Zhu-Lin (Sam) Xie

Assistant Professor
Department of Chemistry and Biochemistry
Charles E. Schmidt College of Science
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Professional Experiences

Florida Atlantic University, Boca Raton, FL — 2023-present
Assistant professor
Department of Chemistry and Biochemistry

Argonne National Laboratory, Lemont, IL — 2019 – 2023
Postdoctoral Researcher
Chemical Sciences and Engineering Division
Supervisor: Dr Karen L. Mulfort
Research topics: ***a***) Photochemistry and photophysics of Ru, Os and Cu complexes; ***b***) High-energy X-ray scattering/pair distribution analysis (HEXS/PDF) for studying supramoleular structure of transition metal complexes; ***c***) CO_2 capture and reduction by molecular catalysts

University of Texas at Austin, Austin, TX — 2013 – 2019
PhD, Chemistry
Advisor: Michael J. Rose
Thesis: Bio-inspired iron pincers: from [Fe]-hydrogenase mimics to hydrogen activation reactivity

University of Jinan, Jinan, China — 2008 – 2012
BS, Chemistry

Honors and Awards

Leon O. Morgan Fellowship, **2018**, UT Austin
Ethel Gene Kahmer Endowed Presidential Fellowship, **2018**, UT Austin
Professional Development Award, **2016**, conference travel grant, UT Austin

Publications

1. L. Wang*, M. Shao, Z.-L. Xie*, K. L. Mulfort*. Recent Advances in Immobilizing and Benchmarking Molecular Catalysts for Artificial Photosynthesis. *Langmuir*, **2024**, 40, 46, 24195–24215.
2. Brian T. Phelan†, Zhu-Lin Xie†, Xiaolin Liu, Xiaosong Li, Karen L. Mulfort*, and Lin X. Chen*. Photodriven electron-transfer dynamics in a series of heteroleptic Cu(I)-anthraquinone dyads. *Journal of Chemical Physics*, **2024**, 160, 144905. (**†co-first author**)
3. Elizabeth Ryland, Xiaolin Liu, Gaurav Kumar, Sumana Raj, Zhu-Lin Xie, Alexander Mengele, Sven Fauth, Kevin Siewerth, Benjamin Dietzek-Ivanšić, Sven Rau, Karen L. Mulfort, Xiaosong Li, and Amy Cordones*. Site-specific electronic structure of covalently linked bimetallic dyads from nitrogen K-edge X-ray absorption spectroscopy. *Journal of Chemical Physics*, **2024**, 160, 084307.
4. Justin M. Hoffman, Niklas B. Thompson, Olaf Borkiewicz, Xiang He, Samuel Amsterdam, Zhu-Lin Xie, Aaron Taggart, Karen L. Mulfort, Alex B. F. Martinson, Lin X. Chen*, Uta Ruett*, and David M. Tiede*. Orientational analysis of atomic pair correlations in nanocrystalline indium oxide thin films. *IUCrJ*, **2024**, 11, 120-128.
5. Zhu-Lin Xie, Nikita Gupta, Jens Niklas, Oleg G. Poluektov, Vincent M. Lynch, Ksenija D. Glusac and Karen L. Mulfort*. Photochemical charge accumulation in a heteroleptic copper(I)-anthraquinone molecular dyad via proton-coupled electron transfer. *Chemical Science*, **2023**,14, 10219-10235.
6. Lei Wang,* Zhu-Lin Xie, Xin Li, Vincent M. Lynch and Karen L. Mulfort*. Optical detection of alcohols with a Cu(I)HETPHEN complex by reversible aldehyde to hemiacetal conversion. *Analyst*, **2023**, 148, 4274-4278.

7. Lei Wang, Zhu-Lin Xie, Brian T. Phelan, Vincent M. Lynch, Lin X. Chen, and Karen L. Mulfort*. Changing Directions: Influence of Ligand Electronics on the Directionality and Kinetics of Photoinduced Charge Transfer in Cu(I)Diimine Complexes. *Inorganic Chemistry*, **2023**, 62, 35, 14368–14376.

8. Zhu-Lin Xie, Xiaolin Liu, Andrew J. S. Valentine, Vincent M. Lynch, David M. Tiede, Xiaosong Li*, and Karen L. Mulfort*. Bimetallic Copper/Ruthenium/Osmium Complexes: Observation of Conformational Differences Between the Solution Phase and Solid State by Atomic Pair Distribution Function Analysis. *Angewandte Chemie International Edition*, **2022**, 61, e202111764. (**ACIE hot paper and journal cover**)

9. Michael W. Mara*, Brian T. Phelan, Zhu-Lin Xie, Tae Wu Kim, Darren J. Hsu, Xiaolin Liu, Andrew J. S. Valentine, Pyosang Kim, Xiaosong Li, Shin-ichi Adachi, Tetsuo Katayama, Karen L. Mulfort* and Lin X. Chen*. Unveiling ultrafast dynamics in bridged bimetallic complexes using optical and X-ray transient absorption spectroscopies. *Chemical Science*, **2022**, 13, 1715-1724.

10. William V. Taylor,† Brenna K. Cashman,† Zhu-Lin Xie, Karen K. Ngo, and Michael J. Rose*. Synthesis and Magnetic Properties of Antimony-Ligated Co (II) Complexes: Stibines versus Phosphines. *Inorganic Chemistry*, **2022**, 61, 18, 6733–6741**. (†co-first author)**

11. Da Xie, Meng Yu, Zhu-Lin Xie, Rahul T. Kadakia, Chris Chung, Lauren E. Ohman, Kamyab Javanmardi, and Emily L. Que*. Versatile Nickel (II) Scaffolds as Coordination-Induced Spin-State Switches for ^{19}F Magnetic Resonance-Based Detection. *Angewandt Chemie International Edition*, **2020**, 59, 22523-22530.

12. Zhu-Lin Xie, Wenrui Chai, Spencer A. Kerns, Graeme A. Henkelman, and Michael J. Rose*. Bioinspired CNP Iron(II) Pincers Relevant to [Fe]-Hydrogenase (Hmd): Effect of Dicarbonyl versus Monocarbonyl Motifs in H_2 Activation and Transfer Hydrogenation. *Inorganic Chemistry*, **2020**, 59, 2548–2561.

13. Zhu-Lin Xie, Doran L. Pennington, Dylan G. Boucher, James Lo, and Michael J. Rose*. Effects of Thiolate Ligation in Monoiron Hydrogenase (Hmd): Stability of the $\{Fe(CO)^2\}^{2+}$ Core with NNS Ligands. *Inorganic Chemistry*, **2018**, 57, 10028-10039.

14. William V. Taylor, Zhu-Lin Xie, Nicholas I. Cool, Sofia A. Shubert, and Michael J. Rose*. Synthesis, Structures and Characterization of Nickel(II) Stibines: Steric and Electronic Rationale for Metal Deposition. *Inorganic Chemistry*, **2018**, 57, 10364-10374.

15. Zhu-Lin Xie, Gummadi Durgaprasad, Azim K. Ali, and Michael J. Rose*. Substitution reactions of iron(II) carbamoyl-thioether complexes related to mono-iron hydrogenase. *Dalton Transactions*, **2017**, 46, 10814-10829.

16. Subramaniam Kuppuswamy, Joshua D. Wofford, Chris Joseph, Zhu-Lin Xie, Azim K. Ali, Vincent M. Lynch, Paul A. Lindahl, and Michael J. Rose*. Structures, Interconversions and Spectroscopy of Iron Carbonyl Clusters with an Interstitial Carbide: Localized Metal Center Reduction by Overall Cluster Oxidation. *Inorganic Chemistry*, **2017**, 56, 5998-6012.

17. Gummadi Durgaprasad†, Zhu-Lin Xie† and Michael. J. Rose*. Iron Hydride Detection and Intramolecular Hydride Transfer in a Synthetic Model of Mono-Iron Hydrogenase with a CNS Chelate. *Inorganic Chemistry*, **2016**, 55, 386-389. **(†co-first author)**

18. Keren A. Thomas Muthiah, Gummadi Durgaprasad, Zhu-Lin Xie, Owen M. Williams, Christopher Joseph, Vincent M. Lynch, Michael J. Rose*. Mononuclear Iron(II) Dicarbonyls Derived from NNS Ligands: Structural Models Related to a Possible "Pre-Acyl" Active Site of Mono-Iron (Hmd) Hydrogenase. *European Journal of Inorganic Chemistry*, **2015**. 1675-1692.

19. Zhu-Lin Xie, Yong-Rong Xie, Guo-Hai Xu, Zi-Yi Du, Zhong-Gao Zhou, Wu-Leng Lai. Four novel alkaline-earth metal coordination polymers with networks controlled by the diverse coordination modes of amino-sulfonate ligand: Synthesis, crystal structures and luminescent properties. *Inorganica Chimica Acta*, **2012**, 384, 117-124.

20. Zhu-Lin Xie, Wu-Leng Lai, Rui-Qing Yang, Y.-R. Xie*. Poly[aqua(μ_{11}-4, 6-dihydroxybenzene-1, 3-disulfonato)-dipotassium], *Acta Crystallographic*, **2011**, E67, m1745.

21. Yong-Rong Xie*, Ting-Ting Liao, Zhu-Lin Xie, Xi-Yun He, Rui-Qing Yang. Synthesis and crystal structure of novel samarium coordination polymer derived from sulfonic acid ligand, *Journal of Rare Earths*, **2010**, 28, 456-459.

Oral Presentations

1. Zhu-Lin Xie, Unleashing the Power of Transition Metal Complexes for Chemical Transformations Relevant to Energy Conversion: a Tale of Structure and Function, University of Nevada Reno (Reno, NV), 3/29/2023 (invited).

2. Zhu-Lin Xie, Unleashing the Power of Transition Metal Complexes for Chemical Transformations Relevant to Energy Conversion: a Tale of Structure and Function, Florida Atlantic University (Boca Raton, FL), 3/16/2023 (invited).
3. Zhu-Lin Xie, Unleashing the Power of Transition Metal Complexes for Chemical Transformations Relevant to Energy Conversion: a Tale of Structure and Function, Binghamton University (Binghamton, NY), 2/15/2023 (invited).
4. Zhu-Lin Xie, Niklas Thompson, Xiaolin Liu, Andrew J. S. Valentine, Vincent M. Lynch, David M. Tiede, Xiaosong Li, Karen L. Mulfort*, High-Energy X-ray Scattering and Pair Distribution Function Analysis: An Emerging Tool to Reveal (Supra)molecular Structure of Transition Metal Complex in Solution Phase, ACS National Meeting (Chicago, IL), Aug. 2022.
5. Zhu-Lin Xie, Brian T. Phelan, Nikita Gupta, Ksenija Glusac, Lin X. Chen, and Karen L. Mulfort*, Building a Cu(I) HETPHEN Anthraquinone Supramolecular Assembly for Investigating Key Charge Accumulation Pathways in Solar Energy Conversion, ACS National Meeting (Atlanta, GA & Virtual), Fall 2021.
6. Zhu-Lin Xie, Brian T. Phelan, Lin X. Chen, and Karen L. Mulfort*. Building a Cu(I) HETPHEN Anthraquinone Supramolecular Assembly for Investigating Key Charge Accumulation Pathways in Solar Energy Conversion. Argonne Postdoctoral Research and Career Symposium (Lemont, IL), Fall 2020.

Poster Presentations

1. Zhu-Lin Xie, Brian T. Phelan, Lin X. Chen, Karen L. Mulfort*. Building a Cu(I) HETPHEN Anthraquinone Supramolecular Assembly for Investigating Key Charge Accumulation Pathways in Solar Energy Conversion, ACS National Meeting (Chicago, IL), Aug. 2022. (Poster)
2. Zhu-Lin Xie, Brain T. Phelan, Lin X. Chen, Karen L. Mulfort*. Building a Cu(I) HETPHEN Anthraquinone Supramolecular Assembly for Investigating Key Charge Accumulation Pathways in Solar Energy Conversion, Gordon Research Conference: Electron Donor-Acceptor Interactions (Newport, RI), Aug. 2022. (Poster)
3. Zhu-Lin Xie, and Michael J. Rose*. Substitution Reactions of Iron(II) Carbamoyl-thioether Complexes Related to Mono-Iron Hydrogenase. ACS National Meeting (Washington, DC), Mar. 2017. (Poster)
4. Zhu-Lin Xie, Gummadi Durgaprasad and Michael J. Rose*. Synthetic Modeling of Mono-Iron Hydrogenase: CNS Chelates Supporting an Iron-Hydride Species, Substitution Reactions and C–H Activation of TMAO. ACS National Meeting (San Diego, CA), Mar. 2016. (Poster)
5. Zhu-Lin Xie, Gummadi Durgaprasad, Subramaniam Kuppuswamy and M. J. Rose*. Iron-Hydride Detection and Intramolecular Hydride Transfer in a Mono-Iron (Hmd) Hydrogenase Mimic Supported by a CNS Chelate. Green Chemistry Symposium (Austin, TX), Jul. 2015. (Poster)

Grants

External

1. DoD, HBCUMI (Myeongsub Kim PI, Zhu-Lin Xie Co-PI) 10/2025-9/2026, $ 392,018.00, "Acquisition of a Magnetron Sputtering System for Defense-Oriented Materials and Sensor Research and Integrated Education" (pending)
2. DoD, HBCUMI (Vivian Merck PI, Zhu-Lin Xie Co-PI) 6/1/2024-5/31/2025, $ 238,187.00, "X-ray Powder Diffraction: An indispensable tool for research and education in science and engineering" (awarded)
3. DoD, HBCUMI (Myeongsub Kim PI, Zhu-Lin Xie Co-PI) 6/1/2024-5/31/2025, $ 512,696.27, "Acquisition of an X-ray Micro Computed Tomography (micro-CT) System for Multidisciplinary Research and Integrated Education" (awarded)

Teaching Experience

Florida Atlantic University

Course Number	Course Title	Credits	Sem/Year	Number of Students
CHM3609L	Inorganic Chemistry Laboratory	1	Spring 2025	19
CHM3609	Inorganic Chemistry	3	Spring 2025	18
CHM3609	Inorganic Chemistry	3	Spring 2024	21

University of Texas at Austin

Teaching Assistant
Lab Courses: General Chemistry Lab (four semesters), Descriptive Inorganic Chemistry (one semester)
Lecture Courses: Principles of Chemistry I (one semester), Principles of Chemistry II (two semester), Intro to Chemical Practice (one semester), Bio-inorganic Chemistry (graduate class, two semesters)

Mentoring

Postdoctoral

Laxmi Devkota	Summer 2024 – Summer 2025, Scientist at Waste Management (Arlington, Oregon)

Graduate Students

Popy Rani Paul	Fall 2024 – present
Muhammad Shahid	Fall 2024 – present

Undergraduate

Sandra Dickson	Spring 2025-present
Rafael Fanjul	Fall 2024 – present
Jonas Putigna	Fall 2024 – present
Juan Delfin	Spring 2024 – present
Shaaz Mumtazali	Fall 2023 – Spring 2025
Jordan Deblasis	Fall 2023 – Spring 2025

Services

Florida Atlantic University

Graduate Committee	Summer 2024 – present	Mohammed Selim
Departmental	Spring 2024	Faculty Searching Committee. Tenure-track Environmental Chemistry,
College	May 2025	Faculty Marshal, CoS commencement
University	March 2025	Reviewer for Summer Undergraduate Research Fellowship (SURF)

University of Texas at Austin

Lab Assistant, Departmental Electron Paramagnetic Resonance Facility (2016 – 2019)
Duties: Kept the EPR instrument functioning by timely maintenance; Successfully led and implemented the instrument relocation project; Provided training session for users; Offered EPR measurement services for external users.

Journal Reviewer

Journal of the American Chemical Society
Chemical Science
Inorganic Chemistry
Journal of Catalysis
Journal of Material Chemistry A
Zeitschrift für anorganische und allgemeine Chemie
ChemistrySelect
Materials Today Sustainability

Grant Reviewer

- March 2025, American Chemistry Society Petroleum Research Fund (ACS PRF)
- August 2024, Reaching a New Energy Sciences Workforce (RENEW) Program, US Department of Energy

Outreach

- Spring 2024, Explore FAU Outreach Event: representing the department at student recruiting and retention