



Dr. Shuhei Furukawa

Associate Professor of Chemistry

Institute for Integrated Cell-Material Sciences (iCeMS)

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Education:

2000 B.Sc. Kyoto University, Japan

2005 Ph.D. Kyoto University, Japan. Supervisor: Susumu Kitagawa

Professional Career:

2005-2007 Postdoc. Katholieke Universiteit Leuven, Belgium Supervisors: Frans De Schryver, Steven De Feyter

2007 Assistant Professor, Graduate School of Engineering, Kyoto University, Japan

2008-2013 Group Leader, ERATO Kitagawa Integrate Pores Project, JST, Japan

2010-2017 Associate Professor, WPI-iCeMS, Kyoto University, Japan

2017-present Associate Professor (PI), WPI-iCeMS, Kyoto University, Japan

Scientific Activities:

2018-present Associate Editor, APL Materials (American Institute of Physics)

2016-present Next Generation Advisor, Chem (Cell Press)

2019-present Member of IZA Commission on Metal-Organic Frameworks

Research Interests:

Coordination chemistry, Soft matter, Supramolecular chemistry, Self-assembly, Porous materials

Honors:

2017 The Representative of Japan for the 2017 APEC Science Prize for Innovation, Research and Education (ASPIREPrize)

2017 The Young Scientists' Prize for Science and Technology by MEXT

2014 Rising Stars, 41st International Conference on Coordination Chemistry

2014 The Chemical Society of Japan Award for Young Chemists

2012 PCCP Prize 2012 by the Royal Society of Chemistry

Selected Papers:

1. A. Legrand, G. A. Craig, M. Bonneau, S. Minami, K. Urayama, S. Furukawa, *Chemrxiv*.9746177.
2. A. Carné-Sánchez, G. A. Craig, P. Larpent, V. Guillerme, K. Urayama, D. Maspoch, S. Furukawa, *Angew. Chem. Int. Ed.* **2019**, *58*, 6347.
3. A. Carné-Sánchez, J. Albalad, T. Grancha, I. Imaz, J. Juanhuix, P. Larpent, S. Furukawa, D. Maspoch, *J. Am. Chem. Soc.* **2019**, *141*, 4094.
4. A. Carné-Sánchez, G. A. Craig, P. Larpent, T. Hirose, M. Higuchi, S. Kitagawa, K. Matsuda, K. Urayama, S. Furukawa, *Nat. Commun.* **2018**, *9*, 2506.
5. R. Kawano, N. Horike, Y. Hijikata, M. Kondo, A. Carné-Sánchez, P. Larpent, S. Ikemura, T. Osaki, K. Kamiya, S. Kitagawa, S. Takeuchi, S. Furukawa, *Chem* **2017**, *2*, 393.

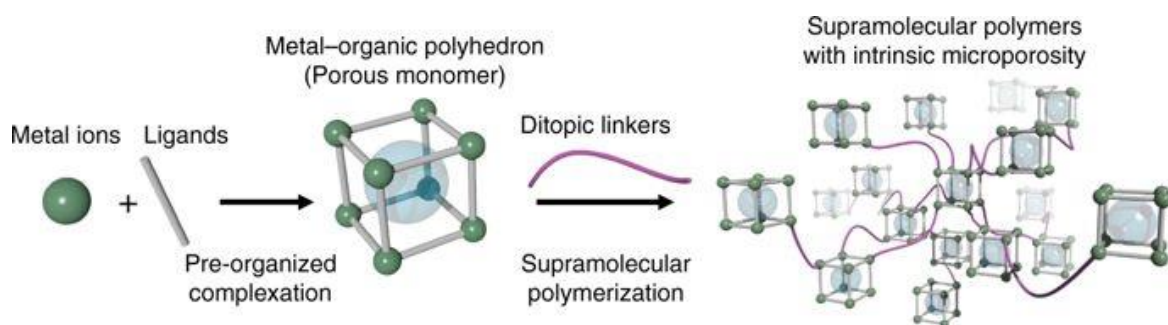
Porous Soft Matter Based on Metal-Organic Polyhedra

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Designed porosity in coordination materials relies on highly ordered crystalline networks, which provide stability upon solvent removal. However, the requirement for crystallinity often impedes control of higher degrees of morphological versatility, or materials processing. Herein, we describe a supramolecular approach to the synthesis of amorphous polymer materials with controlled microporosity. The strategy entails the use of robust metal-organic polyhedra (MOPs) as porous monomers in the supramolecular polymerization reaction. Detailed analysis of the reaction mechanism of the MOPs with imidazole-based linkers revealed the polymerization to consist of three separate stages: nucleation, elongation, and cross-linking. By controlling the self-assembly pathways, we successfully tuned the resulting macroscopic form of the polymers, from spherical colloidal particles to colloidal gels with hierarchical porosity. The resulting materials display distinct microporous properties arising from the internal cavity of the MOPs. This synthetic approach could lead to the fabrication of soft, flexible materials with permanent porosity.





Dr. Chia-Her Lin

Professor

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Research Interests:

1. Synthesis and Structural Characterization of New MOFs
2. MOFs for Selective Gas Adsorption and Separation (CO₂ capture, H₂ and CH₄ storage)
3. MOFs for Enzyme Immobilization
4. MOFs for Mixed Matrix Membranes (MMMs)

Awards:

2014 Outstanding Research Award, Chung Yuan Christian University

Selected Publications:

1. Duraisamy Senthil Raja, Chih-Chiung Pan, Chia-Wei Chen, Yu-Hao Kang, Jiun-Jen Chen* and Chia-Her Lin*. Synthesis of Mixed Ligand and Pillared Paddlewheel MOFs using Waste Polyethylene Terephthalate Material as Sustainable Ligand Source. *Microporous and Mesoporous Materials*, **2016**, *231*, 186-191.
2. Ming-Jhe Sie, Chia-Her Lin*, Sue-Lein Wang*. Polyamine-Cladded 18-Ring-Channel Gallium Phosphites with High-Capacity Hydrogen Adsorption and Carbon Dioxide Capture. *J. Am. Chem. Soc.*, **2016**, *138*, 6719–6722.
3. Sheng-Han Lo, Duraisamy Senthil Raja, Chia-Wei Chen, Yu-Hao Kang, Jiun-Jen Chen*, Chia-Her Lin*. Waste polyethylene terephthalate (PET) materials as sustainable precursors for the synthesis of nanoporous MOFs, MIL-47, MIL-53(Cr, Al, Ga) and MIL-101(Cr). *Dalton Trans.*, **2016**, *45*, 9565–9573.
4. Yung-Han Shih, Chien-Ping Fu, Wan-Ling Liu, Chia-Her Lin*, Hsi-Ya Huang* and Shengqian Ma*. Nanoporous Carbons Derived from Metal-Organic Frameworks as Novel Matrices for Surface-Assisted Laser Desorption/Ionization Mass Spectrometry. *Small*, **2016**, *12*, 2057–2066.

Defect and Desolvation-Triggered Domino Lattice Rearrangement in a Metal-Organic Framework

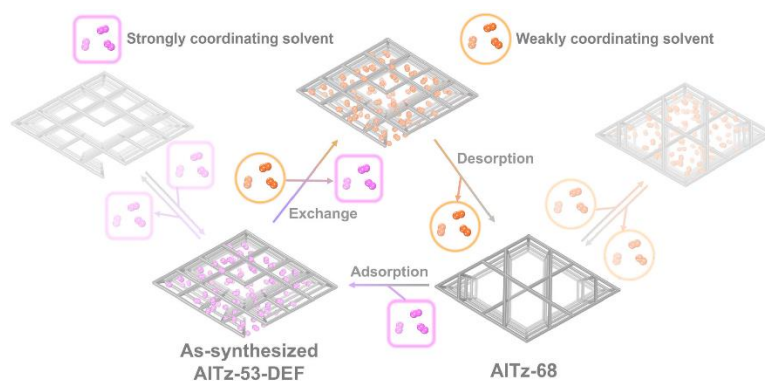
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Topological transitions between significantly different phases typically require extreme conditions to collectively break chemical bonds and overcome the stress caused to the original structure by altering its correlated bond environment. In this work, we present a case system that can achieve rapid rearrangement of the whole lattice of a metal–organic framework (MOF) through a ‘domino’ alteration of the bond connectivity under mild conditions. The system transforms from a disordered amorphous MOF with low porosity to a highly porous and crystalline isomer within 40 seconds upon activation (solvent exchange and desorption), resulting in a significant increase in surface area, from 725 to 2,749 m²/g. Spectroscopic measurements show that this counter-intuitive lattice rearrangement involves a metastable intermediate that results from solvent removal on coordinately unsaturated metal sites. This amorphous–crystalline switch between two topological distinct MOFs is shown to be reversible over four cycles through activation and re-immersion in polar solvents.



References:

1. Sheng-Han Lo, Ching-Hsuan Chien, Yu-Lun Lai, Chun-Chuen Yang, Jey Jau Lee, Duraisamy Senthil Raja, and Chia-Her Lin*, “A mesoporous aluminium metal–organic framework with 3 nm open pores”, *J. Mater. Chem. A*, **2013**, *1*, 324–329.
2. Sheng-Han Lo, Liang Feng, Kui Tan, Zhehao Huang, Shuai Yuan, Kun-Yu Wang, Bing-Han Li, Wan-Ling Liu, Gregory S. Day, Songsheng Tao, Chun-Chuen Yang, Tzuoo-Tsair Luo, Chia-Her Lin*, Sue-Lein Wang*, Simon J. L. Billinge, Kuang-Lieh Lu*, Yves J. Chabal*, Xiaodong Zou, and Hong-Cai Zhou* (2019, Dec). Desolvation-Triggered Domino Lattice Rearrangement in a Metal-Organic Framework. *Nature Chemistry* Accepted.



Dr. Hoi Ri Moon

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Department of Chemistry

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Research Interests:

1. Coordination chemistry
2. Metal-organic frameworks
3. Gas storage and separation
4. Energy-related materials

Awards:

2018 Excellent Research Award, *Deputy Prime Minister and Minister of Education*

2017 Young Inorganic Chemist Award, *KCS Division of Inorganic Chemistry*

2016 Outstanding Teaching Award, *UNIST*

2009 Overseas Postdoctoral Fellowship, *National Research Foundation of Korea*

2006 Best Poster Presentation Award, *The 98th Annual Meeting of the Korean Chemical Society*

2005 Young Scientist Awards for Best Poster Presentations, *The 11th Asian Chemical Congress*

Selected Publications:

1. Ohmin Kwon, Jin Yeong Kim, Sungbin Park, Jae Hwa Lee, Junsu Ha, Hyunsoo Park, Hoi Ri Moon**, and Jihan Kim*. Computer-aided Discovery of Connected Metal-Organic Frameworks. *Nature Commun.* **2019**, 10, 3620.
2. Kwanghyo Son, Jin Yeong Kim, Gisela Schütz, Sung Gu Kang,* Hoi Ri Moon*, and Hyunchul Oh*. Coordinated Molecule-Modulated Magnetic Phase and Metamagnetism in Metal Organic Frameworks. *Inorg. Chem.* **2019**, 58, 8895-8899.
3. Sungeun Jeoung, Songho Lee, Jae Hwa Lee, Soochan Lee, Wonyoung Choe, Dohyun Moon,* and Hoi Ri Moon**. Tuning of the Flexibility in Metal-Organic Frameworks based on Pendant Arm Macrocycles. *Chem. Commun.* **2019**, 55, 8832-8835.
4. Jae Hwa Lee, Sungeun Jeoung, Yongchul G. Chung,* and Hoi Ri Moon**. Elucidation of Flexible Metal-Organic Frameworks: Research Progresses and Recent Developments. *Coord. Chem. Rev.* **2019**, 389, 161-188.

Rational Design of MOF@MOF

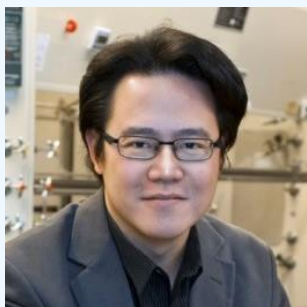
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Composite metal-organic frameworks (MOFs) are comprised of one MOF and another material with noticeably different properties. In general, MOFs are viewed as attractive candidates to construct new composite materials given their facile synthesis and a large library of synthesized MOFs (over 70,000) that can be used as building blocks. As such, many researchers have integrated MOFs with other classes of materials (e.g. other MOFs, carbonbased materials, oxides, metal nanoparticles, polymers) to produce new structures with synergetic properties. Unfortunately, in many of these composite MOFs, the precise nature of the interaction and the bonding at the interface between the two materials is unknown and cannot be characterized well with any of the known methods. One major drawback that stems from this “black box interface” is the loss in tunability and control that prevents facile optimization of MOFs, given the nebulous nature of the interactions at the atomic and the molecular scales.

To remedy this drawback, one can envision a more *rational* approach where the materials are *a priori* designed with the molecular interactions between the two materials mapped out prior to their synthesis. In this talk, we present a joint computational/experimental workflow that screens thousands of metal-organic frameworks (MOFs) and identifies the optimal MOF pairs that can seamlessly “connect” to one another by taking advantage of the fact that the metal nodes of one MOF can form coordination bonds with the linkers of the second MOF. Six MOF pairs (HKUST-1@MOF-5, HKUST-1@IRMOF-18, UiO-67@HKUST-1, PCN-68@MOF-5, UiO-66@MIL-88B(Fe) and UiO-67@MIL-88C(Fe)) yielded from our theoretical predictions were successfully synthesized, leading to clean single crystalline MOF@MOF, demonstrating the power of our joint workflow. Our work can serve as a starting point to accelerate the discovery of novel MOF composites that can potentially be used for many different applications.



Dr. Chia-Kuang (Frank) Tsung

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Short Bio:

Prof. Chia-Kuang Frank Tsung received his undergraduate training at National Sun-Yet Sun University in Taiwan, where he received his B. S. degree. He then moved on to UC Santa Barbara, where he pursued a doctoral degree in the laboratory of Galen D. Stucky. As a graduate student, he carried out research at the forefront of materials chemistry, focusing on the synthesis and characterization of metal and metal oxide nanostructures. After his productive graduate studies, Prof. Tsung moved to UC Berkeley, where he became a postdoctoral fellow with Gabor Somorjai and Peidong Yang. Frank's postdoctoral work centered on the development of high-performance heterogeneous catalysts. Prof. Tsung joined the chemistry faculty at Boston College in the summer of 2010 and has established a compelling research program. Prof. Tsung is interested in identifying new approaches to change the behavior of heterogeneous catalysis in a fundamental way. His research strategy is based on the molecular-level control of the catalytic transformation through tuning of molecule adsorption on active metal surfaces.

Insights into MOF Chemical Biology

Chia-Kuang (Frank) Tsung

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Heterogeneous catalysis is critical for the prosperity of human civilization. It provides access to the range of chemicals, materials, and fuels we use. Understanding and controlling catalytic processes are essential for developing improved energy storage and conversion technologies. Towards this long-term vision of precisely controlling active sites, our group focuses on incorporating catalysts into crystalline nanoporous materials, metal-organic frameworks (MOFs). The precise molecularly-defined pores intrinsic to the MOFs provide a new tool to control the catalytic transformations on the catalysts. We have developed methods to combine organometallic catalysts, enzymes, and nanoparticle catalysts with MOFs of precisely tuned pore structures to manipulate the reactions.



Dr. Dan Zhao

Associate Professor

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National University of Singapore

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Short Bio:

Dan Zhao obtained his PhD degree in Inorganic Chemistry under the supervision of Prof. Hong-Cai Joe Zhou at Texas A&M University in 2010. After finishing his postdoctoral training at Argonne National Laboratory, he joined the Department of Chemical & Biomolecular Engineering at National University of Singapore in July 2012 as an Assistant Professor, and was promoted to Associate Professor with tenure in July 2018. His research interests include advanced porous materials and membranes with the applications in clean energy and environmental sustainability.

Advanced Composite & Porous Membranes for Gas Separation

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The recent decade has witnessed the booming development of advanced porous materials (APMs) such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). Unlike their conventional counterparts (e.g., silica, activated carbon, and zeolite), APMs have crystalline structures, uniform yet tunable pore size, and versatile chemical compositions suitable as membrane materials for separation processes. In this talk, I will introduce our group's work on the fabrication of advanced composite and porous membranes containing APMs for gas separation such as CO₂ capture and natural gas upgrading.



Dr. Fa-Kuen Shieh

Professor

Department of Chemistry, College of Science

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Honors

1. Outstanding Research Award, NCU, 2018
2. Excellent Paper Award-Science College 2017, NCU, 2014-2017
3. 2-year MOST Grant for Excellent Young Scholar, Aug. 2016 - July 2018
4. Excellent Paper Award-Science College 2014-17, National Central University
5. Outstanding Teaching Award-Science College 2011, National Central University
6. The scholarship of government sponsorship for overseas study 1999, period: 2001-2004

Research Interesting

Metal-organic Frameworks (MOFs), MOF Chemical Biology, Enzymology, Biocomposite Synthesis

Selected Publications

1. Tz-Han Wei, Shi-Hong Wu, Yi-Da Huang, Wei-Shang Lo, Benjamin P. Williams, Sheng-Yu Chen, Hsun-Chih Yang, Yu-Shen Hsu, Zih-Yin Lin, Xin-Hua Chen, Pei-En Kuo, Lien-Yang Chou*, Chia-Kuang Tsung * and **Fa-Kuen Shieh***. Rapid Mechanochemical Encapsulation of Biocatalysts into Robust Metal–Organic Frameworks. *Nat. Commun.* **2019**
2. F.-S. Liao, W.-S. Lo, Y.-S. Hsu, C.-C. Wu, S.-C. Wang, **F.-K. Shieh***, J. V. Morabito, L.-Y. Chou, K. C.-W. Wu, and C.-K. Tsung*. Shielding Against Unfolding by Embedding Enzymes in Metal-Organic Frameworks via a de novo Approach. *J. Am. Chem. Soc.* **2017**, *139*, 6530-6533
3. Y.-H. Huang, W.-S. Lo, Y.-W. Kuo, W.-J. Chen, C.-H. Lin and **F.-K. Shieh***. Green and Rapid Synthesis of Zirconium Metal-organic Frameworks via Mechanochemistry: UiO-66 Analog nanocrystals obtained in one hundred seconds. *Chem. Commun.* **2017**, *53*, 5818-5821
4. **F.-K. Shieh***, S.-C. Wang, C.-I. Yen, C.-C. Wu, S. Dutta, L.-Y. Chou, J. V. Morabito, P. Hu, M.-H. Hsu, K. C.-W. Wu*, and C.-K. Tsung*. Imparting Functionality to Biocatalysts via Embedding Enzymes into Nanoporous Materials by a de novo Approach: Size-Selective Sheltering of Catalase in Metal-Organic Framework Microcrystals. *J. Am. Chem. Soc.* **2015**, *137*, 4276-4279.
5. **F.-K. Shieh***, S.-C. Wang, S.-Y. Leo and K. C.-W. Wu*. Water-Based Synthesis of Zeolitic Imidazolate Framework-90 (ZIF-90) with a Controllable Particle Size. *Chem.-Eur. J.* **2013**, *34*, 11139-11142

Insights into MOF Chemical Biology

Fa-Kuen Shieh

Department of Chemistry, College of Science, National Central University

Short Bio:

MOFs have been used in diverse applications including bio-sensing, biomass, and catalysis. This study was introducing a new concept in material biology (MOF Chemical Biology) by studying the change in biological functions of biomolecules such as protein enzymes when they are contained within synthetic MOF biocomposites (termed enzyme@MOFs) obtained by the *de novo* biomineralization synthesis route, performed under mild and aqueous conditions. Those biocomposites are with apertures that allow substrates to move freely and while embedded enzymes or bacterium are confined inside the framework where they are shielded against most structural changes. Remarkably, we successfully demonstrated that catalase (CAT), maintains its biological function in the decomposition of hydrogen peroxide even when exposed to 6 M urea and 80 °C after being embedded in ZIF-90 microcrystals, ZIFs- a subgroup MOFs, via a *de novo* approach. The CAT molecules are confined in the mesoporous cavities in the ZIFs and that the tight confinement limited the structural changes. Moreover, we also demonstrated the first example of encapsulating enzymes into robust metal-organic frameworks (MOFs) via a solid-state mechanochemical process. The mechanochemically encapsulated enzymes retain the desired functionality and show resistance to proteases even under acidic conditions. Those new approaches will provide an alternative system, i.e., structural confinement effect, for broadening MOF applications on the study of biochemistry functionalities to prokaryotes, eukaryotes or mammalian cells etc.

References:

1. F.-K. Shieh and C.-K. Tsung et al. *J. Am. Chem. Soc.*, **2017**, 139, 6530-6533.
2. F.-K. Shieh et al. *Chem. Commun.* **2017**, 5818-5821
3. F.-K. Shieh, Kevin C.-W. Wu and C.-K. Tsung et al. *J. Am. Chem. Soc.*, **2015**, 137, 4276–4279.



Dr. Ryota Sakamoto

Associate Professor

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Graduate School of Engineering

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Diplomas:

1998 – 2002 B. S. The University of Tokyo
2002 – 2004 M. S. The University of Tokyo
2004 – 2007 Ph. D. The University of Tokyo

Research Activities:

2007-2009: Assistant Professor, Department of Chemistry, Tokyo University of Science, Japan
2014-2019: Assistant Professor, Department of Chemistry, The University of Tokyo, Japan
2012: Visiting Professor, Faculty of Chemistry, University of Strasbourg
2019- : Associate Professor, Department of Energy and Hydrocarbon Chemistry, Kyoto University, Japan

Awards:

2018: The Young Scientists' Prize in The 2018 Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Japan.
2016: Chemical Society of Japan Award for Young Chemist

Selected Publications:

1. "A single-stranded coordination copolymer affords heterostructure observation and photoluminescence intensification" Ryojun Toyoda, Ryota Sakamoto, Naoya Fukui, Ryota Matsuoka, Mizuho Tsuchiya, Hiroshi Nishihara, *Science Adv.* **2019**, 5, eaau0637.
2. "Bis(dipyrrinato)zinc(II) Complex Chiroptical Wires: Exfoliation into Single Strands and Intensification of Circularly Polarized Luminescence" Risa Aoki, Ryojun Toyoda, Julius F. Kögel, Ryota Sakamoto, Jatish Kumar, Yasutaka Kitagawa, Koji Harano, Tsuyoshi Kawai, Hiroshi Nishihara, *J. Am. Chem. Soc.* **2017**, 139, 16024-16027.
3. "Coordination Nanosheets Based on Terpyridine-zinc(II) complexes: As Photoactive Host Materials" Takamasa Tsukamoto, Kenji Takada, Ryota Sakamoto, et al. *J. Am. Chem. Soc.* **2017**, 139, 5359-5366.
4. "Crystalline Graphdiyne Nanosheets Produced at a Gas/Liquid or Liquid/Liquid Interface" Ryota Matsuoka, Ryota Sakamoto, Ken Hoshiko, Sono Sasaki, Hiroyasu Masunaga, Kosuke Nagashio, Hiroshi Nishihara, *J. Am. Chem. Soc.* **2017**, 139, 3145–3152.
5. "Dissymmetric Bis(dipyrrinato)zinc(II) Complexes: Rich Variety and Bright Red to Near-Infrared Luminescence with a Large Pseudo Stokes Shift" Ryota Sakamoto, Toshiki Iwashima, Julius F. Kögel, Shinpei Kusaka, Mizuho Tsuchiya, Yasutaka Kitagawa, Hiroshi Nishihara, *J. Am. Chem. Soc.* **2016**, 138, 5666–5677.
6. "A photofunctional bottom-up bis(dipyrrinato)zinc(II) complex nanosheet" Ryota Sakamoto, Ken Hoshiko, Qian Liu, Toshiki Yagi, Tatsuhiro Nagayama, Shinpei Kusaka, Mizuho Tsuchiya, Yasutaka Kitagawa, Wai-Yeung Wong, Hiroshi Nishihara, *Nature Commun.* **2015**, 6, 6713.

Functional Molecule-Based Nanowires and Nanosheets

Ryota Sakamoto

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Although molecule-based bottom-up nanosheets manufactured directly from molecular components can exhibit greater structural diversity than top-down nanosheets, the bottom-up nanosheets reported thus far lack useful functionalities. In this five years, we have created “functional” bottom-up metal complex nanosheets.^{1,2} One such example includes a bottom-up nanosheet featuring a photoactive bis(dipyrrinato)zinc(II) complex motif (Fig. 1a).^{2c,f} A liquid/liquid interfacial synthesis between a three-way dipyrin ligand and zinc(II) ions results in a multi-layer nanosheet, whereas an air/liquid interfacial reaction produces a single-layer or few-layer nanosheet with domain sizes of >10 μm on one side. The bis(dipyrrinato)zinc(II) metal complex nanosheet is easy to deposit on various substrates using the Langmuir-Schäfer process. The nanosheet deposited on a transparent SnO₂ electrode functions as a photoanode in a photoelectric conversion system and is thus the first photofunctional bottom-up nanosheet. Other achievements on one-dimensional coordination nanowires³ and carbonaceous nanosheet graphdiynes⁴ are to be also reported.

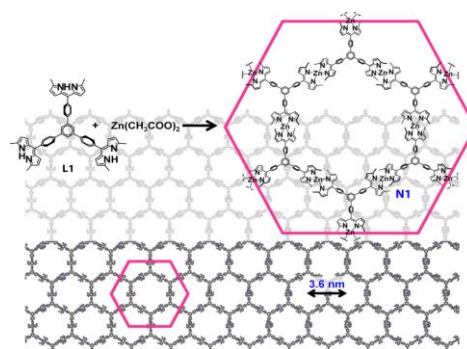


Figure 1.

Bis(dipyrrinato)zinc(II) complex **nanosheet**.

References:

- (a) *Chem. Commun.* **2017**, 53, 5781 (review); (b) *Coord. Chem. Rev.* **2017**, 346, 139 (review); (c) *Chem. Sci.* invited (review).
- (a) *J. Mater. Chem. C* **2019**, 7, 9159; (b) *Chem. Sci.* **2019**, 10, 5218; (c) *Angew. Chem. Int. Ed.* **2017**, 56, 3526; (d) *J. Am. Chem. Soc.* **2017**, 139, 5359; (e) *Chem. Sci.* **2017**, 8, 8078; (f) *Nat. Commun.* **2015**, 6, 6713; (g) *J. Am. Chem. Soc.* **2015**, 137, 4681; (h) *J. Am. Chem. Soc.* **2014**, 136, 14357; (i) *J. Am. Chem. Soc.* **2013**, 135, 2462.
- (a) *Sci. Adv.* **2019**, 5, eaau0637; (b) *J. Am. Chem. Soc.* **2017**, 139, 16024; (c) *Chem. Sci.* **2015**, 6, 2853.
- (a) *J. Am. Chem. Soc.* **2017**, 139, 3145; (b) *Phys. Rev. Mater.* **2018**, 2, 054204; (c) *J. Mater. Chem. A* **2018**, 6, 22189; (d) *ACS Appl. Mater. Interfaces* **2019**, 11, 2730; (e) *Adv. Mater.* 10.1002/adma.201804211 (review).



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Research Fellow/Director

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I. Education

- 1989/04 ~ 1992/03, Ph.D. Department of Chemistry, Tohoku University, Sendai, Japan
1987/04 ~ 1989/03, M.S. Department of Chemistry, Tohoku University, Sendai, Japan
1983/04 ~ 1987/03, B.S. Department of Chemistry, Tohoku University, Sendai, Japan

II. Research & Job Experience

- 2019/07/01-2019/07/31 Visiting Professor
Faculty of Science, Kobe university.
- 2018/08~up to date Director
Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan
- 2018/04/01-2018/07/31 Visiting Professor
Faculty of Science, Kobe university.
- 2007/08~ up to date Research fellow
Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan
- 2007/03 ~ 2008/04, Visiting associate professor
Theoretical and Computational Molecular Science,
Department of Theoretical and Computational Molecular Science,
Institute for Molecular Sciences, National Institute of Natural Sciences,
Okazaki, Japan
- 2003/08 ~ 2007/07 Associate research fellow
Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan
- 2000/08 ~ 2003/07 Assistant research fellow
Center for Condensed Matter Sciences, National Taiwan University, Taipei, Taiwan
- 1994/08 ~ 2000/07 Post doctoral fellow
Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
- 1993 /04 ~ 1994/07 Post doctoral fellow
Department of Chemistry and Biochemistry & Center for Early Events in Photosynthesis,
Arizona State University, Tempe, AZ, USA
- 1992/04 ~ 1993/03 Research fellow
supported by Japan Society for Promotion of Science (JSPS)
Department of Chemistry, Tohoku University, Sendai, Japan

A Quantum Mechanical Simulations Study of Electronic Properties of Selected Noble Metal-Organic Frameworks

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^b Center of Atomic Initiative for New Materials, National Taiwan University

Metal–Organic Frameworks (MOFs) are known as crystalline inorganic–organic hybrid nanomaterials with a uniformed porous structure, high stability and tunable metrics. Due to their unique characteristics, MOFs are exclusively studied for various applications such as gas storage, sensing, chemical separations, catalysis, drug delivery and biomedical imaging. More recently, MOFs are emerging as promising semiconductors and conductors with low-cost, simple fabrication process, stable, and multifunctional tunability. Therefore, MOFs are expecting to have great potential for the advanced applications in electronics. In this regard, the determination of key electronic structures—energy bandgap, band structure, band type, density of states as well as features of the valence band maximum (VBM or HOMO) and conduction band minimum (CBM or LUMO) at band edges—is of prime importance to understand the electrical nature of MOFs. However, accurate estimations of key electronic structures of MOFs are challenging tasks due to their complex structural systems composed of inorganic, organic and solvent molecules. Using by both experimental measurements and theoretical DFT calculations, for the first time, we found the Strontium based MOF (Sr-based MOF) have the semiconducting behavior with relatively narrow bandgap compared with the conventional insulating MOFs due to their unique metal nodes and highly conductive carbon linkers [1]. On the basis of this newly established approach, we have studied noble MOFs. In my presentation, I will talk about the electronic properties for selected MOFs [2,3].

Reference

- [1] M.Usman, S.Mendiratta, S.Batjargal, G.Haider, M.Hayashi, N.R.Gade, J.-W.Chen, Y.-F.Chen, K.-L.Lu*, Semiconductor Behavior of a Three Dimensional Sr-Based Metal–Organic Framework, *ACS Applied Materials & Interfaces*, 7, 22767–22774 (2015).
- [2] Pathak, A., Shen, J.W., Usman, M., Wei, L.F., Mendiratta, S., Chang, Y.S., Sainbileg, B., Ngue, C.M., Chen, R.S., Hayashi, M. and Luo, T.T., Integration of a (-Cu-S-)n plane in a metal-organic framework affords high electrical conductivity. *Nature Communications*, 10, 1721 (2019).
- [3] Usman, M., Bera, K.P., Haider, G., Sainbileg, B., Hayashi, M., Lee, G.H., Peng, S.M., Chen, Y.F. and Lu, K.L., Single-Molecule-Based Electroluminescent Device as Future White Light Source. *ACS Applied Materials & Interfaces*, 11, 4084–4092 (2019).



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Ziqi Sun is currently an Associate Professor and ARC Future Fellow in the Queensland University of Technology (QUT), Australia. His research interest includes developing bio-inspired smart nanomaterials and 2D metal oxide nanomaterials for sustainable energy and environmental applications, such as rechargeable batteries, oil-water separations, and catalysis. Ziqi received his PhD degree on Materials Science and Engineering from Institute of Metal Research, Chinese Academy of Sciences in 2009. After one-year experience as NIMS postdoctoral fellow (Japan) on solid oxide fuel cells, he joined University of Wollongong (UOW), Australia in 2010 and moved to QUT as a faculty member in 2015. Ziqi serves for some prestigious leadership roles in both the academic and professional communities, such as Chair of the Energy Committee TMS, Editors-in-Chief of Sustainable Materials and Technologies (CiteScore = 8.43, Elsevier), Handling Editor of Physics Open (Elsevier), Principal Editor of Journal of Materials Research (MRS), Associate Editor of Surface Innovations (ICE), Editorial Board Member of Scientific Reports, Journal of Materials Science and Technology, and Nano Materials Science.

A Combination of Theoretical and Experimental Study on MOF- Related Materials

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Metal-organic frameworks (MOFs) combining the merits of both organic and inorganic functional building structures are fundamentally important and can meet the requirement of vast scientific and technological applications. Although the primary property of a MOF material is its chemical composition, a number of parameters influence its performance, such as molecular configuration, morphology, size, etc. In this presentation, we intend to design some novel MOF materials with high performance by using a combination of theoretical calculation and experimental study. For example, A new MOF building structure, [Metal–Carbon–(Benzene)_i–Chain]_n ring abbreviated as [M-CB_iC]_n (M = Ti, V, and Cr), to form a ring structure with multi-edges n (= 2–6) and then 2D and 3D structures was proposed based on advanced computational methods. They are thermodynamically stable and chemically and physically versatile with ring shape. The physiochemical properties, such as electronic structures, optical response, and hydrogen evolution properties of this unique MOF structure can be tailored by changing the length of the carbon chain, the edge number of rings, or the type of connecting metal atoms. These well-designed MOF materials offer favorable transport properties, altered electronic coupling properties, and tunable optical properties, and thus have the potential to boost the performance of sustainable energy devices.