



Michael J. Rose

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Education and Research

University of Texas, Austin – (2022 – present) *Director, Center for Electrochemistry*

(2019 – present) *Associate Professor, Department of Chemistry*

(2012 – 2018) *Assistant Professor, Department of Chemistry*

California Institute of Technology – (2009-12) NSF ACC-F Postdoctoral Fellowship (2010-2012); NSF/CCI-Solar Postdoctoral Scholar (2009-2010). Joint appointment in the research groups of Prof Harry Gray and Prof Nate Lewis. Syntheses of Fe, Ni and Co catalysts for H₂ generation and covalent Si-C/C-C attachment of transition metal complexes to silicon photoelectrodes.

University of California, Santa Cruz – Ph.D. Chemistry (2009). Bio-inorganic chemistry, Advisor: Prof Pradip Mascharak. *a)* Syntheses, structures, and biological utility of ruthenium-based NO donors derived from carboxamide ligands and coordinated chromophores. *b)* Synthetic modeling of iron-containing nitrile hydratase: photoregulation of carboxamide/thiolate Fe-active site by NO & effect of S-oxygenation on NO photolability.

Roche Pharmaceuticals (Palo Alto), Inflammatory and Viral Disease Unit (2000-2002) – Research Associate I (2000-2001) / Research Associate II (2001-2002). Drug discovery with purinergic (P₂Y₂/P₂Y₁) and muscarinic (M₁-M₅) G-protein coupled receptors: steady-state and kinetic inhibitors. Development of tissue culture assays for inflammatory mucin production (muc4/5/5ac). Mentor: Dave Swinney, Ph.D.

University of California, Davis – B.S. Fermentation Science (2000). This major incorporates basic and applied chemistry (analytical, organic and biochemistry) in biotechnology and food sciences.

Awards and Fellowships

Ed Stiefel Young Investigator Award & Lecture, Metals in Biology Gordon Conference, January 2017

Cottrell Scholar (2016): Heavy Atom Ligation & Undergraduate Outreach Corps

Teaching Excellence Award, College of Natural Sciences (2015): Teaching & Promoting Undergraduate Research

Office of Naval Research, Young Investigator (2013-2017): Hybrid Molecular/Materials Semiconductors

Ralph Powe Junior Faculty Enhancement Award (2013-2014): Synthetic Modeling of Mono-Iron Hydrogenase

NSF ACC-F Postdoctoral Fellowship (2010-2012): Attachment of Molecular H₂ Catalysts to Semiconductors

NSF/CCI-Solar Postdoctoral Fellowship (2009-2010): A Molecular All-Manganese Water-Splitting Cell

Chancellor's Dissertation Fellowship (2007-2008) UCSC, Thesis research support

Other Notable Funding

Welch Catalyst Grant (2024-2029, co-PI): Artificial Dinitrogen Transferase Enzymes (\$5M)

Keck Foundation (2019-2022, co-PI): Silicon Interfaces to Enable PDI Singlet Fission & Triplet Transfer (\$1M)

Lam Research Corporation (2015-2017): Electroless Metal Deposition on Semiconductor Substrates

Dreyfus Foundation Special Programs (2014-2018): *H₂ from H₂O*, Water-Splitting Outreach Program

Memberships

Subscribing member of American Chemical Society (ACS): Inorganic Division (2003-present)

Publications

	<u>Total</u>	<u>Last 5 Years</u>
<i>h</i>-index:	30	18
<i>i</i>10-index:	59	46
Citations:	2913	1083
Publications:	91	33

[Independent Career — In Revisions, Submitted or Substantially in Progress]

- 1) X. Chen, U. Braga, G. N. Ruiz, J. A. Smolen, K. Wilson, G. Yadav, S. Xiang, H. Kim, A. B. Braunschweig, M. J. Rose, S. T. Roberts and J. D. Batteas*. Substrate Surface Energy Dependent Morphology and Photoluminescence of 5,10,15,20-Tetrakis-(2,3,4,5,6 pentafluorophenyl) Porphyrin Nano-Assemblies. *To be submitted*.
- 2) G. N. Ruiz, S. Vasylevskiy, M. Aubrey and M. J. Rose*. The Real Structure of the First Synthetic Inorganic Compound, Prussian Blue, Revealed by Electron Diffraction Crystallography (MicroED). *To be submitted*.
- 3) A. T. Larson, S. Vasylevskiy, and M. J. Rose*. Distal Scaffold Dynamics Modulates Eyring Activation Parameters in Re(I) Substitution Reactions: A Case for Dynamics as the ‘Third Coordination Sphere’. *To be submitted*.
- 4) J. Labrecque, V. M. Lynch, D. K. McIntosh, J. Horseman and M. J. Rose*. Scaffold Flexibility Increases Biomimetic Reactivity in a Model of [Fe]-Hydrogenase: A Rationally Designed Synthetic Pscychrophile. *To be submitted*.
- 5) B. K. Cashman, R. Mondol, J. P. Shupp, J. Telser, J Krzystek and M. J. Rose*. Enhanced Easy Axis Magnetism in a Heavy Pnictogen (P→Bi) Co^I (*S* = 1) Series Featuring the First Covalent Bismuth-(3*d*)Metal Paramagnet. *To be submitted*.
- 6) C. Cobb and M. J. Rose*. An Authentic Iron-Carbide Cluster Featuring a Ferrous Site Supported by Multi-Phosphide and Hydride Ligation. *To be submitted*.
- 7) C. Joseph, E. J. Dick and M. J. Rose*. Structures, Reactivity and Formation Kinetics of the Fe₄Mo₂ Variant of the Interstitial Carbide Iron Carbonyl Clusters. *To be submitted*.
- 8) C. Cobb, R. K. Ngo, S. Vasylevskiy, J. Balderas, E. J. Dick and M. J. Rose*. Single-Step Access to Thiolate-Supported, Six-Iron Clusters with an Authentic Carbide: Utility of non-PSEPT Anionic Intermediate. *In Revisions at Inorg. Chem.*
- 9) B. R. Pollok, J. R. Brinker, S. G. Lewis, S. Daemi, S. T. Roberts, F. E. Osterloh, J. D. Eaves and M. J. Rose*. Tetracene Functionalized Si(111) Achieves Enhanced Solar to Chemical Energy Conversion with Defect Free TiO₂. *In Revisions*.
- 10) R. Mondol and M. J. Rose*. Antimony-Enhanced Magnetic Anisotropy in a Chelate-Supported Cobalt(II) Iodide: The Heavy Atom Effect. *In Revisions*.

[Independent Career — Published]

- 11) E. E. Stumbo[‡], S. T. Goralski[‡], P. R. Leclair, S. A. Kerns and M. J. Rose*. Two-Site Binding of a Dodecyl-Appended Rhenium Complex to Bovine β-Lactoglobulin. *J. Inorg. Biochem.* Accepted. [‡]equal authorship
- 12) H.-J. Kim and M. J. Rose*. Role of Interfacial Potential Drop on Redox-Couple Dependent Voltages using Hybridized Si(111)-Bis(Anthracene) Photoelectrodes. *ChemElectrochem* **2024**, *11*, e202400468.
- 13) T. Volek, M. A. Verkamp, G. N. Ruiz, A. J. Staat, B. C. Li, M. J. Rose, J. D. Eaves and S. T. Roberts. The Interplay of Singlet Fission and Structural Disorder Controls Triplet Exciton Transport in Ethylphenyl Perylenediimide Crystals. *J. Am. Chem. Soc.* **2024**, *146*, 29575-29587.
- 14) T. Ho, B. J. Lee, T. Buchanan, M. Heikes, R. Steinart, E. Milem, S. T. Goralski, Y.-N. Wang, S.-H. Lee, V. M. Lynch, M. J. Rose, K. Mitchell-Koch and K. Hull. Cu-Catalyzed Three-Component Alkene Carboamination: Insights and Rational Design to Overcome Limitations. *J. Am. Chem. Soc.* **2024**, 25176-25189.

- 15) C. Hallock and M. J. Rose*. Electrochemical Impedance of Well-Passivated Semiconductors Reveals Bandgaps, Fermi Levels & Interfacial Density of States. *J. Am. Chem. Soc.* **2024**, *146*, 18989-18998.
- 16) A. T. Larson, B. Boyle, J. Labrecque, A. Ly, C. Bui, S. Vasylevskiy and M. J. Rose*. Synthesis & Conformational Dynamics of Selenanthrene (Oxides): Establishing an Energetic Flexibility Index for Scaffolds. *Inorg. Chem.* **2024**, *63*, 10240-10250.
- 17) C. R. Cobb, E. J. Dick, K. Ngo and M. J. Rose*. Redox-Promoted Ligand Substitutions on $[\text{Fe}_6(\mu_6\text{-C})(\text{CO})_{16}]^{2-}$: Tripodal Phosphine Supported Iron-Carbide Clusters. *Chem. Sci.* **2024**, 11455-11471.
- 18) M. J. Rose and H. S. White. *Commentary*: Allen J. Bard: Electrochemist who Developed Scanning Electrochemical Microscopy. *Nature* **2024**, *629*, 285.
- 19) J. M. Strain[‡], G. N. Ruiz[‡], S. T. Roberts and M. J. Rose*. Substrate-Induced Thin-Film Crystal Phases of Perylenediimide (PDI): Thin Films on Methylated Silicon(111). *Langmuir* **2024**, *40*, 2519-2530. [‡]equal authorship
- 20) M. J. Rose*. *Perspective*: Semiconductor Band Structure, Symmetry and Molecular Interface Hybridization for the Chemist. *J. Am. Chem. Soc.* **2024**, *146*, 5735-5748.
- 21) J. Labrecque, Y.-I. Cho, F. Agboola, D. McIntosh and M. J. Rose*. Distal Scaffold Flexibility Accelerates Ligand Substitution Kinetics in Manganese(I) Tricarbonyls: Flexible Thianthrene vs Rigid Anthracene. *Dalton Trans.* **2023**, *52*, 4028-4037.
- 22) S. T. Goralski, K. M. Cid-Seara, J. J. Jarju, A. LaGrow, M. J. Rose* and L. M. Salonen*. Threefold Reactivity of a COF-Embedded Rhenium Catalyst: Reductive Etherification, Oxidative Esterification or Transfer Hydrogenation. *Chem. Commun.* **2022**, 12074-12077.
- 23) J. M. Gurrentz, K. A. Jarvis, I. R. Gearba-Dolocan and M. J. Rose*. Atomic Layer Deposited Al_2O_3 as a Protective Overlayer for Focused Ion Beam Preparation of Plan-View STEM Samples. *Ultramicroscopy* **2022**, 113562.
- 24) W. V. Taylor, B. K. Cashman, Z.-L. Xie, K. K. Ngo and M. J. Rose*. Synthesis and Magnetic Properties of Antimony-Ligated Co(II) Complexes: Stibines versus Phosphines. *Inorg. Chem.* **2022**, *61*, 6733-6741.
- 25) S. T. Goralski and M. J. Rose*. Emerging Artificial Metalloenzymes Asymmetric Hydrogenation Reactions. *Curr. Opin. Chem. Biol.* **2021**, 102096.
- 26) S. A. Kerns[#], J. Seo[#], V. M. Lynch, J. Shearer, S. T. Goralski, E. R. Sullivan and M. J. Rose*. Scaffold-based [Fe]-Hydrogenase Model: H_2 Activation Initiates Fe(0)-hydride Extrusion and Non-biomimetic Hydride Transfer. *Chem. Sci.* **2021**, 12838-12846. [#]Equal contributions
- 27) J. M. Gurrentz and M. J. Rose*. Covalent Attachment of Polyoxometalates to Passivated Si(111) Substrates: A Stable and Electronic Defect-Free Si|POM Platform. *J. Phys. Chem. C.* **2021**, *125*, 14287-14298.
- 28) D. G. Boucher, K. L. Kearney, E. Ertekin and M. J. Rose*. Tuning *p*-Si(111) Photovoltage via Molecule|Semiconductor Electronic Coupling. *J. Am. Chem. Soc.* **2021**, *143*, 2567-2580.
- 29) C. Joseph, C. R. Cobb and M. J. Rose*. Single-Step Insertion of Sulfides and Thiolate into Iron Carbide-Carbonyl Clusters: Unlocking the Synthetic Door to FeMoco Analogues. *Angew. Chem. Intl. Ed.* **2021**, *133*, 3475-3479.
- 30) C. Joseph, J. P. Shupp, C. R. Cobb and M. J. Rose*. Construction of Synthetic Models for Nitrogenase Relevant Ni_2Fe Biogenesis Intermediates and Iron-Carbide-Sulfide Clusters. *Catalysts* (Bio-Inorganic Special Edition) **2020**, *10*, 1317.
- 31) S. A. Kerns and M. J. Rose*. Scaffold-based Functional Models of [Fe]-Hydrogenase: Building the Bridge between Biological Structure and Molecular Function. *Acc. Chem. Res.* **2020**, *53*, 1637-1647.
- 32) M. J. Rose*. [Fe]-Hydrogenase (Hmd): Insights from Enzyme Structure, Spectroscopy and Synthetic Models. *Comprehensive Coordination Chemistry III* **2020**.
- 33) J. M. Gurrentz and M. J. Rose*. Non-Catalytic Benefits of Ni(II) Binding to an Si(111)-PNP Construct for Photoelectrochemical Hydrogen Evolution: Metal Ion Induced Flat Band Potential Modulation. *J. Am. Chem. Soc.* **2020**, *142*, 5657-5667.

- 34) R. T. Perarek, D. G. Boucher, N. R. Neale and M. J. Rose*. Energetic Tug-of-War between Pt and Leaky TiO₂: Positive and Negative Effects on the Function of Molecularly Modified p-Si(111)|TiO₂|Pt Photocathodes. *ChemElectroChem* **2020**, *7*, 1048-1056.
- 35) S. T. Goralski, T. A. Manes, S. E. A. Lumsden, V. M. Lynch and M. J. Rose*. Divergent Solution and Solid State Structures of Mono- and Dinuclear Nickel(II) Pyridone Complexes. *Organometallics* **2020**, *39*, 1070-1079.
- 36) Z.-L. Xie, W. Chai, S. A. Kerns, G. A. Henkelman and M. J. Rose*. Bio-inspired CNP Iron(II) Pincer Relevant to [Fe]-Hydrogenase: Effect of Dicarbonyl versus Monocarbonyl Motifs in H₂ Activation and Transfer Hydrogenation. *Inorg. Chem.* **2020**, *59*, 2548-2561.
- 37) J. P. Shupp and M. J. Rose*. Facile Hydrogen Atom Abstraction and Sulfide Formation from a Methyl-Thiolate Capped Iron-Sulfur-Carbonyl Cluster. *Dalton Trans.* **2020**, *49*, 23-26
- 38) B. K. Cashman, K. M. Sandmann and M. J. Rose*. Isolation and X-Ray Structure of Dialkylbismuth(III) Iodo 'Nanosquare': Breaking the Mold of Polymeric R₂BiX. *Inorg. Chem.* **2019**, *58*, 13751-13754.
- 39) J. McGale, G. E. Cutsail III, C. Joseph, M. J. Rose and S. DeBeer*. Spectroscopy and Mössbauer Characterization of M₆ and M₅ Iron(Molybdenum) Carbide Clusters: High Carbide-Iron Covalency Enhances Local Iron Site Electron Density Despite Oxidation. *Inorg. Chem.* **2019**, *58*, 12918-12932
- 40) Y. I. Cho, G. Durgaprasad and M. J. Rose*. Unexpected Facial Ligation in a CNP Iron(II) 'Pincer' and the Consistent Role of Methenyl(acyl) Unit as a Pendant Base in H₂ Heterolysis in Model Complexes of Mono-Iron Hydrogenase (Hmd). *Inorg. Chem.* **2019**, *58*, 12689-12699.
- 41) W. V. Taylor, C. X. Cammack, S. A. Shubert and M. J. Rose*. Thermoluminescent Antimony-Supported Copper-Iodo Cuboids: Approaching NIR Emission via High Crystallographic Symmetry. *Inorg. Chem.* **2019**, *58*, 16330-16345. *Invited Complementary Front Cover; Editors Choice ACS 365*
- 42) D. G. Boucher, J. R. Speller, R. Han, F. E. Osterloh and M. J. Rose*. Decoupling Effects of Surface Recombination and Barrier Height on p-Si(111) Photovoltage in Semiconductor|Liquid Junctions via Molecular Dipoles and Metal Oxides. *ACS Appl. Energy Mater.* **2019**, *2*, 66-79.
- 43) R. T. Pekarek, K. L. Kearney, B. M. Simon, E. Ertekin, A. Rockett and M. J. Rose*. Identifying Charge Transfer Mechanisms at Semiconductor Heterojunctions with Molecular Surface Dipoles and Multiscale Computational Modeling. *J. Am. Chem. Soc.* **2018**, *140*, 13223-13232.
- 44) J. Imbrogno, R. C. Ferrier Jr, B. K. Wheatle, M. J. Rose, N. Lynd*. Decoupling Catalysis and Chain-Growth Functions of Mono(μ -alkoxo)-Di(alkylaluminums) in Epoxide Polymerization: Emergence of the N/Al Adduct Catalyst. *ACS Catalysis* **2018**, *8*, 8796-8803.
- 45) Z.-L. Xie, D. L. Pennington, D. G. Boucher, J. Lo and M. J. Rose*. Effects of Thiolate Ligation in Mono-Iron Hydrogenase (Hmd): Stability of the {Fe(CO)₂}²⁺ Core with NNS Ligands. *Inorg. Chem.* **2018**, *57*, 10028-10039.
- 46) W. V. Taylor, Z.-L. Xie, N. I. Cool, S. A. Shubert and M. J. Rose*. Syntheses, Structures and Characterization of Nickel(II) Stibines: Steric and Electronic Rationale for Metal Deposition. *Inorg. Chem.* **2018**, *57*, 10364-10374.
- 47) R. T. Pekarek, A. L. Bleier, E. R. Sullivan, E. A. Bevan, O. Ursi, T. H. Rose and M. J. Rose*. H₂fromH₂O: A Water-Splitting Kit with Instructional Applications in Secondary Education. *J. Lab. Chem. Ed.* **2018**, *6*, 47-59.
- 48) R. T. Pekarek, H. Celio and M. J. Rose*. Synthetic Insights into Surface Functionalization of Si(111)-R Photoelectrodes: Steric Control and Deprotection of Molecular Passivating Layers. *Langmuir* **2018**, *34*, 6328-6327.
- 49) S. Kerns, A.-C. Magtaan, P. Vong and M. J. Rose*. Functional Hydride Transfer by a Thiolate-Containing Model of Mono-Iron Hydrogenase featuring an Anthracene Scaffold. *Angew. Chem. Int. Ed.* **2018**, *57*, 2855-2858.
- 50) C. Joseph, S. Kuppaswamy, V. M. Lynch and M. J. Rose*. Fe₅Mo Cluster with Iron-Carbide and Molybdenum-Carbide Bonding Motifs: Structure and Selective Alkyne Reductions. *Inorg. Chem.* **2018**, *57*, 20-23.
- 51) D. W. Redman, M. J. Rose and K. J. Stevenson*. Electrodeposition of Amorphous Molybdenum Chalcogenides from Ionic Liquids and Their Activity for the Hydrogen Evolution Reaction. *Langmuir* **2017**, *33*, 9354-9360.

- 52) 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.
- 53) J. Seo, T. E. Sotman, E. Sullivan, B. D. Ellis, T. Phung and M. J. Rose*. Structural and Electronic Modification of Pyridones and Pyrones via Regioselective Bromination and Trifluoromethylation. *Tetrahedron.* **2017**, *73*, 4519-4528.
- 54) J. P. Shupp, A. R. Rose and M. J. Rose*. Synthesis and Interconversions of Reduced, Alkali-Metal Supported Iron-Sulfur-Carbonyl Complexes. *Dalton Trans.* **2017**, *46*, 9163-9171.
- 55) T. A. Manes and M. J. Rose*. Rigid Scaffolds for the Design of Molecular Catalysts and Biomimetic Active Sites: A Case Study of Anthracene-based Ligands for Modeling Mono-Iron Hydrogenase (Hmd). *Coord. Chem. Rev.* **2017**, *353*, 295-308.
- 56) S. Kuppuswamy, J. D. Wofford, C. Joseph, Z.-L. Xie, A. K. Ali, V. M. Lynch, P. A. Lindahl, and M. J. Rose*. Structures, Interconversions and Spectroscopy of Carbonyl Clusters with an Interstitial Carbide: Localized Metal Center Reduction via Cluster Oxidation. *Inorg. Chem.* **2017**, *56*, 5998-6012.
- 57) J. Seo, T. A. Manes and M. J. Rose*. Structural & Functional Synthetic Model of Mono-Iron Hydrogenase Featuring an Anthracene Scaffold. *Nature Chem.* **2017**, *9*, 552-557.
- 58) H. J. Kim, K. L. Kearney, L. H. Le, Z. J. Haber, A. A. Rockett and M. J. Rose*. Charge-Transfer through Ultrathin Film TiO₂ on *n*-Si(111) Photoelectrodes: Experimental and Theoretical Investigation of Electric Field-Enhanced Transport with a Non-Aqueous Redox Couple. *J. Phys. Chem. C* **2016**, 25697-25708.
- 59) Y. I. Cho, M. L. Ward and M. J. Rose*. Substituent Effects of N4 Schiff Base Ligands on the Formation of Fluoride-Bridged Dicobalt(II) Complexes via B-F Abstraction: Structures and Magnetism. *Dalton Trans.* **2016**, *45*, 13466-13476.
- 60) T. A. Manes and M. J. Rose*. Mono- and Dinuclear Manganese Carbonyls Supported by Novel 1,8-Disubstituted (L = Py, S^{Me}, SH) Anthracene Ligand Scaffolds. *Inorg. Chem.* **2016**, *55*, 5127-5138.
- 61) O. M. Williams, J. W. Shi and M. J. Rose*. Photoelectrochemical Study of *p*-GaP(100)|ZnO|Au-NP Devices: Strategies for Enhanced Electron Transfer and Aqueous Catalysis. *Chem. Commun.* **2016**, *52*, 9145-9148.
- 62) W. V. Taylor, U. H. Soto, V. M. Lynch and M. J. Rose*. Antimony-Supported Cu₄I₄ Cuboid with Short Cu-Cu Bonds: Structural Basis for Far-Visible/NIR Thermoluminescence. *Inorg. Chem.* **2016**, *55*, 3206-32087.
- 63) D. R. Redman, H. J. Kim, K. J. Stevenson and M. J. Rose*. Photo-Assisted Electrodeposition of MoS_x from Ionic Liquid on Organic-Functionalized Silicon Photoelectrodes for H₂ Generation. *J Mater. Chem. A* **2016**, 7027-7035.
- 64) 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.
- 65) H. J. Kim, J. Seo and M. J. Rose*. H₂ Photogeneration Using a Phosphonate-Anchored Ni-PNP Catalyst on a Band-Edge-Modified *p*-Si(111)|AZO Construct. *ACS Appl. Mater. Interfaces* **2016**, *8*, 1061-1066.
- 66) T. A. Manes and M. J. Rose*. Redox Properties of a Bis-pyridine Rhenium Carbonyl Derived from an Anthracene Scaffold. *Inorg. Chem. Commun.* **2015**, *61*, 221-224.
- 67) F. Li, V. M. Basile and M. J. Rose*. Electron Transfer through Surface-Grown, Ferrocene-Capped Oligophenylene Molecular Wires (5–50 Å) on *n*-Si(111) Photoelectrodes. *Langmuir*, **2015**, *31*, 7712-7716.
- 68) J. Seo, R. T. Pekarek and M. J. Rose*. Photoelectrochemical Operation of a Surface-Bound, Nickel Phosphine H₂ Evolution Catalyst on *p*-Si(111): A Molecular Semiconductor|Catalyst Construct. *Chem. Commun.* **2015**, *51*, 13264-13267.
- 69) O. M. Williams, A. H. Cowley and M. J. Rose*. Structural and Electronic Characterization of Multi-Electron Reduced Naphthalene(BIAN)-Cobaloximes. *Dalton. Trans.* **2015**, *44*, 13017-13029.
- 70) H. J. Kim, K. L. Kearney, L. H. Le, R. T. Pekarek and M. J. Rose*. Platinum-Enhanced Electron Transfer and Surface Passivation through Ultrathin Film Aluminum Oxide (Al₂O₃) on Si(111)-CH₃ Photoelectrodes. *ACS Appl. Mater. Intfc.* **2015**, *7*, 8572-8584.
- 71) J. Seo, H. J. Kim, R. T. Pekarek and M. J. Rose*. Hybrid Organic/Inorganic Band-Edge Modulation of *p*-Si(111) Photoelectrodes: Effects of R, Metal Oxide and Pt on H₂ Generation. *J. Am. Chem. Soc.* **2015**, *137*, 3173-3177.

- 72) K. A. Thomas Muthia, G. Durgaprasad, C. Joseph, V. M. Lynch and M. J. Rose*. Mononuclear Iron(II) Dicarbonyls Derived from NNS Ligands – Structural Models Related to a ‘Pre-Acyl’ Active Site of Mono-Iron (Hmd) Hydrogenase. *Eur. J. Inorg. Chem.* **2015**, 1675-1691.
- 73) F. Li, V. M. Basile, R. T. Pekarek and M. J. Rose*. Steric Spacing of Molecular Linkers on Passivated Si(111) Photoelectrodes. *ACS Appl. Mater. Interfaces* **2014**, *6*, 20557-20568.
- 74) J. Seo, A. K. Ali and M. J. Rose*. Novel Ligand Architectures for Metalloenzyme Modeling: Anthracene-based Ligands for Synthetic Modeling of Mono-[Fe] Hydrogenase. *Comments Inorg. Chem.* **2014**, *34*, 103-113.
- 75) S. E. A. Lumsden, G. Durgaprasad, Z.-L. Xie, O. M. Williams, K. A. Thomas Mutiah and M. J. Rose*. Tuning Coordination Modes of Pyridine/Thioether Schiff Base (NNS) Ligands to Mononuclear Manganese Carbonyls. *Dalton Trans.* **2014**, *43*, 10725.
- 76) Y. I. Cho, D. M. Joseph and M. J. Rose*. ‘Criss-Crossed’ Dinucleating Behavior of an N4 Schiff Base Ligand: Formation of a μ -OH, μ -O₂ Dicobalt(III) Core via O₂ Activation. *Inorg. Chem.* **2013**, *52*, 13298-13300.

[Postdoctoral]

- 77) J. R. McKone, S. Ardo, J. D. Blakemore, P. J. Bracher, J. L. Dempsey, T. V. Darnton, M. C. Hansen, W. H. Harman, M. J. Rose, M. G. Walter, S. Dasgupta, J. R. Winkler, and H. B. Gray*. The Solar Army: A Case Study in Outreach Based on Solar Photoelectrochemistry. *Rev. Adv. Sci. Eng.* **2014**, *3*, 288-303.
- 78) L. E. O’Leary, M. J. Rose, T. X. Ding, E. Johansson, B. S. Brunschwig and N. S. Lewis*. Heck Couplings of Small Molecules to Mixed Methyl/Thienyl Monolayers at Low Defect Density Si(111). *J. Am. Chem. Soc.* **2013**, *135*, 10081.
- 79) M. J. Rose, J. R. Winkler and H. B. Gray*. Hydrogen Generation Catalyzed by Fluorinated Diglyoxime-Iron Complexes at Low Overpotentials. *J. Am. Chem. Soc.* **2012**, *134*, 8310.
- 80) M. J. Rose, J. R. Winkler and H. B. Gray*. Four-Iron Cluster and a Buckled Macrocyclic Complex from Reduction of [(dmgBF₂)Fe(L)₂] (L = MeCN, ^tBuNC). *Inorg. Chem.* **2012**, *51*, 1980.
- 81) M. J. Rose, D. E. Bellone and H. B. Gray*. Spectroscopic and Magnetic Characterization of an Iodo Co(I) Tripodal Phosphine Complex. *Dalton Trans.* **2012**, *41*, 11788.
- 82) Q. Dong, M. J. Rose*, W.-Y. Wong* and H. B. Gray*. Dual Coordination Modes of Ethylene Linked NP2 Ligands with Cobalt(II) and Nickel(II) Iodides. *Inorg. Chem.* **2011**, *50*, 10213.

[Graduate]

- 83) M. J. Rose, N. M. Betterley, A. Oliver, and P. K. Mascharak*. Binding and Photorelease of Nitric Oxide (NO) to a Synthetic Model of Iron-Containing Nitrile Hydratase (Fe-NHase). *Inorg. Chem.* **2010**, *49*, 1854-1864.
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[Industry]

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Funding

Pending

Department of Energy, Basic Energy Sciences

Solar Photochemistry \$575,000 (PI) 2025-2028

Insights to Facet-Selective Charge Transfer from Semiconductor Planewave Symmetry and Molecular Hybridization

National Science Foundation(CHE) \$525,000 (PI) 2025-2028

Flexible Scaffolds & Protein Host for [Fe]-Hydrogenase and FeMoco Mimics: Dynamics as the Thematic 'Third Coordination Sphere'

Welch Foundation \$300,000 (PI) 2025-2028

Harnessing the Extreme Spin-Orbit Coupling of Bismuth: Bi-3d(Metal) Complexes for Unique Magnetic & Spectroscopic Properties

Current

Welch Foundation

Catalyst Grant Program \$5,000,000 2024-2029

Rose Portion \$1,000,000

Artificial Dinitrogen Transferase Enzymes

Department of Energy, Basic Energy Sciences

Solar Photochemistry \$475,000 (PI) 2022-2025

Elucidating Design Principles of Semiconductor|Molecule Electronic Coupling for Improved Photoelectrochemical Function

National Science Foundation(CHE) \$450,000 (PI) 2021-2025 (NCE)

Scaffold-based Biomimetics of Fe-Hydrogenase and Nitrogenase (FeMoco): Interrogating Dynamics, Protein Matrix Effects, and Carbide Motifs

Welch Foundation \$300,000 (PI) 2022-2025

Elucidating Design Principles for Semiconductor | Molecule Electronic Coupling

CNS Spark Grant \$200,000 (PI) 2022-2025

Heavy-Atom (Bismuth) Ligation to 3d Metals for Molecular Magnets and Data Storage

Past Major Grants

Welch Foundation

WelchX Collaborative Grant \$100,000 2023-2024

Rose Portion: \$45,000

Detection & Extraction of Hot Carriers in Silicon by Ultrafast Electron Diffraction

W.M. Keck Foundation \$1,000,000 (co-PI) 2019-2023

Rose Portion: \$400,000

Uncovering Design Principles for Energy Transfer across Organic | Inorganic Interfaces

Welch Foundation \$240,000 (PI) 2019-2022

Earth Abundant Elements for Energy-Related Energy Conversions

National Science Foundation \$420,000 (PI) 2018-2021

Scaffold-based Synthetic Models of Mono-Iron Hydrogenase: Structure and Dynamics

Welch Foundation \$240,000 (PI) 2016-2019

Earth Abundant Metal Catalysts for Energy-Related Chemical Transformations

Cottrell Scholar (RCSA) \$100,000 (PI) 2015-2017

Imparting Precious Metal Properties to First-Row Metals with Heavy Atom Ligands, and Connecting Undergraduates to Outreach Activities via 'Undergraduate Outreach Corps'

Office of Naval Research \$540,000 (PI) 2013-2017

A Hybrid Molecular/Materials Approach to Semiconductor Surface Passivation and Catalyst Attachment for a Solar Fuels Device

Welch Foundation \$180,000 (PI) 2013-2016

Imparting Precious Metal Properties to First-Row Metals for C-H Activation: Ligation to Inexpensive, Heavy Main Group Donors

ACS Petroleum Research Fund \$100,000 (PI) 2013-2016

Imparting Precious Metal Properties to First-Row Metals for C-H Activation: Ligation to Inexpensive, Heavy Main Group Donors

Dreyfus Foundation \$25,000 (PI) 2013-2016

H₂fromH₂O: A Water-Splitting Outreach Kit for High School Chemistry Instructors

Teaching Experience

UT Austin (Instructor)

Inorganic Chemistry, CH 431 (2019-present). Undergraduate Junior-level Inorganic Chemistry

Materials Chemistry, CH XXX (2018-19). Co-listed Grad/UG course in Materials, Crystalline and Nano Chemistry

Organometallics & Catalysis, CH XXX (2015, 2017) Co-listed Grad/UG course in modern catalysis

Bio-Inorganic Chemistry, CH XXX (2014-2018, 2020, 2024) Graduate course for biological inorganic chemistry and spectroscopy

Advanced Inorganic Lab Techniques, CH 341 (need-to-check). Upper division undergraduate laboratory

Advanced Group Theory Seminar (Spring 2020). Informal advanced topics in group theory (1×/week)

UC Santa Cruz (TA)

Advanced Inorganic Chemistry Laboratory. Syntheses and characterization of metal complexes

Instrumental Analysis. Analytical principles and instrumental analysis

Organic Chemistry. Organic chemistry lab

General Chemistry. General chemistry, lab and lecture

Science in the Community | Outreach

Undergraduate Outreach Corps (2016-present): Funded by Research Corporation for Scientific Advancement, this program aims to involve undergraduates in department-wide (and eventually college-wide) outreach activities.

H₂fromH₂O, (2010-present): Funded by Dreyfus Foundations and initiated with an NSF ACC/F postdoctoral fellowship. A water-splitting outreach program designed to engage students in chemistry at the middle school and high school level. The program has partnered with organizations such as GirlStart, UTeach and Hot Science Cool Talks (UT).

Pasadena High School, (2010-2012): After-school outreach program with 4-6 HS students using SHArK Kit for discovery of novel mixed metal oxides for photochemical water splitting.

Pasadena High School, (2010-2012): In-class outreach program consisting of laboratory exercises in electrochemical water-splitting to H₂ and O₂ using electrodes and solar hobby kits.

Muir High School in Pasadena, (2009-2010): outreach program consisting of laboratory exercises in light absorption, solar energy and assembling blackberry TiO₂ solar cells.

Santa Cruz County Science Fair, (Judge, Chemistry and Biochemistry; 2008)

Santa Cruz County Science Fair, (Judge, Biology and Biochemistry; 2007)