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

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. **Z.-L. Xie**, N. Gupta, J. Niklas, O. G. Poleuktov, V. M. Lynch, K. D. Glusac, K. L. Mulfort*. Photochemical charge accumulation in a heteroleptic copper(I)-anthraquinone molecular dyad via proton-coupled electron transfer. *Chem. Sci.*, **2023**, in press
2. L. Wang, **Z.-L. Xie**, X. Li, V. M. Lynch, K. L. Mulfort*. Optical detection of alcohols with a Cu(i)HETPHEN complex by reversible aldehyde to hemiacetal conversion. *Analyst*, **2023**, 148, 4274-4278
3. L. Wang, **Z.-L. Xie**, B. T. Phelan, V. M. Lynch, L. X. Chen, K. L. Mulfort*. Changing Directions: Influence of Ligand Electronics on the Directionality and Kinetics of Photoinduced Charge Transfer in Cu(I)Diimine Complexes. *Inorg. Chem.*, **2023**, 62, 35, 14368–14376
4. **Z.-L. Xie**, X. Liu, A. J. S. Valentine, V. M. Lynch, D. M. Tiede, X. Li*, K. L. Mulfort*. Bimetallic Copper/Ruthenium/Osmium Complexes: Observation of Conformational Differences Between the Solution Phase and Solid State by Atomic Pair Distribution Function Analysis. *Angew. Chem. Int. Ed.*, **2022**, 61, e202111764. (**ACIE hot paper and journal cover**)
5. M. W. Mara, B. T. Phelan, **Z.-L. Xie**, T. W. Kim, D. J. Hsu, X. Liu, A. J. S. Valentine, P. Kim, X. Li, S. Adachi, T. Katayama, K. L. Mulfort*, L. X. Chen*. Unveiling ultrafast dynamics in bridged bimetallic complexes using optical and X-ray transient absorption spectroscopies. *Chem. Sci.*, **2022**, 13, 1715-1724.
6. W. V. Taylor†, B. K. Cashman†, **Z.-L. Xie**, K. K. Ngo, M. J. Rose*. Synthesis and Magnetic Properties of Antimony-Ligated Co (II) Complexes: Stibines versus Phosphines. *Inorg. Chem.*, **2022**. 61, 18, 6733–6741. **(†co-first author)**
7. D. Xie, M. Yu, **Z.-L. Xie**, R. Kadakia, C. Chung, L. Ohman, K. Javanmardi, E. Que*. Versatile Nickel (II) Scaffolds as Coordination-Induced Spin-State Switches for ^{19}F Magnetic Resonance-Based Detection. *Angew. Chem. Int. Ed.*, **2020**, 59, 22523-22530.

8. **Z.-L. Xie**, W. Chai, G. A. Henkelman, M. 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. *Inorg. Chem.* **2020**, 59, 2548–2561.
9. **Z.-L. Xie**, D. Pennington, J. Lo, D. Boucher and M. J. Rose*. Effects of Thiolate Ligation in Monoiron Hydrogenase (Hmd): Stability of the $\{Fe(CO)^2\}^{2+}$ Core with NNS Ligands. *Inorg. Chem.* **2018**. 57, 10028-10039.
10. W. V. Taylor, **Z.-L. Xie**, N. I. Cool, S. A. Shubert and M. J. Rose* Synthesis, Structures and Characterization of Nickel(II) Stibines: Steric and Electronic Rationale for Metal Deposition. *Inorg. Chem.* **2018**. 57, 10364-10374.
11. **Z.-L. Xie**, G. Durgaprasad, A. K. Ali and M. J. Rose*. Substitution reactions of iron(II) carbamoyl-thioether complexes related to mono-iron hydrogenase. *Dalton Trans.* **2017**. 46, 10814-10829.
12. S. Kuppuswamy, J. Wofford, C. Joseph, **Z.-L. Xie**, A. K. Ali, V. M. Lynch, P. A. Lindahl, and M. J. Rose*. Structures, Interconversions and Spectroscopy of Iron Carbonyl Clusters with an Interstitial Carbide: Localized Metal Center Reduction by Overall Cluster Oxidation. *Inorg. Chem.* **2017**, 56, 5998-6012.
13. G. Durgaprasad†, **Z.-L. Xie**† and M. J. Rose*. Iron Hydride Detection and Intramolecular Hydride Transfer in a Synthetic Model of Mono-Iron Hydrogenase with a CNS Chelate. *Inorg. Chem.* **2016**, 55, 386-389. **(†co-first author)**
14. K. A. Thomas Muthiah, G. Durgaprasad, **Z.-L. Xie**, O. M. Williams, C. Joseph, V. M. Lynch and M. 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. *Eur. J. Inorg. Chem.* **2015**. 1675-1692.
15. **Z.-L. Xie**, Y.-R. Xie*, G.-H. Xu, Z.-Y. Du, Z.-G. Zhou, W.-L. 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. *Inorg. Chim. Acta*. **2012**, 384, 117-124.
16. **Z.-L. Xie**, W.-L. Lai, R.-Q. Yang, Y.-R. Xie*. Poly[aqua(μ_{11}-4, 6-dihydroxybenzene-1, 3-disulfonato)-dipotassium], *Acta Cryst.*, **2011**, E67, m1745.
17. Y.-R. Xie*, T.-T. Liao, **Z.-L. Xie**, X.-Y. He, R.-Q. Yang. Synthesis and crystal structure of novel samarium coordination polymer derived from sulfonic acid ligand, *J. Rare Earths*, **2010**, 28, 456-459.

Oral Presentations

1. **Z.-L. 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. **Z.-L. 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. **Z.-L. 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. **Z.-L. Xie**, N. Thompson, X. Liu, A. J. S. Valentine, V. M. Lynch, D. M. Tiede, X. Li, K. 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. **Z.-L. Xie**, B. T. Phelan, N. Gupta, K. Glusac, L. X. Chen, and K. 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. **Z.-L. Xie**, B. T. Phelan, L. X. Chen, and K. 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. **Z.-L. Xie**, B. T. Phelan, L. X. Chen, K. 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. **Z.-L. Xie**, B. T. Phelan, L. X. Chen, K. 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. **Z.-L. Xie**, and M. J. Rose*. Substitution Reactions of Iron(II) Carbamoyl-thioether Complexes Related to Mono-Iron Hydrogenase. ACS National Meeting (Washington, DC), Spring **2017**. (Poster)
4. **Z.-L. Xie**, G. Durgaprasad and M. 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), Spring **2016**. (Poster)
5. **Z.-L. Xie**, G. Durgaprasad, S. 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), Summer **2015**. (Poster)

Teaching

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)

University Services

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 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