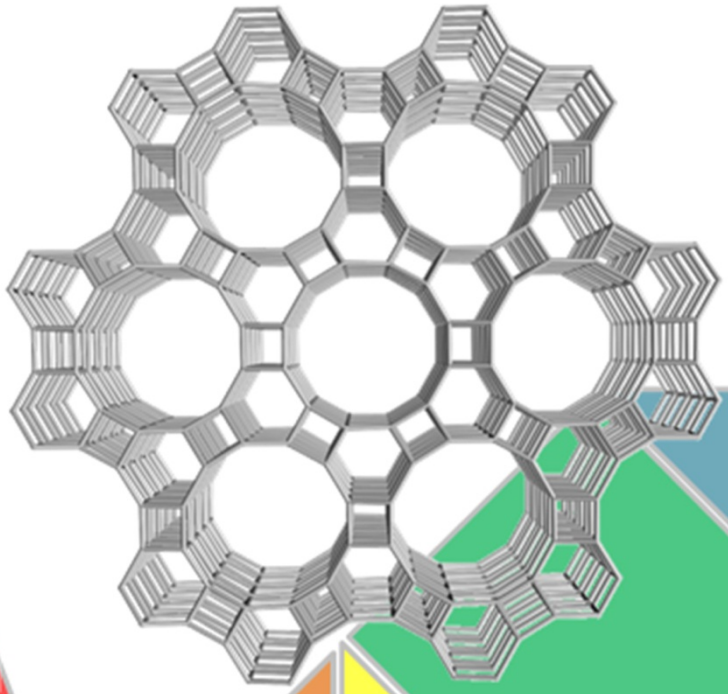
吉林大学
Jilin University

"111" Project Workshop (II)

NEW PERSPECTIVES OF FUNCTIONAL NANOPOROUS MATERIALS



PROGRAM

Changchun, China

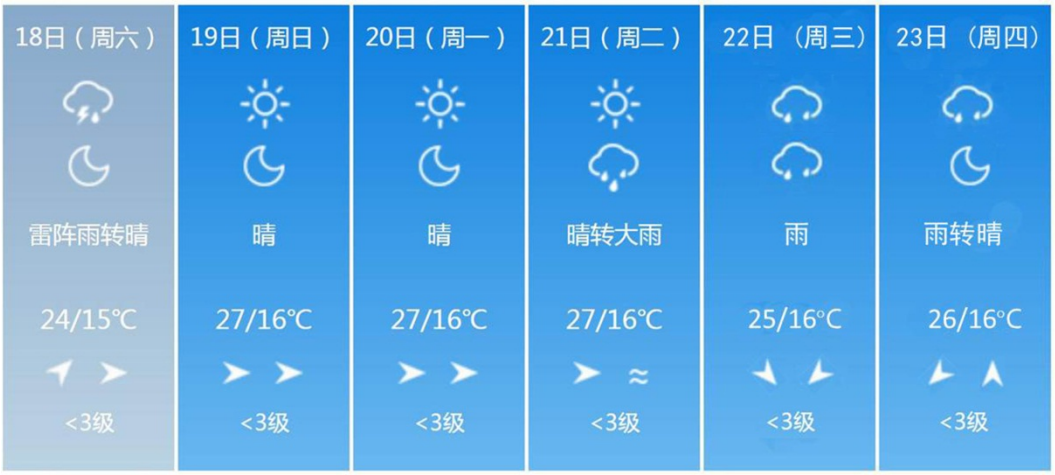
20-22 August, 2018

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 18-23 August, 2018:



August	18	19	20	21	22	23

Contacts:

Yunling Liu (130 3900 5641)

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Please meet at the lobby of the hotel at 08:00 on 21 August and 08:30 on 22 August.

WORKSHOP PROGRAM

Tuesday, 21 August, 2018, Lecture Hall (II), Auditorium

Time	Speaker	Title	Chairperson
08:30 - 08:40	Opening Ceremony	Jihong Yu	
08:40 - 09:10	Avelino Corma	Well Defined Single Site Solid Catalysis: Influence of Short and Long Range Interactions	Jihong Yu
09:10 - 09:40	Christine E. A. Kirschhock	Zeolites from Inorganic Media: Thoughts and Observations	
09:40 - 10:10	Yan Xu	Bioinspired Organized Matter	
10:10 - 10:30	Coffee Break		
10:30 - 11:00	Suk Bong Hong	Embedded Isoreticular Zeolites	Ben Slater
11:00 - 11:30	Chia-Her Lin	Polyamine-Cladded 18-Ring Channel Gallium Phosphites with High- Capacity Hydrogen Adsorption and Carbon Dioxide Capture	
11:30 - 12:00	Yunling Liu	Isoreticular synthesis of Zeolite-like Supramolecular Assemblies (ZSAs) and Their Application in Gas Adsorption and Separation	
12:00 - 12:20	Group Photo		
12:20 - 14:00	Lunch		
14:00 - 14:30	Robert Raja	Predictive Molecular Design of Multifunctional Solid Catalysts	Suk Bong Hong
14:30 - 15:00	Yi Li	High-throughput computational zeolite structure prediction	
15:00 - 15:30	Zhen-An Qiao	Nanoscaled Mesoporous Materials: Designed Synthesis and Applications	Bao-Lian Su

15:30 - 16:00	Qinfen Gu	Tackling Material Research Puzzles by Synchrotron Based Techniques	
16:00 - 16:20	Coffee Break		
16:20	Laboratory and Campus Tour		
18:00	Dinner		

Wednesday, 22 August, 2018, Lecture Hall (II), Auditorium

Time	Speaker	Topic	Chairperson
09:00 - 09:30	Jihong Yu	Emerging Applications of Zeolitic Nanoporous Materials	Robert Raja
09:30 – 10:00	Ben Slater	Defects and Disorder in Framework Materials	
10:00 - 10:30	Mercedes Boronat	Combined Theoretical and Spectroscopic Study of the Low Temperature Formation of Nitrites and Nitrates on Cu-CHA Catalysts, and its Implications for the NH_3-SCR-NO_x Reaction Mechanism	
10:30 - 10:50	Coffee Break		
10:50 - 11:20	Jin Shang	Active Adsorbents for Molecular Separation	Christine E. A. Kirschhock
11:20 - 11:50	Bao-Lian Su	Single-Cell Yolk-Shell Encapsulation for Long-Term Viability with Size-Dependent Permeability and Molecular Recognition	
11:50 - 12:20	Duoduo Liang	Publishing in Wiley Materials Science Journals	
12:20 - 12:30	Closing Remarks	Jihong Yu	
12:30	Lunch and Free Discussion		
14:00	Excursion		
18:00	Dinner		

Well defined single site solid catalysis: influence of short and long range interactions

Avelino Corma

Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas

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The preparation of solid catalysts with well-defined single sites generated from molecular catalysts and metals will be presented. Their catalytic activity and unique selectivity will be shown, and differences between single metal atoms, metal clusters and nanoparticles will correlated with their electronic structure and adsorption properties.

Finally, the activity of single isolated acid sites in microporous materials will be introduced and the contribution of the active site and the confinement effects on acidic properties measures by probe molecules and catalytic behavior will be uncoupled.

Avelino Corma

- **EDUCATION**

1974 Valencia University Degree Chemical Sciences
1976 Complutense Madrid University PhD Doctor of Chemical Sciences

- **CURRENT POSITION(S)**

Research Professor

- **RESEARCH INTERESTS**

Catalysis, Catalyst Synthesis, Meso and Microporous Materials, Zeolites and Zeotypes, Cascade Reactions, Petrochemistry, Fine Chemistry, Nanomaterials

- **AWARDS**
  - Chinese government's Friendship Award (2017)
  - IZA Award of the International Zeolite Association (2016)
  - Spiers Memorial Award of the Royal Society of Chemistry (2016)
  - Prince of Asturias Award for Technical & Scientific Research (2014)
  - Honour Medal to the Invention from the Fundación García Cabrerizo (Spain) (2012)
  - Grande Medaille de l´Académie des Sciences (2011)
  - Gold of Medal for Chemistry Research Career 2001-2010 (2010)
  - Eni Award (2010)
  - Centenary Prize of the Royal Society of Chemistry (2010)
  - Rhodia Pierre-Gilles de Gennes Prize for Science and Industry (now Solvay Award) (2010)
  - Bourdart Award in Advanced Catalysis (2009)
  - A. V. Humboldt - J. C. Mutis Research Award (2009)
  - Gabor A. Somorjai Award of the American Chemical Society for Creative Research in Catalysis (2008)
  - National Award on Science and Technology of México (2006)
  - Alwin Mittasch Award of Dechema (2006)
  - Paul Sabatier Award of the French Society of Chemistry (2006)
  - Iberoamerican Fedaration of Catalysis Societies Award (FISOCAT) (2006)

- Gold of Medal of the Royal Society of Chemistry of Spain (2005)
- Breck Award of the International Zeolite Association (IZA) (2004)
- Eugene J. Houdry Award of the American Catalysis Society in Applied Catalysis (2002)
- F. Gault European Award on "Catalysis" (2001)
- King Jaime I Award on "New Technologies" (2000)

- **SELECTED PUBLICATIONS**

1. F. R. Fortea-Pérez, M. Mon, J. Ferrando-Soria, A. Leyva-Pérez, A. Corma, J. M. Herrera, D. Osadchii, J. Gascon, D. Armentano, E. Pardo, "MOF-Driven Synthesis of Ultrasmall Palladium Clusters and Their Unique Reactivity for Carbene–Mediated Reactions", *Nature Mater.* **2017**, 16, 760-766.
2. E. M. Gallego, M. T. Portilla, C. Paris, A. Leon-Escamilla, M. Boronat, M. Moliner, A. Corma, ""Ab initio" synthesis of zeolites for preestablished catalytic reactions", *Science* **2017**, 355, 1051-1054.
3. G. D. Feng, P. Cheng, W. F. Yan, M. Boronat, X. Li, J. H. Su, J. Y. Wang, Y. Li, A. Corma, R. R. Xu, Yu, J. H. "Accelerated crystallization of zeolites via hydroxyl free radicals", *Science* **2016**, 351, 1188-1191.
4. L. C. Liu, U. Diaz, R. Arenal, G. Agostini, P. Concepcion, A. Corma, "Generation of subnanometric platinum with high stability during transformation of a 2D zeolite into 3D" *Nature Mater*. **2017**, 16, 132-138.
5. P. Garcia-Garcia, J. M. Moreno, U. Diaz, M. Bruix, A. Corma, "Organic-inorganic supramolecular solid catalyst boosts organic reactions in water" *Nature Commun*. **2016**, 7, 10835.
6. T. Rodenas, I. Luz, G. Prieto, B. Seoane, H. Miro, A. Corma, F. Kapteijn, I. X. Llabres, X. Francesc, J. Gascon, "Metal-organic framework nanosheets in polymer composite materials for gas separation" *Nature Mater*. **2015**, 14, 48-55.
7. A. Leyva-Perez, A. Domenech-Carbo, A. Corma, "Unique distal size selectivity with a digold catalyst during alkyne homocoupling" *Nature Commun*. **2015**, 6, 6703.
8. M. Mifsud, S. Gargiulo, S. Iborra, I. Arends, F. Hollman, A. Corma, "Photobiocatalytic chemistry of oxidoreductases using water as the electron donor" *Nature Commun*. **2014**, 5, 4145.
9. R. Martinez-Franco, M. Moliner, Y. Yifeng, S. Juliang, W. Wei, X. Zou. A. Corma, "Synthesis of an extra-large molecular sieve using proton sponges as organic structure-directing agents" *Proc. Nat. Acad. Sci.* **2013**, 110, 3749-3754.
10. A. Corma, P. Concepcion, M. Boronat, M. J. Sabater, J. Navas, M. Yacaman, E. Larios, A. Posadas, A. M. Lopez-Quintela, D. Buceta, "Exceptional oxidation activity with size-controlled supported gold clusters of low atomicity" *Nature Chem*. **2013**, 5, 775-781.
11. J. Oliver-Meseguer, J. R. Cabrero-Antonino, I. Dominguez, A. Leyva-Perez, A. Corma, "Small Gold Clusters Formed in Solution Give Reaction Turnover Numbers of 107 at Room Temperature" *Science* **2012**, 338, 1452-1455.
12. A. Leyva-Perez, A. Corma, "Similarities and Differences between the "Relativistic" Triad Gold, Platinum, and Mercury in Catalysis" *Angew. Chem. Int. Ed*. **2012**, 51, 614-635.
13. J. Jiang, J. L. Jorda, J. H. Yu, L. Baumes, E. Mugnaioli, M. J. Diaz-Cabanas, U. Kolb, A. Corma, "Synthesis and structure determination of the hierarchical meso-microporous zeolite ITQ-43" *Science* **2011**, 333, 1131-1134.
14. A. Corma, P. Serna, "Chemoselective Hydrogenation of Nitro Compounds with Supported Gold Catalysts" *Science* **2006**, 313, 332-334.
15. A. Abad, P. Concepción, A. Corma, H. García, "A collaborative effect between gold and a support induces the selective oxidation of alcohols" *Angew. Chem. Int. Ed*. **2005**, 44, 4066-4069.

Zeolites from inorganic media: thoughts and observations

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Centre for Surface Chemistry and Catalysis - Characterisation and Application Team, KU Leuven, Celestijnenlaan 200f, 3001 Leuven, Belgium

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How do zeolites form? Porous structures during growth depend on species, not connected to the framework but still interacting with it, to fill the voids in the structures. In presence of organic structure directing agents this role is taken by the organic cations and quite often shape and size of the channels and cavities reflects the molecule geometry. Naively seen, in the final outcome the zeolite separates the aqueous, hydrophilic environment from a more hydrophobic assembly containing the organic species. In a way the zeolite therefore can be described as a mediator between regions of varying hydrophilicity.

However, zeolites also form in absence of organics. Only in rare cases organics are involved in natural zeolite formation. Also the early pioneers in zeolite science focused on purely inorganic synthesis mixtures. A clue on how porosity is achieved in these environments is the simple assessment of the as made zeolite structure, including the content of the pores: water and inorganic cations. Also here, the phase found in the zeolites is different from the composition of the environment. In the case of typical zeolite syntheses in inorganic media, the ionic density inside the zeolites exceeds by far the concentration in the remaining fluid. As a consequence, the Si/Al ratio in the obtained zeolites is quite low, compared to the situation where organic templates are applied. Furthermore, the most common products are small pore zeolites with channel sizes not exceeding 8-membered rings, though Faujasite, with its 12-ring windows and large supercages, readily can be formed from inorganic systems.

Interestingly, the topology of the frameworks also is governed by the type of the cation, an observation often employed in zeolite synthesis. So asides a pure phase separating process occurring during zeolite growth into zones with different ionic strength and hydrophilicity, also structure directing effects need to be identified.

Two limiting cases in the composition of inorganic zeolite synthesis mixtures will be discussed:
The highly diluted case in zeolite transformations and the extremely concentrated case in hydrated silicate ionic liquids. Both systems are characterized by their absence of a gel phase, greatly facilitating observation of zeolite formation by monitoring the emerging solid zeolite and remaining synthesis composition.
For both cases the effect of type of inorganic cation, concentration of framework elements and supersaturation will be highlighted.

Christine E. A. Kirschhock

- **EDUCATION**

Master in Chemistry and Chemical Engineering
PhD in material Sciences

- **CURRENT POSITION(S)**

Professor at KU Leuven, Belgium

- **RESEARCH INTERESTS**

Porous, functional materials: Physicochemical characterization, optimization, and understanding their formation.

- **TRACK-RECORD**

1988 Bachelor (Chemistry) TU Darmstadt
1990 Dipl. Chem. Thesis TU Darmstadt; Thesis:
"Dynamics of guest molecules in zeolites by solid state NMR"
1995 Ph.D Material Sciences TU Darmstadt; Summa Cum Laude; Thesis:
"Localisation of guest species and charge-transfer complexes in zeolites by diffraction and spectroscopy"
1996-1997 Postdoctorate TU Darmstadt; Material Science
1997-2002 Research assistant KU Leuven; Material Science
2002-2005 Postdoctorate FWO KU Leuven; Centre for Surfacechemistry and Catalysis (COK)
2003-2005 Docent
2005-2011 Professor at COK (Hoofddocent BOF)
2011- Full Professor at COK (Hoogleraar)

- **SELECTED PUBLICATIONS**

1. E. Verheyen, L. Joos, K. Van Havenbergh, E. Breynaert, N. Kasian, E. Gobechiya, K. Houthoofd, C. Martineau, M. Hinterstein, F. Taulelle, V. Van Speybroeck, M. Waroquier, S. Bals, G. Van Tendeloo, C. Kirschhock, J. Martens, Design of zeolite by inverse sigma transformation. *Nature Mater*. **2012**, 11-12(12), 1059-1064.
2. L. Van Tendeloo, M. Haouas, J. Martens, C. Kirschhock, E. Breynaert, F. Taulelle, Zeolite synthesis in hydrated silicate ionic liquids. *Faraday Discuss*. **2015**, 179, 437-449
3. L. Van Tendeloo, W. Wangermez, A. Vandekerkhove, T. Willhammar, S. Bals, A. Maes, J. Martens, C. Kirschhock, E. Breynaert, Postsynthetic High-Alumina Zeolite Crystal Engineering in Organic Free Hyper-Alkaline Media. *Chem. Mater.* **2017**, 29, 629-638.
4. L. Van Tendeloo, B. de Blochouse, D. Dom, J. Vancluysen, R. Snellings, J. Martens, C. Kirschhock, A. Maes, E. Breynaert, Cation exchange properties of zeolites in hyper alkaline aqueous media. *Environ. Sci. Technol*. **2015**, 49, 1729-1737.
5. L. Van Tendeloo, E. Gobechiya, E. Breynaert, J. Martens, C. Kirschhock, Alkaline cations directing the transformation of FAU zeolite into five different framework types. *Chem. Commun*. **2013**, 49, 11737-11739.

Bioinspired Organized Matter

Yan Xu
State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, China
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Understanding how complex hybrid materials are organized through synergistic self-assembly and chemical synthesis across extended and multiple length scale is of growing interest in materials science and technologies. This talk will highlight some recent advances in the synthetic construction of macroscopic bulk materials under equilibrium conditions. We focus on organization of higher-order architectures from inorganic nanophases using cellulose self-assembly to coordinate the nucleation, growth and transformation. We examine a range of synthetic modalities that give rise to extended length-scale organization of matter spanning from molecular to macroscopic level.[1-3] Of particular interest is a helical superstructure of cellulose by entropic process to facilitate its use as functional nanobuilding bloack for extended scale architecturation with anisotropic properties and chiroptical activity.[4,5] Key elements of the constructional codes associated with these processes are identified with regard to existing knowledge, and presented as a heuristic guideline for the rational organization of advanced nanomaterials that hold promising potentials in photonic, environmental and energy applications.[6]

References:

1. G. N. Li, H. B. Huang, B. W. Yu, Y. Wang, J. W. Tao, Y. X. Wei, S. G. Li, Z. M. Liu, Y. Xu, R. R. Xu, *Chem. Sci*. **2016**, 7, 1582
2. X. T. Ma, G. N. Li, J. W. Tao, P. Li, H. Z. Zheng, S. G. Li, Y. Xu, *Chem. Eur. J.* **2018**, 24, 1.
3. H. B. Huang, Y. Yang, L. H. Chen, Y. Wang, S. Z. Huang, J. W. Tao, X. T. Ma, Tawfique Hasan, Y. Li, Y. Xu, B. L. Su, *Nanoscale*, **2016**, 8, 10928.
4. G. Chu, D. Qu, E. Zussman, Y. Xu, *Chem. Mater*, **2017**, 29, 3980.
5. G. Chu, X. S. Wang, H. J. Jiang, T. R. Chen, J. X. Gao, D. Qu, Y. Xu, ACS *Appl. Mater. Interf*, **2015**, 7, 21797.
6. H. Z. Zheng, W. R. Li, W. Li, X. J. Wang, Z. Y. Tang, S. X-A Zhang, Y. Xu, *Adv. Mater.* **2018**, 30, 1705948.

Yan Xu

- **EDUCATION**

PhD Imperial College London, UK
BSc Jilin University, China

- **CURRENT POSITION(S)**

Professor
State Key Laboratory of Inorganic Synthesis and Preparative Chemistry
Jilin University, China

- **RESEARCH INTERESTS**

Based on bioinspired concepts, we seek to advance a new integrative approach to the synthetic construction of macroscale bulk materials with embedded complexity, higher-order architectures and integrated functions from multi-scale building blocks, and emergence of complex forms of organized matter. We aim to explore new scientific and technological horizons based on the understanding of living systems which are capable of collective behaviors through matter and energy exchange.

- **TRACK-RECORD**

2011- Professor, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin Univeristy
2001-2010 Senior Research Scientist, Grenidea Technologies, Singapore
1996-1999 Assistant Professor, Department of Chemistry, Nanyang Technological University, Singapore
1992-1995 Postdoctoral Research Fellow, Department of Chemistry, National University of Singapore, Singapore
1987-1991 PhD Imperial College London, UK

- **SELECTED PUBLICATIONS**

Adv. Mater. **2018**, 30, 1705948; *Modern Inorganic Synthetic Chemistry*, ELSEVIER **2017**, ISBN 9780444635914; *Angew. Chem. Int. Ed.* **2017**, 56, 1; *Chem. Mater.* **2017**, 29, 3980; *Chem. Sci.* **2016**, 7, 1582; *J. Mater. Chem. A* **2015**, 3, 1709; *J. Mater. Chem. A* **2014**, 2, 12442.

Embedded Isoreticular Zeolites

Suk Bong Hong

Center for Ordered Nanoporous Materials Synthesis, Division of Environmental Science and Engineering, POSTECH, Pohang, Gyeongbuk, 37673, Korea.

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Zeolites are a unique class of crystalline microporous solids with very high surface areas, being a consequence of well-defined cavities and channels of molecular dimensions that enable a variety of commercial applications, including ion exchange, separation, and catalysis. This is largely due to the continual discovery of zeolites with novel framework structures and/or compositions.

We have recently discovered a novel zeolite family with increasing structural complexity and embedded isoreticular structures, denoted the RHO family.[1-8] Zeolite Rho (IZA code RHO), consisting of 10-hedral ($[4^8 8^2]$) double 8-ring (*d8r*) and 26-hedral ($[4^{12}6^8 8^6]$) *lta* cages, is its first generation. The isoreticular expansion of scaffolds in the RHO family of embedded isoreticular zeolites (EIZs) includes the insertion of a pair of *d8r* and 18-hedral ($[4^{12}8^6]$) *pau* cages along each unit-cell edge. The space between the scaffolds is filled by four other cage types. Here we describe the structure solution, prediction, and synthesis of the RHO family of EIZs and their CO_2 adsorption properties.

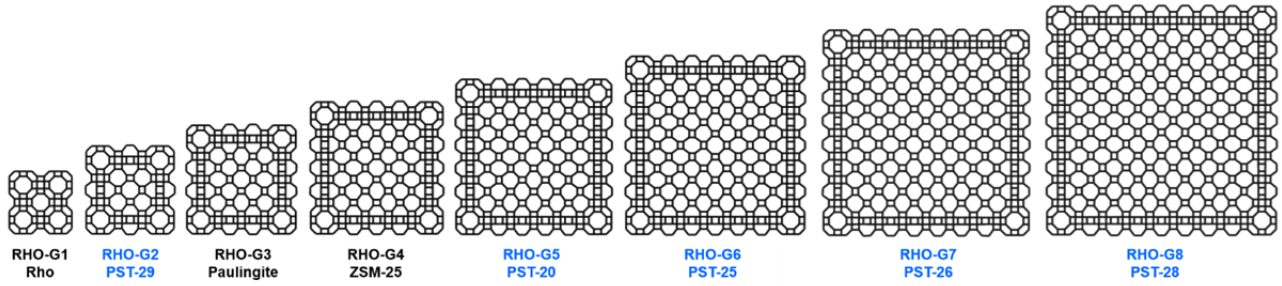

Figure 1. Framework representations of cross-sections (circa 12 Å thick) of the RHO family of EIZs.

References:

1. P. Guo, J. Shin, A. G. Greenaway, J. G. Min, J. Su, H. J. Choi, L. Liu, P. A. Cox, S. B. Hong, P. A. Wright, X. Zou, *Nature* **2015**, 524, 74.
2. A. G. Greenaway, J. Shin, P. A. Cox, E. Shiko, S. P. Thompson, S. Brandani, S. B. Hong, P. A. Wright, *Z. Kristallogr.* **2015**, 230, 223.
3. J. Shin, H. Xu, S. Seo, P. Guo, J. G. Min, J. Cho, P. A. Wright, X. Zou, S. B. Hong, *Angew. Chem. Int. Ed.* **2016**, 55, 4928.
4. A. Mayoral, J. G. Min, S. B. Hong, *Microporous Mesoporous Mater*. **2016**, 236, 129.
5. J. Cho, H. J. Choi, P. Guo, J. Shin, X. Zou, S. B. Hong, *Chem. Eur. J.* **2017**, 23, 15922.
6. J. G. Min, H. J. Choi, J. Shin, S. B. Hong, *J. Phys. Chem. C* **2017**, 121, 16342.
7. J. G. Min, K. C. Kemp, S. B. Hong, *J. Phys. Chem. C* **2017**, 121, 3404.
8. H. Lee, J. Shin, W. Choi, H. J. Choi, T. Yang, X. Zou, S. B. Hong, submitted.

Suk Bong Hong

- **EDUCATION**

  1979-1983 B.S. Chemical Engineering, Hanyang University

  1983-1985 M.S. Chemistry, Seoul National University

  1989-1992 Ph.D. Chemical Engineering, Virginia Tech

- **CURRENT POSITION(S)**

  Director, National Creative Research Initiative Center for Ordered Nanoporous Materials Synthesis, NRF, Korea

  Professor, Environmental Science and Engineering, POSTECH, Pohang 37673, Korea

- **RESEARCH INTERESTS**

  Synthesis, and Characterization of Ordered Nanoporous Materials and Their Uses in the Development of Sustainable and Green Chemical Processes.

- **PUBLICATIONS**

  > 190 Research Papers, 4 Review Articles, and > 20 Patents.

Polyamine-Cladded 18-Ring Channel Gallium Phosphites with High- Capacity Hydrogen Adsorption and Carbon Dioxide Capture

Ming-Jhe Sie[1], Chia-Her Lin[2,*] and Sue-Lein Wang[1,*]

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In this study, we synthesized a unique inorganic framework bearing the largest 18-membered-ring channels in gallium phosphites, denoted as NTHU-15, which displayed genuine porosity even though large organic templates were present. The idea of using the "template cladded" strategy succeeded in releasing channel space of up to ~24% of unit-cell volume as highly-positive-charged organic templates were manipulated to cling to anionic inorganic walls. NTHU-15 showed high H_2 uptake of 3.8 mmol/g at 77 K, and effective CO_2 absorption of ~2.4 mmol/g at 298 K, which surpassed all other known extra-large-channel inorganic framework compounds. NTHU-15 has been successful at overcoming the long-standing problem of organic-templated extra-large-channel structures as opposed to a “true open” framework. Moreover, it realized practical gas sorption functionality in innovated metal phosphites. Considering its high stability in hot water and high selectivity in CO_2 adsorption, NTHU-15 may be the first novel inorganic framework material to be applied to the field of flue gas cleaning.[1]

References:

1. M.-J. Sie, C.-H. Lin, S.-L. Wang, *J. Am. Chem. Soc.* **2016**, 138, 6719–6722.

Chia-Her Lin

- **EDUCATION**

PhD, Department of Chemistry, National Tsing Hua University

- **CURRENT POSITION(S)**

Professor, Department of Chemistry, Chung Yuan Christian University

- **RESEARCH INTERESTS**

Synthesis and Structural Characterization of New MOFs
MOFs for Selective Gas Adsorption and Separation
MOFs for Enzyme Immobilization
MOFs for Mixed Matrix Membranes (MMMs)

- **TRACK-RECORD**

Deputy Director, R&D Center for Membrane Technology, Chung Yuan Christian University
International Zeolite Association, Commission on Metal Organic Frameworks Members

- **AWARDS**

2014 Outstanding Research Award, Chung Yuan Christian University

- **SELECTED PUBLICATIONS**

1. M.-J. Sie, C.-H. Lin*, S.-L. Wang*, *J. Am. Chem. Soc.* **2016**, 138, 6719-6722.
2. S.-H. Lo, D. S. Raja, C.-W. Chen, Y.-H. Kang, J.-J. Chen*, C.-H. Lin*, *Dalton Trans*. **2016**, 45, 9565-9573.
3. Y.-H. Shih, C.-P. Fu, W.-L. Liu, C.-H. Lin*, H.-Y. Huang*, S. Q. Ma*, *Small* **2016**, 12, 2057-2066.
4. D. S. Raja, I.-H. Chang, Y.-C. Jiang, H.-T. Chen*, C.-H. Lin*, *Micropor. Mesopor. Mater*. **2016**, 216, 20-26.
5. W.-L. Liu, N.-S. Yang, Y.-T. Chen, S. Lirio, C.-Y. Wu, C.-H. Lin*, H.-Y. Huang*, *Chem. Eur. J*. **2015**, 21, 115-119.
6. W.-L. Liu, C.-Y. Wu, C.-Y. Chen, B. Singco, C.-H. Lin,* H.-Y. Huang*, *Chem. Eur. J*. **2014**, 20, 8923-8928.
7. C.-L. Lin, S. Lirio, Y.-T. Chen, C.-H. Lin*, H.-Y. Huang*, *Chem. Eur. J*. **2014**, 20, 3317-3321.
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10. H.-Y. Lin, H.-L. Huang, C.-Y. Chin, X. H. Bu, K.-H. Lii, L.-H. Huang, C.-H. Lin, S.-L. Wang*, *Science*, **2013**, 339, 811-813.
11. W.-L. Liu, S.-H. Lo, B. Singco, C.-C. Yang, H.-Y. Huang*, C.-H. Lin*, *J. Mater. Chem. B*, **2013**, 1, 928-932.
12. S.-H. Lo, C.-H. Chien, Y.-L. Lai, C.-C. Yang, J. J. Lee, D. S. Raja, C.-H. Lin*, *J. Mater. Chem. A*, **2013**, 1, 324-329.

Isoreticular synthesis of Zeolite-like Supramolecular Assemblies (ZSAs) and Their Application in Gas Adsorption and Separation

Yunling Liu

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, P. R. China

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Zeolite-like metal-organic frameworks (ZMOFs), a special subclass of metal-organic frameworks (MOFs), is of particular interest and offer great prospective for applications pertaining to gas adsorption/separation.[1, 2] A survey of zeolite topologies revealed that the four-membered ring (4R) is the most abundant secondary building unit (SBU) in conventional zeolites. Thus, functional metal-organic squares (MOSs) would be logical targets as rigid and directional square building units for the synthesis of new zeolite-like supramolecular assemblies (ZSAs) if the MOSs can be designed and programmed to contain complementary peripheral functional groups that can permit and direct their assembly into zeolite-like topologies via supramolecular interactions (e.g. hydrogen bonding).

Inspired by the above consideration, we opted to use imidazoledicarboxylate-like ligands as bridging linkers and bis(monodentate) diamines as capping ligands (Figure 1). Indeed, reactions of 4,5-imidazoledicarboxylic acid (H_3ImDC), $Co(CH_3COO)_2 \bullet 4H_2O$ and 1,2-propanediamine (1,2-PDA) yielded **ZSA-1** which possessed a supramolecular 3D network with the zeolite GIS topology.[3] Furthermore, systematic functionalization was performed by altering the substitutional groups of ligands (-CH_3, CH_2CH_3, -Pr, -NH_2, -CH_2OH), in combination with distinct bis(monodentate) amines (1,2-PDA, En), resulting in series of isoreticular ZSAs named **ZSA-3-9**.[4, 5]

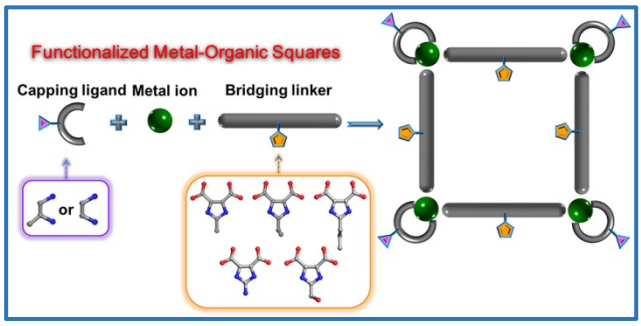

Figure 1. Representation of the synthetic strategy for the construction of MOS-based ZSAs.

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Yunling Liu

- **EDUCATION**

PhD Degree of Chemistry

- **CURRENT POSITION(S)**

Professor of College of Chemistry, Jilin University

- **RESEARCH INTERESTS**

Our main research interest is focused on the design and synthesis of porous zeolite-like metal-organic frameworks and exploring their gas storage and separation properties. Metal-organic frameworks (MOFs) materials, which offer large surface areas, high void volumes, tunable pore sizes and chemical tenability, have been actively pursued on account of their potential applications in industry, such as gas storage and separation and natural gas purification. With respect to designing and synthesizing optimal MOFs with excellent gas separation capabilities, different strategies including those based on secondary building units (SBUs), supermolecular building blocks (SBBs), Lewis basic sites (LBSs), open metal sites (OMSs) (interaction), and ionic skeletons (charge-induce force) have been frequently employed. We have successfully synthesized a series of porous zeolite-like MOFs (ZMOFs) materials for gas storage and separation applications by using different synthesis strategies.

- **TRACK-RECORD**

2008-	Professor of Chemistry, Jilin University
2010-2012	Research Scientist, King Abdullah University of Science and Technology
2004-2008	Associate Professor, Jilin University
2000-2004	Assistant Professor, Jilin University
2003-2005	Postdoc, University of South Florida
2001-2002	Research Associate, The University of Hong Kong
1997-2000	Ph.D. College of Chemistry, Jilin University

- **SELECTED PUBLICATIONS**

1. S. Wang, T. Zhao, G. Li, L. Wojtas, Q. Huo, M. Eddaoudi,* Y. Liu*, *J. Am. Chem. Soc*. **2010**, 132, 18038–18041.
2. X. Luo, Y. Cao, T. Wang, G. Li, J. Li, Y. Yang, Z. Xu, J. Zhang, Q. Huo, Y. Liu*, M. Eddaoudi*, *J. Am. Chem. Soc.* **2016**, 138, 786-789.
3. X. Hang,[‡] B. Liu,[‡] X. Zhu, S. Wang, H. Han, W. Liao,* Y. Liu,* C. Hu*, *J. Am. Chem. Soc.* **2016**, 138, 2969-2972.
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5. Y. Liu, J. F. Eubank, A. Cairns, J. Eckert, V. Ch. Kravtsov, R. Luebke, M. Eddaoud,* *Angew. Chem. Int. Ed.* **2007**, 46, 3278-3283.
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Predictive Molecular Design of Multifunctional Solid Catalysts

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The ability to design and engineer multifunctional active sites at the nanoscale, by drawing on the intricate ability of enzymes to evolve single-sites with distinctive catalytic function, has prompted complimentary and concordant developments in the field of catalyst design and in situ operando spectroscopy.[1] The choice and proximity of these multifunctional sites coupled with their propensity to modify and tailor the local-structural environment in their immediate vicinity has since instigated the predictive design of novel heterogeneous solids for targeted catalysis. By aligning the synthetic strategy with in situ spectroscopic and structural methods, the nature of these active sites can be probed at the molecular level to provide synergistic enhancements in catalytic activity and selectivity. These characterization tools have facilitated robust structure-property correlations to be established, which have enabled the rational design of highly active and selective catalysts for selective oxidation and acid-catalysed processes. Innovations in design-application approach have led to a more fundamental understanding of catalytic processes at the nanoscale, which has facilitated the dextrous manipulation and predictive fabrication of targeted sites for catalysis.[2,3]

This talk will highlight some recent advances in our design strategy for tailoring active sites within microporous and hierarchical architectures and how operando tools can be used for monitoring diffusion pathways during catalysis.[4] It will further illustrate the potential of hierarchically porous catalysts to host a plethora of different types of active sites, found traditionally within the microporous architectures, for expanding substrate scope in catalysis.[5] Strategies for the integration and amalgamation of these developments leading to the discovery and design of novel microporous and hierarchical architectures for sustainable catalytic transformations will also be discussed.

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Robert Raja, FRSC

- **EDUCATION**

MSc (HONS) Chemistry, PhD

- **CURRENT POSITION(S)**

Professor of Materials Chemistry and Catalysis, Co-Chair Clean Carbon Strategic Research Group, Head of Teaching

- **RESEARCH INTERESTS**

The focal theme of our current research is in the discovery, design and fabrication of novel catalytic materials, for application as heterogeneous catalysts in chemical, pharmaceutical, environmental and energy technologies. Our current research efforts are focused on understanding the atomic and molecular basis of catalytic action by nanoporous and nanoparticulate solids, based on the structural and spectroscopic understanding of the nature of the active sites, the mode of activation of catalyst precursors, and the secrets of their selectivity and durability. The diversity of our current research on advanced catalytic materials has also been pivotal in expanding scope to the rational design of hierarchical architectures, where we are investigating a range of topics on CO2 storage and utilisation.

- **TRACK-RECORD**

2016-	Professor of Materials Chemistry & Catalysis
2015-	Head of Teaching, University of Southampton
2012-2015	Director of Admissions, Chemistry, University of Southampton, UK
2011-2016	Chair: Energy Strategic Research Group, University of Southampton, UK
2006-2015	Associate Professor, University of Southampton, UK.
2003-2006	Senior Research Associate, Department of Chemistry, University of Cambridge, UK.
2001-2003	Senior Research Chemist, Bayer Chemicals, Leverkusen, Germany & University of Cambridge (UK).
1999-2001	Postdoctoral Research Fellow, Department of Chemistry, University of Cambridge, UK.
1997-1999	1851 Exhibition Research Fellow, Davy-Faraday Research Lab. Royal Institution of Great Britain, UK.
1994-1997	Ph.D. National Chemical Laboratory, University of Pune, India.

- **AWARDS**

2016	Eminent Visiting Scientist, Institute for Materials Research & Engineering, Singapore
2015	SCI Industrial Inventor Award
2013	Honeywell Inventors Award
2011	Santander Universities Educational and Entrepreneurial Award, Brussels, Europe.
2008	Erskine Fellow & Scholarship, University of Canterbury, New Zealand.
2005	RSC/SCI Barrer Award '*for contributions to preparative materials chemistry & industrial catalysis*.'
2004	International Association of Catalysis Societies, Young Scientist Award.
1997	1851 Exhibition Research Fellowship awarded by the Royal Commission for the Exhibition of 1851.

- **SELECTED PUBLICATIONS**

Select reviews: *Proceedings of The Royal Society A*, **2016**, *472*, 20160095; *Chem. Commun. Feature Article*, **2014**, *50*, 5940-5957; *Topics in Catalysis*, **2009**, *52*, 322-332; *Acc. Chem. Res*. **2008**, *41*, 708-720; *Angew. Chem. Intl. Ed.* **2005**, *44*, 6456-6482; *Annual Rev. Mater. Res.* **2005**, *35*, 315-350.

High-throughput computational zeolite structure prediction

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Zeolites have been widely used in the fields of catalysis, separation, and ion-exchange because of their microporous framework structures.[1] To date, over 200 distinct zeolite framework types have been discovered, but they cannot meet the rapidly growing demand from various industrial fields for new zeolites with superior physical and chemical properties. Computer simulation and modeling provides a new direction in the discovery of new zeolite structures.[2,3] However, high-throughput prediction of not-yet-discovered hypothetical zeolite structures is challenging because of their intrinsic structural complexity and diversity.

We have developed two computational approaches, i.e., the Monte Carlo simulation approach and the high-throughput genomic approach. The Monte Carlo simulation approach is implemented in our homemade computer program, FraGen, which is based on a parallel tempering global optimization algorithm.[4] In comparison with previous structure prediction algorithm, FraGen is more efficient for configuration space searching. With its featured capability to fix the Wyckoff position for each T atom, FraGen is able to find more hypothetical zeolite structures than previous approaches under the same conditions. The genomic approach is designed for ABC-6 zeolite structures, which enumerates all of the combinations of 6-rings that represents a feasible ABC-6 zeolites via a ternary coding system.[5,6] Using this approach, we have enumerated nearly 90,000 hypothetical ABC-6 zeolite structures constructed from ≤16 layers of 6-rings, and identified about 1,000 ABC-6 structures that are the most realizable in experiment.[5] We have built a database collecting all hypothetical structures generated by these two approaches.

In addition to structure prediction, we have developed several approaches for structure evaluation and screening, such as the local interatomic distance criteria and the closest non-adjacent O…O pair criteria.[7,8] Using these criteria, many unfeasible hypothetical zeolite structures that are deemed feasible according to previous structure evaluation methods can be screened out. Furthermore, we have developed a topologic approach, which analyzes the channel network of zeolites. Via this approach, hypothetical zeolites with promising adsorption, diffusion, and catalytic properties can be immediately identified among a large number of hypothetical candidates.

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4. Y. Li, J. Yu, R. Xu, *J. Appl. Cryst* **2012**, 45, 855-861.
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8. J. Lu, L. Li, H. Cao, Y. Li, J. Yu, *Phys. Chem. Chem. Phys*. **2017**, 19, 1276-1280.

Yi Li

- **EDUCATION**

2005-2006 Guest Student Department of Materials, ETH Zurich, Switzerland;
2003 Research Associate Department of Chemistry, The Hong Kong University of Science and Technology, Hong Kong;
2001-2006 Ph.D. State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University, China;
1997-2001 B.Sc. College of Chemistry, Jilin University, China.

- **CURRENT POSITION(S)**

Professor of Inorganic Chemistry, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University

- **RESEARCH INTERESTS**

Cheminfomatics of functional nanoporous materials:

1. Computational prediction of nanoporous crystalline structures
2. High-throughput screening of nanoporous materials according to their properties
3. Database development for nanoporous materials
4. Machine learning of the structure-property relationships and reaction mechanisms of porous materials

- **TRACK-RECORD**

2017- Deputy Director, International Center of Future Science, Jilin University
2014- Professor, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University
2009-2014 Associate Professor, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University
2006-2009 Lecturer, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University

- **AWARDS**

2016 Recipient of the Excellent Young Scientists Fund (NSFC)
2012 Second Prize of National Natural Science Award, 4th achiever

- **SELECTED PUBLICATIONS**

1. Y. Li, H. Cao, J. Yu*, *ACS Nano*, **2018**, 12, 4096-4104.
2. Y. Li, L. Li, J. Yu*, *Chem*, **2017**, 3, 928-949.
3. Y. Li, J. Yu*, *Chem. Sci.* **2016**, 7, 3472-3481.
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6. Y. Li, J. Yu*, R. Xu, *Angew. Chem. Int. Ed.* **2013**, 52, 1673-1677.

Nanoscaled Mesoporous Materials: Designed Synthesis and Applications

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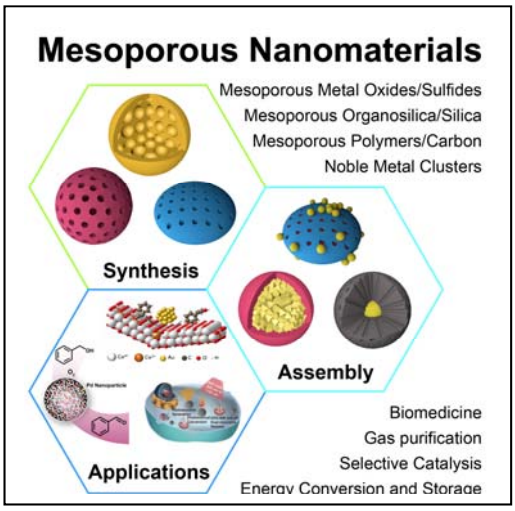
Significant research efforts in recent years have been devoted to the development of nanoparticles with mesostructures for applications in diverse fields.[1] Their nanoscaled size, high surface area and large porosity make mesoporous nanoparticles useful in adsorption, catalysis, energy storage, controlled drug release and cellular delivery.[2] The composition and structure of the nanoparticles are key to the achievable properties. Among mesoporous nanoparticles, mesoporous silica nanoparticles, mesoporous metal oxides, mesoporous carbons have been extensively synthesized by a well-controllable sol-gel process. Compared with bulk materials, which are above a micrometer in size, nanometer-sized mesoporous particles not only have the advantages mentioned above, but additional properties, such as fast mass transport, effective adhesion to substrates, and good suspension in solution. For example, mesoporous carbon nanomaterials are a large class of new materials, and have great potential applications in advanced electrodes for energy conversion and storage, catalysis and nanomedicinal therapy.[3] On the consideration of the preparation methods for mesoporous nanomaterials, we are planning to develop new low cost strategies to directly synthesize nanomaterials with certain mesoporous structure. Meanwhile we will investigate the formation mechanisms and the relationship of the pore structures and properties of the obtained functionalized mesoporous materials. Thus, in our group, we not only focus on the synthesis of mesoporous nanomaterials but also provide some references and guidances to their practical applications in energy conversion and storage, catalysis and nanomedicinal therapy.



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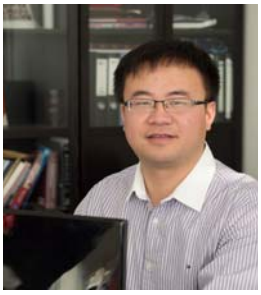
Zhen-An Qiao



- **EDUCATION**

2002-09 to 2006-06 | Bachelor (Department of Chemistry)
Jilin University: Changchun, Jilin, China
2006-09 to 2011-06 | Doctor (State Key Laboratory of Inorganic Synthesis and Preparative Chemistry)
Jilin University: Changchun, Jilin, China
2011-06 to 2012-08 | Postdoc (Department of Chemistry)
University of Tennessee: Knoxville, TN, United States
2012-08 to 2015-05 | Postdoc (Chemical Science Division)
Oak Ridge National Laboratory: Oak Ridge, TN, United States

- **CURRENT POSITION(S)**

Professor of Inorganic Chemistry

- **RESEARCH INTERESTS**

Designed Synthesis and Properites of Mesoporous Materials;
Mesoporous Materials for Catalysis, Electrical Energy Storage, Separation and Bioscience.

- **TRACK-RECORD**

2015-09 to present | Professor (State Key Laboratory of Inorganic Synthesis and Preparative Chemistry)
Jilin University: Changchun, Jilin, China

- **AWARDS**

Young Thousand Talented Program (2014)

- **SELECTED PUBLICATIONS**

1. Libo Zhou, Ying Jing, Yubin Liu, Zhihe Liu, Duyang Gao, Haobin Chen, Weiye Song, Tao Wang, Xiaofeng Fang, Weiping Qin, Zhen Yuan, Sheng Dai, Zhen-An Qiao*, Changfeng Wu*, *Theranostics*, **2018**, 8, 663-675.
2. Tao Wang, Pengfei Zhang, Yan Sun, Bing Liu, Yali Liu, Zhen-An Qiao*, Sheng Dai, *Chem. Mater*. **2017**, 29, 4044-4051.
3. Zhen-An Qiao,* Songhai Chai, Kimberly Nelson, Zhonghe Bi, Jihua Chen, Shannon M. Mahurin, Xiang Zhu, Sheng Dai*, *Nat. Commun*. **2014**, 5, 3705.
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5. Zhen-An Qiao, Bingkun Guo, Andrew J. Binder, Jihua Chen, Gabriel M. Veith, Sheng Dai*, *Nano Lett.* **2013**, 13, 207−212.
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7. Zhen-An Qiao, Suree S. Brown, Jamie Adcock, Gabriel M. Veith, J. Chris Bauer, E. Andrew Payzant, Raymond R. Unocic, Sheng Dai*, *Angew. Chem. Int. Ed*. **2012**, 51, 2888–2893.

Tackling material research puzzles by synchrotron based techniques

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X-ray is an excellent probe for studying the electronic and crystallographic structure, microstructure, dynamic and kinetic processes of materials. In an application, what makes one material better than another? Scientists and engineers can employ X-ray methods to understand how such materials and even devices work. Using specific designed in-situ setups, materials or components can be subjected to conditions designed to mimic their true operating conditions. For these types of work, making use of large scale facilities such as Australian Synchrotron (ANSTO) is essential.

Synchrotron radiation with high flux and high resolution gives us information that would not be possible from laboratory X-ray instruments. X-rays are electromagnetic radiation emitted from electrons that are circulated in a central storage ring before being directed to an experimental station; a beamline. The main advantages of synchrotron radiation are high parallelism, high intensity, and tuneable energy. Synchrotron X-rays are available as an extremely intense beam that allow fast scattering or diffraction studies. At synchrotron sources various techniques at different beamlines offer structural and chemical information on different time and length scales. For example, in-situ X-ray powder diffraction (XRPD) uses the high intensity and resolution of synchrotron radiation for fast studies of phase transitions and detailed structure solution of novel compounds, while small-angle X-ray scattering (SAXS) provides information on particle size and shape. X-ray absorption spectroscopy (XAS) uses the energy tunability properties of synchrotron radiation to provide inter atomic distances, bonding valence, and oxidation states of the samples. Here we describe a collection of applications with synchrotron based techniques which have been used in variety of materials and energy research. Combining synchrotron radiation with various sample environment setups we are able to demonstrate the power of the method.

Qinfen Gu

- **EDUCATION**

2005 – 2008 ETH Zurich, Switzerland, Department of materials, PhD
2003 – 2005 Chalmers University of Technology (CTH), Sweden, Department of materials, Master
2002 - 2003 Utrecht University of Applied Sciences, Holland, Department of Engineering management, Master
1997 - 2002 Shanghai University, Department of material science and engineering, Bachelor

- **CURRENT POSITION(S)**

2018-now, Australian Synchrotron (ANSTO), Acting principal scientist
2015-now, Melbourne University, Adjunct Senior Research Fellow

- **RESEARCH INTERESTS**

Synchrotron X-ray diffraction/scattering, X-ray absorption spectroscopy, small angle X-ray scattering techniques, energy storage materials (including hydrogen storage materials), metal-organic frameworks and zeolites, material under extreme conditions (high pressure & high temperature).

- **TRACK-RECORD**

I have been awarded 3 ARC grants and in charge of several ANSTO research grants over past 10 years.

- **AWARDS**

Finalist for ANSTO Awards in Nuclear Science and Technology (2017)
Finalist of NSW Energy Future Collaborative Innovation Award, Australia (2014)

- **SELECTED PUBLICATIONS**

1. Y. Jiang, Y. Song, Z. Pan, Y. Meng, L. Jiang, Z. Wu, P. Yang, Q. F. Gu*, D. Sun*, L. Hu*, ACS Nano **2018**.
2. Z. Pan, Y. Jiang, P. Yang, Z. Wu, W. Tian, L. Liu, Y. Song, Q. F. Gu*, D. Sun*, L. Hu*, *ACS Nano* **2018**, 12, 2968-2979.
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9. Q. F. Gu, G. Krauss, W. Steurer, F. Gramm, A. Cervellino, *Phys. Rev. Lett.* **2008**, 100, 045502.
10. Q. F. Gu, G. Krauss, W. Steurer, W. *Adv. Mater.* **2008**, 20, 3620.

Emerging Applications of Zeolitic Nanoporous Materials

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Zeolites are a fascinating class of materials which are actively involved in various processes of our current interest, such as energy saving catalytic processes, environmentally benign sorbents, storage materials for waste and energy, and other emerging applications. In recent decade, zeolite chemistry has witnessed significant advance in the aspect of synthesis and mechanistic study, structure characterization, computation and catalysis [1-5]. Strikingly, zeolites are finding many new applications that are beyond their traditional applications. In this presentation, I will first present some recent advances in zeolite chemistry, and then demonstrate some new applications of zeolites. For instance, utilizing zeolites as a host matrix, we have successfully embedded ultrasmall metal nanoclusters in zeolites, which can act as highly-efficient nanocatalysts for hydrogen generation from formic acid (FA) [6-8]. Taking advantage of the nano-confinement effect, we have developed a “dots-in-zeolites” strategy to in-situ confine carbon dots (CDs) in zeolitic matrices during hydrother-mal/solvothermal crystallization to generate ultralong-lifetime room temperature thermally activated delayed fluorescence (TADF) materials and phosphorescence materials [9]. Thanks to the excellent chemical, thermal, and mechanical stability of zeolites, we have fabricated zeolite-coated mesh films for gravity-driven oil-water separation [10]. Furthermore, we have introduced a polarity-based protocol to regulate the wetting behavior of the superamphiphilic porous nanofibrous membranes by infusing the high polar-component-of-surface-energy (PSE) liquid into the membranes to repel the immiscible low PSE liquid [11]. In addition, we have prepared bioactive 3D printed porous titanium implants with strontium (Sr) ions incorporated zeolite coatings (SZCs) to improve the osteogenesis and osteointegration capacity. It is believed that zeolites as a new platform may boost many new applications in the future.

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1. B. M. Weckhuysen, J. H. Yu, *Chem. Soc. Rev.* **2015**, 44, 7022.
2. Y. Li, L. Li, J. H. Yu, *Chem* **2017**, 3, 928.
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6. N. Wang, Q. M. Sun, J. H. Yu, *Adv. Mater.* **2018**, in press.
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10. Y. Wang, J. C. Di, L. Wang, X. Li, N. Wang, B. X. Wang, Y. Tian, L. Jiang, J. H. Yu, *Nature Commun.* **2017**, 8, 575.

Jihong Yu

- **EDUCATION**

1992-1995 Ph.D. Department of Chemistry, Jilin University
1989-1992 M.S. Department of Chemistry, Jilin University
1985-1989 B.S. Department of Chemistry, Jilin University

- **CURRENT POSITION(S)**

Academician of Chinese Academy of Sciences, Fellow of TWAS, Professor of State Key Laboratory of Inorganic Synthesis and Preparative Chemistry & College of Chemistry, Director of International Center of Future Science, Jilin University.

- **RESEARCH INTERESTS**

Rational synthesis and application of zeolitic nanoporous materials in energy, environment and other emerging fields:

1) Synthesis: synthesis of new zeolites, developing new synthetic routes, mechanistic study
2) Applications: catalysis, separation, host-guest assembly, biomedicine, etc.

- **TRACK-RECORD**

2016- Director of Center of Future Science, Jilin University, Changchun, China
2011-2015 Chief Scientist of the 973 Project of China
2007-2010 Cheung Kung Professorship, Ministry of Education of China
1999- Professor of Department of Chemistry, Jilin University, Changchun, China
1997-1998 Associate Professor of Department of Chemistry, Jilin University, Changchun, China
1995-1996 Assistant Professor of Department of Chemistry, Jilin University, Changchun, China
05-08/2004 Guest Professor of Department of Chemistry, Stockholm University, Sweden
1997-1998 CREST Foreign Researcher of Physics Department, Tohoku University, Sendai, Japan
1996-1997 Postdoctoral Fellow of Department of Chemistry, The Hong Kong University of Science and Technology, Hongkong

- **AWARDS**

2017 IUPAC Distinguished Women in Chemistry/Chemical Engineering Award
2014 National Key Talent Project-Young and Middle Aged Experts with Outstanding Contributions
2013 National High-Level Talents Special Support Plan
2012 National Prize for Natural Science (II)
2012 Science & Technology Innovation Team Award for Young and Middle-aged Talents of Jilin Province
2010 The Bau Family Award in Inorganic Chemistry
2009 The 6th China Young Female Scientists Award
2008 National Natural Science Award (I) of Jilin Province
2007 The 10th China Youth Science and Technology Award
2006 National Prize for Natural Science (II)
2001 National Outstanding Youth Science Foundation of China
2000 The Teaching and Research Award Program for Outstanding Young Teachers in Higher Education Institutions of MOE, China

Defects and disorder in framework materials

Ben Slater
Department of Chemistry, UCL, London, UK
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In this talk, I will summarise our recent work centred on zeolites and MOFs, focusing on efforts to better understand the driving forces for order and disorder in these materials. More specifically, I will discuss how the distribution of aluminium in zeolites is affected by extra framework countercations and templates and show how aluminium zoning can arise. A new insight is that I will argue that zeolites are an example of a frustrated framework material and that this frustration may play a role in foreshortening the lifetime of zeolite catalysts on-stream. Part of our efforts to understand heterogenous distribution of aluminium is made possible through a recent collaboration to exploit machine learning approaches and I will show some initial results which allow us to model more representative models of zeolites containing 10s of 1000s of atoms and lengthscales approaching 10nm and beyond. In the second half of the talk, I will concentrate on defects in MOFs, their characterisation, their distribution in common MOFs and the impact of defects on physical and chemical properties.

Ben Slater

- **EDUCATION**

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)

- **CURRENT POSITION(S)**

Professor, Dept. of Chemistry, University College London

- **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. High performance computing.

- **TRACK-RECORD**

>£15m of research funding from various research bodies including EPSRC, NSF, Leverhulme and Royal Society. Currently a Royal Society Industry Fellow in collaboration with Johnson Matthey.

- **AWARDS**

RSC/SCI Barrer prize (2008), Royal Society of Chemistry for “innovative contributions tothe 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”

- **SELECTED PUBLICATIONS**

1. J. J. Shephard, B. Slater, P. Harvey, M. Hart, C. L. Bull, S. T. Bramwell, C. G. Salzmann, “Doping-induced disappearance of ice II from water’s phase diagram” *Nature Phys.* **2018**, 1, doi:10.1038/s41567-018-0135-7.
2. J. Witman, S. Ling, P. Boyd, S. Barthel, M. Haranczyk, B. Slater, B. Smit, “Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of 2D Zeolites” *ACS Central Sci.* **2018**, *4*, 235-245.
3. R. E. Fletcher, S. Ling, B. Slater, “Violations of Löwenstein's rule in zeolites” *Chem. Sci.* **2017**, 8, 7483-7491.
4. M. Witman, S. Ling, S. Jawahery, P. G. Boyd, M. Haranczyk, B. Slater, B. Smit, “The Influence of Intrinsic Framework Flexibility on Adsorption in Nanoporous Materials” *J. Am. Chem. Soc.* **2017**, 139, 5547-5557.
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6. S. Ling, B. Slater, “Dynamic acidity in defective UiO-66” *Chem. Sci.* **2016**, 7, 4706-4712.
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Combined theoretical and spectroscopic study of the low temperature formation of nitrites and nitrates on Cu-CHA catalysts, and its implications for the NH_3-SCR-NO_x reaction mechanism

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The selective catalytic reduction of nitrogen oxides with ammonia, NH_3-SCR-NO_x reaction, using small pore Cu-CHA zeolite as catalyst, is one of the most efficient technologies to reduce NO_x emissions from diesel vehicles.[1-3] But despite the intense investigation in the field, neither the complete reaction mechanism nor the exact nature of the active sites under reaction conditions are clearly established.[4,5]

In situ EPR and IR techniques combined with DFT calculations have been applied to the study of the oxidation half-cycle of the NH_3-SCR-NO_x reaction on Cu-SSZ-13 and Cu-SAPO-34 catalysts. EPR and IR spectroscopies unambiguously show that Cu^+ is oxidized to Cu^{2+} at room temperature in the presence of a mixture of NO and O_2, producing adsorbed NO_2, nitrites and nitrates. Several pathways are proposed from DFT calculations to oxidize Cu^+ to Cu^{2+} either by NO_2 alone or by a mixture of NO and O_2, with activation energy barriers lower than 70 kJ/mol. The non-negligible role of the non-catalyzed disproportionation of NO into N_2O + NO_2 in this process is theoretically and experimentally evidenced.

The results presented here will show that, in the absence of NH_3, non-solvated Cu^+ cations located in the 6R rings of the CHA structure and directly attached to framework oxygen atoms can be oxidized to Cu^{2+} by NO, NO_2 or NO + O_2, generating adsorbed NO_2 and nitrite species at room temperature.

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MERCEDES BORONAT

- **EDUCATION**

DOCTOR IN CHEMISTRY, UNIVERSITY OF VALENCIA

- **CURRENT POSITION(S)**

TENURED SCIENTIST, INSTITUTO DE TECNOLOGIA QUIMICA, UNIVERSITAT POLITECNICA DE VALENCIA - CSIC

- **RESEARCH INTERESTS**

Theoretical Modeling of Heterogeneous Catalysis. Electronic and structural properties of solid catalysts including zeolites, metal particles and clusters, and metal oxides. Theoretical studies of solid-catalyzed reaction mechanisms. Application of DFT to the rationalization of the catalytic behavior of solid materials and the identification of active and selective centers for hydrogenation, oxidation and organic reactions. Modelling of spectroscopic properties like IR vibrational frequencies, NMR shifts and EPR parameters.

- **TRACK-RECORD**
- 2007 - present Científico Titular CSIC, Instituto Tecnología Química, UPV-CSIC
- 2003-2007 Titulado Superior Investigación y Laboratorio, Instituto Tecnología Química, UPV-CSIC
- 2001-2003 Junior Researcher, Fundación CEAM (Centro de Estudios Ambientales del Mediterráneo)
- 1999-2001 Post-doc Instituto Tecnología Química, UPV-CSIC
- 1999 Ph.D. Thesis, Univ. de Valencia

- **SELECTED PUBLICATIONS**

1. C. Li, C. Paris, J. Martinez-Triguero, M. Boronat, M. Moliner, A. Corma, " Synthesis of reaction-adapted zeolites as methanol to olefins catalysts with mimics of reaction intermediates as organic structure-directing agents" *Nature Catal*. **2018**, just accepted.
2. F. R. Fortea-Pérez, M. Mon, J. Ferrando-Soria, M. Boronat, A. Leyva-Pérez, A. Corma, J. M. Herrera, D. Osadchii, J. Gascon, D. Armentano, E. Pardo, "The MOF-driven synthesis of supported palladium clusters with catalytic activity for carbine-mediated chemistry" *Nature Mater*. **2017**, 16, 760.
3. P. Concepción, M. Boronat, S. García-García, E. Fernández, A. Corma, "Enhanced stability of copper clusters of low atomicity against oxidation. Effect on the catalytic redox process" *ACS Catal*. **2017**, 7, 3560-3568.
4. E. M. Gallego, M. T. Portilla, C. Paris, A. León-Escamilla, M. Boronat, M. Moliner, A. Corma, "Ab initio synthesis of zeolites for preestablished catalytic reactions" *Science* **2017**, 355, 1051.
5. G. Feng, P. Cheng, W. Yan, M. Boronat, X.Li, J. Su, J. Wang, Y. Li, A. Corma, R. Xu, J. Yu, "Accelerated crystallization of zeolites via hydroxyl free radicals" *Science* **2016**, 351, 1188.
6. M. Boronat, A. Leyva-Pérez, A. Corma, "Theoretical and Experimental Insights into the Origin of the Catalytic Activity of Subnanometric Gold Clusters: Attempts to Predict Reactivity with Clusters and Nanoparticles of Gold" *Acc. Chem. Res.* **2014**, 47, 834.
7. A. Corma, P. Concepción, M. Boronat, M. J. Sabater, J. Navas, M. J. Yacamán, E. Larios, A. Posadas, M. A. López-Quintela, D. Buceta, E. Mendoza, G. Guilera y A. Mayoral, "Exceptional Oxidation Activity with Size-Controlled Supported Gold Clusters of Low Atomicity" *Nature Chem*. **2013**, 5, 775.
8. M. Boronat, C. Martinez-Sanchez, A. Corma, "Enzime-like specificity in zeolites: A unique position in mordenite for selective carbonylation of methanol and dimethyl ether with CO" *J. Am. Chem. Soc*. **2008**, 130, 16316.

Active Adsorbents for Molecular Separation

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Molecular separation plays a key role in energy and environmental technologies. Here we present our recent discovery of a new “active” molecular sieving mechanism – “molecular trapdoor” – in a class of chabazite zeolites through combined experimental and atomistic simulation works. These trapdoor chabazite absorbents have their eight-membered-ring (8MR) aperture (the only possible gas passage) blocked by some extraframework cations. Some specific gas molecules can interact with the aperture-keeping cations to induce temporary and reversible cation deviation from the center of 8MR aperture, allowing for the gas admission. The different chemical/physical interaction capability of various gas molecules with the aperture-keeping cations endows a selective gas admission, which is in striking contrast to conventional sieving mechanism where the molecular size plays a decisive role. A novel absorption model is developed to quantitatively describe the isobar adsorption curves (i.e. adsorption amount as a function of temperature) for our “active” trapdoor chabazites.

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2. J. Shang, G. Li, Q. Gu, R. Singh, P. Xiao, J. Z. Liu, P. A. Webley, *Chem. Commun.* **2014**, 50, 4544.
3. G. Li, J. Shang, Q. Gu, R. V. Awati, A. Grant, N. Jensen, X. Zhang, D. S. Sholl, J. Z. Liu, P. A. Webley, E. May, *Nature Commun*. **2017**, 8, 15777.

Jin Shang

- **EDUCATION**

Postdoctoral Fellow, Georgia Institute of Technology, 2016-2016
Postdoctoral Fellow, The University of Melbourne, 2013-2016
Ph.D. in Chemical Engineering, The University of Melbourne, 2009-2013
Master in Environmental Engineering, Northeastern University, 2007-2009
Bachelor in Environmental Engineering, Northeastern University, 2003-2007

- **CURRENT POSITION(S)**

Assistant Professor, City University of Hong Kong

- **RESEARCH INTERESTS**

Gas adsorption, separation, storage

- **TRACK-RECORD**

Principle Investigator, National Natural Science Foundation of China Research Grants (RMB 250, 000), 01/2018-12/2020
Principle Investigator, Hong Kong Research Grants Council General Research Fund-Early Career Scheme (HKD 600, 577), 01/2018-12/2020
Principle Investigator, Basic Research Free Exploration Program in Shenzhen Grant (RMB 500, 000), 06/2017-05/2019

- **AWARDS**

The Chancellor's Prize for Excellence in the PhD Thesis, The University of Melbourne, Australia, 2014
John Melvin Memorial Prize for Best PhD Thesis in the School of Engineering 2013, The University of Melbourne, Australia, 2013
Chinese Government Award for Outstanding Self-Financed Students Abroad, 2013

- **SELECTED PUBLICATIONS**

1. J. Shang,* G. Li, Q. Gu, R. Singh, P. Xiao, J. Z. Liu,* P. A. Webley*, *Chem. Commun*. **2014**, 50, 4544.
2. J. Shang, G. Li, R. Singh, P. Xiao, J. Z. Liu, P. A. Webley, *J. Phys. Chem. C* **2013**, 117, 12841.
3. J. Shang, G. Li, J. Li, L. Li, P. A. Webley, J. Z. Liu, *J. Phys. Chem*. *C* **2015**, *119*, 27449.
4. G. Li,[#] J. Shang,[#] Q. Gu, R. V. Awati, A. Grant, N. Jensen, X. Zhang, D. S. Sholl, J. Z. Liu, P. A. Webley, E. May, *Nature Commun.* **2017**, 8, 15777.
5. T. Du, X. Fang, L. Liu, J. Shang, B. Zhang, Y. Wei, H. Gong, S. Rahman, E. F. May, P. A. Webley, G. Li, *Chem. Commun.* **2018**, 54, 3134-3137.
6. J. Shang, G. Li, R. Singh, Q. Gu, K. Nairn, T. Bastow, N. Medhekar, C. Doherty, A. Hill, J. Z. Liu, P. A. Webley, *J. Am. Chem. Soc.* **2012**, *134*, 19246.
7. A. Cao, W. Zhu, J. Shang, J. H. Klootwijk, E. J. R. Sudhölter, J. Huskens, L.C.P.M. de Smet, *Nano Lett.* **2017**, 17, 1-7.
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9. Y. He, J. Shang,* Q. Gu, G. Li, J. Li, R. K. Singh, P. Xiao, P. A. Webley*, *Chem. Commun.* **2015**, 51, 14716.
10. J. Shang,* G. Li, R. Singh, P. Xiao, D. Danaci, J. Z. Liu,* P. A. Webley*, *J. Chem. Phys.* **2014**, 140, 084705.

Single-Cell Yolk-Shell Encapsulation for Long-Term Viability with Size-Dependent Permeability and Molecular Recognition

Bao-Lian Su

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Like nanomaterials, bacteria have been unknowingly used for centuries and hold significant economic potential for fuel and medicinal compound production. Their full exploitation, however, is impeded by the low biological activity and stability in industrial reactors. Though cellular encapsulation addresses these limitations, cell survival is usually compromised due to shell-to-cell contacts and low permeability. Here, we report protamine-assisted, ordered packing of silica nanocolloids with tunable and uniformly organized nanoporosities for single cyanobacterium encapsulation. A void between the capsule shell and cell is created by the controlled internalization of protamine acting as an electrostatic template for the ordered porous shell formation. These unprecedented ordered yolk-shell nanostructures provide long-term cell viability with superior photosynthetic activities and resistance in hostile environments. Engineering the colloidal packing allows tunable shell-pore diameter for size-dependent permeability and introduction of new functionalities for specific molecular recognition. Our strategy could significantly enhance the activity and stability of bacteria for various nanobiotechnological applications.

Bao-Lian Su

Member of the European Academy of Sciences
Member of the Royal Academy of Belgium

- **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 Mesostructured 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.

Publishing in Wiley Materials Science Journals

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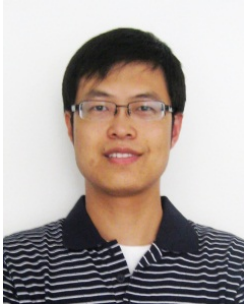
A highly competitive research environment with increasingly limited research funding has created a "Publish or Perish" attitude among scientists who are judged on both the quantity and the quality of their research articles. This presentation provides a brief overview of Wiley materials science journal profile, and how manuscripts are handled by in-house editorial staff (including prescreening, finding referees and making decision on referee reports). Tips will be presented on how to select an appropriate journal for your paper, what aspects of preparation and presentation to focus on from an editor's and referee's perspective, and hints for increasing the discoverability of your paper after publication.

Duoduo Liang



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Duoduo Liang studied materials science and engineering at the University of Science and Technology Beijing, China and earned his PhD from the University of Antwerp, Belgium. He had been a postdoc researcher at Tsinghua University in Beijing prior to joining Wiley Beijing office in 2010. He is currently one of the deputy editors of Advanced Materials; he also handles the peer review of Advanced Science, Advanced Optical Materials and Particle & Particle Systems Characterization.

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