International Microsymposium: 13.-14.3.2017, TU Dresden

Switchability in Porous Metal-Organic Frameworks

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Chair: S. Kaskel

Organizing Committee: E. Brunner, A. Eychmüller, G. Seifert

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Scope:

Porous materials play a key role in gas and liquid phase separations, energy storage, as catalysts and for optical and chemical sensing. Metal-Organic Frameworks (MOFs) stand out among other porous materials due to their extremely high porosity and modular tunability. While the majority of porous solids (and MOFs) is *rigid*, a novel and unique class of *switchable* MOFs was discovered in recent years. These materials only open their pores dynamically, as a response to the presence of gases or liquids at a characteristic concentration associated with unprecedented, step-wise unit cell volume changes (more than 240 %) during gas uptake. Such *switchable MOFs* are able to specifically respond or even recognize certain types of molecular species by opening their pores, resulting in a step-wise change of physical (i.e. magnetism, optical density, bulk density, etc.) and chemical characteristics (catalytic activity, reactivity). Moreover, they reversibly close their pores in the absence of the respective species. A principle understanding of the dynamic phenomena in such materials would represent a unique technological basis for the design of switchable catalysts, filters, threshold sensors, or stimulus induced drug delivery by receptor systems with integrated key-lock functionality. However, so far the discovery of switchable MOFs (also named gating, or breathing MOFs) was essentially accidental but recently an increasing number of such compounds are being discovered. Currently, it is still impossible to rationally predict new switchable structures, because the underlying microstructural principles, responsible for such a high degree of flexibility, are not understood. For the technological development of switchable MOFs in separation, catalysis, or sensing, a fundamental understanding of the underlying structural principles and gas-solid interaction mechanisms is needed. The symposium primarily addresses the *fundamentals of porosity switching* phenomena in the solid state and the underlying principles. Experimental and theoretical approaches in order to derive a predictive model for framework flexibility will be presented, as well as parallelized physical characterization tools will be established enabling the application of *in situ* global scattering techniques (XRD) and *in situ* local probe spectroscopies (NMR, EPR, EXAFS) in order to analyze the microscopic structural transformations and dynamics induced by host/guest interactions during adsorption/desorption. Only an interdisciplinary discussion will promote this new field to develop a predictive framework for switchable MOFs fostering an intense cooperation of theoreticians, synthetic chemists, and physicists.

Monday, March 13th:

Location: TU Dresden, Bergstr. 66, 01069 Dresden
Neubau Chemische Institute, Lecture Hall S89

Time	Program
8.30	*Registration*
9.00	S. Kaskel: *Welcome and Introduction*
	Chair: S. Kaskel
9.10	"Natural Gas Storage in Metal-Organic Frameworks" J. A. Mason, M. K. Taylor, J. Oktawiec, M. I. Gonzalez, T. Runčevski, J. E. Bachman, R. L. Siegelman, **J. R. Long** (Berkeley)
10.00	"Breathing MOFs for energy-related applications" P. Yot, A. Ghoufi, P.L. Llewellyn, **G. Maurin** (Montpellier)
10.30	"Structure, Disorder and Function in Flexible MOFs" C. Tschense, T. W. Kemnitzer, J. Wack, Y. A. Avadhut, C. D. Keenan, **J. Senker** (Bayreuth)
11.00	*Coffee Break*
	Chair: E. Brunner
11.40	"Flexibility, Defects and Disorder in Soft Porous Crystals: Molecular Insight from Computational Chemistry" A. H. Fuchs, A. Boutin, **F.-X. Coudert** (Paris)
12.10	"Pressure Amplification by Negative Gas Adsorption in the Switchable Metal-Organic Framework DUT-49" **S. Krause**, V. Bon, I.Senkovska, U. Stoeck, D. Wallacher, D. M. Többens, R. S. Pillai, G. Maurin, F.-X. Coudert, S. Kaskel (Dresden)
12.30	"Framework Flexibility by Molecular Buckling" **J. D. Evans**, L. Bocquet, F-X. Coudert (Paris)
12.50	Lunch (Mensa)
	Chair: R. Schmid
14.00	"Particle size effects and tunability of switching in DUT-8 architectures". H. Miura, N. Kavoosi, V. Bon, I. Senkovska, **S. Kaskel** (Dresden)
14.30	"Investigation of Structural Transformations and Defects in Flexible MOFs by Electron Paramagnetic Resonance Spectroscopy" **A. Pöppl**, M. Mendt, M. Šimėnas (Leipzig)
15.00	"On the flexibility in DUT-8: the role of conformational isomerism" P. Petkov, **T. Heine** (Leipzig)
15.30	"On the Control of Multifaceted Structural Flexibility in Functionalized Pillared-Layered MOFs by the Choice of Metal Center" **R. A. Fischer**, A. Schneemann, G. Kieslich, P. Vervoorts (München)
16.00	*Coffee Break*
	Chair: R. A. Fischer
16.40	"*In Situ* NMR Spectroscopy of Flexible MOFs" **E. Brunner**, S. Paasch, M. Rauche, M. Sin (Dresden)
17.10	"Using ab-initio calculations to explain the measured ^{129}Xe chemical shift in UiO-66 and UiO-67" **G. Seifert**, K. Trepte, E. Brunner (Dresden)
17.40	"First-principles derived force fields for the understanding of structural transformations in flexible MOFs" **R. Schmid,** J. P. Dürholt, J. Keupp, M. Dyga, R. Amabile, M. Alaghemandi (Bochum)
18.10 - 21.10	Buffet Dinner, Beer, and Poster Session

Please allow 5 minutes time for questions!

Tuesday, March 14th:

Location: TU Dresden, Bergstr. 66, 01069 Dresden
Neubau Chemische Institute, Lecture Hall S89

Time	Program
	Chair: T. Düren
9.00	"Functions Integration in Flexible MOFs for Molecular Separation" **R. Matsuda**, M. Foo, Y. Ma, A. Hori (Nagoya)
9.30	"Selective Adsorption on Flexible Layer-Based MOFs" **A. Kondo**, H. Tanaka, T. Ohkubo, H. Kajiro, H. Kanoh, K. Kaneko, K. Maeda (Tokyo)
10.00	"Flow Microreactor Synthesis of Elastic Layer-structured MOF (ELM-12) with Controlled Size and Gate Adsorption Characteristics" **S. Watanabe**, A. Fukuta, H. Tanaka, M.T. Miyahara (Kyoto)
10.30	"Triazolyl Isophthalate MOFs: Structural Flexibility and in situ PXRD studies" **H. Krautscheid**, M. Kobalz, O. Erhart, H. Preissler (Leipzig)
11.00	*Coffee Break*
	Chair: S. Kaskel
11.30	"Photoswitchable MOF Thin Films" Z. Wang, A. Knebel, S. Grosjean, C. Wöll, S. Bräse, J. Caro, **L. Heinke** (Karlsruhe)
12.00	"Group theory to generate and rationalize interpenetrated MOFs" **I. Baburin** (Dresden)
12.30	"Insight into guest-induced flexibility in metal-organic frameworks by combing high pressure crystallography and molecular simulation" C. Hobday, C. Morrison, S. Moggach, **T. Düren** (Bath)
13.00	Lunch (Mensa)
14.00	Optional: Lab visits, individual discussions
15.00	End

Please allow 5 minutes time for questions!

Locations:

- **Neubau Chemische Institute: Bergstr. 66**

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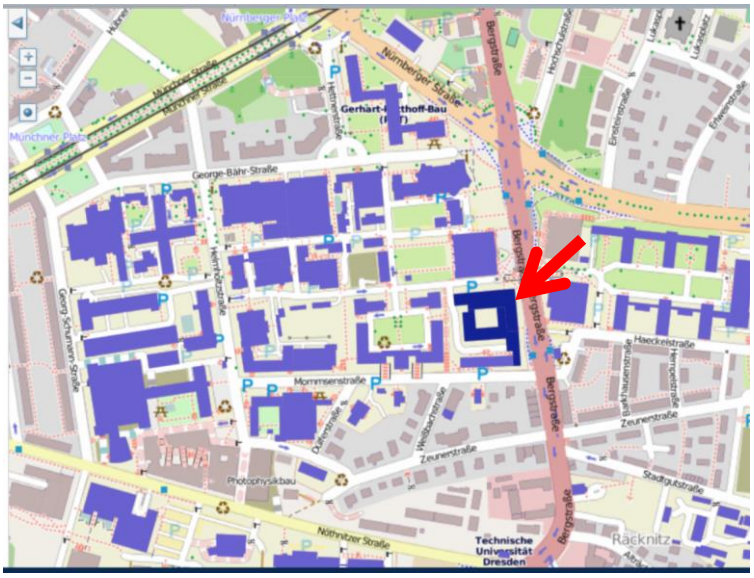

- **Lecture Hall S90 (K level):**

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