

# Hannah S. Shafaat

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## Education

- 2011:** Ph.D., *University of California at San Diego (UCSD)*, Chemistry  
Thesis: Spectroscopy and dynamics of amino acid radical intermediates in electron transfer processes  
Advisor: Professor Judy E. Kim
- 2008:** M.S., *University of California at San Diego (UCSD)*, Chemistry
- 2006:** B.S., *California Institute of Technology (Caltech)*, Chemistry, with honors  
Advisor: Professor Harry B. Gray and Dr. Adrian Ponce (*Jet Propulsion Laboratory*)

## Professional Experience

- 2019 – present:** Associate Professor, Department of Chemistry and Biochemistry  
*The Ohio State University (OSU), Columbus, OH, USA*
- 2013 – 2019:** Assistant Professor, Department of Chemistry and Biochemistry  
*The Ohio State University (OSU), Columbus, OH, USA*
- 2011 – 2013:** Alexander von Humboldt Postdoctoral Fellow  
*Max Planck Institute for Chemical Energy Conversion,  
Mülheim an der Ruhr, Germany*
- Projects: Characterization of [NiFe] and [NiFeSe] hydrogenases and models, Mn/Fe oxidases  
Advisor: Director Wolfgang Lubitz

## Honors and Awards

- 2019:** Kavli Fellow (*Korean-American Kavli Frontiers of Science Symposium*)
- 2019:** Selected for *JACS Young Investigators Virtual Issue*
- 2019:** Ed Stiefel Young Investigator Award (*Metals in Biology GRC*)
- 2018:** National Institutes of Health R35 MIRA Award for New and Early Stage Investigators
- 2018:** Alfred P. Sloan Research Fellow in Chemistry
- 2018:** OSU University Laboratory Safety Committee Excellence in Safety Award
- 2017:** Department of Energy Office of Science Early Career Award
- 2017:** Selected for *ACS Select Virtual Issue on Engineered Biomolecular Catalysts*
- 2015:** National Science Foundation CAREER Award
- 2015:** Selected for *ACS Select Virtual Issue on Emerging Investigators in Bioinorganic Chemistry*
- 2014:** OSU Biophysics Program Plenary Faculty Speaker

### *Prior to appointment at OSU:*

- 2012:** Young Researcher Participant at 62<sup>nd</sup> Lindau Nobel Laureate Meeting
- 2011:** Alexander von Humboldt Postdoctoral Research Fellowship recipient
- 2007:** NDSEG Fellowship recipient
- 2007:** NSF Graduate Research Fellowship recipient
- 2006:** Richard P. Schuster award for excellence in Chemistry, Caltech

## Professional Activities

- 2022:** Chair, Bioinorganic Subcommittee, *American Chemical Society*, Division of Inorganic Chemistry
- 2021:** Chair-Elect, Bioinorganic Subcommittee, *American Chemical Society*, Division of Inorganic Chemistry
- 2020 – 2022:** Editorial Advisory Board, *Inorganic Chemistry*
- 2017 – 2019:** *National High Magnetic Field Laboratory* User Program Advisory Committee (EMR Sub-committee)
- 2016 – 2019:** *American Society for Biochemistry and Molecular Biology* Membership committee

<b>2016 – 2018:</b>	American Chemical Society Division of Inorganic Chemistry Alternate Councilor
<b>2019:</b>	DOE Basic Energy Sciences (BES) Roundtable on Liquid Solar Fuels Participant
<b>2017:</b>	DOE Bioenergy Technologies Office (BETO) Engineered Carbon Reduction Workshop Participant
<b>2015 – present:</b>	Chemistry Women Mentorship Network Faculty ChemWMN mentor
<b>2017 – present:</b>	OSU NIH Molecular Biophysics Training Program
<b>2013 – 2017:</b>	OSU NIH Chemistry-Biology Interface Training Program
<b>2016:</b>	NSF Mid-Scale Workshop for Instrument Development in Chemistry
<b>2015:</b>	ACS Postdoc-to-Faculty Workshop Faculty Mentor and Panelist
<b>2016 – 2019:</b>	Proposal Reviewer for NRC Research Associateship Program
<b>Ongoing</b>	Proposal Reviewer for NSF, DOE, NIH, ACS PRF, Swiss National Science Foundation, Swedish Energy Agency, Ohio Cancer Society, SSRL, OSU Institute for Materials Research Seed Grant Program
	Paper Reviewer for <i>Science</i> , <i>PNAS</i> , <i>JACS</i> , <i>Nature Chemistry</i> , <i>Nature Catalysis</i> , <i>Nature Chemistry Reviews</i> , <i>Chem. Rev.</i> , <i>Acc. Chem. Res.</i> , <i>Inorg. Chem.</i> , <i>JPC A</i> , <i>JPC B</i> , <i>ACS Catal.</i> , <i>Chem. Sci.</i> , <i>Biochemistry</i> , <i>ChemBioChem</i> , <i>ChemPlusChem</i> , <i>ChemComm</i> , <i>CHEM</i> , <i>Chem. Phys. Lett.</i> , <i>Dalton Trans.</i> , <i>J. Inorg. Biochem.</i> , <i>Biophys. J.</i> , <i>Inorg. Chim. Acta</i> , <i>Angew. Chem. Int. Ed.</i>

### Independent Publications

Key to contributors: †Undergraduate student, §Graduate student, &Postdoctoral scholar, @Collaborator, #Equal contribution, \*Corresponding author

32. Treviño, R. E.; § **Shafaat, H.S.**\* Protein-based models offer mechanistic insight into complex nickel metalloenzymes. *Curr. Opinion in Chemical Biology* **2022**, 67, 102110. DOI: 10.1016/j.cbpa.2021.102110.
31. Tao, W.; @ Yerbulekova, A.; § Moore, C.; @ **Shafaat, H.S.**;\* Zhang, S.\* @ Controlling the direction of S-nitrosation vs. denitrosation: reversible cleavage and formation of S-N bond within a dicopper center. *J. Am. Chem. Soc.*, just accepted.
30. **Shafaat, H.S.**\*, Yang, J.Y.\* @ Uniting Biological and Chemical Strategies for Selective CO<sub>2</sub> Reduction. *Nature Catalysis* **2021**, 4, 928-933. DOI: 10.1038/s41929-021-00683-1.
29. Wang, H.; @ Cleary, M. B.; @ Lewis, L. C.; § Bacon, J. W.; @ Caravan, P.; @ **Shafaat, H. S.**; Gale, E. M.\* @ Enzyme Control Over Ferric Iron Magnetostructural Properties. *Angewandte Chemie International Edition* **2021** DOI: 10.1002/anie.202114019.
28. Lewis, L.C.; § **Shafaat, H.S.**\* Reversible electron transfer and substrate binding support [NiFe<sub>3</sub>S<sub>4</sub>] ferredoxin as a protein-based model for [NiFe] carbon monoxide dehydrogenase. *Inorg. Chem.* **2021**, 60 (18), 13869-13875. DOI: 10.1021/acs.inorgchem.1c01323. **\*Featured in Forum Issue on Small Molecule Activation Reactions.**
27. Naughton, K. J.; † Treviño, R. E.; § Moore, P. J.; † Wertz, A. E.; § Dickson, J. A.; † Shafaat, H. S.\* *In Vivo* Assembly of a Genetically Encoded Artificial Metalloenzyme for Hydrogen Production. *ACS Synthetic Biology* **2021**, 10 (8) 2116-2120. DOI: [10.1021/acssynbio.1c00177](https://doi.org/10.1021/acssynbio.1c00177).
26. Gardner, E.J.; @ Marguet, S.C.; § Cobb, C.R.; @ Pham, D.M.; @ Beringer, J.A.M.; @ Bertke, J.A.; @ **Shafaat, H.S.**\*; Warren, T.H.\* @ Uncovering Redox Non-Innocent H-Bonding in Cu(I)-Diazene Complexes. *J. Am. Chem. Soc.* **2021**, 143 (39), 15960-15974. DOI: 10.1021/jacs.1c04108.
25. Nichols, A. W.; @ Cook, E. N.; @ Gan, Y. J.; § Miedaner, P. R.; @ Dressel, J. M.; @ Dickie, D. A.; @ **Shafaat, H. S.**; Machan, C. W. @\* Pendent Relay Enhances H<sub>2</sub>O<sub>2</sub> Selectivity during Dioxygen Reduction Mediated by Bipyridine-Based Co–N<sub>2</sub>O<sub>2</sub> Complexes. *J. Am. Chem. Soc.* **2021**, 143 (33), 13065-13073. DOI: [10.1021/jacs.1c03381](https://doi.org/10.1021/jacs.1c03381).
24. Kisgeropoulos, E.C.; § Manesis, A.C.; §# **Shafaat, H.S.**\* (2021) Ligand field inversion as a mechanism to gate bioorganometallic reactivity: Investigating a biochemical model of acetyl CoA synthase using spectroscopy and computation. *J. Am. Chem. Soc.*, 143 (2), 849-867. DOI: 10.1021/jacs.0c10135.
23. **Shafaat, H.S.**\* [NiFe] Hydrogenases: A Paradigm for Bioinorganic Hydrogen Conversion. In *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier. In press. DOI: 10.1016/B978-0-08-102688-5.00056-8 **\*Invited contribution.**
22. Treviño, R.E.; § Slater, J.W.; § **Shafaat, H.S.**\* (2020) Robust carbon-based electrodes for hydrogen evolution through site-selective covalent attachment of an artificial metalloenzyme. *ACS Applied Energy Materials*, 3 (11), 11099-11112. DOI: 10.1021/acsaem.0c02069.

21. Wang, H.; Wong, A.; Lewis, L.C.; Nemeth, G.; Jordan, V.C.; Bacon, J.; Caravan, P.; **Shafaat, H.S.**; Gale, E.M.\* (2020). Rational ligand design enables pH control over aqueous iron magnetostructural dynamics and relaxometric properties. *Inorg. Chem.*, 59 (23), 17712 – 17721. DOI: 10.1021/acs.inorgchem.0c02923.
20. Kisgeropoulos, E.C.; Griese, J.J.; Smith, Z.R.; Branca, R.M.M.; Schneider, C.R.; Högbom, M.; **Shafaat, H.S.**\* (2020). Key Structural Motifs Balance Metal Binding and Oxidative Reactivity in a Heterobimetallic Mn/Fe Protein. *J. Am. Chem. Soc.*, 142 (11), 5338–5354. DOI: 10.1021/jacs.0c00333.
19. Yu, Z.; Thompson, Z.; Behnke, S. L.; Fenk, K. D.; Huang, D.; **Shafaat, H. S.**; Cowan, J. A.\* Metalloglycosidase Mimics: Oxidative Cleavage of Saccharides Promoted by Multinuclear Copper Complexes under Physiological Conditions. *Inorg. Chem.* 2020, 59, 11218–11222. DOI: 10.1021/acs.inorgchem.0c01193.
18. Dhakal, S.\*; **Shafaat, H.S.**; Balasubramaniam, V. M.\* Thermal and high-pressure treatment stability of egg-white avidin in aqueous solution. *J. Food Proc. Eng.* 2020, 43, e13481. DOI: 10.1111/jfpe.13481
17. McGarry, K. G.\*; Lalis, R. F.\*; Moyer, R. A.\*; Johnson, K. M.\*; Tallan, A. M.\*; Winters, T. P.\*; Taris, J. E.\*; McElroy, C. A.\*; Lemmon, E. E.\*; **Shafaat, H. S.**; Fan, Y.\*; Deal, A.\*; Marguet, S.C.\*; Harvilchuck, J.A.\*; Hadad, C.M.\*; Wood, D.W.\* A Novel, Modified Human Butyrylcholinesterase Catalytically Degrades the Chemical Warfare Nerve Agent, Sarin (2020). *Toxicol Sci*, 174 (1), 133–146. DOI: 10.1093/toxsci/kfz251.
16. Marguet, S.C.\*; Stevenson, M.J.\*; **Shafaat, H.S.**\* (2019) Intramolecular Electron Transfer Governs Photoinduced Hydrogen Evolution by Nickel-Substituted Rubredoxin: Resolving Elementary Steps in Solar Fuel Generation. *J. Phys. Chem. B.*, 123 (46), 9792-9800. DOI: 10.1021/acs.jpcc.9b08048.
15. Schneider, C.R.\*; Lewis, L.C.\*; **Shafaat, H.S.**\* (2019) The good, the neutral, and the positive: buffer identity impacts CO<sub>2</sub> reduction activity by nickel(II) cyclam. *Dalton Trans.*, 48, 15810-15821. DOI: 10.1039/C9DT03114F. **\*Selected as Dalton Transactions HOT Article.**
14. Slater, J.W.\*; Marguet, S.C.\*; Gray, M.E.\*; Monaco, H.A.\*; Sotomayor, M.\*; **Shafaat, H.S.**\* (2019) The Power of the Secondary Sphere: Modulating Hydrogenase Activity in Nickel-Substituted Rubredoxin. *ACS Catalysis*, 9 (10), 8928-8942. DOI: 10.1021/acscatal.9b01720.
13. Manesis, A.C.\*; Musselman, B.W.\*; Keegan, B.\*; Shearer, J.\*; Lehnert, N.\*; **Shafaat, H.S.**\* (2019) A Biochemical Nickel(I) State Supports Nucleophilic Alkyl Addition: A Roadmap for Methyl Reactivity in Acetyl Coenzyme A Synthase. *Inorg. Chem.*, 58 (14), 8969-8982. DOI: 10.1021/acs.inorgchem.8b03546. **\*Selected as ACS Editor's Choice; \*Selected for Front Cover Feature; \*Selected for IC Virtual Issue on "Modern Spectroscopy in Inorganic Chemistry"**
12. Behnke, S.L.\*; Manesis, A.C.\*; **Shafaat, H.S.**\* (2018) Spectroelectrochemical investigations of nickel cyclam indicate different reaction mechanisms for electrocatalytic CO<sub>2</sub> and H<sup>+</sup> reduction. *Dalton Trans.*, 47, 15206-15216. DOI: 10.1039/C8DT02873G.
11. Slater, J.W.\*; Marguet, S.C.\*; Monaco, H.A.\*; **Shafaat, H.S.**\* (2018) Going beyond Structure: Nickel-Substituted Rubredoxin as a Mechanistic Model for the [NiFe] Hydrogenases. *J. Am. Chem. Soc.*, 140 (32), 10250-10262. DOI: 10.1021/jacs.8b05194.
10. Schneider, C.R.\*; Manesis, A.C.\*; Stevenson, M.J.\*; **Shafaat, H.S.**\* (2018) A Photoactive Semisynthetic Metalloenzyme Exhibits Complete Selectivity for CO<sub>2</sub> Reduction in Water. *Chem. Commun.* 54, 4681 - 4684. DOI: 10.1039/C8CC01297K.
9. Maugeri, P.T.\*; Griese, J.J.\*; Branca, R.\*; Miller, E.K.\*; Smith, Z.R.\*; Eirich, J.\*; Högbom, M.\*; **Shafaat, H.S.**\* (2018) Driving protein conformational changes with light: Photoinduced structural rearrangement in a heterobimetallic oxidase. *J. Am. Chem. Soc.* 140 (4), 1471-1480. DOI: 10.1021/jacs.7b11966. **\*Selected for 2019 JACS Young Investigator Virtual Issue.**
8. Stevenson, M.J.\*; Marguet, S.C.\*; Schneider, C.R.\*; **Shafaat, H.S.**\* (2017) Light-driven hydrogen evolution by nickel-substituted rubredoxin. *ChemSusChem*. 10 (22), 4424-4429. DOI: 10.1002/cssc.201701627.
7. Manesis, A. C.\*; O'Connor, M. J.\*; Schneider, C. R.\*; **Shafaat, H. S.**\* (2017) Multielectron Chemistry within a Model Nickel Metalloprotein: Mechanistic Implications for Acetyl-CoA Synthase. *J. Am. Chem. Soc.* 139 (30), 10328 - 10338. DOI: 10.1021/jacs.7b03892.
6. Miller, E. K.\*; Trivelas, N. E.\*; Maugeri, P. T.\*; Blaes, E. J.\*; **Shafaat, H. S.**\* (2017) Time-Resolved Investigations of Heterobimetallic Cofactor Assembly in R2lox Reveal Distinct Mn/Fe Intermediates. *Biochemistry* 56 (26), 3369–3379 DOI: 10.1021/acs.biochem.7b00403.
5. Slater, J. W.\*; Marguet, S. C.\*; Cirino, S. L.\*; Maugeri, P. T.\*; **Shafaat, H. S.**\* (2017) Experimental and DFT Investigations Reveal the Influence of the Outer Coordination Sphere on the Vibrational

- Spectra of Nickel-Substituted Rubredoxin, a Model Hydrogenase Enzyme. *Inorg. Chem.* 56 (7), 3926–3938 DOI: 10.1021/acs.inorgchem.6b02934. **\*Selected as feature article in ACS Select Virtual Issue on Engineered Biomolecular Catalysts.**
4. Schneider, C. R.,<sup>§</sup> **Shafaat, H. S.\*** (2016). An Internal Electron Reservoir Enhances Catalytic CO<sub>2</sub> Reduction by a Semisynthetic Enzyme. *Chem. Commun.* 52, 9889–9892. DOI: 10.1039/C6CC03901D.
  3. Behnke, S.L.,<sup>§</sup> **Shafaat, H.S.\*** (2016). Heterobimetallic Models of the [NiFe] Hydrogenases: A Structural and Spectroscopic Comparison. *Comments on Inorganic Chemistry*, 36 (3), 123-140. DOI:10.1080/02603594.2015.1108914. **\*Invited Review**
  2. Slater, J.W.,<sup>§</sup> **Shafaat, H.S.\*** (2015). Nickel-Substituted Rubredoxin as a Minimal Enzyme Model for Hydrogenase. *J. Phys. Chem. Lett.*, 6 (18), 3731-3736. DOI: 10.1021/acs.jpcclett.5b01750.
  1. Manesis, A.C.,<sup>§</sup> **Shafaat, H.S.\*** (2015). Electrochemical, Spectroscopic, and Density Functional Theory Characterization of Redox Activity in Nickel-Substituted Azurin: A Model for Acetyl-CoA Synthase. *Inorg. Chem.*, 54 (16), 7959-7967. DOI: 10.1021/acs.inorgchem.5b01103.

### **Publications Prior to OSU (†Publication after faculty appointment)**

22. Rivera, J.J., Liang, J.H., Shimamura, G.R., **Shafaat, H.S.**, Kim, J.E. (2019). Raman and Quantum Yield Studies of Trp48-d<sub>5</sub> in Azurin: Closed-Shell and Neutral Radical Species. *J. Phys. Chem. B*, 123 (30), 6430-6443. DOI: 10.1021/acs.jpcc.9b04655.†
21. Katz, S., Noth, J., Horch, M., **Shafaat, H.S.**, Happe, T., Hildebrandt, P., Zebger, I. (2016). Vibrational spectroscopy reveals the initial steps of biological hydrogen evolution. *Chem. Sci.*, 7, 6746-6752. DOI: 10.1039/C6SC01098A.†
20. Kutin, Y., Srinivas, V., Fritz, M., Kositzki, R., **Shafaat, H. S.**, Birrell, J., Bill, E., Haumann, M., Lubitz, W., Högbom, M., Griese, J. J., Cox, N. (2016). Divergent Assembly Mechanisms of the Manganese/Iron Cofactors in R2lox and R2c Proteins. *J. Inorg. Biochem.*, 162, 164–177. DOI: 10.1016/j.jinorgbio.2016.04.019.†
19. Hugenbruch, S.; **Shafaat, H. S.**; Krämer, T.; Delgado-Jaime, M. U.; Weber, K.; Neese, F.; Lubitz, W.; DeBeer, S. (2016). In Search of Metal Hydrides: An X-Ray Absorption and Emission Study of [NiFe] Hydrogenase Model Complexes. *Phys. Chem. Chem. Phys.*, 18 (16), 10688-10699. DOI: 10.1039/C5CP07293J.† **Featured Cover Article**
18. Rapatskiy, L. Ames, W.M. Perez-Navarro, M. Savitsky, A., Griese, J.J. Weyhermuller, T. **Shafaat, H.S.**, Högbom, M., Neese, F. Pantazis, D.A., Cox, N. (2015). Characterization of Oxygen Bridged Manganese Model Complexes using Multifrequency <sup>17</sup>O-hyperfine EPR Spectroscopies and Density Functional Theory. *J. Phys. Chem. B.*, 119 (43), 13904-13921. DOI: 10.1021/acs.jpcc.5b04614.†
17. Larson, B. C., Pomponio, J. R., **Shafaat, H. S.**, Kim, R. H., Leigh, B. S., Tauber, M. J., Kim, J. E. (2015). Photogeneration and quenching of tryptophan radical in azurin. *J. Phys. Chem. B.*, 119 (29), 9438–9449. DOI: 10.1021/jp511523z.†
16. **Shafaat, H. S.**, Griese, J. J., Pantazis, D. A., Roos, K., Andersson, C. S., Popović-Bijelić, A., Gräslund, A., Siegbahn, P. E. M., Neese, F., Lubitz, W., Högbom, M., Cox, N. (2014). Electronic structural flexibility of heterobimetallic Mn/Fe cofactors: R2lox and R2c proteins. *J. Am. Chem. Soc.*, 136 (38), 13399-13409. DOI: 10.1021/ja507435t.†
15. **Shafaat, H.S.**, Kim, J.E. (2014). Resonance Raman Analysis of the Tryptophan Cation Radical. *J. Phys. Chem. Lett.*, 5, 3009-3014. DOI: 10.1021/jz5012324.†
14. Riethausen, J., Rüdiger, O., Gaertner, W., Lubitz, W., **Shafaat, H.S.\*** (2013). Spectroscopic and electrochemical characterization of the [NiFeSe] hydrogenase from *Desulfobivrio vulgaris* Miyazaki F: Reversible redox behavior and interactions between electron transfer centers. *ChemBioChem*, 14, 1714-1719. DOI: 10.1002/cbic.201300120.
13. Griese, J.J., Roos, K., Cox, N., **Shafaat, H.S.**, Branca, R. M. M., Lehtiö, J., Gräslund, A., Lubitz, W., Siegbahn, P.E.M., Högbom, M. (2013). Direct observation of structurally encoded metal discrimination and ether bond formation in a heterodinuclear metalloprotein. *PNAS*, 110 (43), 17189-17194. DOI: 10.1073/pnas.1304368110.
12. **Shafaat, H.S.**, Rüdiger, O., Ogata, H., Lubitz, W. (2013). [NiFe] hydrogenases: a common active site for hydrogen metabolism in diverse environments. *BBA-Bioenergetics*, 1827, 986-1002. DOI: 10.1016/j.bbabi.2013.01.015.

11. **Shafaat, H.S.**, Weber, K., Petrenko, T., Neese, F., Lubitz, W. (2012). Key hydride vibrational modes in [NiFe] hydrogenase model compounds studied by resonance Raman spectroscopy and density functional calculations. *Inorg. Chem.*, 51, 11787-11797. DOI: 10.1021/ic3017276.
10. Weber, K., Kraemer, T., **Shafaat, H.S.**, Weyhermuller, T., Bill, E., van Gestel, M., Neese, F., Lubitz, W. (2012). A functional [NiFe]-hydrogenase model compound that undergoes biologically relevant reversible thiolate protonation. *J. Am Chem. Soc.*, 134, 20745-20755. DOI: 10.1021/ja309563p.
9. McLaughlin, M., Retegan, M., Bill, E., Payne, T., **Shafaat, H.S.**, Peña, S., Sudhamsu, J., Ensign, A., Crane, B., Neese, F., Holland, P. (2012). Azurin as a protein scaffold for a low-coordinate non-heme iron site with a small-molecule binding pocket. *J. Am. Chem. Soc.*, 134, 19746-19757. DOI: 10.1021/ja308346b.
8. Stoll, S., **Shafaat, H.S.**, Krzystek, J., Ozarowski, A., Tauber, M.J., Kim, J.E., Britt, R.D. (2011). Hydrogen bonding of tryptophan radicals revealed by EPR at 700 GHz. *J. Am Chem. Soc.*, 133, 18098-18101. DOI: 10.1021/ja208462t.
7. **Shafaat, H.S.**, Leigh, B.S., Tauber, M.J., Kim, J.E. (2010). Spectroscopic comparison of photogenerated tryptophan radicals in azurin: Effects of local environment and structure. *J. Am. Chem. Soc.*, 132, 9030-9039. DOI: 10.1021/ja101322g.
6. **Shafaat, H.S.**, Sanchez, K.M., Neary, T.J., Kim, J.E. (2009). Ultraviolet resonance Raman spectroscopy of a beta-sheet peptide: A model for membrane protein folding. *J. Raman Spectrosc.* 40, 1060-1064. DOI: 10.1002/jrs.2237.
5. **Shafaat, H.S.**, Leigh, B.S., Tauber, M.J., Kim, J.E. (2009). Resonance Raman Characterization of a Stable Tryptophan Radical in an Azurin Mutant. *J. Phys. Chem. B* 113 (1): 382-388. DOI: 10.1021/jp809329a.
4. Yung, P.T., **Shafaat, H.S.**, Connon, S.A., Ponce, A. (2007). Quantification of viable endospores from a Greenland ice core. *FEMS Microbial Ecology* 59 (2): 300-306. DOI: 10.1111/j.1574-6941.2006.00218.x.
3. Connon, S.A., Lester, E.D., **Shafaat, H.S.**, Obenhuber, D.C., Ponce, A. (2007). Bacterial diversity in hyperarid Atacama Desert soils. *J. Geophys. Res—Biogeosciences* 112 (G4): G04S17. DOI: 10.1029/2006JG000311.
2. **Shafaat, H.S.**, Ponce, A. (2006). Applications of a Rapid Endospore Viability Assay for Monitoring UV Inactivation and Characterizing Arctic Ice Cores. *Appl. Environ. Microbiol.* 72: 6808-6814. DOI: 10.1128/AEM.00255-06.
1. **Shafaat, H.S.**, Cable, M.L., Ikeda, M.K., Kirby, J.P., Pelletier, C.C., Ponce, A. (2005). Towards an *in situ* endospore detection instrument. Aerospace, 2005 IEEE Conference: 660-669.

## **External Support**

### **Current Research Support**

“Elucidating mechanisms of biological hydrogen conversion through model metalloenzymes”; NSF (CHE-2108684); Hannah S. Shafaat (PI); \$429,000 total direct and indirect costs; 10/1/2021 – 9/30/2024.

“NSF-DFG EChem: CAS: Mechanistic interrogation of electrocatalytic hydrogen evolution by an artificial hydrogenase”; NSF (CHE-2140211); Hannah S. Shafaat (Co-PI), Corinna Hess (Co-PI, Technical University of Munich), Olaf Rüdiger (Co-PI, Max Planck Institute for Chemical Energy Conversion); \$350,125 total direct and indirect costs; 12/1/2021 – 11/30/2024.

“Development of robust catalysts for sustainable H<sub>2</sub> evolution”; IIT Bombay-Ohio State Frontier Center; Arnab Dutta (PI, IITB), Hannah S. Shafaat (co-PI); \$18,000 total direct costs; 7/1/2021-6/30/2022.

“Bringing Inorganic Carbon to Life: Developing Model Metalloenzymes for C1 Conversion Reactions”; Department of Energy (DOE) Early Career Research Program Award (DE-SC0018020); Hannah S. Shafaat (PI); \$750,000 total direct and indirect costs; 9/1/2017 – 8/31/2022.

Alfred P. Sloan Research Fellowship 2018; Sloan Foundation; Hannah S. Shafaat (PI); \$65,000 total direct and indirect costs; 9/1/2018 – 8/31/2022 (Two-year no-cost extension granted).

“Metallobiochemistry of Mn/Fe protein cofactors”; NIH R35 Maximizing Investigators’ Research Award for Early Stage Investigators (GM128852-01); Hannah S. Shafaat (PI); \$1,879,182 total direct and indirect costs; 9/1/2018 – 8/31/2023.

### Completed Research Support

“CAREER: Metalloenzyme mechanisms probed by resonance Raman spectroscopy”; NSF Faculty Early Career Development Program (1454289); Hannah S. Shafaat (PI); \$650,000 total direct and indirect costs; 7/1/2015-9/30/2021 (No-cost extension granted).

“Artificial metalloenzymes for sustainable H<sub>2</sub> production in biological systems”; Ohio State Sustainability Research Seed Grant (FY20); Patrice Hamel (PI, OSU), Hannah S. Shafaat (co-PI), Alexandra Dubini (co-PI, University of Cordoba, Spain); \$50,000 total direct costs; 7/1/2020-6/30/2021.

“A Macromolecular Nickel Catalyst for Carbon-Carbon Bond Formation from C1 Precursors”; American Chemical Society Petroleum Research Fund (ACS PRF) Doctoral New Investigators (57403-DNI6); Hannah S. Shafaat (PI); \$110,000 total direct and indirect costs; 6/1/2017 – 8/31/2019.

Breakfast of Science Champions Program Grant; OSU Office of Outreach and Engagement; Hannah S. Shafaat (PI) and Courtney Price (co-organizer); \$4,000 total direct costs; 11/2016.

“Developing electrodes for hydrogen production based on robust biological catalysts”; OSU Materials Research Seed Grant Program, Exploratory Materials Research Grant; \$40,000 direct costs; 9/1/2015 – 8/31/2016.

“Biomaterials for the Efficient Production of Hydrogen Gas from Water: Towards Solar Fuels”; OSU Institute for Materials Research Facility Grant Award; Hannah S. Shafaat (PI); \$2,000 total direct costs; 7/1/2014-6/30/2015.

### Supercomputer Grants

“Mechanistic investigations of small molecule activation reactions in model nickel metalloenzymes through computationally-guided spectroscopy”; Ohio Supercomputer Center; 100,000 Resource Units; awarded February 2018.

“Investigation of small molecule activation reactions in model metalloenzymes by computationally-guided resonance Raman spectroscopy”; Ohio Supercomputer Center; 100,000 Resource Units; 10/2016 – 02/2018.

“Development and application of computationally-guided resonance Raman spectroscopy to study small molecule activation reactions in model bioinorganic systems”; Ohio Supercomputer Center; 30,000 Resource Units; 08/2015 – 10/2016.

### Invited Talks and Seminars

#### 2021

Department of Chemistry and Biochemistry, Colorado School of Mines: “*What’s a Nickel Worth? Elucidating mechanistic principles of complex metalloenzymes through protein-based models*”

Department of Chemistry, University of Kentucky: “*What’s a Nickel Worth? Elucidating mechanistic principles of complex metalloenzymes through protein-based models*”

Department of Chemistry, Queen’s University Belfast (Virtual presentation): “*What’s a Nickel Worth? Elucidating mechanistic principles of complex metalloenzymes through protein-based models*”

Department of Chemistry and Chemical Biology, Woodward CCB Departmental Colloquium, Harvard University (Virtual presentation): “*Elucidating mechanistic principles of complex metalloenzymes through protein-based models*”

Department of Biochemistry, University of São Paulo (Virtual presentation): “*‘Metalling’ with Nature: Harnessing Bioinorganic Chemistry for Small Molecule Activation*”

#### 2020

Department of Chemistry seminar, Washington State University (Virtual presentation): “*‘Metalling’ with Nature: Harnessing Bioinorganic Chemistry for Small Molecule Activation*”

Department of Chemistry seminar, Trinity University (Virtual presentation): “*‘Metalling’ with Nature: Harnessing Bioinorganic Chemistry for Small Molecule Activation*”

Department of Chemistry seminar, University of Miami: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

### 2019

Department of Chemistry seminar, Yale University: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

Department of Chemistry seminar, University of Kansas: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

Structural and Quantitative Biology (SQB) Seminar Series, University of California at Berkeley: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

Department of Chemistry seminar, University of Pennsylvania: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

Department of Chemistry seminar, Binghamton University: *“Looking to the future by modeling the past: Design and characterization of engineered metalloenzymes for small molecule activation”*

Department of Chemistry seminar, Johns Hopkins University: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Department of Chemistry seminar, University of Colorado, Boulder: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Department of Chemistry and Biochemistry seminar, University of Notre Dame: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Department of Chemistry seminar, University of Georgia: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Center for Diagnostics and Therapeutics colloquium speaker, Georgia State University: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

### 2018

Department of Chemistry seminar, University of British Columbia: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Department of Chemistry seminar, Simon Fraser University: *“Metalling’ with Nature: Design and characterization of model metalloenzymes for small molecule activation”*

Molecular Biophysics Training Program Inaugural Symposium student-selected talk, Ohio State University: *“Model nickel metalloenzymes for energy conversion”*

Department of Chemistry seminar, University of Utah: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Villers Wilson Meloche Lectureship, University of Wisconsin- Madison: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Biochemistry seminar, University of California at San Diego: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry seminar, University of California at Irvine: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Chemical Engineering seminar, California Institute of Technology: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry seminar, University of Washington: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Biochemistry seminar, University of Texas: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Biochemistry seminar, Texas A&M University: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry seminar, Bowling Green State University: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Chemical Biology seminar, Cornell University: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry and Biochemistry seminar, University of Rochester: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

School of Chemical Sciences seminar, Arizona State University: *“Rebuilding ancient pathways: Model metalloenzymes for energy conversion”*

Department of Chemistry seminar, University of Arizona: *"Rebuilding ancient pathways: Model metalloenzymes for energy conversion"*

#### 2017

Department of Chemistry and Biochemistry seminar, Auburn University: *"Rebuilding ancient pathways: Model metalloenzymes for energy conversion"*

Department of Chemistry and Biochemistry seminar, Wayne State University: *"Rebuilding ancient pathways: Model metalloenzymes for energy conversion"*

Department of Chemistry seminar, University of Michigan: *"Rebuilding ancient pathways: Model metalloenzymes for energy conversion"*

Invited speaker, 13<sup>th</sup> Annual Mini-Symposium on Metals in Biological and Chemical Systems, Duquesne University: *"Rebuilding ancient pathways: Model nickel metalloenzymes for energy conversion"*

Department of Chemistry seminar, Rice University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, University of Houston: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, Indiana University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, University of Florida: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, University of Akron: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Student Affiliates of the American Chemical Society Annual Colloquium, Kent State University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, Youngstown State University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, University of Illinois Urbana-Champaign: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry seminar, Michigan State University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

#### 2016

Department of Chemistry seminar, Wright State University: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry and Biochemistry seminar, Hope College: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry and Biochemistry seminar, Calvin College: *"Teaching old proteins new tricks: Engineering metalloenzymes for energy conversion reactions"*

Department of Chemistry and Biochemistry seminar, Miami University: *"Transforming workhorse electron transfer proteins into energy-converting metalloenzymes"*

Department of Chemistry and Biochemistry seminar, Western Kentucky University: *"Transforming workhorse electron transfer proteins into energy-converting metalloenzymes"*

#### 2015

Keynote Speaker, Cleveland State Interdisciplinary Research Conference: *"Small molecule activation in bioinorganic systems: From characterization of Nature's active sites to design of next generation enzymes"*

Department of Chemistry seminar, Marshall University: *"Small molecule activation in bioinorganic systems: From characterization of Nature's active sites to design of next generation enzymes"*

Department of Chemistry seminar, Kenyon College: *"Small molecule activation in bioinorganic systems: From characterization of Nature's active sites to design of next generation enzymes"*

Battelle Lecture Series Invited Speaker, Departments of Computational Science and Chemistry, Capital University: *"Small molecule activation in bioinorganic systems: From characterization of Nature's active sites to design of next generation enzymes"*

#### 2014



Department of Chemistry seminar, Baldwin Wallace University: *"Small molecule activation in bioinorganic systems: From characterization of Nature's active sites to design of next generation enzymes"*

Molecular Life Sciences Interdisciplinary Graduate Program Symposium Biophysics Faculty plenary speaker, The Ohio State University: *"Small molecule activation in metalloproteins: From hydrogenases to oxidases"*

### 2013

Department of Chemistry seminar, National Taiwan University: *"Heterobimetallic protein cofactors: Nature's tool for small-molecule activation"*

## **Invited Presentations at Professional Meetings**

### 2023

(Forthcoming, postponed from 2021) Oral presentation at Telluride Science Research Center (TSRC) Workshop "Redox Biochemistry: From Enzymes to Models"

### 2022

(Forthcoming) Plenary speaker, 13<sup>th</sup> International Hydrogenase Conference

(Forthcoming, postponed from 2020) Oral presentation at 2022 Metallocofactors Gordon Research Conference

(Forthcoming, postponed from 2020) Oral presentation at 2022 Organometallics Gordon Research Conference

(Forthcoming, postponed from 2020) Oral presentation at 2022 Molecular Basis of Microbial One-Carbon Metabolism Gordon Research Conference

(Forthcoming, postponed from 2020) Oral presentation at 2022 Electron Donor-Acceptor Interactions Gordon Research Conference

### 2021

Oral presentation in 6<sup>th</sup> Gateway NMR Conference (Hosted by Miami University): *"Uncovering biochemical ligand field inversion using pulsed EPR spectroscopy"*

Oral presentation in Reactions in Time and Space: Future Opportunities for Spectroscopy and Beyond - CHESS 2030 Workshop: *"Reconstructing primordial energy conversion processes in model metalloproteins"*

Oral presentation at ACS Fall 2021 Virtual Meeting Inorganic Lectureship Award Symposium in honor of Jenny Yang: *"One carbon at a time: Modeling carbon monoxide dehydrogenase in robust metalloprotein scaffolds"*

Oral presentation in JBIC Virtual Symposium on Energy Conversion inspired by Bioinorganic Chemistry: *"Reconstructing primordial energy conversion processes in model metalloproteins"*

Global Inorganic Discussion Weekdays Virtual Symposium: *"Emergent Complexity: Reconstructing primordial energy conversion processes in model metalloproteins"*

Oral presentation at ACS Spring 2021 Virtual Meeting in Fresenius Award Symposium in honor of Kyle Lancaster: *"Uncovering Ligand Field Inversion in a Biochemical Model of Acetyl Coenzyme A Synthase using Pulsed EPR Spectroscopy"*

Keynote speaker at "Metalloproteins at the crossroads of design and nature" virtual symposium (Hosted by Rutgers University): *"Emergent Complexity: Reconstructing primordial energy conversion processes in model metalloproteins"*

### 2020

Oral presentation at 2nd Frontiers in Photochemistry Conference: *"Artificial Metalloenzymes For Light-Driven Hydrogen Evolution And Carbon Dioxide Reduction"*

### 2019

Oral presentation at Wolfgang Lubitz' 70<sup>th</sup> Birthday Symposium: *"Pulsed EPR: An ideal tool to probe electronic structures of cofactor assembly intermediates in Mn/Fe R2lox"*

Oral presentation at 2019 International Conference on Biological Inorganic Chemistry (ICBIC-19): *"Inspired by Nature: Model Metalloenzymes for Energy Conversion"*

- Oral presentation at ACS Fall 2019 National Meeting in Symposium on “Learning from Nature: Earth-Abundant Metals for Oxidation Catalysis”: *“Spectroscopic investigations of metal binding and oxygen activation in the heterobimetallic Mn/Fe R2lox proteins”*
- Oral presentation at Telluride Science Research Center (TSRC) Workshop “Biological and Bioinspired Redox Catalysts”: *“Model nickel metalloproteins for small molecule activation”*
- Oral presentation at Kavli Frontiers of Science Symposium (Fourth Korean-American Symposium): *“Learning from Nature: Building Artificial Metalloenzymes for Energy Conversion and Storage”*
- Oral presentation at Central Regional ACS Meeting: *“Developing model nickel metalloenzymes for energy conversion”*
- Oral presentation at CANBIC-7: *“Metal binding and O<sub>2</sub> activation in heterobimetallic Mn/Fe R2lox”*
- Oral presentation at 2019 International Hydrogenase Conference: *“Learning from the Best: Model Metalloenzymes that Imitate Hydrogenase and Carbon Monoxide Dehydrogenase”*
- Oral presentation at 2019 Inorganic Reactions Mechanisms Gordon Research Conference: *“Bioorganometallic Chemistry Within a Model Nickel Enzyme”*
- Oral presentation at 2019 Metals in Biology Gordon Research Conference (Ed Stiefel Award Lecture): *“If I had a nickel... Model metalloenzymes for energy conversion”*

### 2018

- Oral presentation at 2018 Department of Energy Physical Biosciences Biennial Meeting: *“Bringing Inorganic Carbon to Life: Developing Model Metalloenzymes for C1 Conversion Reactions”*
- Oral presentation at 2018 EURO-BIC meeting, Birmingham, England, UK: *“Model nickel metalloenzymes for energy conversion”*
- Oral presentation at 2018 International Conference on Coordination Chemistry (ICCC), Sendai, Japan: *“Model nickel metalloenzymes for H<sub>2</sub> generation (and CO<sub>2</sub> fixation)”*
- Oral presentation at 2018 Centre for Sustainable Chemical Technologies Summer Showcase, Bath, England, UK: *“Model nickel metalloenzymes for energy conversion”*
- Oral presentation at 2018 North American/Greece/Cyprus Workshop on Paramagnetic Materials: *“EPR spectroscopic investigations of metal binding specificity and oxygen activation in heterobimetallic Mn/Fe proteins”*
- Discussion Leader for Metallocofactors Gordon Research Conference: *“Carbon Transformations: CO, formate, and C-C bonds”*
- Oral presentation at 2018 Penn State Bioinorganic Workshop: *“Resonance Raman Spectroscopy: From Structure to Reactivity”*
- Oral presentation at 2018 7th Bluegrass Molecular Biophysics Symposium, University of Kentucky: *“Nickel-substituted rubredoxin as an artificial hydrogenase: Experiment and theory”*
- Oral presentation at Solar Fuels Gordon Research Conference: *“Model metalloenzymes for CO<sub>2</sub> fixation and H<sub>2</sub> evolution: Towards liquid fuels”*

### 2017

- Oral presentation at Telluride Science Research Center (TSRC) Workshop “Control of Proton and Electron Transfers in Redox Catalysis”: *“Towards a mechanistic understanding of catalytic hydrogen production by nickel-substituted rubredoxin”*
- Oral presentation at 20<sup>th</sup> International Society of Magnetic Resonance and Rocky Mountain Conference on EPR (ISMAR/RMC-EPR): *“Model nickel metalloenzymes for energy conversion”*
- Session speaker at 2<sup>nd</sup> International Solar Fuels conference (ISF-2): *“Model Nickel Enzymes for Photogenerated Fuels”*
- Oral presentation at 2017 Joint North American/Greece/Cyprus Workshop on Paramagnetic Materials and Current Trends in Molecular and Nanoscale Magnetism (NAGC/CTMNM): *“Model nickel metalloenzymes for energy conversion reactions”*
- Oral presentation at 253<sup>rd</sup> ACS National Meeting: *“Protein-based models of carbon monoxide dehydrogenase/acetyl coenzyme A synthase”*
- Oral presentation at The Fifth Symposium on Advanced Biological Inorganic Chemistry (SABIC-2017) “Young, Outstanding, Upcoming” symposium, Kolkata, India *Declined*

### 2016

- Oral presentation at 2016 SSRL/LCLS Users’ Meeting: *“Electrocatalytic hydrogen evolution by nickel-substituted rubredoxin, a model hydrogenase enzyme”*

Oral presentation at 252<sup>th</sup> ACS National Meeting: *“Transforming workhorse electron transfer proteins into energy-converting metalloenzymes”*

#### 2015

Oral presentation at 250<sup>th</sup> ACS National Meeting: *“Developing functional metalloenzyme mimics using model protein scaffolds”*

Oral presentation at Telluride Science Research Center Workshop “Structure and Function of Hydrogenase Mimics”: *“Hydrogen Production in Engineered Metalloprotein Scaffolds”*

Oral presentation at CANBIC-5: *“Using resonance Raman spectroscopy to investigate catalytic metalloenzyme intermediates”*

#### 2014

Oral presentation at 248<sup>th</sup> ACS National Meeting: *“Small molecule activation in bioinorganic systems: From characterization of Nature’s active sites to design of next-generation enzymes”*

Oral presentation at First Ohio Conference on the Sustainable Use of Greenhouse Gases: *“Design and characterization of metalloprotein scaffolds for activation of greenhouse gases”*

### **Contributed Presentations at Professional Meetings**

#### 2020

Poster presentation at GRC Metals in Biology: *“From Structure to Function: Multifrequency Pulsed EPR Investigations of Assembly Intermediates in Mn/Fe R2lox”*

#### 2018

Poster presentation at GRC Metals in Biology: *“Model metalloenzymes for CO<sub>2</sub> fixation and H<sub>2</sub> generation”*

#### 2017

Oral presentation in Spotlight Session: Biocatalysts, ASBMB 2017 Annual Meeting: *“Protein-based Models of Nickel Metalloenzymes”*

Selected oral presentation at GRC Metals in Biology: *“Unraveling the Mn/Fe lipid-binding oxidases: An investigation of metal specificity and cofactor assembly in R2lox”*

Poster presentation at GRC Metals in Biology: *“Investigating metal specificity and cofactor assembly in R2lox, a novel heterobimetallic Mn/Fe protein”*

#### 2016

Oral presentation at 11<sup>th</sup> International Hydrogenase Meeting: *“Nickel-substituted rubredoxin as a functional enzyme model for hydrogenase”*

Poster presentation at GRC Microbial Basis of One-Carbon Metabolism: *“Nickel-Substituted Azurin as a Protein-Based Mimic of the Active Site in Acetyl-CoA Synthase”*

Participant in workshop on Research Opportunities in Photochemistry, Solar Energy & Advanced X-ray Methods, SSRL: *“Studying H<sub>2</sub> conversion at metalloprotein active sites”*

Poster presentation at GRC Metals in Biology: *“Repurposing workhorse electron transfer proteins for energy storage reactions”*

#### 2015

Oral presentation at Pacificchem-2015: *“Developing functional hydrogenase mimics using model metalloprotein scaffolds”*

Oral presentation at Pacificchem-2015: *“Development and application of computationally-guided resonance Raman spectroscopy to investigate metalloenzyme intermediates”*

Poster presentation at Center for Sustainable Use of Greenhouse Gases Industry Planning Conference: *“Design and characterization of metalloprotein scaffolds for activation of wasted carbon”*

Oral presentation at 249<sup>th</sup> ACS National Meeting: *“Electrocatalytic hydrogen production performed by model protein scaffolds”*

Poster presentation at GRC Metals in Biology: *“Small molecule activation in bioinorganic systems: Designing new functionality into model protein scaffolds”*

2014

Oral presentation at ElectrochemOhio: *“Electrocatalytic hydrogen production performed by model protein scaffolds”*

Poster presentation at Catalytic Systems for Chemical Energy Conversion Symposium: *“Probing the electronic structure of the heterobimetallic Mn/Fe cofactor of the R2lox proteins using advanced EPR techniques”*

Prior to faculty appointment

**Oral presentation** at 3<sup>rd</sup> Hydrogenase Meeting (2013)

Poster presentation at ICBIC-16 (2013)

**Oral presentation** at 244<sup>th</sup> ACS National Meeting (Fall 2012)

Poster presentation at 244<sup>th</sup> ACS National Meeting (Fall 2012)

Poster presentation at Penn State Bioinorganic Workshop (2012)

**Oral and poster presentations** at Alexander von Humboldt Network Meeting (2012)

Poster presentation at Faraday Discussions 150: Frontiers in Spectroscopy (2011)

Poster presentation at GRC Metals in Biology (2011)

**Oral presentation** at 239<sup>th</sup> ACS National Meeting (Spring 2010)

Poster presentation at GRC Protein Cofactors, Radicals, and Quinones (2010)

**Oral and poster presentations** at ICBIC-14 (2009)

**Oral presentation** at 236<sup>th</sup> ACS National Meeting (Fall 2008)

Two poster presentations at 232<sup>nd</sup> ACS National Meeting (Fall 2006)

Poster presentation at 106<sup>th</sup> General ASM Meeting (2006)

**Oral presentation** at 231<sup>st</sup> ACS National Meeting (Spring 2006)

Teaching ExperienceOSU Department of Chemistry and Biochemistry

*CHEM 1220* — General Chemistry II (Undergraduate)

Spring 2020 (307 students)

*CHEM 4310* — Physical Chemistry II (Undergraduate; thermodynamics and statistical mechanics)

Spring 2015 (38 students), Spring 2016 (53 students), Spring 2017 (54 students)

*CHEM 6330* — Group Theory and Bonding (Graduate)

Fall 2019 (32 students), Fall 2021 (18 students)

*CHEM 6520* — Thermodynamics (Graduate)

Fall 2013 (27 students), Fall 2014 (33 students), Fall 2015 (22 students), Fall 2016 (34 students), Fall 2017 (29 students)

*CHEM 6530* — Kinetics (Graduate)

Fall 2013 (20 students), Fall 2014 (30 students), Fall 2015 (20 students), Fall 2016 (33 students), Fall 2017 (32 students), Fall 2018 (33 students), Fall 2019 (40 students)

*CHEM 6782* — Ethics in Research (Graduate)

Spring 2020 (71 students)

*CHEM 8399* — Special Topics—The Inorganic Chemistry of Bioinspired Energy Conversion (Graduate)

Spring 2019 (13 students)

OSU Ohio State Biochemistry Program

*OSBP 7700* — Student Seminar course. Fall 2014 (32 students), Spring 2019 (21 students).

OSU Teaching Enrichment Activities

*University Center for the Advancement of Teaching Course Design Institute*—Fall 2017

*Ohio State University Institute for Teaching and Learning (UITL) Endorsement: Course Design Institute*

Penn State Bioinorganic Workshop

*(Forthcoming) Resonance Raman Spectroscopy* — Practical and lecture, Summer 2022

*Resonance Raman Spectroscopy* — Practical and lecture, Summer 2018 (45 students)

Mentoring (Current members in bold)

*Postdoctorate:*

**Adam Jenkins (2021 – present)**

Chandradeep Ghosh (2018 – 2020) [Postdoctoral Scholar, TAMU, Bankaitis lab]

Michael Stevenson (2016 – 2017) [Assistant Professor, University of San Francisco]

*Graduate:*

**Josephine Gan (2020 – present)**

**Joseph Hazel (2019 – present)**

**Luke Lewis (2019 – present)**

**Regina Treviño (2017 – present)**

**Ashlee Wertz (2020 – present)**

**Alina Yerbulekova (2019 – present)**

Effie Kisgeropoulos (2015 – 2020) [Ph.D.; Postdoctoral Researcher, National Renewable Energy Laboratory, King group]

*Dissertation Title: From Structure to Function: Utilizing the Biophysical Toolbox to Interrogate a Novel Class of Mn/Fe Proteins*

Sean Marguet (2015 – 2020) [Ph.D.; Geo. Pfau Sons Co. Inc.]

*Dissertation Title: Mechanistic Investigation of Light-driven Hydrogen Production by Nickel-substituted Rubredoxin: A Solar Fuel Photocatalyst*

Shelby Behnke (2014 – 2019) [Ph.D.; Process Engineer, Intel Corporation]

*Dissertation Title: Investigating Mechanistic Pathways: A Spectroelectrochemical Study of [Ni(cyclam)]<sup>2+</sup>*

Camille Schneider (2015 – 2019) [Ph.D.; Data Scientist, Chemical Abstract Services]

*Dissertation Title: Modeling Complexity: Development and Characterization of a Carbon Monoxide Dehydrogenase Mimic to Identify Key Factors for Reactivity*

Jeffrey Slater (2014 – 2018) [Ph.D.; Postdoctoral Researcher, Penn State University, Bollinger/Krebs group]

*Dissertation Title: Nickel-Substituted Rubredoxin as a Protein-Based Enzymatic Mimic for [NiFe] Hydrogenase*

Anastasia Manesis (2014 – 2018) [Ph.D.; Postdoctoral Researcher, Northwestern University, Rosenzweig group]

*Dissertation Title: Bioorganometallic Chemistry within Nickel-Substituted Azurin: From Protein Design to Reactivity*

Pearson Maugeri (2014 – 2017) [Ph.D.; Process Engineer, Intel Corporation]

*Dissertation Title: Applications of resonance Raman spectroscopy to the study of bioinorganic macromolecules*

Clayton Wilson (2017 – 2019) [M.S.; Teacher, Greensboro Day School]

*Thesis Title: Effects of Outer Sphere Mutations on CO Binding to Nickel-Substituted Azurin and Implications for Acetyl Coenzyme A Synthase Substrate Channeling*

James York-Winegar (2013 – 2014)

*Undergraduate:*

**Jonathan Henry (2021 – present)**

**Riley Stein (2020 – present)**

**Peter Moore (2019 – present)**

Sophia Sterling (2021)

Sierra Cady (2019 – 2021)

Ella Troy (2019 – 2020)

Kassandra Naughton (2017 – 2019) [Graduate Student, University of Kentucky]

Pathorn Teptarakulkarn (Summer 2019)

John Nugent (Summer 2019)

Kiara Devese (2018)

Aryn Hubbard (2018)

Zachary Smith (2016 – 2018)

Ayla Robinson (2017 – 2018)

Jessica Fulton (2018)

Jack Eifert (2017-2018)

Tim O'Connor (2017) [Quality Control Chemist, Scientific Protein Laboratories]

Alex Leveto (2016 – 2017)

Nicholas Trivelas (2014 – 2016) [Medical Student, Kansas City University]

Matthew O'Connor (2014 – 2016) [High school chemistry teacher, Columbus, OH]  
Haleigh Monaco (2014 – 2015) [Graduate Student, University of Colorado]  
Sabrina Cirino (2013 – 2014) [Masters of Science in Anesthesia Program, Case Western Reserve University]  
Casey Flowers (Summer 2014)  
Guanyu Hu (Summer 2014)

*High School:*

Maizy Pratt (2019 – 2020)  
Isaac Bamba (2020 – 2020)  
Alexander Dickson (Summer 2018, 2019)  
Peter Moore (Summer 2017, 2018) [Undergraduate Student, Ohio State University]  
Prapti Dalal (Summer 2015, Summer 2016) [Undergraduate and Medical Student, NEOMED]  
Charlie Marshall (Summer 2015) [Undergraduate Student, Northwestern University]

*Research Scientists:*

Haleigh Monaco (2015 – 2016) [Graduate Student, University of Colorado]

## **Service**

### Conferences and Workshops

*2023 (Forthcoming, postponed from 2021)*

Co-organizer of Telluride Science Research Center (TSRC) Workshop: “Redox Biochemistry: From Enzymes to Models”

*2022 (Forthcoming, postponed from 2020)*

Lead instructor for Resonance Raman section at Penn State Bioinorganic Chemistry Workshop

*2021*

Lead organizer for Pacificchem 2021 Symposium: “New Frontiers in Bioinorganic Chemistry: Combining Synthesis, Spectroscopy, and Enzymology to Understand Dynamic Interplay across Time and Length Scales”—*Cancelled due to COVID-19 pandemic*

*2019*

Co-organizer of Telluride Science Research Center (TSRC) Workshop: “Biological and Bioinspired Redox Catalysts”

*2018*

Co-organizer and moderator of ICCO 2018 session: “Metal mediated hydrogen production and activation inspired by Nature”

Lead instructor for Resonance Raman section at 2018 Penn State Bioinorganic Chemistry Workshop  
Chair of session “Chemistry and Biochemistry of Nickel”, Frontiers in Metallobiochemistry Symposium  
OSU Delegate for Centre for Sustainable Chemical Technologies Advisory Board meeting, Bath, England, UK

Discussion leader at Metals in Biology Gordon Research Conference “Power Hour”

Discussion leader at Solar Fuels Gordon Research Conference “Power Hour”

*2017*

Organizer of regional “Ohio Inorganic Weekend” Conference with approx. 250 attendees

Session chair for Telluride Science Research Center Workshop (TSRC) “Control of Proton and Electron Transfers in Redox Catalysis”

Session moderator and discussion chair for 2<sup>nd</sup> International Solar Fuels conference (ISF-2):  
Bioinspired Approaches

Session chair at 20<sup>th</sup> International Society of Magnetic Resonance and Rocky Mountain Conference on EPR

2016

Co-organizer (with Stefan Stoll) of ACS PHYS symposium for 251<sup>st</sup> National Meeting: "How Enzymes Work" ("Understanding Enzymatic Catalysis across Multiple Timescales: Experiment and Theory")

2015

Round table discussion leader at Telluride Science Research Center Workshop "Structure and Function of Hydrogenase Mimics": *"Catalytic and Outer Coordination Sphere Studies to Understand the Function of Hydrogenases"*

Faculty mentor volunteer and panelist at ACS Postdoc-to-Faculty workshop

2014

Invited discussion leader for session "Bioinorganic Chemistry of Renewable Energy" at Gordon Research Seminar in Bioinorganic Chemistry

Chair of session "Hydrogenases", Frontiers in Metallobiochemistry Symposium

### The Ohio State University

#### *College of Arts and Sciences (ASC)*

2020 – present      ASC Strategic Plan Work Group

2019 – present      Sustainability Committee

2019-2020:          Science Sundays Committee

#### *Department of Chemistry and Biochemistry*

2021 – present      Chair, Safety Committee

2021 – present      Graduate Admissions Committee

2019 – 2020          Chair, Safety Committee

2019 – 2020          Publicity Committee

2019:                  *Ad hoc* Admissions Committee reviewer

2018-2019:          Department Chair Search Committee

2016:                  Judge, Denman Undergraduate Research Forum

2016:                  Panelist and Presenter, Pre-Denman Presentation Workshop

2016:                  Judge, Chemistry Club Poster Competition with Columbus ACS Section

2015:                  OSU Fulbright Panel Selection Committee

2015:                  Panel Volunteer, Summer Research Opportunities Program

2014, 15, 17, 19:      Judge, Dow Poster Competition

2014 – 2018:          Graduate Admissions Committee

2013 – 2016:          Spectroscopy Research Focus Group seminar coordinator

2013 – 2017:          Safety Committee

2013 – 2015:          Committee for Research Support Services

#### *The Ohio State Biochemistry Program*

2015 – 2018:          Molecular Life Sciences Seminar Series selection committee

2014 – 2018:          Presentation judge at Annual Molecular Life Sciences Interdisciplinary Graduate Program Symposium

Fall 2014:              Faculty leader for Student Seminar course

#### *OSU Chemical Physics Program*

2015 – present:      Chemical Physics program graduate committee

2015 – present:      Frontiers in Spectroscopy seminar committee

#### *OSU Biophysics Program*

2015 – 2017:          Faculty leader for Bioinorganic Subgroup Literature Series

#### *Office of Diversity and Inclusion*

2016– present:      Faculty LSAMP mentor

#### *OSU Graduate School*

Candidacy examination committees: 39

Masters thesis examination committees: 1  
Dissertation examination committees: 18

### External Service

National High Magnetic Field Laboratory NSF Site Visit User Presentation (2021)  
National High Magnetic Field Laboratory NSF Site Visit User Presentation (2020)  
NIH Scientific Review Group 2022/01 MSFA (*ad hoc* member, 10/2021)  
NIH ZRG1 F04B-H (20) L Fellowships: Chemistry, Biochemistry and Biophysics Study Section (2021)  
NIH F04B 2021/01 ZRG1 BCMB-N (02) M: Special Emphasis Panel (2021)  
Department of Energy Basic Energy Sciences Review Panel  
National Science Foundation Proposal Review Panel  
External Examiner for Ph.D. Dissertation, I.I.T. Ghandinigar (2021)

### Notable Student Accomplishments

#### *Graduate Students*

Department of Energy Office of Science Graduate Student Research Awardee (2021): Regina Treviño  
ACS Division of Inorganic Chemistry Young Investigator Award (2021): Effie Kisgeropoulos  
Simons Fellow of the Life Sciences Research Foundation (2020 – 2023): Anastasia Manesis  
F32 Kirschstein-NRSA Postdoctoral Fellowship (2020 – 2023): Anastasia Manesis (*declined*)  
F32 Kirschstein-NRSA Postdoctoral Fellowship (2020 – 2023): Jeffrey Slater  
SACNAS National Diversity in STEM Conference Presentation Award (2019): Regina Treviño  
Molecular Biophysics NIH T32 Training Grant (2019 – 2021): Joseph Hazel  
Pelotonia Graduate Fellowship (2018 – 2020): Effie Miller  
College of Arts and Sciences Graduate Studies Travel Award (2019): Regina Treviño  
College of Arts and Sciences Graduate Student Award for Mentoring Excellence (2018): Anastasia Manesis  
OSU Presidential Fellowship Awardee (2018 – 2019): Camille Schneider  
Bioinorganic Chemistry Gordon Research Seminar Vice-Chair (2018) and Chair (2019): Anastasia Manesis  
Ohio PEO Scholarship Awardee (2018): Anastasia Manesis  
Ray Travel Fellowship Awardee (2017): Anastasia Manesis  
GAANN Fellowship Awardee (2017-2018): Regina Treviño  
Second Place Poster Award Winner at Interdisciplinary Graduate Program (2017): Anastasia Manesis  
Materials Week Best Poster Awards (2017): Shelby Behnke and Jeffrey Slater  
Dow Poster Award Winner (2016): Camille Schneider  
First Place Poster Award Winner at Ohio Supercomputer Center Statewide Users' Meeting (2016): Sean Marguet  
Robin C. Burrell Memorial Fund Travel Grant (2016): Anastasia Manesis  
Chemistry Biology Interface Program Training Fellowship (2015-2017): Camille Schneider  
National Science Foundation Graduate Fellowship Honorable Mention (2015): Anastasia Manesis  
Dow Poster Award Winner (2015): Anastasia Manesis  
Robin C. Burrell Memorial Fund Travel Grant (2015): Jeffrey Slater  
Cellular, Molecular, and Biochemical Sciences NIH T32 Training Grant (2014 – 2015): Pearson Maugeri  
Dow Poster Award Finalist (2014): Jeffrey Slater

#### *Undergraduate Students*

OSU Undergraduate Research Apprenticeship Program Fellow (2021): Riley Stein  
Ohio Inorganic Weekend Poster Session 1<sup>st</sup> Place Awardee (2018): Cassandra Naughton  
Ohio Inorganic Weekend Poster Session 3<sup>rd</sup> Place Awardee (2017): Zachary Smith  
Denman Undergraduate Research Forum 2<sup>nd</sup> Place Awardee (2016): Nicholas Trivelas  
Denman Undergraduate Research Forum Honorable Mention (2016): Matthew O'Connor  
Pelotonia Undergraduate Fellowship (2015-2016): Nicholas Trivelas  
ASC Undergraduate Research Scholarship (2015): Matthew O'Connor  
Undergraduate Summer Research Fellowship (2015): Matthew O'Connor, Nicholas Trivelas



SOLAR Fund Undergraduate Research Award (2015): Nicholas Trivelas  
OSU Research Scholar Award (2015): Nicholas Trivelas  
Undergraduate Summer Research Fellowship (2014): Sabrina Cirino

### **Outreach and Broader Impacts**

- Columbus Alternative High School Internship Experience Host Site
- Coordinator of OSU Breakfast of Science Champions program with ~500 middle-school participants across and liaison with Columbus City School District coordinator (2016-2018)
- OSU Department of Chemistry and Biochemistry and Joint Safety Team Safety Award (2016-2017)
- Laboratory Safety Dean's List award (2017 - present)
- Co-coordinator for Breakfast of Science Champions event across OSU and liaison with Columbus City School District coordinator (2016)
- Lead Site Organizer for Chemistry and Biochemistry Department Breakfast of Science Champions event (2015-present)
- Development and implementation of Summer Internship Program within research laboratory (2015-present)
- "Meet a Scientist" Event Contributor through Portal to the Public program at Columbus Museum of Science and Industry (COSI, 2015)
- Workshop for attendees of Sally Ride Science Festival (2011)
- Workshop for local San Diego Brownie Troop (2011)
- Hosted high school class, gave demonstration of laser spectroscopy (2010)
- Workshop for attendees of Sally Ride Science Festival (2008)

### **Professional Affiliations**

- American Chemical Society (since 2007)
- Society for Biological Inorganic Chemistry (since 2008)
- Ohio State Biochemistry Program (OSBP) (since 2013)
- OSU Biophysics Program (since 2013)
- OSU Chemical Physics Program (since 2013)
- OSU Institute for Materials Research (since 2014)
- American Society for Biochemistry and Molecular Biology (since 2016)