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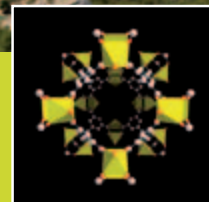
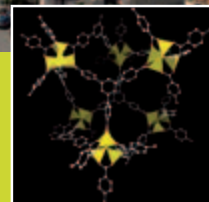
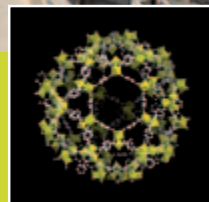
Micromeritics manufactures a number of instruments suitable for characterizing metal organic frameworks. The ASAP 2020 Accelerated Surface Area and Porosimetry System can be used to determine the microporosity and hydrogen storage capacity of such materials. Hydrogen adsorption isotherms can easily be obtained on MOFs, zeolites, and activated carbons. Both the Micromeritics ASAP 2050 Xtended Pressure Sorption Analyzer and the Particulate Systems HPVA-100 High Pressure Volumetric analyzer are ideally suited for determining the storage capacity and heat of adsorption for MOFs, as well as other materials such as zeolites, carbons, and novel crystalline materials.



2nd International Conference on Metal-Organic Frameworks and Open Framework Compounds

September 5 – 8, 2010 · Palais du Pharo

Marseille/France



PROGRAMME

COMMITTEES / ORGANIZER

LOCAL ORGANIZING COMMITTEE

Sandrine Bourrelly	CNRS – Aix-Marseille University/F
G�rard F�rey	Universit� de Versailles/F
Martin Hartmann	University of Erlangen-Nuremberg/D
Stefan Kaskel	Dresden University of Technology
Philip Llewellyn	CNRS – Aix-Marseille University/F (Chairman)
Guillaume Maurin	CNRS-Institut Charles Gerhardt Universit� Montpellier2/F
Silke Megelski	DECHEMA e.V., Frankfurt am Main/D

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Pascal Dietzel	SINTEF Materials and Chemistry, Oslo/N
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Makoto Fujita	University of Tokyo/J
Joseph T. Hupp	Northwestern University, Evanston, IL/USA
Katsumi Kaneko	Chiba University/J
Kimoon Kim	Pohang University of Science & Technology/ROK
Susumu Kitagawa	Kyoto University/J
Wenbin Lin	University of North Carolina, Chapel Hill, NC/USA
Jeffrey Long	University of California, Berkeley, CA/USA
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Ulrich M�ller	BASF SE, Ludwigshafen/D
Michael O’Keefe	Arizona State University, Tempe, AZ/USA
Matthew Rosseinsky	University of Liverpool/UK
Randall Snurr	Northwestern University, Evanston, IL/USA
Maria Vallet-Regi	Universidad Complutense de Madrid/E
Jaume Veciana	Institut de Ci�ncia de Materials de Barcelona (CSIC)/E
Richard Willis	UOP Research Center, Des Plaines, IL/USA
Jihong Yu	Jilin University, Changchun/PRC

UNDER THE AUSPICES OF



CONFERENCE ORGANIZER



DECHEMA e.V.
Society for Chemical Engineering
and Biotechnology
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/D

INVITATION

Porous solids and particularly metal-organic frameworks are strategic materials in numerous applications concerning energy, sustainable development and health. MOF2010 will be held between 5th and 8th September 2010.

This conference will follow the very successful 2008 conference held in Augsburg. The 2010 conference will be organized in Marseille at a central location overlooking the old port. The aims of MOF2010 are to address all questions concerning the community working with metal-organic frameworks, metal coordination compounds and related materials.

The spectrum of topics to be treated range from synthesis and characterization of new materials to properties of materials towards potential applications in biology/medicine, catalysis, magnetism, luminescence and sorption. Both experimental and theoretical aspects will be dealt with, along with key questions pertaining to potential industrial applications of this fascinating family of materials.

As in Augsburg, a single strand oral session will be maintained allowing attendees to view the various aspects of scientific research on these materials. As such, a strong emphasis will be given to the poster presentation. DECHEMA and the IZA therefore extend a cordial invitation to any colleagues interested in MOF research to attend this meeting.

PROGRAMME AT A GLANCE

Sunday, Sept 5, 2010		Monday, Sept 6, 2010	
		8:30	Welcome + Introduction P. Llewellyn
		<i>Chairs:</i>	<i>M.J. Rosseinski</i> <i>G. Férey</i>
		9:00	INVITED LECTURE M. Fujita
		9:45	P. Behrens
		10:10	M. Kandiah
		10:35	Coffee Break with Exhibition and Posters
		11:00	H. Bux
		11:25	J.C. Tan
		11:50	D. Sholl
		12:15	R.A. Fischer
		12:40	Lunch Break
		<i>Chairs:</i>	<i>J. Hupp</i> <i>S. Kitagawa</i>
		14:10	C. Sanchez
		14:35	H. Sato
		15:00	R.R. Willis
		15:25	J.A. Real
16:00	Registration open	15:50	Coffee Break with Exhibition and Posters
		16:20	INVITED LECTURE M.J. Rosseinsky
		17:05	End of the 1st conference day
		19:00 – 23:30	Conference Dinner at the "Fort Ganteaume"
18:00 – 21:00	Welcome Reception Get Together		

PROGRAMME AT A GLANCE

Tuesday, Sept 7, 2010		Wednesday, Sept 8, 2010	
<i>Chairs:</i>	<i>M. Fujita</i> <i>M. Hartmann</i>	<i>Chairs:</i>	<i>C. Zhong</i> <i>R.E. Morris</i>
8:30	INVITED LECTURE J. Hupp	8:30	INVITED LECTURE C. Serre
9:15	M. Savonnet	9:15	N. Rosi
9:40	S.M. Cohen	9:40	M. Haja Mohideen
10:05	M. Goesten	10:05	R. Ameloot
10:30	Coffee Break with Exhibition and Posters	10:30	Coffee Break with Exhibition and Posters
11:00	P. Nachtigall	11:00	J. Seo
11:25	L. Alaerts	11:25	A. Pöpl
11:50	D. Volkmer	11:50	A. Martinez-Joaristi
12:15	N. Maksimchuk	12:15	P.D.C. Dietzel
12:40	Lunch Break	12:40	Lunch Break
<i>Chairs:</i>	<i>M.D. Allendorf</i> <i>R. Snurr</i>	<i>Chairs:</i>	<i>C. Serre</i> <i>S. Kaskel</i>
14:10	INVITED LECTURE C. Zhong	14:10	M. Thommes
		14:35	A. Dailly
14:55	Y. Chen	15:00	K. Sillar
15:20	G. Maurin	15:25	INVITED LECTURE M.D. Allendorf
15:45	Coffee Break with Exhibition and Posters	16:10	Coffee Break with Exhibition and Posters
16:15	S. Kaskel	16:20	End of Conference
16:40	A. Vimont		
17:05	A.F.P. Ferreira		
17:30 – 20:00	Poster Party		
20:00	End of the 2nd conference day		

LECTURE PROGRAMME

MONDAY, SEPTEMBER 6, 2010

08:30	Welcome + Introduction P. Llewellyn, CNRS – Aix-Marseille University/F
Chairs:	<i>M.J. Rosseinski, University of Liverpool/UK G. Férey, Université de Versailles/F</i>
09:00	INVITED LECTURE Crystalline molecular flasks M. Fujita, University of Tokyo/J
09:45	Zr-based metal-organic frameworks: from nano to single crystals via a modulation approach P. Behrens, 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
10:10	Tagged Zr-metal organic frameworks and their post synthetic modifications and applications M. Kandiah, S.U. Nanot, N.H. Nilsen, S. Jakobsen, U. Olsbye, M. Tilset, K.P. Lillerud, University of Oslo/N
10:35	Coffee Break with Exhibition and Posters
11:00	Zeolitic imidazolate framework-8 molecular sieve membrane: from molecular modelling to membrane permeation H. Bux, J. Caro, F.Y. Li, J. Cravillon, M. Wiebcke, C. Chmelik, J. Kärger, S. Fritzsche, L. Hertäg, University of Hanover/D; Y.S. Li, Dalian Institute of Chemical Physics/PRC
11:25	Mechanical properties of zeolitic imidazolate frameworks (ZIFs) J.C. Tan, T.D. Bennett, A.K. Cheetham, University of Cambridge/UK
11:50	Using multiple levels of computer modeling to accelerate development of MOFs for membrane applications D. Sholl, T. Watanabe, E. Haldoupis, S. Nair, Georgia Institute of Technology, Atlanta, GA/USA
12:15	Directing the orientation of layer-based SURMOFs on SAMs R.A. Fischer, D. Zacher, K. Yussenko, A. Bétard, S. Henke, T. Lahnorg, Ruhr-Universität Bochum/D; O. Shekhah, C. Woell, KIT - Karlsruhe Institute of Technology/D; A. Terfort, Frankfurt University/D
12:40	Lunch Break

LECTURE PROGRAMME

MONDAY, SEPTEMBER 6, 2010

Chairs:	<i>J. Hupp, Northwestern University, Evanston, IL/USA S. Kitagawa, Kyoto University/J</i>
14:10	Elaboration and adsorption properties of hierarchically structured optical thin films of MOFs A. Demessence, Université Pierre et Marie Curie, Paris and Université de Versailles/F; L. D'Arras, C. Boissière, D. Grosso, Université Pierre et Marie Curie, Paris/F; P. Horcajada, C. Serre, G. Férey, Université de Versailles/F; C. Sanchez, Université Pierre et Marie Curie, Paris/F
14:35	Photo-responsive porous coordination polymers H. Sato, R. Matsuda, Japan Science and Technology Agency, Kyoto/J; S. Kitagawa, University of Kyoto/J
15:00	Hydrothermal stability of PCPs: theory matches experiment A.I. Benin, P. Jakubczak, J.F. Abrahamian, J.J. Low, R.R. Willis, UOP LLC, Des Plaines, IL/USA
15:25	Chemo-responsive switching of spin state in Hofmann-like porous metal-organic frameworks J.A. Real, University of Valencia/E; M.C. Muñoz, Universidad Politécnica de Valencia/E; A.B. Gaspar, F.J. Muñoz-Lara, University of Valencia/E; S. Kitagawa, M. Ohba, University of Kyoto/J
15:50	Coffee Break with Exhibition and Posters
16:20	INVITED LECTURE Sorption and structure in biologically-derived MOF materials M.J. Rosseinski, University of Liverpool/UK
17:05	End of the 1st conference day
19:00	Conference Dinner at "Fort Ganteaume"
23:30	

LECTURE PROGRAMME

TUESDAY, SEPTEMBER 7, 2010

Chairs:	<i>M. Fujita, The University of Tokyo/J</i> <i>M. Hartmann, University of Erlangen-Nuremberg/D</i>
08:30	INVITED LECTURE Designing catalytic metal-organic frameworks J. Hupp, Northwestern University, Evanston, IL/USA
09:15	Tailor-made multifunctional MOF via a generic post-functionalization route for acid/base catalysis M. Savonnet, IRCELYON, Villeurbanne/F; D. Bazer-Bachi, N. Bats, V. Lecocq, IFP-LYON, Solaize/F; C. Pinel, D. Farrusseng, IRCELYON, Villeurbanne/F
09:40	Postsynthetic modification of MOFs: a general strategy to control MOF structure and function Z. Wang, K. Tanabe, S. Garibay, C. Volkringer, J. Nguyen, S.M. Cohen, U.C. San Diego, La Jolla/USA
10:05	Sulfonate post-functionalised metal-organic frameworks: a new class of strong acid catalysts and proton conducting materials M. Goesten, J. Juan-Alcañiz, E.V. Ramos-Fernandez, J. Gascon, F. Kapteijn, TU Delft/NL
10:30	Coffee Break with Exhibition and Posters
11:00	On the accuracy of theoretical methods for the description of MOFs P. Nachtigall, L. Grajciar, University of Prague/CZ; M. Rubes, O. Bludsky, IOCB, Prague/CZ
11:25	Active site engineering on metal-organic frameworks for Diels-Alder catalysis L. Alaerts, R. Matthessen, F. Vermoortele, B. Carlier, R. Ameloot, D.E. De Vos, Katholieke Universiteit Leuven/B
11:50	Catalytic oxidation reactions by cobalt(II)-containing metal-organic frameworks D. Volkmer, M. Tonigold, Ulm University/D; A. Mavrantoukakis, J. Sauer, Humboldt University of Berlin/D
12:15	Hybrid polyoxometalate/MIL-101 catalysts for liquid phase selective oxidation N.V. Maksimchuk, O.A. Kholdeeva, Boreskov Institute of Catalysis, Novosibirsk/RUS; K.A. Kovalenko, V.P. Fedin, Nikolaev Institute of Inorganic Chemistry, Novosibirsk/RUS
12:40	Lunch Break

LECTURE PROGRAMME

TUESDAY, SEPTEMBER 7, 2010

Chairs:	<i>M.D. Allendorf, Sandia National Laboratories, Livermore, CA/USA</i> <i>R. Snurr, Northwestern University, Evanston, IL/USA</i>
14:10	INVITED LECTURE Understanding mixture separation in MOFs by computer modelling C. Zhong, Beijing University of Chemical Technology/PRC
14:55	Adsorption and separation of CH₃OH/H₂O and CO₂/CH₄ in a highly hydrophobic metal-organic framework Zn(BDC)(TED)_{0.5} Y. Chen, National University of Singapore/SGP; J.Y. Lee, University of New Jersey, Newark, NJ /USA; R. Babarao, National University of Singapore/SGP; J. Li, University of New Jersey, Newark, NJ/USA; J.W. Jiang, National University of Singapore/SGP
15:20	Computational study of the structural grafting effects on natural gas upgrading in metal-organic frameworks Q. Yang, G. Maurin, N. Ramsahye, CNRS-Institut Charles Gerhardt Université Montpellier2/F; A. Wiersum, P. Llewellyn, CNRS – Aix-Marseille Université/F; F. Ragon, H. Chevreau, S. Miller, P. Horcajada, T. Devic, C. Serre, Université de Versailles/F
15:45	Coffee Break with Exhibition and Posters
16:15	Metal-organic frameworks based on BTB linkers and their application in gas storage and catalysis K. Gedrich, N. Klein, Dresden University of Technology/D; M. Heitbaum, A. Notzon, University of Münster/D; I. Senkovska, Dresden University of Technology/D; F. Glorius, University of Münster/D; S. Kaskel, Dresden University of Technology/D
16:40	Metal-organic framework with reducible open metal sites: <i>in situ</i> FTIR characterization of Fe²⁺/Fe³⁺ CUS sites; interactions with CO₂, propane, propylene and propyne A. Vimont, H. Leclerc, S. Wuttke, P. Bazin, J.C. Lavalley, M. Daturi, EnsiCAEN, CNRS - University of Caen/F; P. Horcajada, C. Serre, G. Férey, CNRS – Université de Versailles/F; P. Llewellyn, S. Bourrelly, CNRS- Aix-Marseille University/F; J.S. Chang, Catalysis Center for Molecular Engineering, Daejeon/ROK
17:05	Process development of propane/propylene separation using CuBTC extrudates N. Lamia, A.F.P. Ferreira, M.G. Plaza, J.C. Santos, A.E. Rodrigues, LSRE - Laboratory of Separation Reaction Engineering, FEUP, Porto/P
17:30	Poster Party
20:00	End of the 2nd conference day

LECTURE PROGRAMME

WEDNESDAY, SEPTEMBER 8, 2010

Chairs:	<i>C. Zhong, Beijing University of Chemical Technology/PRC</i> <i>R.E. Morris, University of St. Andrews/UK</i>
08:30	INVITED LECTURE BioMOFs for the delivery of active molecules <i>C. Serre, Université de Versailles/F</i>
09:15	Porous Metal-Adeninate MOFs: design, preparation, and biomedical and environmental applications <i>J. An, N. Rosi, University of Pittsburgh, PA/USA</i>
09:40	Protecting group and pore-discriminating adsorption properties of a hydrophilic-hydrophobic metal-organic framework <i>M. Haja Mohideen, B. Xiao, P. Wheatley, Y. Li, A. Slawin, University of St. Andrews/UK; N. Cessford, T. Düren, University of Edinburgh/UK; X. Zhao, R. Gill, M. Thomas, Newcastle University/UK; J. Griffin, S. Ashbrook, D. Aldous, R.E. Morris, University of St. Andrews/UK</i>
10:05	Hollow metal-organic framework capsules with crystalline walls showing selective permeability <i>R. Ameloot, W. Vanhove, L. Alaerts, M.B.J. Roeffaers, B.F. Sels, D.E. De Vos, Katholieke Universiteit Leuven, Heverlee/B</i>
10:30	Coffee Break with Exhibition and Posters
11:00	Multi-step and gate-opening type adsorption on a porous coordination polymer possessing gated channels <i>J. Seo, R. Matsuda, C. Bonneau, Japan Science and Technology Agency (JST), Kyoto/J; S. Kitagawa, Kyoto University/J</i>
11:25	Temperature-driven structural phase transition in chromium-doped MIL-53(Al) – an electron spin resonance spectroscopy study <i>M. Mendt, B. Jee, A. Pöppl, University of Leipzig/D; N. Stock, Universität zu Kiel/D; M. Hartmann, D. Himsel, University of Erlangen-Nuremberg/D</i>
11:50	Electrochemical synthesis of metal-organic frameworks and their application in coatings and membranes <i>A. Martinez Joaristi, J. Gascon, F. Kapteijn, Delft University of Technology/NL</i>

LECTURE PROGRAMME

WEDNESDAY, SEPTEMBER 8, 2010

12:15	A new series of isorecticular honeycomb-like coordination polymers with high density of open metal sites <i>P.D.C. Dietzel, M. Frøseth, R. Blom, SINTEF Materials and Chemistry, Oslo/N; R.E. Johnsen, H. Fjellvåg, University of Oslo/N</i>
12:40	Lunch Break
Chairs:	<i>C. Serre, Université de Versailles/F</i> <i>S. Kaskel, Dresden University of Technology /D</i>
14:10	Adsorption behavior and textural characterization of novel open metal-organic frameworks (MOFs) <i>J. Moellmer, INC, Leipzig/D; C. Thibault, Quantachrome, Boynton Beach, FL/USA; R. Luebke, A. Cairns, F. Nour, University of South Florida, Tampa, FL/USA; M. Eddaoudi, King Abdullah University of Science and Technology, Thuwal/SAR; R. Staudt, INC, Leipzig/D; M. Thommes, Quantachrome, Boynton Beach, FL/USA</i>
14:35	Research status of metal-organic frameworks as adsorbent materials for on-board H₂ storage applications <i>A. Dailly, General Motors LLC, Warren, MI/USA</i>
15:00	Ab initio prediction of methane adsorption isotherms for CPO-27-Mg <i>K. Sillar, J. Sauer, Humboldt University of Berlin/D</i>
15:25	INVITED LECTURE Manipulation of MOFs for device fabrication <i>M.D. Allendorf, B. Jacobs, R. Houk, Sandia National Laboratories, Livermore, CA/USA; Y. Kobayashi, B. Wiers, J. Long, University of California, Berkeley, CA/USA; A. Talin, National Institute of Standards and Technology, Gaithersburg, MD/USA; P. Hesketh, J.H. Lee, A. Venkatasubramanian, Georgia Institute of Technology, Atlanta, GA/USA</i>
16:10	Poster Awards Closing Remarks
16:20	End of the Conference

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. Berni, 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

POSTER PROGRAMME

- 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

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- 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

POSTER PROGRAMME

- 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. Dulcevsciaia, 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. Firlej, 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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. Mavrantonas, K. Vogiatzis, W. Kloppe,
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

POSTER PROGRAMME

- 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. Civaleri, 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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. Shekhah, 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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

POSTER PROGRAMME

- 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.

Please note: the registration fee cannot be waived for authors.

EXHIBITION / ACKNOWLEDGEMENT

EXHIBITION

In parallel to the scientific sessions, companies are invited to present products, processes and services in the field of MOFs. The exhibition area is close to the lecture and poster hall and allows an ideal integration of lectures, poster discussions as well as company and product presentations. As exhibition space is strictly limited, we recommend you to reserve your space as soon as possible. For stand application and further details concerning the organization please contact the congress office.

The following companies have already registered:

- Micromeritics, Verneuil en Halatte/F
- Rubotherm GmbH, Bochum/D in cooperation with:
APOLLO Instruments, Compiègne/F and BEL Japan Inc., Osaka/J
- Setaram Instrumentation, Caluire/F

A frequently updated list is available at www.mof-conf.org

ACKNOWLEDGEMENT

The main sponsor of the conference is:



Micromeritics,
Verneuil en Halatte/F

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IFP, Institute Français du Pétrole,
Rueil-Malmaison/F



Royal Society of Chemistry,
Cambridge/UK



Rubotherm GmbH,
Bochum/D in cooperation with:
APOLLO Instruments, Compiègne/F
and **BEL Japan Inc., Osaka/J**



Setaram Instrumentation,
Caluire/F

SOCIAL PROGRAMME

SOCIAL PROGRAMME

Sunday, September 5, 2010

18:00 – 21:00

Welcome reception

There will be an informal gathering at the Palais du Pharo to welcome the participants to the conference. Drinks and snacks will be served.

Free of charge, registration is required.

Monday, September 6, 2010

19:00 – 23:30

Conference dinner

The conference dinner will take place at “Fort Ganteaume”.

The conference dinner will be held on the Monday evening at the Military Garrison, Fort Ganteaume which is at the very entrance of Marseilles Old Port. The Fort dates back to 1664 as a place for Louis XIV to place soldiers in order to assert his authority on a population which were not particularly royalist. It is within walking distance of all of the main conference hotels and the conference site. The dinner itself will aim to capture the flavour of Southern France. ... and for those of you who have had enough of MOFs, it is possible to sign up to the French Foreign Legion there.

Cost per person: 52,00 € (plus 19,6% VAT.)
incl. dinner and drinks
Registration is required.

Meeting point: The Meeting point and time will be announced onsite in Marseille.



Tuesday, September 7, 2010

17:30 – 20:00

Poster party

In order to give each participant an adequate opportunity for an intensive discussion of the poster contributions a poster party will take place. Poster authors are requested to be present at their posters.

Free of charge, registration is required.

GENERAL INFORMATION

CONFERENCE VENUE

The conference will be held at:
Palais du Pharo
58, Boulevard Charles-Livon
13007 Marseille/France



Gifted to Napoleon III by Marseille, this area of land, set on the Maure promontory overlooking the Château d'If (famous for its prison) and the entrance to the old harbour, enabled the emperor to fulfill his plans for a waterfront residence. Built by the architects Lefuel and Vaucher between 1858 and 1870, Napoleon's wife, empress Eugenie de Montijo, left the palace to the city in 1883. An auditorium and several halls have been built beneath the garden.

For details please visit <http://palaisdupharo.marseille.fr>

History of Marseille

With 2600 years of history, Marseille has preserved its traditions and unique lifestyle over the centuries.

Marseilles invites you to take a walk down the legendary Canebière, to stroll around the Old Harbour with its fish market and take a ride on the famous ferry-boat.



GENERAL INFORMATION

Marseille is the capital of soap-making and the home of the world-famous santons (Christmas crib figures representing well-known figures in Provençal life).

Marseilles is an ideal starting point for discovering the beautiful villages and historic traditions of Provence. You can take your pick of the tours offered in Marseille: e.g. the cliffs of Cassis, the harbour of Martigues and the Blue Coast, the windmills at Allauch; Aubagne and Le Garlaban, La Sainte-Baume and Sainte-Victoire; Aix-en-Provence, Saint-Rémy de Provence, the citadel of Les Baux de Provence, the Alpilles hills, the town of Arles and the Camargue, and many more.

For detailed information and tour bookings please contact:

Ms. Laurence Berthelier
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33 cours Pierre Puget
13006 Marseille

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Fax: +33 (0)496 102482

E-Mail: laurence.berthelier@matheztravel.com

Internet: www.matheztravel.com

The European Capital of Culture 2013

On September 16, 2008, Marseille was designated European Capital of Culture 2013 along with the Slovak city of Kosice. In 2013, the two cities will become the windows on European cultural activities for the eyes of the world.

The title European Capital of Culture was created in 1985 by the European Union with a view to bringing Europeans closer together and asserting the central role cities play in arts and culture.

Throughout the year 2013, they will be hosting a programme of extraordinary cultural events, expositions, performances, workshops and festivals.

GENERAL INFORMATION

ACCOMMODATION

Accommodation in various hotels, categories and at special rates has been reserved for conference participants.

In order to get choice and availability, we highly recommend to book your hotel room at your earliest convenience via the conference website or directly at www.matheztravel.com/mof2010. Room reservations are binding. Charges for rooms which will not be used, or cancelled too late, must be paid by the participant.

Room reservation will be made by:

Ms. Laurence Berthelier
Voyages C. Mathez
33 cours Pierre Puget
13006 Marseille

Phone: +33 (0)496 102480

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E-Mail: laurence.berthelier@matheztravel.com

Internet: www.matheztravel.com

REGISTRATION FOR PARTICIPATION

Please complete the online registration form via

www.mof-conf.org.

An automatically generated confirmation of receipt will be sent to you by email directly after getting your online registration. You will receive a separate invoice by post after your registration has been booked in. The conference ticket, the list of participants, book of abstracts, CD and name tag will be available at the Palais du Pharo in Marseille at office hours.

In general there is no registration deadline as long as free capacity is available. Please note: registrations made after **August 15, 2010** are not guaranteed to appear in the list of participants.

GENERAL INFORMATION

REGISTRATION FEES ¹⁾

	Members ²⁾	Regular
Participant from Industry	€ 670,00	€ 685,00
Participant from Academia	€ 520,00	€ 535,00
Student/Pensioner (proof of status required)	€ 260,00	€ 275,00

1) plus 19,6% VAT

2) Personal DECHEMA members and EFC/EFCE passport holders

The fee includes the book of abstracts, a CD with extended abstracts (as far as submitted by the authors), the list of participants and beverages during the coffee breaks, but no lunch.

REMITTANCE OF FEES

Fees should be remitted on receipt of the invoice in favour of DECHEMA e.V. to one of the DECHEMA accounts as stated on the invoice. When you authorise the payment for the invoice, please be sure to note as the reason for payment your complete invoice number.

CANCELLATIONS AND REFUNDS

€ 30,00 plus 19,6% VAT for administrative costs will be charged for cancellations received by **August 15, 2010**. Thereafter 80% plus 19,6% VAT of the registration fees will be invoiced; however, the book of abstracts and the CD will be mailed. Only written cancellations will be accepted. If the event is cancelled by DECHEMA e.V. the whole fees will be refunded. Further claims for compensation are excluded.

LUNCH

Lunch will be available at the Palais du Pharo or in the local restaurants and pubs nearby the conference centre. Participants are expected to pay their lunch themselves.

GENERAL INFORMATION

VISA FORMALITIES

Participants from a number of countries may need an entry visa for the Republic of France. It is recommended to apply for a visa well in advance of the conference.

If a formal invitation letter is needed, please order it via conference website www.mof-conf.org in good time.

INSURANCE

The organizers cannot accept responsibility for loss or damage to the private property of participants and accompanying persons which may occur either during or arising from the conference. Participants should therefore take whatever steps they consider necessary regarding insurance.

CONFERENCE OFFICE

DECHEMA e.V.
Research Management & Conferences
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Theodor-Heuss-Allee 25
60486 Frankfurt am Main/Germany

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Fax: +49 (0)69 7564-304
E-mail: geiling@dechema.de
Internet: www.mof-conf.org

Office hours onsite in Marseille

Sunday, September 5, 2010	16:00 h – 21:00 h
Monday, September 6, 2010	07:30 h – 17:05 h
Tuesday, September 7, 2010	08:00 h – 20:00 h
Wednesday, September 8, 2010	08:30 h – 16:30 h
Phone: +49 (0)162/4141-162	

GENERAL INFORMATION

HOW TO GET TO MARSEILLE

Marseille is reachable by air, by sea, by train (also on the TGV Méditerranée high-speed train) and by car.

Connections between Airport and Marseille city centre:By bus from the airport to Marseille

Shuttle service is provided every 20 minutes from 5:10 h to 0:10 h. After 0:10 h, additional coach services are organized according to scheduled flight arrivals.

Journey time: 25 minutes – direct by motorway

Fare (one way): € 8.50.

Phone: +33 (0)442 143127

From Marseille city centre back to the airport:

Departure from St. Charles railway station

Shuttle service every 20 minutes from 4:30 h to 23:30 h

Phone: +33 (0)491 505934

Connections between St. Charles train station and Marseille Old Pier:

Marseille train station is located in the city centre at 15 minutes walk to the Old Pier. Direct connection by tube in 5 minutes.

Taxi service

Groupement Taxis Tupp Radio

Phone: +33 (0)491 058080

Fax: +33 (0)491 503739

E-Mail: info@taxis-tupp.com

Internet: www.taxis-tupp.com

24-hour service:

Phone: +33 (0)4 42 14 24 44

Fax: +33 (0)4 42 88 04 77

E-Mail: taxisaeroport@tiscali.fr

Internet: www.taxis.aeroport.com

Between the airport and the city centre, the fare is about € 40,00 in the daytime and about € 50,00 at night. Night fare is applicable from 19:00 to 7:00 and on sundays and holidays all day long.

