



Xiaoyu Wu

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PROFESSIONAL INTERESTS

Computational chemistry, molecular simulation, artificial intelligence, and reticular materials informatics; metal-organic frameworks, covalent organic frameworks, and nanoporous materials; adsorption and membrane separations; carbon dioxide capture, gas upgrading, hydrocarbon separations, and radioactive iodine capture; high-throughput screening; structure–property relationships; inverse design and machine-learning potentials.

EDUCATION AND ACADEMIC POSITIONS

2023-	National University of Singapore, Singapore	Research Fellow
2018-2023	University of Liverpool, United Kingdom	Ph.D., Chemistry
2014-2018	Nanjing Tech University, China	B.Sc., Chemistry

PROFESSIONAL MEMBERSHIPS AND SERVICE

Member	Royal Society of Chemistry (RSC) American Institute of Chemical Engineer (AIChE)
Reviewer	Chemical Engineering Journal; Water Research; Journal of Colloid and Interface Science; Computational Materials Science; ACS Journal of Chemical Information and Modeling; The Journal of Physical Chemistry B and C; ACS Applied Materials & Interfaces; Energy Conversion and Management; Chemical Physics; and other journals.

PEER-REVIEWED PUBLICATIONS

*29 publications; 18 first-author, equal-first-author, or corresponding-author papers. Xiaoyu Wu is shown in bold. † Equal contribution; * corresponding author.*

29. Pore Space Partition in an indolo[3,2-b]carbazole-based Zr-MOF via Post-Synthetic Linker Installation for Enhanced Selective Ethane/Ethylene Separation, H.-O. Qi†, **X. Wu**†, J. Pang, G. Liu, L. Ding*, and L.-B. Sun*, *Inorg. Chem.*, **2026**, provisionally accepted.

- 28 Efficient CO₂ Capture and Conversion from Flue Gas Enabled by an Indolo[3,2-b]carbazole-Based Copper Metal-Organic Framework, H.-O. Qi†, X.-H. Li†, Z.-J. Diao, F. Li, **X. Wu**, L. Ding, G. Liu*, and L.-B. Sun*,
ACS Mater. Lett., **2026**, DOI: 10.1021/acsmaterialslett.6c00577.
- 27 Interrogating Synthetic Likelihood of Metal-Organic Frameworks: A Digital Discovery Perspective, **X. Wu** and J. Jiang*,
Chem. Sci., **2026**, 17, 12635–12646. (Cover Article).
- 26 Stability-Aware, Transferable Discovery of Metal-Organic Frameworks for Selective Adsorption of C6 Alkane Isomers by Machine Learning, **X. Wu**, Q. Liu, R. Zheng, and J. Jiang*,
Chem. Eng. J., **2026**, 538, 176943.
- 25 Double-Shell Enhanced CO₂ Capture in Metal-Organic Cage-Based Porous Liquids, M. Zuo†, **X. Wu**†, M. K. Dinker*, M. Zhang, Z. Wu, L. Zhao, C. Li, T. Guo, L. Chen, L.-B. Sun*, and L. Ding*,
Sep. Purif. Technol., **2026**, 399, 138319.
- 24 CO₂ Adsorption-Induced Anisotropic Mechanical Response in an 8-Fold Interpenetrated Diamondoid Metal-Organic Framework, R. Zheng, S. A. Mohamed, Q. Liu, **X. Wu***, and J. Jiang*,
J. Mater. Chem. A, **2026**, 14, 15721–15734.
- 23 Machine Learning Guided Discovery of Water Stable Metal-Organic Frameworks for Photocatalytic Hydrogen Production, X. Niu, Z. Zhang, **X. Wu**, Y. Liu, Y. Cui*, and J. Jiang*,
Chem. Sci., **2026**, 17, 5376–5386 (Cover Article).
- 22 Breathing Pores Orchestrated by Multifunctional Chemical Sites in Graphene-Based Conjugated Microporous Polymer Membranes for Efficient H₂ Purification, Q. Liu*, R. Zheng, Z. Liang, L. Sun, **X. Wu***, and G. Liu,
Fuel, **2026**, 421, 138985.
- 21 Digital Discovery of Synthesizable Metal-Organic Frameworks via Molecular Dynamics-Informed, High-Fidelity Deep Learning, **X. Wu**, R. Zheng, Q. Liu, and J. Jiang*,
Adv. Funct. Mater., **2026**, 36, e19565 (Cover Article).
- 20 Supramolecular Framework Crystallinity Engineering via Surface-Confined Polymerization for Enhanced C₃H₆/C₂H₄ Separation, G. Liu, F. Li, Z.-J. Diao, H.-D. Li, **X. Wu**, H.-O. Qi, L. Ding, and L.-B. Sun*,
J. Mater. Chem. A, **2025**, 13, 29016–29026.
- 19 From Chemisorption to Physisorption: A Synergistic Computational Screening Approach to Exploit N-Rich Covalent Organic Frameworks for Methyl Iodide Capture, T. Guo, **X. Wu***, C. Li, L. Zhao, M. Zuo, L. Liu, L.-B. Sun*, and L. Ding*,
Chem. Eng. J., **2025**, 525, 170758.
- 18 Discovering Robust Metal-Organic Frameworks with Open Copper Sites for Precombustion CO₂ Capture: Data-Efficient Exploration and Exploitation by Active Learning, **X. Wu**, Q. Liu, and J. Jiang*,
Chem. Eng. J., **2025**, 521, 167021.
- 17 Machine-Learning-Aided Design of Two-Dimensional C60 Membranes for Molecular-Orientation-Directed CO₂/C₂H₂ Separation, Q. Liu*, **X. Wu**, R. Zheng, G. Liu, and J. Jiang*,
J. Membr. Sci., **2025**, 736, 124655.

- 16 Optimization of Chitosan-Based Demulsifiers via Interfacial Displacement: A Molecular Dynamics and Principal Component Analysis Approach, Y. Yu, X. Song*, X. Yang, C. Wang, **X. Wu**, Y. Wang, W. Xiang, S. Zhao, and H. Liu, *Sep. Purif. Technol.*, **2025**, 365, 132693.
- 15 Graphene Oxide Membranes with Engineered Pocket Suction Water Environments for Selective C1-C2 Alcohol Dehydration, Q. Liu*, Z. Liang, **X. Wu**, Z. Yang, and G. Liu, *ACS Sustain. Chem. Eng.*, **2025**, 13, 14630–14640.
- 14 Unraveling Guest-Induced Structural Transition in a Flexible Metal-Organic Framework for C4 Alkane/Alkene Separation, R. Zheng†, **X. Wu**†, S. A. Mohamed, and J. Jiang*, *Chem. Mater.*, **2025**, 37, 4807–4817.
- 13 Discovering Ultra-Stable Metal-Organic Frameworks for CO₂ Capture from a Wet Flue Gas: Integrating Machine Learning and Molecular Simulation, Z. Zhang, A. S. Palakkal, **X. Wu**, J. Jiang*, and Z. Jiang*, *Environ. Sci. Technol.*, **2025**, 59, 9123–9133.
- 12 Can Large Language Models Predict the Hydrophobicity of Metal-Organic Frameworks?, **X. Wu** and J. Jiang*, *J. Mater. Chem. A*, **2025**, 13, 19307–19315 (Cover Article).
- 11 MOF-KAN: Kolmogorov-Arnold Networks for Digital Discovery of Metal-Organic Frameworks, **X. Wu**, X. Song, Y. Yue, R. Zheng, and J. Jiang*, *J. Phys. Chem. Lett.*, **2025**, 16, 2452–2459.
- 10 Computational Screening Guiding the Development of a Covalent-Organic Framework-Based Gas Sensor for Early Detection of Lithium-Ion Battery Electrolyte Leakage, L. Zhao, C. Yu, **X. Wu**, M. Zuo, Q. Zhang, Q. Dong*, and L. Ding*, *ACS Appl. Mater. Interfaces*, **2025**, 17, 10108–10117.
- 9 Leveraging Cross-Diversity Machine Learning to Unveil Metal-Organic Frameworks with Open Copper Sites for Biogas Upgrading, **X. Wu**†, R. Zheng†, and J. Jiang*, *J. Chem. Theory Comput.*, **2025**, 21, 900–911.
- 8 Accurate and Interpretable Machine Learning with Pore+ Descriptors for Iodide Capture in Metal-Organic Frameworks, **X. Wu**, X. Song, L. Chen*, C. Yu, L. Zhao, M. Zuo, C. Li, H. Choi, J. Jiang*, and L. Ding*, *Sep. Purif. Technol.*, **2025**, 360, 130933.
- 7 Precision-Engineered Metal-Organic Frameworks: Fine-Tuning Reverse Topological Structure Prediction and Design, **X. Wu** and J. Jiang*, *Chem. Sci.*, **2024**, 15, 16467–16479 (Cover Article).
- 6 Topological Isomerism Design of Demulsifiers: A Fusion of Molecular Dynamics Simulation and Experiment, C. Wang, P. Liu, J. Zhao, J. Du, X. Chen, **X. Wu***, X. Song*, G. Wang, J. Liu, and Y. Xiao*, *J. Mol. Liq.*, **2024**, 404, 125000.
- 5 Design of a MOF Based on Octa-Nuclear Zinc Clusters Realizing Both Thermal Stability and Structural Flexibility, Y. Ma, X. Tang, M. Chen, A. Mishima, L. Li, A. Hori, **X. Wu**, L. Ding, S. Kusaka, and R. Matsuda*, *Chem. Commun.*, **2022**, 58, 1139–1142.
- 4 Mapping the Porous and Chemical Structure-Function Relationships of Trace CH₃I Capture by Metal-Organic Frameworks Using Machine Learning, **X. Wu**, Y. Che, L. Chen*, E. J. Amigues, R. Wang, J. He, H. Dong, and L. Ding*, *ACS Appl. Mater. Interfaces*, **2022**, 14, 47209–47221.

- 3 In Silico Tuning of the Pore Surface Functionality in Al-MOFs for Trace CH₃I Capture, **X. Wu**, L. Chen*, E. J. Amigues, R. Wang, Z. Pang, and L. Ding*, *ACS Omega*, **2021**, 6, 18169–18177.
- 2 Unconventional Pyridyl Ligand Inclusion within a Flexible Metal–Organic Framework Bearing an *N,N'*-Diethylformamide (DEF)-Solvated Cd₅ Cluster Secondary Building Unit, M.-Y. Chao, J. Chen, **X. Wu**, R.-Y. Wang, P.-P. Wang, L. Ding*, D. J. Young, and W.-H. Zhang*, *ChemPlusChem*, **2020**, 85, 503–509.
- 1 Understanding Water Adsorption and the Impact on CO₂ Capture in Chemically Stable Covalent Organic Frameworks, Y. Ge, H. Zhou, Y. Ji, L. Ding*, Y. Cheng, R. Wang, S. Yang, Y. Liu, **X. Wu**, and Y. Li*, *J. Phys. Chem. C*, **2018**, 122, 27495–27506.

ACADEMIC CONFERENCES

4 main presenter, 3 poster presentations, 2 oral presentations. Xiaoyu Wu is shown in bold.

- 5 Rejuvenating Digital Discoveries of Metal–Organic Frameworks: In Silico Screening, Fine-Tuned Featurization, and Diversity-Driven Machine Learning, **X. Wu** and J. Jiang. AIChE Annual Meeting, Boston, MA, USA, Oral Presentation, 2025.
- 4 Unraveling Guest-Induced Structural Transition in a Flexible Metal–Organic Framework for C₄ Alkane/Alkene Separation, R. Zheng, **X. Wu** and J. Jiang. AIChE Annual Meeting, Boston, MA, USA, Oral Presentation, 2025.
- 3 Large Language Models Help Predict the Hydrophobicity of Metal–Organic Frameworks, **X. Wu** and Jianwen Jiang. AIChE Annual Meeting, Boston, MA, USA, Poster Presentation, 2025.
- 2 Cross-Database Discovery of Metal–Organic Frameworks with Open Cu(II) Sites for Biogas Upgrading through Machine Learning, **X. Wu** and Jianwen Jiang. AIChE Annual Meeting, San Diego, CA, USA, Poster Presentation, 2024.
- 1 Constructions of hypothetical metal-organic frameworks driven by reticular design, **X. Wu** and Jianwen Jiang. MOF2024, Singapore, Singapore, Poster Presentation, 2024

RESEARCH FUNDING

Research contributor for the following Singapore government funded projects

LCERFI01-0015 U2102d2004	Framework materials for CO ₂ capture. SGD 23,481,120
NRF-CRP26-2021RS-0002	Advanced porous materials for alkane separation. SGD 8,871,670
LCERFI01-0015 Phase 2	Closed-Loop Carbon Capture and Utilisation: SGD 21,909,400

TEACHING AND MENTORING

2023-	Mentoring during postdoctoral training: 2 PhD students. 6 MSc students.
2018-2023	Teaching assistant during doctoral training: Introduction to Chemistry; Introductory Inorganic Chemistry; Introductory Physical Chemistry; Introductory Organic Chemistry I and II; Laboratory Techniques; Preparative Chemistry; and Analytical Chemistry