Zhu-Lin (Sam) Xie

Assistant Professor
Department of Chemistry and Biochemistry
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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

Publications

1. 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**)
2. 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.
3. 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.
4. 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.
5. 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.
6. 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.
7. 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**)
8. 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.

9. 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)**
10. 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.
11. 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.
12. 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.
13. 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.
14. 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.
15. 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.
16. 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)**
17. 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.
18. 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.
19. 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.
20. 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. Oak Ridge Associated Universities, Ralph E. Powe Junior Faculty Enhancement Awards (Zhu-Lin Xie PI), 6/1/24-5/31/25, $10,000, “Electrocatalytic CO_2 Reduction Promoted by Dinuclear Transition Metal Complexes: Synergistic Effects of Metals” (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" (pending)
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" (pending)
4. FAU tech fee program, (Maciej Stawikowski, Zhu-Lin Xie, Renjie Wang, multiple PI), 6/1/2024-5/31/2025, $79,902.48, “Fluorescence spectroscopy for undergraduate laboratories” (declined)

Internal

1. Charles E. Schmidt College of Science, Jumpstart Postdoctoral Program (Zhu-Lin Xie PI), 5/24-5/26, $ 140,000, "Electrocatalytic CO_2 Reduction Promoted by Dinuclear Transition Metal Complexes: Synergistic Effects of Metals and Integration with CO_2 Capture" (declined)
2. Charles E. Schmidt College of Science, Science Fellow Grant (Zhu-Lin Xie PI), 10/1/23-6/30/24, $50,000, "Bimetallic Molecular Catalysts for Electro/Photocatalytic CO_2 Reduction Generating Value-Added Products" (declined)

Teaching

Florida Atlantic University *Assistant Professor* 2023-Present
Lecture Courses:
CHM3609 *Inorganic Chemistry* (2024 spring). Undergraduate Junior-level Inorganic Chemistry
Lab Courses:
CHM3609L *Inorganic Chemistry Laboratory*. Undergraduate Junior-level Inorganic Chemistry

University of Texas at Austin *Teaching Assistant* 2013-2019
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 (2024 summer)

Undergraduate: Juan Delfin (2024 spring), Shaaz Mumtazali (2023 fall), Jordan Deblasis (2023 fall)

Services

Florida Atlantic University

- Faculty Searching Committee. Tenure-track Environmental Chemistry. 2024

University of Texas at Austin, Austin, TX 2016 – 2019

Lab Assistant, Departmental Electron Paramagnetic Resonance Facility
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

Professional Training Workshops and Seminars

- Ultrafast X-ray Summer School, PULSE Institute, Stanford University 6/15/2020 – 6/22/2020
- Rigaku School for Practical Crystallography, Rigaku 6/1/2020 – 6/12/2020
- IES/SharedEPR Summer School for EPR Spectroscopy, International EPR Society 7/17/2019 – 7/21/2019
- ExxonMobil Partners in Academic Laboratory Safety (PALS) Workshop, ExxonMobil 6/5/2018 – 6/7/2018

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