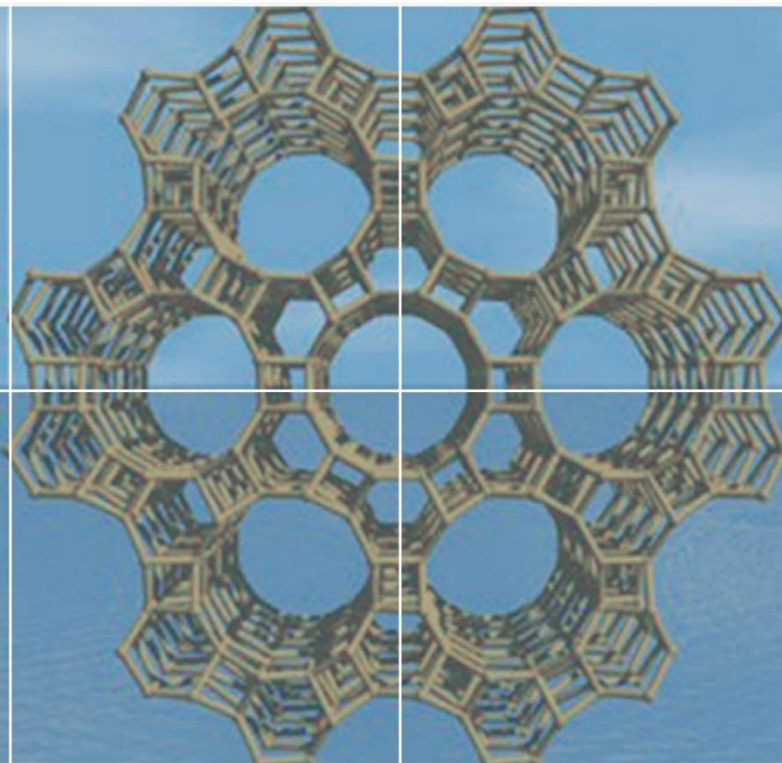




JILIN UNIVERSITY

Workshop on Functional Nanoporous Materials

NEW PERSPECTIVES OF FUNCTIONAL NANOPOROUS MATERIALS



PROGRAM

Jilin University, Changchun, China
13-16 June, 2017

Hotel: The Abritz Hotel
 Address: 888 Guigu Street, Changchun, 130012



Direction from Hotel to Venue: Follow the green line and arrows.
 Weather in Changchun during 13-16 June, 2017: No rain, very comfortable.



June 13 14 15 16 17

Contacts:

Yunling Liu (130 3900 5641)
 Wenfu Yan (138 4308 4682)

Please meet at the lobby of the hotel at 08:00 on 14 June and 08:20 on 15 June.

WORKSHOP PROGRAM

Wednesday, 14 June, 2017, Lecture Hall (II), Auditorium

Time	Speaker	Title	Chairperson
08:30 - 08:40	Opening Ceremony		Jihong Yu
08:40 - 09:15	Stefan Kaskel	New Metal-Organic Frameworks with Ultrahigh Porosity, Switchability and Functionality	Guangshe Li
09:15 - 09:50	Fabrizio Cavani	Mixed Metal Oxides for Gas-phase Reactions: Bio-alcohols and Polyols Transformation to Added Value Chemicals	
09:50 - 10:20	Coffee Break		
10:20 - 10:55	Gopinathan Sankar	On the Formation of Zeolites through in situ and ex situ X-ray Techniques	Jean-Pierre Gilson
10:55 - 11:30	Peng Zhang	X-ray Spectroscopy of Some Metal Nanostructures	
11:30 - 11:50	Group Photo		
12:00	Lunch		
13:30 - 14:05	Fei Wei	Hierarchical Zeolite Structures and Their Application on Methanol to Propylene and Aromatics	Sheng Dai
14:05 - 14:40	Jean-Pierre Gilson	Designer Zeolites: Better, Smaller, More Accessible and... Cheap	
14:40 - 15:10	Coffee Break		
15:10 - 15:45	Bao-Lian Su	Natural Law of Hierarchizing Holds Key to Enhancing Photocatalysis, Amplifying Gas Sensing and Extending Battery Life	Gopinathan Sankar
15:45 - 16:20	Jihong Yu	Zeolitic Materials: Prediction, Synthesis and Application	
16:20	Laboratory and Campus Tour		
18:00	Dinner		

Thursday, 15 June, 2017, Lecture Hall (II), Auditorium

Time	Speaker	Topic	Chairperson
08:50 - 09:25	Sheng Dai	Porous Ionic Liquids: Challenges and Opportunities	Justin D. Holmes
09:25 - 10:00	Guangshan Zhu	Targeted Synthesis of Porous Aromatic Frameworks: From Structure Design to Advanced Application	
10:00 - 10:30	Coffee Break		
10:30 - 11:05	Lixin Wu	Supramolecular Self-Assembly of Inorganic Clusters for Soft Frameworks	Bao-Lian Su
11:05 - 11:40	Justin D. Holmes	Nanoparticle Promoters in Organic and Inorganic Reactions	
12:00	Lunch		
13:30 - 14:05	Xiulian Pan	Porous Materials and Selectivity Control in Syngas Conversion	Guangshan Zhu
14:05 - 14:40	Ben Slater	Computational Modelling Signposts New Directions in Porous Materials	
14:40 - 15:15	Sanliang Ling	Computational Studies of Metal-Organic Frameworks: Defects, Electronic Properties and Gas Adsorptions	
15:15 - 15:25	Closing Remarks		Jihong Yu
15:25	Coffee and Free Discussion with Faculties and Students		
18:00	Dinner		

New Metal-Organic Frameworks with Ultrahigh Porosity, Switchability and Functionality

Stefan Kaskel

Department of Chemistry, Technische Universität Dresden, Germany

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Metal-Organic Frameworks have received considerable attention in recent years because they provide extremely high specific surface areas exceeding traditional adsorbents such as zeolites and activated carbon. Especially mesoporous MOFs provide a wide range of options for further functionalization and even chiral groups can be incorporated rendering such materials as potential candidates for gas storage, enantioselective separation, catalysis and sensing. In recent years, exciting developments have pushed the limits of materials performance to ever higher surface areas up to 7000 m²/g and pore sizes unattained so far in traditional porous solids such as zeolites or activated carbons. DUT-49 (DUT = Dresden University of Technology) is a mesoporous flexible MOF composed of connected Metal-Organic Polyhedra (MOPs) and has the highest gravimetric methane uptake among all known MOFs (308 mg/g at 298 K). Chiral mesoporous MOFs were synthesized. A unique phenomenon observed only in a limited number of materials is *porosity switching in the crystalline solid state*. Such flexibility was predicted 1998 for MOFs by Kitagawa and later termed “3rd Generation MOFs”. Despite these early discoveries, among the about 20.000 coordination network structures only few compounds reveal substantial switching or breathing transitions or related stimuli responsive properties. In order to characterize the adsorbate-induced structural transformations, it is necessary to capture local and global structural information under variable, externally applied gas pressures *in situ*. The development of such *in situ* characterization techniques is essential (EXAFS, XRD, NMR, EPR) to monitor switching during adsorption/desorption cycling. A new phenomenon recently encountered by *in situ* methods is *Negative Gas Adsorption (NGA)*, for the first time detected in a switchable (breathing) mesoporous MOF named DUT-49. While the mechanism could be explained by the aid of theoretical DFT and GCMC calculations, yet the underlying principles to predict such a phenomenon in other MOFs are unknown. For technological applications this effect could have wide implications as it represents a new counterintuitive phenomenon that could be used for pressure amplification.

References:

1. K. Gedrich, I. Senkovska, N. Klein et al, *Angew. Chem. Int. Ed.* **2010**, 49, 8489.
2. K. Gedrich, M. Heitbaum, A. Notzon et al, *Chem. Eur. J.* **2011**, 17, 2099.
3. M. Padmanaban, P. Muller, Ch. Liede et al, *Chem. Commun.* **2011**, 47, 12089.
4. H. Herbert, B. Assfour, F. Epperlein et al, *J. Am. Chem. Soc.* **2011**, 133, 8681.
5. V. Bon, S. Kaskel et al, *Chem Commun.* **2012**, 448, 8407.
6. U. Stoeck, S. Kaskel et al, *Chem. Commun.* **2012**, 48, 1084.
7. V. Bon, I. Senkovska, S. Kaskel et al, *CrystEngComm* **2013**, 15, 9572.
8. G. Nickerl, A. Notzon, M. Heitbaum et al, *Crystal Growth & Design* **2013**, 13, 198.
9. G. Nickerl, U. Stoeck, U. Burkhardt et al, *J. Mater. Chem. A* **2014**, 2, 144.
10. R. Gruenker, V. Bon, P. Mueller et al, *Chem. Commun.* **2014**, 50, 3450.
11. A. Schneemann, V. Bon, I. Schwedler et al, *Chem. Soc. Rev.* **2014**, 43, 6062.
12. V. Bon, I. Senkovska, D. Wallacher et al, *Microporous Mesoporous Mater.* **2014**, 188, 190.
13. U. Stoeck, I. Senkovska, V. Bon et al, *Chem. Commun.* **2015**, 51, 1046.
14. D. Wisser, F. M. Wisser, S. Raschke et al, *Angew. Chem. Int. Ed.* **2015**, 54, 12588.
15. P. Müller, F. M. Wisser, V. Bon et al, *Chem. Mater.* **2015**, 27, 2460.
16. S. Krause, V. Bon, I. Senkovska et al, *Nature*, **2016**, 532, 348.

Kaskel, Stefan



• EDUCATION

- 1997 PhD in Inorganic Chemistry
Chemistry Department, Eberhard Karls University Tübingen/ Germany
- 1995 Diploma in Chemistry
Chemistry Department, Eberhard Karls University Tübingen/ Germany

• CURRENT POSITION(S)

- 2004 – Full Professor, Inorganic Chemistry
Department of Chemistry / Technische Universität Dresden / Germany
- 2008 – Head of Business Unit *Chemical Surface and Reaction Technology*, Fraunhofer Institute
Materials and Beam Technology, Dresden, Germany (part-time)

• PREVIOUS POSITIONS

- 2000 – 2004 Group leader, Department of Heterogeneous Catalysis (F. Schüth), Max-Planck Institute for
Coal Research, Mülheim a.d. Ruhr; Habilitand at Ruhr-Universität Bochum (R. A. Fischer)
- 1998 – 2000 Post-Doc, Department of Solid State Chemistry (J. D. Corbett), Ames Laboratory and Iowa
State University, USA

• FELLOWSHIPS AND AWARDS

- 2017 ERC Advanced Grant
- 2016 Highly cited researcher by Thomson Reuters
- 2015 Research Award, Japan Society for the Promotion of Science (JSPS)
- 2003 Young Scientist Award Nanotechnology, German Federal Ministry of Education and Research,
Germany
- 2000 – 2002 Reimar Lüst-Fellowship of the Max Planck Society, Germany
- 1998 – 2000 Feodor Lynen Research Fellow of the Alexander von Humboldt-Foundation, Ames
Laboratory and Iowa State University, USA

• PUBLICATIONS (392 publications with 13385 citations, h-index 62)

1. S. Krause, V. Bon, S. Kaskel et al, *Nature* **2016**, 532, 348. (7 citations)
2. D. Wisser, F. M. Wisser, S. Kaskel et al, *Angew. Chem. Int. Ed.* **2015**, 54, 12588. (13 citations)
3. J. Brueckner, S. Thieme, S. Kaskel et al, *Adv. Funct. Mater.* **2014**, 24, 1284. (40 citations)
4. K. Sakaushi, E. Hosono, S. Kaskel et al, *Nat. Commun.* **2013**, 4, 1485. (65 citations)
5. J. C. Wang, S. Kaskel, *J. Mater. Chem.* **2012**, 22, 23710. (296 citations)
6. K. Gedrich, I. Senkovska, S. Kaskel et al, *Angew. Chem. Int. Ed.* **2010**, 49, 8489. (77 citations)
7. P. Küsgens, M. Rose, S. Kaskel et al, *Microporous Mesoporous Mater.* **2009**, 120, 325. (306 citations)
8. N. Klein, I. Senkovska, S. Kaskel et al, *Angew. Chem., Int. Ed.* **2009**, 48, 9954. (150 citations)
9. A. Henschel, K. Gedrich, R. Kraehnert and S. Kaskel, *Chem. Commun.* **2008**, 4192. (245 citations)
10. H. Althues, J. Henle, S. Kaskel, *Chem. Soc. Rev.* **2007**, 36, 1454. (238 citations)

Mixed Metal Oxides for Gas-phase Reactions: Bio-alcohols and Polyols Transformation to Added Value Chemicals

Fabrizio Cavani

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Multicomponent mixed metal oxides are used as catalysts for several chemical processes. Examples include multimetal molybdates for allylic oxidation and ammoxidation, phosphomolybdoxovanadates for aldehydes oxidation, rutile-type mixed oxides and vanadyl pyrophosphate for alkanes oxidation and ammoxidation. In recent years, the attention of researchers has been focused on multicomponent systems showing bifunctional properties, i.e., catalysts possessing both acid (or basic) and redox properties. These peculiar chemical-physical features allow to carry out complex, multi-step transformations using a single catalyst.

Here we report about two different classes of mixed metal oxides:

- (a) Catalysts based on MgO, modified by incorporation of ions such as Si^{4+} , Fe^{3+} , Ga^{3+} and Cr^{3+} , showing both basic and dehydrogenating or Lewis-acid properties. These catalysts have been used for several reactions in the gas-phase, i.e., the methylation of phenolics, the reduction of aldehydes and ketones with alcohols via H-transfer, and the transformation of ethanol to either 1-butanol (Guerbet reaction) or butadiene (Lebedev reaction). We investigated in detail the mechanism of the reactions and the role of each catalyst component by combining reactivity experiments, in-situ spectroscopy and DFT calculations.¹
- (b) Catalysts based on WO_3 with hexagonal structure (tungsten bronzes, HTBs), with in-framework or extra-framework V ions and/or Nb ions. These systems show both acidic and redox properties; they were used for the oxidehydration of glycerol to acrylic acid. Combining results of reactivity experiments with those acquired from an in-situ FTIR spectroscopy study it was possible to draw conclusions on the role played by the various physicochemical features of the different components in terms of reactants adsorption and surface reactions.²

References:

1. (a) J. Velasquez Ochoa, C. Bandinelli, O. Vozniuk, A. Chierigato, A. Malmusi, C. Recchia, F. Cavani, *Green Chem.* **2016**, 18, 1653; (b) L. Grazia, A. Lolli, F. Folco, Y. Zhang, S. Albonetti, F. Cavani, *Catal. Sci. Technol.* **2016**, 6, 4418; (c) A. Chierigato, J. Velasquez Ochoa, C. Bandinelli, G. Fornasari, F. Cavani, M. Mella, *ChemSusChem* **2015**, 8, 377.
2. (a) A. Chierigato, C. Bandinelli, P. Concepcion, M. Dolores Soriano, F. Puzzo, F. Basile, F. Cavani, J. M. Lopez Nieto, *ChemSusChem* **2017**, 10, 234; (b) A. Chierigato, M. Dolores Soriano, E. Garcia-Gonzalez, G. Puglia, F. Basile, P. Concepcion, C. Bandinelli, J. M. Lopez Nieto, F. Cavani, *ChemSusChem* **2015**, 8, 398.

Fabrizio Cavani

- **EDUCATION**

Fabrizio Cavani received the PhD in Industrial Chemistry from the University of Bologna in 1986.

From 1986 until 1990 he worked in the Catalysis Center of EniChem, in Milan.



- **CURRENT POSITION(S)**

Since 1990 he is working at the Department of Industrial Chemistry, University of Bologna, where currently is Full Professor of Industrial Chemistry.

- **RESEARCH INTERESTS**

His main field of interest is catalysis for the transformation of renewable raw materials into fuels and chemicals.

On the Formation of Zeolites through *in situ* and *ex situ* X-ray Techniques

Gopinathan Sankar

Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK

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Within the family of heterogeneous catalytic systems, porous materials are of a great interest due to their ability to interact with ions and molecules not only on their surface but throughout their bulk. To produce these microporous materials it is inevitable to use hydrothermal methods. Although, preparation of both the open and dense framework solids require considerable amount of effort to optimise the conditions, recent developments in the *in situ* methods, in particular X-ray scattering methods, offer considerable advantage in determining accurately the conditions required to produce phase pure materials and furthermore these methods allow the understanding of the mechanism of formation of these solids under operating conditions. Recent advances in these techniques allows us to collect high-quality time-resolved data to obtain the kinetics of crystallisation of solids prepared from amorphous gel mixtures. Here we will discuss the processes that take place during the crystallisation of open framework structures under hydrothermal conditions by taking examples in the synthesis of microporous aluminosilicate materials. In addition, how the understanding of the structures of precursor species enabled us to design synthesis of zeolites through zeolite-zeolite transformation will be discussed.

Gopinathan Sankar

- **EDUCATION**

Educated in India - PhD (Indian Institute of Science, Bangalore). In 1990 joined Professor John Thomas group at the Royal Institution of GB, London where he held several positions, which includes PDRA, Assistant Director of DFRL, Leverhulme Senior Research Fellow and Professor of Materials Chemistry. In 2007 he moved to Department of Chemistry, University College London as Professor of Solid-State Chemistry where he continues his research in the following areas.



- **RESEARCH INTERESTS**

My Research Group have been involved in the use of advanced characterization methods to investigate (a) formation nanoporous materials, dense and nano metal cluster systems, (b) structure of these catalytic materials at various length scales and (c) designing catalytic reaction based on the structure determined from various characterisation techniques. Majority of the characterisation is carried out using *in situ* and *ex situ* methods using Synchrotron Radiation techniques combining with optical spectroscopies.

- **FELLOWSHIPS AND AWARDS**

Sankar was awarded a Royal Society Industry Fellowship to carry out collaborative research with Johnson Matthey plc. and he continue to closely work with scientists at Johnson Matthey. He has supervised more than 40 PhD and Post-Doctoral researchers. He has over 250 publications and his current H-index is 51.

X-ray Spectroscopy of Some Metal Nanostructures

Peng Zhang

Department of Chemistry and School of Biomedical Engineering, Dalhousie University, Halifax, NS, B3H4R2, Canada

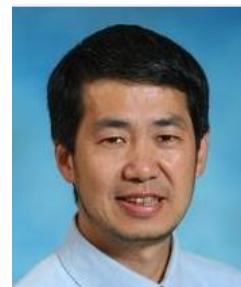
E-mail: peng.zhang@dal.ca

Synchrotron X-ray absorption spectroscopy and associated techniques are useful tools for the element-specific analysis of structure and properties of materials. In this talk, the application of these techniques in the study of some noble metal nanostructures will be presented. Materials of interest include nanocrystals, nano-alloys, nanoclusters and single-atom catalysts. It will be demonstrated that the X-ray spectroscopy methods can sensitively probe the structural and property changes induced by the effects such as metal composition, protecting ligands, nanocrystal shape and alloy bonding. The structural information revealed by the X-ray techniques may also be useful in the catalytic and biomedical applications of these materials.

Peng Zhang

PERSONAL INFORMATION

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RESEARCH INTERESTS

Synchrotron X-ray Spectroscopy, Physical Chemistry of Nanomaterials and Biomaterials, Energy-related and Biomedical Applications of Nanomaterials

WORKING AND EDUCATION EXPERIENCE

2015- Professor, Department of Chemistry, Dalhousie University, Canada
2013- Cross-appointed Professor, School of Biomedical Engineering, Dalhousie University
2011-2015 Associate Professor, Dept. of Chemistry, Dalhousie University, Canada
2005-2011 Assistant Professor, Dept. of Chemistry, Dalhousie University, Canada
2003-2005 NSERC PDF, Department of Chemistry, McGill University, Canada
1999-2003 Ph.D., Department of Chemistry, Western University, Canada
1993-1997 M.Sc. Department of Chemistry, Jilin University, China
1989-1993 B.Sc. Department of Chemistry, Jilin University, China

SELECTED AWARDS AND HONOURS:

2017 Japan Society for Molecular Science Distinguished Lecture Award
2016-2019 Mt. Changbai Professor, Jilin Normal University (China)
2014-2017 Tang Aoqing Professor, Jilin University (China)
2014-2016 iCHEM Professor, Xiamen University (China)
2014-2015 Faculty of Science Killam Prize, Dalhousie University
2012-2014 Harry Shirreff Prize for Excellence in Research in Chemistry, Dalhousie University
2012 Lectureship, Taiwan National Science Council
2012-2014 PCOSS Fellowship, Xiamen University
2008 Dalhousie Innovation Award for "Concepts in Chemistry" textbook (as a coauthor)
2006 Canada Foundation for Innovation (CFI) Leaders Opportunity Fund award
2003-2005 NSERC Postdoctoral Fellowship
2001-2003 Ontario Graduate Scholarship
2001-2002 R.R. Lumsden Fellowship, Western University
2000-2001 R.R. Lumsden Award, Western University
2001 Poster Award, 84th Canadian Society for Chemistry Conference, Montreal

Hierarchical Zeolite Structures and Their Application on Methanol to Propylene and Aromatics

Fei Wei

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Here we started from the overall product distribution of olefins, and noticed the Anderson-Schulz-Flory distribution is validated in MTO process. The single acid site is the main active sites for forming carbon pool to catalysis MTO reaction, while close acid sites were the main active sites for hydrogen transfer and oligomerizations which increase the selectivity of by-product propane and coke; as a result the life time and the selectivity of olefins decrease. The close acid sites accelerate the generation of anthracene, phenanthrene and naphthalene and other polycyclic aromatic products in the cage of SAPO-34, which leads the product diffusion channel blockage and rapid deactivation of SAPO-34. Hierarchical cross-like SAPO-34 catalysts with different pore size distributions were obtained by hydrothermal synthesis with polyethylene glycol (PEG) as the mesopore-generating agent. The cross-like SAPO-34 catalysts had enriched multi-porosity with their mesopores size ranging from 10 to 50 nm. Both the mesoporous structures and morphologies of the hierarchical SAPO-34 can be further tuned by the amount of PEG. The as-obtained SAPO-34 showed dramatic catalytic performance in methanol conversion into olefins. A maximum selectivity of olefins of 96% was achieved, which was attributed to the rapid transport of the reactants and products in zeolitic micropores through mesopores. A methylbenzenes intermediates equilibrium analysis (MIEA) shows the olefins product distribution is controlled by a 0.42 eV energy barrier of cracking. A clear essence of hydrocarbon pool is illustrated. We reviewed some other chain growth process including Fischer-Tropsch Synthesis, polymerization, methanol-to-gasoline, and a general energy barrier of chain growth exists. Such study will not only bring new challenges into MTO studies but also open new methodologies to other chain growth process.

We have built a discrete Ising model for deactivation considering the cage connectivity, inspired by the game of Go. An analytical solution for a simplistic 1D model is found, and it shows good consistency with the experimental results over ZSM-12. Some anomalous pseudo-phase transition phenomena in the deactivation process and in the acid density are presented by modeling the deactivation of SAPO-34. This model may bring new methodologies to research on the zeolite deactivation mechanism.

References:

1. T. Wang, X. Tang, X. Huang, W. Qian, Y. Cui, X. Hui, W. Yang, F. Wei, *Catal. Today* **2014**, 233, 8.
2. Y. Cui, Q. Zhang, J. He, Y. Wang, F. Wei, *Particuology* **2013**, 11, 468.
3. K. Shen, N. Wang, W. Qian, Y. Cui, F. Wei, *Catal. Sci. Technol.* **2014**, 4, 3840.
4. Y. Li, M. Zhang, D. Wang, F. Wei, Y. Wang, *J. Catal.* **2014**, 311, 281.

Fei Wei

- **CURRENT POSITION(S)**

Fei Wei Cheungkong scholar Professor, Director of Beijing key lab of green chemical reaction engineering and technology

- **EDUCATION**

Fei Wei obtained his PhD in chemical engineering from China University of Petroleum in 1990. After a postdoctoral fellowship at Tsinghua University (China), he was appointed an associate professor in 1992 and professor of chemical engineering of Tsinghua University (China) in 1996.

- **RESEARCH INTERESTS**

His scientific interests are technological applications of chemical reaction engineering, multiphase flow, carbon nano materials, and sustainable energy.

- **TRACK-RECORD**

He has designed and successfully running over 30 industrial fluidized bed reactors, and authored three books and over 500 refereed publications with more than 24000 citations with H index 77



Designer Zeolites: Better, Smaller, More Accessible and... Cheap

Jean-Pierre GILSON

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Caen, France*

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Zeolites are still fast growing materials, 55 years after their revolutionary introduction in oil refining and petrochemistry. I will concentrate on the “Zeolite Crystal Engineering”, i.e. the fine tuning of the properties of known zeolites to meet exacting requirements of modern processes. I will describe fundamental work on nucleation that opened the door to the preparation of inexpensive, template-free, nanosized FAU (X & Y variety) with outstanding catalytic performances. I will describe other fundamental studies on the controlled removal of defects in existing zeolites that lead also to vastly superior catalysts and probably adsorbents. Finally, I will discuss the so-called embryonic zeolites, probably the last frontier between organized and disorganized materials and touch a bit the understudied but critical topic of the chemical interactions between a zeolite and its binder during a shaping process (e.g. extrusion).

Jean-Pierre GILSON

- **CURRENT POSITION(S)**

Jean-Pierre GILSON, currently Distinguished Professor at ENSICAEN (France) is also Joint-Professor at DICP, Dalian (China) and invited Professor at Jilin University (China). He teaches mainly physical chemistry (thermodynamics, surface chemistry), catalysis, oil refining processes and petrochemistry of olefins and aromatics.



- **EDUCATION**

He received his PhD at the University of Namur (Belgium) under the guidance of Prof. Eric Derouane with a grant from Haldor Topsøe. Immediately thereafter he started an industrial career in the US (UOP, Grace) and Europe (Shell in The Netherlands and France). After 15 years in industry he moved to Caen where he headed the Laboratory of Catalysis & Spectrochemistry for 3 terms of 4 years spaced by an attachment to Total Refining (4 years) as Director of their academic cooperations. In 2009, he established a new group in Caen with Dr. Svetlana Mintova and Dr. Valentin Valtchev, dedicated to the so-called Zeolite Crystal Engineering, where the properties of zeolites (particle size & shape, hierarchization, composition...) and their interaction with a binder during shaping processes are fine-tuned to meet the very stringent requirements of zeolite catalysts and adsorbents in the fields of oil refining, petrochemicals, gas and biomass valorization.

- **TRACK-RECORD**

He is author or co-author of about 80 papers, 1 book, 37 patents and 3 commercially successful catalytic processes (light paraffins isomerization, aromatics upgrading, FT waxes upgrading to fuels and lubes). He collaborates and consults extensively with major oil, catalysts and process licensing companies.

Natural Law of Hierarchizing Holds Key to Enhancing Photocatalysis, Amplifying Gas Sensing and Extending Battery Life

Bao-Lian Su

¹ *State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Loushi Road 122, Wuhan 430070, China.*

² *Laboratory of Inorganic Materials Chemistry, University of Namur, 61 rue de Bruxelles, B-5000, Namur, Belgium.
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Both plants and animals possess analogous tissues containing hierarchical networks of pores, with pore size ratios that have evolved to maximize mass transport and rates of reactions. The underlying physical principles of this optimized hierarchical design are embodied in Murray's law. However, we are yet to realize the benefit of mimicking nature's Murray networks in synthetic materials due to the challenges in fabricating vascularized structures. Here we emulate optimum natural systems following Murray's law using a bottom-up approach. Such bio-inspired materials, whose pore sizes decrease across multiple scales and finally terminate in size-invariant units like plant stems, leaf veins and vascular and respiratory systems provide hierarchical branching and precise diameter-ratios for connecting multi-scale pores from macro to micro levels. Our Murray material mimics enable highly enhanced mass exchange and transfer in liquid-solid, gas-solid and electrochemical reactions and exhibit enhanced performance in photocatalysis, gas sensing and as Li-ion battery electrodes.

Bao-Lian Su

- **EDUCATION**

Member of the Royal Academy of Belgium, Fellow of the Royal Society of Chemistry and Clare Hall Life Member, University of Cambridge, Prof. Su held “Belgian Francqui Chaire”. He earned his Doctorate from the University Pierre and Marie Curie, Paris, France in 1992. After a post-doctoral stay at the University of Namur, Belgium and then as Project leader at Catalytica Inc., California, USA, he joined the faculty of the University of Namur in Sept. 1995 and created the Laboratory of Inorganic Materials Chemistry. In 2002, he was promoted to Professor and in 2004 again promoted to Full Professor. He served as the Council member of the International Zeolite Association since 2007 and the Council member of the International Mesoporous Materials Association since 2008. He is the President of the Graduate School of Science and Engineering of Materials, Interfaces and Nanostructures (MAIN), Belgium.



- **FELLOWSHIPS AND AWARDS**

Prof. Su has received a series of major awards such as the “First Class Invention Award of Sinopec” in 1992, the “China Patent Excellence Award” in 1994, the “Adolphe Wetrems Prize” of the Royal Academy of Belgium in 2007 and the “Distinguished Award for Novel Materials and their Synthesis” by the International Union of Pure and Applied Chemistry (IUPAC) in 2011.

- **TRACK-RECORD**

He has published 420 SCI papers (with more than 12500 citations and an H index of 60) and book chapters and is the editor of one Wiley-VCH book and four special issues of high profile journals. He also holds 5 international and 20 national patents. He was invited to give more than 80 Plenary, Keynote, Featured and Invited lectures at international high impact congresses during last five years. He is coordinator and principle leader of more than 70 research and collaborative projects within the context of Europe, NATO, Belgian Government, National Science Foundation and Belgian Wallonia Region.

- **RESEARCH INTERESTS**

Prof. Su’s current research fields include the synthesis, the property study and the molecular engineering of nanostructures and highly organized and hierarchically porous materials, bio-integrated living and bio-inspired materials and biomaterials for catalysis, photocatalysis, artificial photosynthesis, nanotechnology, biotechnology, information technology, energy storage and conversion and cell therapy.

Zeolitic Materials: Prediction, Synthesis and Application

Jihong Yu

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun
130012, P. R. China.
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Zeolitic materials with nanoporous architectures are involved in various processes of current interest, such as energy saving catalytic processes, environmentally benign sorbents, storage materials for waste and energy, etc. In recent years, we have been devoting our efforts to the computational prediction, rational synthesis and application of zeolitic materials. In this lecture, I will present in-silico prediction of zeolitic materials with desirable porous architectures and properties. Toward the rational synthesis, we have developed three main strategies on the basis of pre-designed organic structure-directing agent, the heteroatom substitution and computational data mining. By utilization of these synthetic strategies, novel zeolitic materials with desired porous structures and excellent properties have been successfully synthesized. Furthermore, we have discovered that the zeolite synthesis mechanism can be promoted through free radicals, which shed a new light on zeolite crystallization. Taking advantage of their confined nanopores and unique properties, we have also explored some new applications of zeolitic materials in H₂ production, liquid separation and light emitting that are beyond their traditional applications.

References:

1. Y. Li, J. H. Yu, *Chem. Rev.* **2014**, 114, 7268.
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Jihong Yu

Prof. Jihong Yu is from the State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, and is the director of International Center of Future Science, Jilin University. She received her PhD degree under Prof. Ruren Xu from Jilin University in 1995, and worked as a postdoctoral fellow first at the Hong Kong University of Science and Technology with Prof. Ian D. Williams and then at Tohoku University in Japan with Prof. Osamu Terasaki during 1996-1998. She has been a full Professor in the Chemistry Department, Jilin University since 1999. She was awarded the Cheung Kong Professorship in 2007 and elected as the member of the Chinese Academy of Sciences in 2015 and the Fellow of TWAS in 2016. Her main research interest is in the designed synthesis and application of zeolitic nanoporous materials. She has co-authored over 300 research papers; obtained over 20 authorized Chinese Invention Patents; edited 7 books. She was the winners of the National Prize for Natural Science, Distinguished Women in Chemistry/Chemical Engineering Award, Bau Family Award, etc. Currently, she serves as the Associate Editor of *Chemical Science*, and Editorial Board Members of *Materials Horizons*, *Materials Chemistry Frontiers*, *Solid State Sciences*, *National Science Review*, etc.. She is a Council Member of International Zeolite Association and Chinese Chemical Society, and Fellow of the Royal Society of Chemistry.



Porous Ionic Liquids: Challenges and Opportunities

Sheng Dai

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Functional materials using or in the presence of ionic liquids represents a burgeoning direction in materials chemistry. Ionic liquids are a family of non-conventional molten salts that can act as both functional materials and solvents. They offer many advantages, such as negligible vapor pressures, wide liquidus ranges, good thermal stability, tunable solubility of both organic and inorganic molecules, and ion conductivity. The unique solvation environment of these ionic liquids provides new reaction and separation media for controlling many energy-related processes. We have recently developed a class of ionic liquids with intrinsic porosities based on nanoscopic building blocks.¹ Challenges and opportunities in synthesizing and using these porous ionic liquids in energy-related applications will be discussed.

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Sheng Dai

- **EDUCATION**

Dr. Sheng Dai obtained his B.S. degree (1984) and M.S. degree (1986) in Chemistry at Zhejiang University, Hangzhou, China and his Ph.D. (1990) in Chemistry at the University of Tennessee, Knoxville.

- **CURRENT POSITION(S)**

He is currently a corporate fellow and group leader at the Oak Ridge National Laboratory (ORNL) and a Professor of Chemistry at the University of Tennessee, Knoxville (UTK).

- **RESEARCH INTERESTS**

His current research interests include ionic liquids, porous carbon and oxide materials, advanced materials and their applications for separation sciences and energy storage as well as catalysis by nanomaterials.

- **TRACK-RECORD**

He has published more than 600 peer-review papers and received 28 patents. His papers have been cited more than over 27,000 with an h-index of 82 according to Web of Science, Thomson Reuters. He holds over 28 U.S. patents in the areas of ionic liquids, molten salts, porous materials, and their uses in energy-related applications.

- **AWARDS**

His research has led to Battelle S&T Challenges Award (2002), six R&D100 Awards (2010, 2011, two in 2014, 2015, 2016), and a Battelle Distinguished Inventor Award.



Targeted Synthesis of Porous Aromatic Frameworks: From Structure Design to Advanced Application

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Porous organic frameworks (POFs) have been developed greatly as new family of porous materials owing to their high stability, high surface area, tuning pore size, and adjustable skeletons, etc. Nowadays, POFs have been attracted great attentions in the field of gas storage and separation, sensors, and catalysis^{1,2}. To obtain POFs with pre-determined structures and tunable property, it is important to select the suitable building blocks and effective reaction. With the aid of computational design, we have successfully synthesized a series of porous aromatic framework (PAF) materials. Because of the flexibility of building blocks, the functional groups are decorated into PAF skeletons, and then their corresponding post-modified products are obtained. We focus our research on gas (CH₄, CO₂, H₂, C₂H₄, C₂H₆, C₃H₆, I₂, etc.) adsorption and separation.³⁻⁷

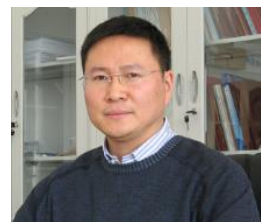
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2. G. S. Zhu, H. Ren, Springer, **2015**, ISBN, 978-3-662-45455-8.
3. H. P. Ma, H. Ren, X. Q. Zou, F. X. Sun, Z. J. Yan, K. Cai, D. Y. Wang, G. S. Zhu, *J. Mater. Chem. A* **2013**, 1, 752.
4. H. P. Ma, H. Ren, X. Q. Zou, F. X. Sun, G. S. Zhu, *Polym. Chem.* **2014**, 5, 144.
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7. Z. J. Yan, Y. Yuan, Y. Y. Tian, D. M. Zhang, G. S. Zhu, *Angew. Chem. Int. Ed.* **2015**, 127, 12924.

Guangshan Zhu

• EXPERIENCE

- Since 2015.8 Professor, Chief Director, Key Laboratory of Polyoxometalate Science of the Ministry of Education, Faculty of Chemistry, Northeast Normal University
- 2001.10–2015.07 Professor, State Key Lab of Inorganic Synthesis and Preparative Chemistry, Jilin University
- 2000.09–2001.09 Associate Professor, State Key Lab of Inorganic Synthesis and Preparative Chemistry, Jilin University
- 1999.09–2000.09 Post-doc Research Associate, Tohoku University, Japan
- 1998.07–2000.08 Assistant Professor, State Key Lab of Inorganic Synthesis and Preparative Chemistry, Jilin University
- 1993.09–1998.06 Ph.D., Inorganic Chemistry, Department of Chemistry, Jilin University
- 1989.09–1993.06 B.Sc., Chemistry, Department of Chemistry, Jilin University



• CURRENT RESEARCH ACTIVITIES

- Targeted synthesis of Porous Aromatic Framework (PAF) materials towards adsorption and separation.
- Synthesis of high quality zeolite large single crystals, oriented membranes, and their applications in micro-devices and gas separation.
- Synthesis of Metal-Organic Framework crystals, membranes, and their utilization in gas adsorption and separation.

• HONORS AND AWARDS

- “Country’s 10,000 Talents Plan”, Ministry of Science and Technology of China, 2012
- Special government allowances of the State Council, 2010
- “Yangzi Scholar”, Ministry of Education of China, 2008
- Second Grade Award for National Natural Science of China, Bureau of National Award of China, 2008
- “Outstanding Young Scientist”, National Natural Science Foundation of China, 2006
- First Grade Award for Progress in Science & Technology of Jilin Province, Bureau of Science & Technology, Jilin Province, twice, 2006 and 2012
- The Elite of New Century in China, Ministry of Education of China, 2005

• PUBLICATIONS

Prof. Guangshan Zhu has published over 300 papers and several reviews. 29 papers have been cited over 100 times and total citation is over 9000 times. His H-index is 51. He wrote a book about “Porous Organic Frameworks: Design, Synthesis and Their Advanced Applications” published by Springer and it has been downloaded for 2952 times. Some of the publications are listed below:

1. G. S. Zhu, H. Ren, *Springer*, **2015**, ISBN: 978-3-662-45456-5.
2. Z. Yan, Y. Yuan, Y. Tian, D Zhang, G. S. Zhu, *Angew. Chem. Int. Ed.*, **2015**, 54, 12733.
3. Y. Yuan, F. Sun, G. S. Zhu, *Nat. Commun.*, **2014**, 5, 4260.
4. X. Gao, X. Zou, H. Ma, S. Meng, G. S. Zhu, *Adv. Mater.*, **2014**, 26, 3644.
5. Y. Yuan, F. Sun, F. Zhang, H. Ren, M. Guo, K. Cai, X. Jing, X. Gao, G. S. Zhu, *Adv. Mater.*, **2013**, 25, 6619.
6. X. Zou, H. Ren, G. S. Zhu, *Chem. Commun.*, **2013**, 49, 3925.

Supramolecular Self-Assembly of Inorganic Clusters for Soft Frameworks

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Nanoporous structures within two and three dimension have attracted huge interest over recent years because of their potentials as advanced materials in fundamental research and industrial applications. Among those known architectures, porous coordination supramolecular polymers and metal organic frameworks (MOFs) exhibit quite uniform pores from less than one to several nanometers. The main drawbacks for the inorganic porous structures, however, are the difficulties to mold thin film in large scale conveniently because the connections between components are normally coordination interaction and/or covalent bond. To overcome the severe challenge, flexible binding such as electrostatic force should be considered. But the issues are its non-saturation and non-preferential binding angles, leading to a key problem in precisely controlling porous structure. Fortunately, polyoxometalates (POMs) as a family of nanosized polyanionic clusters have demonstrated good merits in fabrication of hybrid self-assemblies due to their diverse composition and topology. Importantly, multi-negative charges around the surface of POMs are delocalized, making the clusters ideal candidates as the nodes for soft framework architectures through flexible intermolecular interaction.¹ In this presentation, we succeed in creating flexible single molecular layer ionic POM cluster organic frameworks with unprecedented uniform orthogonal pores in large area. The bolaform cations with azobenzene and flexible spacer are used as the stick bridging POMs via charge compensation.² The soft film bearing well-defined framework structure can be prepared feasibly and the pore size can be modulated for precise size-selective separation of quantum dots. Detailed characterizations and discussions support our conclusion. The present idea is illuminative in supramolecular polymers and porous materials because the obtained single layer ionic cluster-organic framework also demonstrates potentials in absorption-separation, catalysis, and bio-filtration.

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1. L. Yue, H. Ai, Y. Yang, W. Lu, L. X. Wu, *Chem. Commun.* **2013**, 49, 9770.
2. L. Yue, S. Wang, D. Zhou, H. Zhang, B. Li, L. X. Wu, *Nat. Commun.* **2016**, 7, 10742.

Lixin Wu

• EDUCATION and RESEARCH EXPERIENCES

Ph.D. 1993, Institute of Theoretical Chemistry, Jilin University, China.

M.Sc. 1989, Institute of Theoretical Chemistry, Jilin University, China.

B. Sc. 1982, Department of Chemistry, Heilongjiang University, China.

1993-present, Lecturer (1993), Associate Professor (1997), Professor (2000), Jilin University, China

2002-2003, DFG Visiting Professor, Institute of Physics, University of Muenster, Germany.

1997-1998, Research associate, Department of Chemistry, University of Hong Kong, China.

1996-1996, JSPS postdoctoral fellow, Research Inst. for Elec. Sci., Hokkaido University, Japan.

1995-1997, Postdoctoral fellow, Changchun Institute of Physics, CAS, China.



• CURRENT RESEARCH INTEREST

- Assembled structure and functionalization of amphiphilic inorganic/organic supramolecular reversed micelles.
- Self-assembly and nanostructure of block amphiphilic supramolecular polymers.
- Surface patterning and stimulus-responsibility of small molecule/bio-macromolecule composited systems.
- Supramolecular crystals engineer based on inorganic/organic complexes.

• SELECTIVE PUBLICATIONS

1. Y. Liang, S. Wang, D. Zhou, H. Zhang, B. Li, L. X. Wu, *Nat. Commun.* **2016**, 7, 10742.
2. L Shi, B. Li, L. X. Wu, *Chem. Commun.* **2015**, 51, 172.
3. S. Wang, H. Li, D. Li, T. Xu, S. Zhang, X. Dou, L. X. Wu *ACS Macro Lett.* **2015**, 4, 974.
4. B. Zhang, L. Yue, Y. Wang, Y. Yang, L. X. Wu, *Chem. Commun.* **2014**, 50, 10823.
5. L. Yue, H. Ai, Y. Yang, W. Lu, L. X. Wu, *Chem. Commun.* **2013**, 49, 9770.
6. Y. Yang, B. Wang, Y. Wang, L. Yue, W. Li, L. X. Wu, *J. Am. Chem. Soc.* **2013**, 135, 14500.

Nanoparticle Promoters in Organic and Inorganic Reactions

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Metal nanoparticles have long been used as model systems for studying catalytic reactions. The emergence of shape controlled nanocrystals with well-defined morphologies, from simple geometries to complex shapes such as high index surface facets, has led to intensive studies of shape-dependent catalytic activity. Controllable nanoparticle synthesis also enables reaction pathways to be manipulated for a range of applications. This talk will highlight some of the research going on within my group on the use of nanoparticle catalysts in cross coupling chemical reactions and semiconductor nanowire synthesis.

Justin D. Holmes

- **CURRENT POSITION(S) AND RESEARCH INTEREST**

Justin D. Holmes is Professor of Nanochemistry in the Department of Chemistry at University College Cork (UCC). He leads the Materials Chemistry & Analysis Group (MCAG), conducting research on the development of chemical methods for synthesising and assembling nanostructured materials for electronic, sensing, energy and catalytic applications. Prof. Holmes is also Group Leader and Principal Investigator at the Tyndall National Institute in Cork, where his research focuses on investigating nanoscale materials for electronic applications, particularly their in-depth characterisation by advanced electron microscopy techniques. He is a Principal Investigator within the Centre for Adaptive Nanostructures and Nanodevices (CRANN), and the Advanced Materials and Bioengineering Research Centre (AMBER) based at Trinity College Dublin. Within these Centres Prof. Holmes is working on a platform project to develop electronic devices from nanowire networks. Prof. Holmes has also been successful at commercialising research from his laboratory and is co-founder and currently chair of the Scientific Advisory Board for the UCC spin-out company Glantreo Ltd. Prof. Holmes was elected as a member of the Royal Irish Academy in 2016, which is considered to be one of Ireland's highest academic honours.



Porous Materials and Selectivity Control in Syngas Conversion

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Light olefins containing two to four carbon atoms ($C_2=C_4$) are key chemical feedstocks for manufacture of plastics, synthetic fibers and drugs. They can be produced from various sources depending on different regions, for example, from the naphtha fraction of crude oil in Asia and Europe but natural gas condensates (principally ethane and propane) in the Mideast and US. Alternatively, they can be produced from other carbon resources such as coal and biomass via synthesis gas (syngas, a mixture of CO and H_2), by modifying the Fischer-Tropsch synthesis catalysts. However, the selectivity remains below 60% due to the limitation of the reaction mechanism of surface polymerization, as predicted by the Anderson-Schultz-Flory (ASF) model^{1, 2}.

We report a composite catalyst comprising zeolites with partially reducible metal oxides, which enables direct conversion of syngas^{3,4}. Following activation of C-O bond on the metal oxides, the subsequent C-C coupling is modulated within the confined acidic pores of zeolites. As a result, a selectivity to light olefins as high as 80% is achieved, which is far beyond the limit predicted by the ASF model in Fischer-Tropsch synthesis³. In addition, CH_4 and C_{5+} hydrocarbon selectivities are both well below 10%, much lower than those in the Fischer-Tropsch approach. By contrast, in Fischer-Tropsch synthesis process, CH_4 and C_{5+} are difficult to suppress at the same time, frequently with one increasing and the other declining. In addition, the catalyst delivers rather stable performance within a 110-h test.

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3. F. Jiao, J. Li, X. Pan, J. Xiao, X. Bao et al, *Science* **2016**, 351, 1065.
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Xiulian Pan

- **CURRENT POSITION(S)**

Xiulian Pan, a professor from the State Key Laboratory of Catalysis and Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences.

- **FELLOWSHIPS AND AWARDS**

She received the award of the Natural Science Fund for Distinguished Young Scholar from the Natural Science Foundation of China 2014.

- **RESEARCH INTERESTS**

She and her team are dedicated to fundamental studies on confined catalysis within nanostructured porous materials such as carbon nanotubes, zeolites and other porous materials in energy conversion-related processes. Particularly, their efforts focus on syngas chemistry and its selective conversion to chemicals, methane catalytic conversion, ammonia synthesis under mild conditions, and acetylene hydrochlorination.



Computational Modelling Signposts New Directions in Porous Materials

Ben Slater

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In this talk, I will speak about our recent work in modelling zeolites and MOFs. In the first part of my talk, I will show that DFT calculations show that the contrary to expectation, protonated zeolites such as H-MOR, H-RHO, H-CHA and H-LTA have a modest but nonnegligible thermodynamic incentive to adopt non-Lowenstein configurations (i.e. Al-O-Al sequences which have been believed to be highly energetically unfavourable)¹. If these forms of zeolites can be made directly or via post-synthetic routes, the distribution of aluminium would be very different to what calculations suggest for alkali metal compensated zeolites and what experiment seems to show. Our calculations show islanding of aluminium in proton exchanged zeolites. The implications of this prediction will be explored in the talk. In the second part of my talk, I will highlight our work on characterising defects in MOFs. In particular, I will focus on a detailed investigation of point defects in UiO-66 (see figure 1)², emphasizing the how a dynamical picture of the crystal structure is essential to fully understand both structure and function of this material. I will then focus on MOF external surfaces and describe the difficulties of characterising and unambiguously establishing the functional groups at the surface of MOFs, focusing on ZIF-8³.

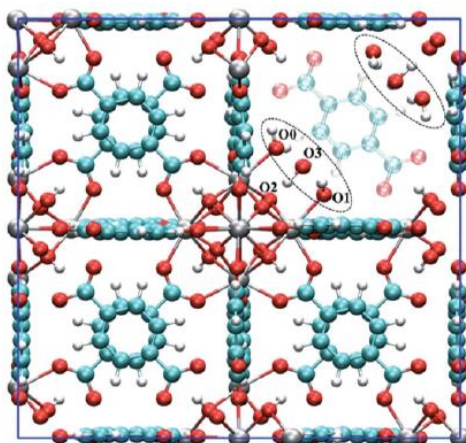


Figure 1: a snapshot of the predicted structure of a missing linker defect in UiO-66, which shows frustrated Lewis pair behaviour.

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1. R. E. Fletcher, S. Ling, B. Slater, arXiv:1612.04162.
2. S. Ling, B. Slater, *Chem. Sci.* **2016**, 7, 4706.
3. B. Slater, S. Ling, *Nat. Mater.* **2017**, 16, 501.

Ben Slater

Professor 2016- Dept. of Chemistry, University College London
 Reader, 2012-2016 Dept. of Chemistry, University College London
 Lecturer, 2007-2012 Dept of Chemistry, University College London
 Davy Faraday Research Fellow, 1999-2007, Royal Institution of Great Britain
 PDRA 1995-1997, Royal Institution of Great Britain/UCL (w/ C. R. A. Catlow/A. M. Stoneham/D.E.Williams)
 PhD (Reading) 1995, BSc(hons) Chemistry 1991 (Nottingham)



Research Interests: Materials chemistry, especially surface and defect chemistry. Porous materials, including zeolites, metal-organic frameworks and water ice. Development and applications of atomistic approaches to modelling.

Awards: RSC/SCI Barrer prize (2008), Royal Society of Chemistry for “innovative contributions to the development and application of computer modelling techniques to the science of microporous materials, especially relating to the surface properties of these materials and to the mechanisms of crystal growth”

Fellowships: Currently a part-time Royal Society Industry fellow in partnership with Johnson Matthey.

Publications: >120 publications including over 100 journal articles in Nature, Nature Materials, PNAS, Angewandte Chemie and Chemical Science. Over 40 publications on porous materials including more than 25 on zeolite or zeotype materials. h-index 34.

External roles: 2015- Executive Editor for AIP Advances. EPSRC college member. Regular EPSRC reviewer and panel member. Reviewer for numerous journals including Nature Materials, Nature Chemistry, PNAS, PRL, Angewandte Chemie and Chemical Science.

Grants: awarded over £ 20m in direct funding from EPSRC, the Leverhulme Foundation and the Royal Society.

Active collaborations: Prof Andrew Goodwin (U of Oxford, UK), Prof Matt Rosseinsky (U of Liverpool, UK), Prof Berend Smit (EPFL, Switzerland), Dr Martin Attfield (U of Manchester, UK) Supervision: PhD supervisor of >15 students. Past first supervisor students include Dr Gareth Tribello, Lecturer (Belfast) and Dr Kim Jelfs, Lecturer (Imperial College). Former PDRA Dr Matt Watkins is now a lecturer at University of Lincoln, Physics.

Selected Recent Talks: 2012 Keynote talk, Zeolite and microporous materials conference, Hiroshima, Japan. 2013 Keynote talk, triennial 17th International Zeolite Conference, Moscow, 2014

Plenary Advanced Materials Symposium, ETH Zurich, 2014 Keynote Czech catalysis society, Prague, Czech Republic

Computational Studies of Metal-Organic Frameworks: Defects, Electronic Properties and Gas Adsorptions

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In this presentation, I will discuss several of our recent computational studies of metal-organic frameworks (MOFs) using density functional theory methods.

I will start with the electronic properties of breathing MOFs,¹ which exhibit dramatic phase change behaviour triggered by the adsorption of guests or other stimuli, for which the MIL-53 material is an archetype. We examine the electronic structure changes associated with changes of phase and density (e.g. large pore of low density and narrow pore of high density), and we find the associated change in band gaps can be larger than 1 eV for known MIL-53 type materials and hypothesized structures. We show that internal pressure (via guest molecules) and external pressure can exert a major influence on the band gap size and gap states. The large response in electronic properties to breathing transitions in MOFs could be exploitable in future applications in resistive switching, phase change memory, piezoresistor, gas sensor, and thermochromic materials.

In the second example, I will discuss defects in MOFs. UiO-66 has emerged as one of the most promising MOF materials due to its thermal and chemical stability and its potential for catalytic applications. Typically, as-synthesised UiO-66 has a relatively high concentration of missing linker defects. The presence of these defects has been correlated with catalytic activity but characterisation of defect structure has proved elusive. We refine a recent experimental determination of defect structure using static and dynamic first principles approaches, which reveals a dynamic and labile acid centre that could be tailored for functional applications in catalysis.²

In the end, I will also briefly discuss our recent work on MOF-74 analogs^{3,4} in collaboration with the groups of Dr Maciej Haranczyk and Prof Berend Smit.

References:

1. S. Ling, B. Slater, *J. Phys. Chem. C* **2015**, 119, 16667.
2. S. Ling, B. Slater, *Chem. Sci.* **2016**, 7, 4706.
3. M. Witman, S. Ling, S. Anderson, L. Tong, K. C. Stylianou, B. Slater, B. Smit, M. Haranczyk, *Chem. Sci.* **2016**, 7, 6263.
4. M. Witman, S. Ling, A. Gladysiak, K. C. Stylianou, B. Smit, B. Slater, M. Haranczyk, *J. Phys. Chem. C* **2017**, 121, 1171.

Sanliang Ling

- **EDUCATION**

Sanliang Ling is a research associate at University College London (UCL). He received his PhD degree from Heriot-Watt University at Edinburgh in 2010, working with Prof Maciej Gutowski on computational and theoretical chemistry. He stayed at Edinburgh for a short period as a postdoctoral research associate, working with Prof Martin Paterson and Prof Ian Galbraith on nonlinear optical properties of conjugated polymers. He then moved to UCL, where he continued to work until now.

- **RESEARCH PROJECTS AND INTERESTS**

At UCL, he has been involved in a range of research projects in several different groups: initially with Prof Alexander Shluger on defects at interfaces in materials for next generation nanoelectronic devices, then with Prof Ben Slater on defects and electronic properties of metal-organic frameworks as well as gas adsorption and separation in flexible metal-organic frameworks, and most recently with Prof Furio Cora on multiferroic and thermoelectric properties of transition metal oxides. His research interests are on first-principles computational materials design, with an emphasis on fundamental understanding of materials properties for energy applications.



JILIN UNIVERSITY