectroscopy**
J. Teufel, K. Manickam, M. Hirscher, Max Planck Institute for Metals Research, Stuttgart/D

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- P 111 **Pyrazolate based metal-organic frameworks for capture and separation of gases and VOCs**
E. Barea, J.A.R Navarro, F. Linares, E. Quartapelle Procopio, C. Montoro, University of Granada/E; S. Galli, N. Masciocchi, Università dell'Insubria, Como/I
- P 112 **Hydrogen adsorption in MOFs studied by low-temperature thermal desorption spectroscopy**
M. Hirscher, I. Krkljus, Max Planck Institute for Metals Research, Stuttgart/D
- P 113 **Hydrogen storage capacity and determination of the heat of adsorption on different MOFs**
N. Klein, I. Senkovska, Dresden University of Technology/D; M. Schlichtenmayer, Max Planck Institute for Metals Research, Stuttgart/D; K. Gedrich, Dresden University of Technology/D; M. Hirscher, Max Planck Institute for Metals Research, Stuttgart/D; S. Kaskel, Dresden University of Technology/D
- P 114 **Simulation of fixed-bed adsorption of CO₂ / CH₄ mixtures on metal-organic frameworks**
M. Schindler, S. Ernst, University of Kaiserslautern/D
- P 115 **Guest-induced structural transformations of flexible porous coordination polymers investigated by coincident adsorption/XRPD measurement**
R. Matsuda, S. Bureekaew, H. Sato, J. Seo, S. Kitagawa, Japan Science and Technology Agency, Kyoto/J
- P 116 **Prediction of adsorption-induced structural transition of a flexible porous coordination polymer**
H. Sugiyama, A. Yamamoto, H. Tanaka, S. Watanabe, T. Fukushima, Y. Hijikata, S. Horike, Kyoto University/J; Y. Kubota, Osaka Prefecture University/J; S. Kitagawa, M. Miyahara, Kyoto University/J
- P 117 **Liquid-phase adsorption on metal-organic frameworks**
A. Henschel, I. Senkovska, S. Kaskel, Dresden University of Technology/D
- P 118 **Synthesis, characterisation and adsorption properties on a new copper-based MOF material**
J. Lincke, D. Lässig, University of Leipzig/D; J. Möllmer, Institut für Nichtklassische Chemie e.V., Leipzig/D; A. Puls, Rubotherm GmbH, Bochum/D; R. Staudt, Institut für Nichtklassische Chemie e.V., Leipzig/D; H. Krautscheid, University of Leipzig/D

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- P 119 **Fundamental relations of hydrogen storage properties to framework topology of MOFs**
B. Streppel, M. Hirscher, Max Planck Institute for Metals Research, Stuttgart/D
- P 120 **Solid-state NMR study on structure and host-guest interactions in MIL53-NH¹³CHO**
J. Wack, University of Bayreuth/D
- P 121 **A comparison of UiO-66(Zr) with CuBTC for the adsorption of CO₂, N₂ and CO₂/N₂ mixtures in presence of water**
E. Soubeyrand-Lenoir, C. Vagner, P. Llewellyn, CNRS – Aix-Marseille University/F; C. Serre, F. Millange, Institut Lavoisier, Université de Versailles/F
- P 122 **Oriented growth of functionalized metal-organic frameworks on SAM-modified gold substrates - vapor sorption isotherms**
F. Hinterholzinger, C. Scherb, University of Munich/D; J.J. Williams, University of Edinburgh/UK; T. Bein, University of Munich/D
- P 123 **In-situ diffraction studies of the structural transition of metal-organic framework Cu-SIP-3**
P.K. Allan, B. Xiao, University of St. Andrews/UK; S.J. Teat, J.W. Knight, Lawrence Berkeley National Laboratory, CA/USA; R.E. Morris, University of St. Andrews/UK
- P 124 **Can the synthesis and activation of MOFs be optimized for gas adsorption?**
C. Palomino Cabello, G. Turnes Palomino, University of the Balearic Islands, Palma de Mallorca/E
- P 125 **Functionalized flexible MIL-53 for the capture of green house gases**
V. Guillerm, C. Serre, T. Devic, G. Férey, Institut Lavoisier, Université de Versailles/F; A. Vimont, M. Daturi, Laboratoire de Catalyse et Spectrochimie, Caen/F; P. Llewellyn, S. Bourrelly, CNRS – Aix-Marseille University/F; G. Maurin, F. Salles, CNRS-Institut Charles Gerhardt Université Montpellier2/F
- P 126 **Thermodynamics of gas adsorption on Mg-MOF-74: combined theoretical and variable-temperature IR spectroscopic studies**
G.T. Palomino, University of the Balearic Islands, Palma de Mallorca/E; S. Bordiga, S. Chavan, L. Valenzano, University of Torino/I; C.O. Areán, University of the Balearic Islands, Palma de Mallorca/E; B. Civalieri, University of Torino/I

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- P 127 **Metal-organic frameworks for the selective removal of N and S compounds from a fuel feed**
M. Maes, F. Vermoortele, S. Schouteden, L. Alaerts, D. De Vos, Katholieke Universiteit Leuven/B
- P 128 **Evaluation of energy heterogeneity in MOF materials: absence of Henry's region in highly flexible MIL-53 and MIL-68 materials?**
M. Pera-Titus, M. Savonnet, D. Farrusseng, Université de Lyon, Villeurbanne/F
- P 129 **Purifying phenolic wastewater using a Cr-based MOF**
M. Maes, S. Schouteden, L. Alaerts, D. De Vos, Katholieke Universiteit Leuven/B
- P 130 **Understanding type V isotherms for H₂O and CO₂ adsorption in MOFs**
M. De Toni, R. Jonchière, S. Paranthaman, F.X. Coudert, A.H. Fuchs, Chimie ParisTech & CNRS/F
- P 131 **Solid state NMR on Cu₃(BTC)₂: adsorption study and resonance assignment**
F. Gul-E-Noor, M. Bertmer, B. Jee, University of Leipzig/D; M. Hartmann, D. Himsl, University of Erlangen-Nuremberg/D
- P 132 **Characterizing molecular transport in MOF ZIF-8**
C. Chmelik, J. Kärger, University of Leipzig/D; H. Bux, J. Caro, University Hanover/D; L. Hertäg, S. Fritzsche, University of Leipzig/D; J.M. van Baten, R. Krishna, University of Amsterdam/NL
- P 133 **Study of water sorption on zinc- and iron-carboxylates for potential heat storage applications**
N. Zabukovec Logar, T. Birska Celic, M. Rangus, G. Mali, M. Mazaj, V. Kaucic, National Institute of Chemistry, Ljubljana/SLO
- P 134 **Tuning polarity by framework functionalization: a new imidazolate based MOF adsorbent, SIM-1**
S. Aguado, D. Farrusseng, IRCELYON-CNRS, Villeurbanne/F
- P 135 **Polarized binding of hydrogen in MOFs as a strategy for building a pragmatic hydrogen storage system**
S. Barman, K. Venkatesan, H. Berke, University of Zürich/CH
- P 136 **Effect of doping MOF-5 metal clusters with Co²⁺ on its hydrogen adsorption capacity**
G. Calleja, J. Botas, Universidad Rey Juan Carlos, Móstoles/E; M. Sánchez-Sánchez, CSIC, Madrid/E; M. Orcajo, Universidad Rey Juan Carlos, Móstoles/E

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- P 137 **Aspects of MOF based chromatography**
F. Mertens, A. Münch, T. Böhle, M. Lohse, D. Schindler, E. Weber, TU Bergakademie Freiberg/D
- P 138 **Absolute adsorption in microporous media**
F. Mertens, TU Bergakademie Freiberg/D
- P 139 **Application of coordination polymers with high density of open metal sites in the separation of carbon dioxide and methane**
P.D.C. Dietzel, F. Schuricht, K.A. Andreassen, R. Blom, SINTEF Materials and Chemistry, Oslo/N
- P 140 **Development of first principle based force fields to describe adsorption and diffusion in MOFs including lattice dynamics**
V. Van Speybroeck, L. Vanduyfhuys, T. Verstraelen, M. Vandichel, J. Van der Mynsbrugge, M. Waroquier, Ghent University/B
- P 141 **Thermodynamics of guest-induced structural transitions in hybrid organic-inorganic frameworks**
F.X. Coudert, C. Triguero, A.H. Fuchs, Chimie ParisTech & CNRS/F; A. Boutin, École normale supérieure, Paris/F; A.V. Neimark, Rutgers University, Piscataway, NJ/USA
- P 142 **Synthesis and functional properties of triazolate-based MOFs**
D. Denysenko, D. Volkmer, University of Ulm/D; B. Streppel, M. Hirscher, Max Planck Institute for Metals Research, Stuttgart/D
- P 143 **Enhancement of hydrogen adsorption in metal-organic frameworks by Mg functionalization. A multiscale computational study**
T. Sterianakos, E. Tylianakis, E. Klontzas, G. E. Froudakis, University of Crete, Heraklion/GR
- P 144 **Gas mixture adsorption in MOFs: predictions from single component data compared with direct experiments**
A. Wiersum, S. Bourrelly, P. Llewellyn, CNRS – Aix-Marseille University/F; F. Ragon, T. Devic, P. Horcajada, F. Millange, C. Serre, Institut Lavoisier, Université de Versailles/F; Y.K. Hwang, J.S Chang, Korea Research Institute of Chemical Technology, Daejeon/ROK

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- P 145 **Influence of metal versus heat and capacity of gas adsorption in various MIL-100 (Fe, Al, Cr) phases**
D. Phanon, A. Wiersum, P. Llewellyn, CNRS – Aix-Marseille University/F; P. Horcajada, C. Serre, Institut Lavoisier, Université de Versailles/F; T. Loiseau, Université de Lille 1/F
- P 146 **Diffusion of pure short n-alkanes and binary mixture with CO₂ in rigid MIL-47(V) and flexible MIL-53(Cr) MOFs**
J. Rosenbach, F. Salles, P. Yot, G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; D. Kolokolov, H. Jobic, IRCE de Lyon/F; A. Ghoufi, Université de Rennes/F; T. Devic, C. Serre, G. Férey, Université de Versailles/F
- P 147 **Structural transition of MIL-53 under pressure: a way to determine the energy of transition between large and narrow pore phases**
M. Boulhout, I. Beurroies, P. Llewellyn, R. Denoyel, CNRS – Aix-Marseille University/F; C. Serre, Institut Lavoisier, Université de Versailles/F
- P 148 **Adsorption of volatile hydrocarbons on MOF-5 studied by means of quasi-equilibrated thermodesorption**
W. Makowski, M. Manko, J. Szklarzewicz, P. Zabierowski, D. Majda, W. Lasocha, Jagiellonian University, Krakow/PL
- P 149 **Adsorption of the aromatic compounds ethylbenzene and styrene on the metal-organic frameworks MIL-47 and MIL-53**
L. Ma, M. van Leuvenhaege, S. Couck, G. Baron, J. Denayer, Vrije Universiteit Brussel/B; M. Maes, F. Vermoortele, L. Alaerts, D. De Vos, Katholieke Universiteit Leuven/B
- P 150 **Hydrogen adsorption in isorecticular metal-organic frameworks based on Zr₆O₄(OH)₄ building block**
S. Chavan, O. Zavorotynska, J.G. Vitillo, S. Bordiga, University of Torino/I; K.P. Lillerud, M.H. Nilsen, S. Jakobsen, University of Oslo/N
- P 151 **Liquid phase separations on MOFs: unsaturated vs saturated alkylaromatics**
M. Maes, F. Vermoortele, L. Alaerts, Katholieke Universiteit Leuven/B; S. Couck, Vrije Universiteit Brussel/B; C. Kirschhock, Katholieke Universiteit, Leuven /B; J. Denayer, Vrije Universiteit Brussel; D. De Vos, Katholieke Universiteit Leuven/B

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- P 152 **Modelling of breakthrough profiles of Amino-MIL-53**
S. Couck, T. Rémy, F. Warnier, G. Baron, J. Denayer, Vrije Universiteit Brussel/B; J. Gascon, F. Kapteijn, Delft University of Technology/NL
- P 153 **DFT and ab-initio study of dihydrogen binding in metal-organic frameworks with exposed metal sites**
A. Mavrantoukakis, K. Vogiatzis, W. Klopffer, KIT - Karlsruhe Institute of Technology/D
- P 154 **Theoretical study for improving hydrogen storage on metal-organic frameworks**
H. Mizuseki, N.S. Venkataramanan, R. Sahara, Y. Kawazoe, Tohoku University, Sendai/J
- P 155 **MOF's characterisation with innovative volumetric/calorimetric techniques**
E. Wirth, R. André, P. Le Parlouër, Setaram Instrumentation, Caluire/F
- P 156 **MOFs as preconcentrator materials**
I. Raible, Y. Joseph, N. Krasteva, Sony Deutschland GmbH, Stuttgart/D
- P 157 **Molecular dynamics investigation of the influence of lattice flexibility and partial charges on the migration of guest molecules in the metal-organic framework ZIF-8**
M. Knauth, K. Kirchner, S. Fritzsche, C. Chmelik, J. Kärger, University of Leipzig/D; T. Remsungnen, Khon Kaen University/THA; K. Seeharmart, University of Leipzig/D; J. Caro, H. Bux, University of Hanover/D
- P 158 **Molecular dynamics investigation of the self-diffusion of guest molecules in the metal-organic framework Zn(tbip) with rigid and flexible framework**
K. Seeharmart, T. Nanok, M. Knauth, S. Fritzsche, C. Chmelik, J. Kärger, University of Leipzig/D; T. Remsungnen, Khon Kaen University/THA; R. Krishna, University of Amsterdam/NL
- P 159 **Structural prediction of dinuclear layer pillar metal-organic frameworks: studied by quantum calculations**
O. Saengsawang, Chulalongkorn University, Bangkok/THA; M. Knauth, University of Leipzig/D; A. Pianwanit, Chulalongkorn University, Bangkok/THA; C. Kritayakornpong, King Mongkut's University of Technology Thonburi, Bangkok/THA; M. Wiebcke, University Hanover/D; S. Fritzsche, University of Leipzig/D; S. Hannongbua, Chulalongkorn University, Bangkok/THA

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- P 160 **IR investigation in operando conditions of CO₂ adsorption in the MIL-53(Cr) using a high pressure variable-temperature cell with a small dead volume: evaluation of quantity adsorbed, nature of adsorption sites and structural evolution**
P. Bazin, H. Leclerc, A. Vimont, M. Daturi, Laboratoire Catalyse et Spectrochimie, Caen/F; S. Bourrelly, P. Llewellyn, Laboratoire Chimie Provence, Marseille/F
- P 161 **Investigation of C3 separation over MIL100-Fe using operando IR spectroscopy: adsorption sites and effect of the temperature of activation**
S. Wuttke, P. Bazin, A. Vimont, M. Daturi, Université de Caen/F; P. Horcajada, C. Serre, G. Férey, Université de Versailles/F; J.S. Chang, Korea Research Institute of Chemical Technology, Daejeon/ROK
- P 162 **Tailoring MOFs for CO₂ capture: the amino-effect**
J.G. Vitillo, S. Chavan, B. Seyyedi, F. Bonino, Université di Torino/I; D. Farrusseng, University Lyon/F; S. Bordiga, Università di Torino/I
- P 163 **Metal-organic frameworks for CO₂ capture incorporating triazamacrocycles and heterodinuclear metallic clusters**
G. Ortiz, S. Brandes, Y. Rousselin, R. Guillard, Université de Bourgogne, Dijon/F
- P 164 **The adsorption of CO and CO₂ on CPO-27-M (M = Mg, Ni, Zn) through quantum mechanical approaches**
B. Civalieri, L. Valenzano, University of Torino/I; K. Sillar, J. Sauer, Humboldt University, Berlin/D
- P 165 **Metal-organic frameworks for CO₂ capture incorporating triazamacrocycles and homodinuclear zinc clusters**
G. Ortiz, S. Brandes, Y. Rousselin, R. Guillard, Université de Bourgogne, Dijon/F
- P 166 **Design of metal-organic frameworks for separation of carbon dioxide from gas mixtures**
Y.S. Bae, C.E. Wilmer, O.K. Farha, B.G. Hauser, J.T. Hupp, R.Q. Snurr, Northwestern University, Evanston, IL/USA
- P 167 **Methane adsorption isotherms of new IRMOFs obtained by Monte Carlo computer simulations**
S. Alves Jr., F.F. Silva, R.L. Longo, D.P. Santos, E.H.L. Falcão, Universidade Federal de Pernambuco, Recife/BR

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- P 168 **Adsorption of long chain n-alkanes in rigid (MIL-47(V)) and flexible functionalized (MIL-53(Fe)) metal-organic frameworks: insights from experiments and molecular simulations**
P. Trems, T. Khuong Trung, I. Deroche, G. Maurin, N.A. Ramsahye, F. Fajula, CNRS-Institut Charles Gerhardt Université Montpellier2/F; T. Devic, C. Serre, P. Horcajada, G. Férey, Institut Lavoisier, Université de Versailles/F
- P 169 **Unusual adsorption behaviour in metal-organic frameworks**
D. Fairen-Jimenez, N.A. Seaton, T. Düren, The University of Edinburgh/UK
- P 170 **What does it take to accurately predict adsorption properties of zeolitic imidazole frameworks?**
D. Fairen-Jimenez, N.A. Seaton, T. Düren, The University of Edinburgh/UK
- P 170A **Hydrogen adsorption in Cu-MOF (Cu(PDC))**
H. Sakai, I. Kanoya, T. Furuta, M. Hosoe, Honda R&D Co. Ltd., Wako, Saitama/J

Topic 3: Novel applications and physical properties

- P 171 **The synthesis, optimal formation conditions and biological activity of oxim pinostrobin copper (II) complex**
O. Loiko, A. Khalitova, Karaganda State University/KAZ; A. Mashentseva, L.N. Cumelev, Eurasian National University, Astana/KAZ; B.I. Tuleuov, SPH „Phytochemistry“, Karaganda/KAZ
- P 172 **Structure and properties of an amorphous metal-organic framework**
T.D. Bennett, University of Cambridge/UK; A.L. Goodwin, University of Oxford/UK; M.T. Dove, University of Cambridge/UK; D.A. Keen, University of Oxford/UK; M.G. Tucker, E.R. Barney, A.K. Soper, ISIS Facility, Oxford/UK; E.G. Bithell, J.C. Tan, A.K. Cheetham, University of Cambridge/UK
- P 173 **Assessment of metal-organic framework membranes and composites for gas separations using computational modeling**
S. Keskin, KOC University, Istanbul/TR; D.S. Sholl, Georgia Institute of Technology, Atlanta, GA/USA

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- P 174 **Analysis of void space of porous materials: from a single structure to database screening**
M. Haranczyk, C.H. Rycroft, Lawrence Berkeley National Laboratory, CA/USA; J. Klotz, G. Carlsson, Stanford University, Palo Alto, CA/USA; J.A. Sethian, B. Smit, University of California, Berkeley, CA/USA
- P 175 **Photochromic hybrid materials**
D. Hermann, U. Ruschewitz, University of Cologne/D
- P 176 **Dense and homogeneous PCPs coatings on oxide surfaces**
A. Betard, O. Vreshch, D. Zacher, K. Yussenko, R.A. Fischer, Ruhr-Universität Bochum/D
- P 177 **Synthesis and luminescence of Zn-based MOFs built up from rod-shaped secondary building units and long oligo(phenyleneethynylene)dicarboxylate linker**
A. Schaate, University Hanover/D; P. Roy, University of Bielefeld; J. Panke, M. Wark, University of Hanover/D; A. Godt, University of Bielefeld/D; P. Behrens, University of Hanover/D
- P 178 **Optoelectrochemical properties of SURMOFs deposited by the layer-by-layer method**
J. Panke, University Hanover/D; D. Zacher, Ruhr-Universität Bochum/D; M. Wark, University of Hanover/D; R.A. Fischer, Ruhr-Universität Bochum/D
- P 179 **Analysis of the formation of mof particles by time resolved scattering including SLS, SAXS and SANS**
 J. Cravillon, M. Wiebcke, University Hanover/D; D. Zacher, R.A. Fischer, Ruhr-Universität Bochum/D; R. Schweins, Institut Laue-Langevin, Grenoble/F; T. Narayanan, European Synchrotron Radiation Facility, Grenoble/F; R. Nayuk, K. Huber, University of Paderborn/D
- P 180 **Solid solutions of soft porous coordination polymers for fine-tunable gate-opening type adsorption profiles**
T. Fukushima, S. Horike, S. Kitagawa, Kyoto University/J
- P 181 **Fine tuned metal-organic framework for high and selective CO₂ uptake: framework reduction of MOFs by organometallics increases the adsorption properties**
M. Meilikhov, K. Yussenko, Ruhr-Universität Bochum/D; A. Torrisi, C. Mellot-Drazniek, University College London/UK; R.A. Fischer, Ruhr-Universität Bochum/D

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- P 182 **Step-by-step growth of the [Cu₃(btc)₂] and [Cu₂(ndc)₂(dabco)] thin films on different bare and fictionalized substrates**
K. Yusenko, M. Meilikhov, Ruhr-Universität Bochum/D; H.J. Buschmann, German Textile Research Center, Krefeld/D; R.A. Fischer, Ruhr-Universität Bochum/D
- P 183 **Modeling NMR and EPR parameters in the metal-organic framework Cu₃(BTC)₂**
N. Vankova, T. Heine, Jacobs University Bremen/D
- P 184 **New studies on metal-organic frameworks**
S.M. Keltie, R.J. Aldus, P.A. Gale, M. Tromp, University of Southampton/UK
- P 185 **Confocal fluorescence microscopy reveals localization of dyes in and on fluorescently modified metal-organic frameworks (MOFs)**
M. Ma, A. Pinto, A. Gross, D. Zacher, R.A. Fischer, N. Metzler-Nolte, Ruhr-Universität Bochum/D
- P 186 **Efficient luminescence in rare earth amide and amine MOFs**
C.J. Höller, A. Zurawski, P. Matthes, K. Müller-Buschbaum, University of Würzburg/D; M. Mai, C. Feldmann, KIT - Karlsruhe Institute of Technology/D
- P 187 **Photoluminescent MOF to gunshot residue identification**
I. Weber, A.J.G. Melo, M.A.M. Lucena, M. Oliveira, S. Alves Jr., Universidade Federal de Pernambuco, Recife/BR
- P 188 **Preparation of proton conductive coordination hybrids**
S. Horike, S. Breekaew, S. Kitagawa, Kyoto University/J
- P 189 **Guest-responsive porous magnetic frameworks based on polycyanometallate building units**
M. Ohba, K. Yoneda, R. Ohtani, Kyoto University/J; A.B. Gaspar, J.A. Real, Universidad de Valencia/E; S. Kitagawa, Kyoto University/J
- P 190 **Thin films of MOFs prepared by liquid-phase epitaxy: suppression of interpenetration and facile determination of diffusion coefficients**
O. Shekha, H. Wang, O. Zybaylo, C. Wöll, KIT - Karlsruhe Institute of Technology/D; D. Zacher, R. Schmid, M. Tafipolsky, R.A. Fischer, Ruhr-Universität Bochum/D

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- P 191 **An entangled porous coordination polymer as a luminescent sensor**
S. Furukawa, Japan Science and Technology Agency, Kyoto/J; Y. Takashima, Kyoto University/J; V. Martinez, University of Basque Country, Bilbao/E; S. Kitagawa, Kyoto University/J
- P 192 **Coordinatively immobilized monolayers on porous coordination polymer crystals**
M. Kondo, Kyoto University/J; S. Furukawa, Japan Science and Technology Agency, Kyoto/J; S. Kitagawa, Kyoto University/J
- P 193 **MOFs as materials for microelectronics: theoretical estimation of dielectric and thermal conductance properties**
K. Zagorodniy, G. Seifert, Dresden University of Technology/D; H. Hermann, IFW Dresden/D
- P 194 **Crystal structure and dielectric property of porous coordination polymers having dipolar rotor**
W. Kosaka, R. Matsuda, S. Kitagawa, Japan Science and Technology Agency, Kyoto/J
- P 195 **Electrical behavior of porous metal-organic frameworks to address their breathing ability, drug encapsulation and ionic exchange properties**
S. Devautour-Vinot, G. Maurin, F. Henn, CNRS-Institut Charles Gerhardt Université Montpellier2/F; P. Horcajada, T. Devic, A. Fateeva, J. Eubank, D. Paula De Cuhna, C. Serre, Institut Lavoisier, Université de Versailles/F
- P 196 **Surface modification of SURMOFs**
B. Liu, D. Zacher, Ruhr-Universität Bochum/D; T. Ladnorg, KIT -Karlsruhe Institute of Technology/D; A. Bétard, Ruhr-Universität Bochum/D; C. Wöll, KIT - Karlsruhe Institute of Technology/D; R. A. Fischer, Ruhr-Universität Bochum/D
- P 197 **A guest-responsive fluorescent 3D microporous metal-organic framework derived from a long lifetime pyrene core**
K.C. Stylianou, R. Heck, S.Y. Chong, J. Bacsá, J. T.A. Jones, Y.Z. Khimiyak, D. Bradshaw, M.J. Rosseinsky, University of Liverpool/UK
- P 198 **Facile preparation of imidazolate based MOF membranes on tubular porous alumina for separation applications**
S. Aguado, C.H. Nicolas, D. Farrusseng, IRCELYON-CNRS, Villeurbanne/F

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- P 200 **NanoMOF: nanoporous metal-organic frameworks for production**
W. Graehlert, Fraunhofer IWS, Dresden/D; P. Collier, Johnson Matthey PLC, Reading/UK; J. Martens, Katholieke Universiteit Leuven/B; J.A.R. Navarro, Universidad de Granada/E; St. Kaskel, Dresden University of Technology/D; P. Dietzel, Stiftelsen SINTEF, Oslo/N; S. Bordiga, Università di Torino/I; D. Farrusseng, IRCELYON-CNRS/F; L. Ouvry, OUVRY SAS, Lyon/F; A. Lang, Norafin GmbH, Allschwil/CH; D. Packet, Oleon NV, Oelegem/B; M. Herskowitz, Ben-Gurion University of the Negev, Beer-Sheva/IL; P. Pataki, Innovatex, Budapest/H; G. Bissolotti, Società Italiana Acetilene e Derivati S.p.A, Bergamo/I; Ph. Martin, TDL Sensors LTD, Manchester/UK; B. Boehringer, Bluecher GmbH, Erkrath/D; A. Gerds, Hollomet GmbH, Dresden/D
- P 201 **Photophysical study of an entangled porous coordination polymer: guest dependent charge transfer complex emission**
V. Martínez, University of Basque Country, Bilbao/E; S. Furukawa, Y. Takashima, Kyoto University/J; I. Lopez Arbeloa, University of Basque Country, Bilbao/E; S. Kitagawa, Kyoto University/J
- P 202 **Investigation of covalent organic frameworks by a first principle derived force field**
S. Amirjalayer, R. Schmid, Ruhr-Universität Bochum/D
- P 203 **Atomic scale modeling of Cu and Zn paddle-wheel metal organic frameworks**
S. Bureekaew, S. Amirjalayer, R. Schmid, Ruhr-Universität Bochum/D; S. Kitagawa, Kyoto University/J
- P 204 **Development and application of a consistent first principles derived force field (MOF-FF) for porous hybrid materials**
 S. Amirjalayer, S. Bureekaew, M. Tafipolsky, R. Schmid, Ruhr-Universität Bochum/D
- P 205 **In vivo toxicity studies of nanoparticles of iron porous MOFs**
P. Horcajada, T. Baati, Université de Versailles/F; R. Gref, Université Paris 11/F; C. Serre, G. Férey, Université de Versailles/F; P. Couvreur, Université Paris 11, Malabry/F

POSTER PROGRAMME

- P 206 **Quantitative structure activity relationship of metal-organic frameworks as potential nanocarriers for drug encapsulation and delivery**
 C. Gaudin, E. Ivanoff, G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; D. Paula de Cuhna, P. Horcajada, C. Serre, Université Versailles/F
- P 207 **Fundamental host-guest interactions in porous metal-organic frameworks**
 M. Wehring, S. Hertel, M. Gratz, F. Stollmach, University of Leipzig/D; S. Amirjalayer, R. Schmid, Ruhr-Universität Bochum/D
- P 210 **Coordination polymers based on carbohydrazone binuclear copper(II) complex bridged by dipyriddy linkers**
D. Dragancea, Academy of Sciences of Moldova, Chisinau/MD; V.B. Arion, University of Vienna/A; S. Shova, Moldova State University, Chisinau/MD; S. Decurtins, University of Bern/CH
- P 211 **Electronic properties of MOFs: an ab-initio investigation**
B. Civaleri, L. Valenzano, S. Novarino, M. Ferrero, University of Torino/I; M. Rerat, University of Pau/F
- P 212 **Flexibility and motion in scandium terephthalates characterised by diffraction and solid state NMR and their consequences for adsorption**
J.P.S. Mowat, P.A. Wright, J.M. Griffin, V.R. Seymour, S.E.M. Ashbrook, University of St. Andrews/UK; S.R. Miller, Institut Lavoisier, Université de Versailles/F

Topic 4: Perspectives in catalysis and engineering aspects

- P 213 **A detailed study of the catalytic performance of V, Co and Cu MOFs in the oxidation of cyclohexene**
K. Leus, I. Muylaert, University of Ghent/B; A. Verberckmoes, University College Ghent/B; G.B. Marin, Y.Y. Liu, V. Van Speybroeck, P. Van Der Voort, University of Ghent/B
- P 214 **The remarkable catalytic activity of the saturated MIL-47 in the oxidation of cyclohexene**
 K. Leus, I. Muylaert, M. Vandichel, G.B. Marin, M. Waroquier, V. Van Speybroeck, P. Van Der Voort, University of Ghent/B

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- P 215 **Cu₃(BTC)₂: metal-organic framework catalyzing Friedländer reaction**
E. Perez-Mayoral, UNED, Madrid/E; K. Sulisz, J. Heyrovsky Institute, Prague/CZ; B. Gil, Jagiellonian University, Cracow/PL; J. Cejka, J. Heyrovsky Institute, Prague/CZ
- P 217 **Au@PCPs – synthesis, characterization and catalytic applications**
M. Müller, D. Esken, Ruhr-Universität Bochum/D; S. Turner, O.I. Lebedev, University of Antwerp/B; R.A. Fischer, Ruhr-Universität Bochum/D
- P 218 **Innovative Ni- and Fe-based alloy metal foams give resistance and flexibility**
R. Poss, A.-S. Dreher, Alantum Europe GmbH, Sauerlach/D
- P 220 **How many CO's can coordinate to Cu-BTC centres?**
P. Petkov, G. Vayssilov, University of Sofia/BG; T. Heine, Jacobs University Bremen/D
- P 221 **New generation of super-acid solid catalysts based on one-pot encapsulation of heteropoly-acids in metal organic frameworks**
J. Juan-Alcañiz, E.V. Ramos-Fernandez, M. Goesten, A. Martinez-Joaristi, J. Gascon, F. Kapteijn, Delft University of Technology/NL
- P 222 **Post-synthetic functionalization of MIL-101 with super bases: grafting on the metal vs covalent bonding on the linker**
M. van Dalen, J. Juan-Alcañiz, E.V. Ramos-Fernandez, J. Gascon, F. Kapteijn, Delft University of Technology/NL
- P 223 **Energy landscapes of imidazolate-based MOFs: a route to understanding structures and optimizing properties**
S. Leoni, I. Baburin, B. Assfour, G. Seifert, Dresden University of Technology/D
- P 224 **Incorporation of iron tetrasulfophthalocyanine within metal-organic framework MIL-101**
O. Zalomaeva, Y. Chesalov, V. Kaichev, M. Melgunov, V. Zaikovskii, O. Kholdeeva, Boreskov Institute of Catalysis, Novosibirsk/RUS; K. Kovalenko, V. Fedin, Nikolaev Institute of Inorganic Chemistry, Novosibirsk/RUS; A. Sorokin, IRCELYON-CNRS, Villeurbanne/F

POSTER PROGRAMME

- P 225 **Metal-organic frameworks as heterogeneous catalysts**
M. Gustafsson, J. Grins, A. Bartoszewicz, B. Martín-Matute, X. Zou, Stockholm University/S
- P 226 **Probing the catalytic properties of MOFs containing redox-active transition metals**
C. Worch, R. Gläser, University of Leipzig/D
- P 227 **Unexpected reversible lattice changes of [Cu₂(1,4-bdc)₂dabco] MOF thin films upon loading with ferrocene**
R. Heck, O. Zybaylo, O. Shekhah, T. Lahnorg, H. Arslan, S. Heissler, P. Weidler, C. Woell, KIT - Karlsruhe Institute of Technology/D
- P 228 **Metal-organic frameworks as heterogeneous catalysts for monosaccharide dehydration**
F. Vermoordele, S. Schouteden, L. Alaerts, D.E. De Vos, Katholieke Universiteit Leuven/B
- P 229 **Functional metal-organic frameworks as heterogeneous basic catalysts**
M. Fischer, M. Hartmann, University of Erlangen-Nuremberg/D
- P 230 **Synthesis optimization of porous known MOFs**
F. Ragon, C. Serre, P. Horcajada, T. Devic, Université de Versailles/F
- P 231 **Hyper hydrophobic imidazolate MOF films by post-functionalization**
S. Aguado, J. Canivet, D. Farrusseng, IRCELYON-CNRS, Villeurbanne/F
- P 232 **How does alkene epoxidation with TBHP occur in MIL-47?**
M. Vandichel, K. Leus, I. Muylaert, P. van Der Voort, M. Waroquier, V. van Speybroeck, Ghent University/B
- P 233 **Biologically inspired MOFs mimicking the Cu-containing active site of particulate methane monooxygenase**
M. Grzywa, B. Breidenkötter, D. Volkmer, University of Ulm/D; J. Sonntag, E. Klemm, University of Stuttgart /D
- P 234 **Computational modelling of O₂ adsorption in a Cobalt(II)-containing metal-organic framework**
A. Mavrantoukakis, J. Sauer, Humboldt-University of Berlin/D; M. Tonigold, D. Volkmer, University of Ulm /D

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- P 235 **Rationalisation of the infra-red frequencies of Brønsted acid sites in the MIL-53 MOF material: role of the pore size and the nature of the metal center**
M. Ben Yahia, G. Maurin, CNRS-Institut Charles Gerhardt Université Montpellier2/F; A. Vimont, J.C. Lavalley, Laboratoire Catalyse et Spectrochimie, Caen/F; F. Millange, T. Devic, G. Férey, C. Serre, Institut Lavoisier, Université de Versailles/F
- P 236 **Stability of MOFs in liquid phase hydrogenation catalysis**
S. Opelt, M. Aimer, E. Klemm, University of Stuttgart/D

POSTER PROGRAMME

POSTER AWARD INFORMATION

A poster prize will be awarded for the best poster. The award will be conferred at the end of the conference before the closing remarks on Wednesday, September 8, 2010 at 16:00 h. All poster authors are asked to attend the session.

LAST MINUTE POSTER SUBMISSION

Further poster contributions can be accepted as last minute posters, subject to approval by the Scientific Committee and as long as free capacity is available. These last minute posters will be announced in the last minute information available at the beginning of the conference.

Submission of last minute posters is possible **until August 10, 2010**, at the latest. **Papers can only be accepted via online submission.**

For full information and submission: www.mof-conf.org.

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