The Ohio State University
Department of Chemistry and Biochemistry

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Hannah S. Shafaat

Academic Background

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

Professional Experience

2013 – present: Assistant Professor, *The Ohio State University, Columbus, OH, USA*
2011 – 2013: Postdoctoral Fellow with Wolfgang Lubitz, *Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany*

Honors and Awards

2015: Selected for *ACS Select Virtual Issue* on Emerging Investigators in Bioinorganic Chemistry
2012: Young Researcher Participant at 62nd 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 Affiliations

- American Chemical Society (since 2007)
- Society for Biological Inorganic Chemistry (since 2008)
- Ohio State Biochemistry Program (since 2013)
- Ohio State Biophysics Program (since 2013)
- Ohio State Chemical Physics Program (since 2013)
- Ohio State Chemistry-Biology Interface Training Program (since 2014)
- Ohio State Institute for Materials Research (since 2014)

External Support

Current Research Support

"CAREER: Metalloenzyme mechanisms probed by resonance Raman spectroscopy"; NSF Faculty Early Career Development Program (1454289); Hannah S. Shafaat (PI); $520,000 total direct and indirect costs; 7/1/2015-6/30/2020.

"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.

Former Research Support

"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

"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; awarded August 2015.

Teaching Experience

4310: Physical Chemistry II (Undergraduate, thermodynamics and statistical mechanics), Spring 2015

6520: Chemical Thermodynamics (Graduate), Fall 2013, Fall 2014, Fall 2015
6530: Chemical Kinetics (Graduate), Fall 2013, Fall 2014

Research Group Members (Current members in bold-face)

Graduate:
James York-Winegar (2013 – 2014)
Anastasia Manesis (2014 – present)
Jeffrey Slater (2014 – present)
Shelby Behnke (2014 – present)
Effie Kisgeropoulos (2015 – present)
Pearson Maugeri (2015 – present)
Camille Schneider (2015 – present)
Undergraduate:
Nicholas Trivelas (2014 – present)
Matthew O'Connor (2014 – present)
Haleigh Monaco (2014 – 2015) [Research Scientist, Shafaat Group, OSU]
Sabrina Cirino (2013 – 2014) [Masters of Science in Anesthesia Program, Case Western Reserve University]
Casey Flowers (Summer 2014)
Guanyu Hu (Summer 2014)
High School:
Prapti Dalal (Summer 2015)
Charlie Marshall (Summer 2015)
Research Scientists:
Haleigh Monaco (2015 – present)

Service

Conferences and Workshops

2015

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

Department of Chemistry and Biochemistry

2015:	OSU Fulbright Panel Selection Committee
2015:	Panel Volunteer, Summer Research Opportunities Program
2014, 2015:	Judge, Dow Poster Competition
2014 – present:	Graduate Admissions committee, physical division
2013 – present:	Spectroscopy Research Focus Group seminar coordinator
2013 – present:	Committee for Research Support Services
2013 – present:	Safety committee

The Ohio State Biochemistry Program

2015 – present:	Molecular Life Sciences Seminar Series selection committee
May 2015:	Presentation judge at Molecular Life Sciences Interdisciplinary Graduate Program Symposium
Fall 2014:	Faculty leader for Student Seminar course
May 2014:	Presentation judge at Molecular Life Sciences Interdisciplinary Graduate Program Symposium

OSU Chemical Physics Program

2015 – present:	Chemical Physics program graduate committee
2015 – present:	Frontiers in Spectroscopy seminar committee

OSU Biophysics Program
2015 – present: Faculty leader for Bioinorganic Subgroup Literature Series

External Service

American Chemical Society
2015 – present: Division of Inorganic Chemistry Alternate Councilor

Invited Talks and Seminars

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

2015

Oral presentation at 250th 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 248th 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"*

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

Contributed Presentations at Professional Meetings

2015

Oral presentation at Pacifichem-2015: *"Developing functional hydrogenase mimics using model metalloprotein scaffolds"*

Oral presentation at Pacifichem-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 249th 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
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"*
Oral presentation at 3rd Hydrogenase Meeting (2013)
Poster presentation at ICBIC-16 (2013)
Oral presentation at 244th ACS National Meeting (Fall 2012)
Poster presentation at 244th 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 239th 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 236th ACS National Meeting (Fall 2008)
Two poster presentations at 232nd ACS National Meeting (Fall 2006)
Poster presentation at 106th General ASM Meeting (2006)
Oral presentation at 231st ACS National Meeting (Spring 2006)

Research Publications (Independent career)

3. Behnke, S.L., **Shafaat, H.S.*** (2015). Heterobimetallic Models of the [NiFe] Hydrogenases: A Structural and Spectroscopic Comparison. *Comments on Inorganic Chemistry*, in press.
2. Slater, J.W., **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.jpclett.5b01750.
1. Manesis, A.C., **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.

Research Publications (Prior to OSU)

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 ^{17}O-hyperfine EPR Spectroscopies and Density Functional Theory. *J. Phys. Chem. B., Article ASAP., DOI*: 10.1021/acs.jpcb.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. Journal Impact Factor: 3.4; Times cited: 0.
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. Journal Impact Factor: 11.4; Times cited: 0
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. Journal Impact Factor: 6.7; Times cited: 0.
14. Riethausen, J., Rüdiger, O., Gaertner, W., Lubitz, W.*, **Shafaat, H.S.*** (2013). Spectroscopic and electrochemical characterization of the [NiFeSe] hydrogenase from Desulfovibrio vulgaris Miyazaki F: Reversible redox behavior and interactions between electron transfer centers. *ChemBioChem*, 14, 1714-1719. *DOI:* 10.1002/cbic.201300120. Journal Impact Factor: 3.7; Times cited: 2.
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. Journal Impact Factor: 9.7; Times cited: 3.

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.bbabio.2013.01.015. Journal Impact Factor: 4.8; Times cited: 34.
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. Journal Impact Factor: 4.6; Times cited: 15.
10. Weber, K., Kraemer, T., **Shafaat, H.S.,** Weyhermuller, T., Bill, E., van Gastel, 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. Journal Impact Factor: 10.7; Times cited: 29.
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. Journal Impact Factor: 10.7; Times cited: 5.
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. Journal Impact Factor: 9.9; Times cited: 11.
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. Journal Impact Factor: 9.0; Times cited: 23.
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. Journal Impact Factor: 3.1; Times cited: 21.
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. Journal Impact Factor: 3.5; Times cited: 21.
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. Journal Impact Factor: 3.0; Times cited: 31.
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. Journal Impact Factor: 3.0; Times cited: 73.
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. Journal Impact Factor: 3.5; Times cited: 32.
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.

Notable Student Accomplishments

Chemistry Biology Interface Program Training Fellowship (2015-2016): Camille Schneider
National Science Foundation Graduate Fellowship Honorable Mention (2015): Anastasia Manesis
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 Experience

- Lead Site Organizer for Chemistry and Biochemistry Department Breakfast of Science Champions event (2015)
- Development and implementation of Summer Internship Program within research laboratory (2015)
- Portal to the Public Volunteer Contributor for 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)