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EDUCATION

- Postdoctoral Fellow** 1/2012–7/2014
Kyoto University, Kyoto, Japan
Advisor: Keiji Morokuma
Research Focus: Computational Studies of Metalloenzymes,
Metallocofactor Model Complexes, and Homogeneous Catalysis
- Ph.D., Inorganic Chemistry** 8/2007–12/2011
Montana State University, Bozeman, MT
Advisor: Robert K. Szilagy
Dissertation: Development of Computational Methods for Iron-
Sulfur Clusters: Application to the Elusive Structure of the
Iron-Molybdenum Cofactor of Nitrogenase
- B.A., Biochemistry, Minor: Japanese Studies (summa cum laude)** 8/2002–12/2006
Willamette University, Salem, OR
Advisor: Karen L. McFarlane Holman
Thesis: X-ray Absorption Spectroscopy on the Ruthenium-Based
Anti-Cancer Drug NAMI-A and Related Compounds

TEACHING

- University of Puget Sound**
Visiting Assistant Professor 8/2015–current
General Chemistry (36 students/section)
General Chemistry Laboratory
Seminars in Scholarly Inquiry II - The Artificial Intelligence Revolution
- State University of New York at Oswego**
Visiting Assistant Professor 8/2014–5/2015
General Chemistry I (130 students)
General Chemistry II (70 students)
Inorganic Chemistry (25 students)
Inorganic Chemistry Laboratory
Computational Methods in Chemistry (10 students)

SERVICE

Head of General Chemistry II Lab Organization and Planning	12/2018–current
Member of Chemistry Department Thesis Committee	8/2016–current
Assistant for Chemistry Department Community Open House	10/2018
Member of Chemistry Department Faculty-Hiring Committee	1/2017–5/2017
Panel Member for Graduate School Advice Night	2015–2017
Reviewer of Summer Research Proposals	3/2016

RESEARCH ADVISING

University of Puget Sound Undergraduate Research Students

Emaleigh Curl 6/2016–5/2018

Poster at 253rd ACS National Meeting, San Francisco, CA, April 2017:
Theoretical Study of Ligand Effects on Homogeneous Hydrogenation
Catalyzed by Iron-Pyridone Complexes

Hoi-Kit Cheung 9/2016–5/2018

Thesis: Computational Insight into the Effects of Substituted
Phosphine Ligands on Iron-Based Hydrogenation Catalysts

Joe Brennan 9–12/2017

Focus: Effect of Pyridine Ligand on an Iron-Based Hydrogenation
Catalyst

Cameron Braithwaite 9/2015–5/2017

Thesis: Developing a Computational Model of the Nitrogenase
Iron-Molybdenum Cofactor

PUBLICATIONS

Journal Articles

- (1) Stratton, A.; Ericksen, M.; Harris, T.V.; Symmonds, N.; Silverstein, T.P. Mercury (II) Binds to Both of Chymotrypsin's Histidines, Causing Inhibition Followed by Irreversible Denaturation/Aggregation. *Prot. Sci.* **2017**, 26 (2), 292.
- (2) Harris, T.V.; Szilagyi, R.K. Protein Environmental Effects on Iron-Sulfur Clusters: A Set of Rules for Constructing Computational Models for Inner and Outer Coordination Spheres. *J. Comput. Chem.* **2016**, 37 (18), 1681.
- (3) Honda, K.; Harris, T.V.; Hatanaka, M.; Morokuma, K.; Mikami, K. Computational SN₂-Type Mechanism for the Difluoromethylation of Lithium Enolate with Fluoroform through Bimetallic C–F Bond Dual Activation. *Chem. Eur. J.* **2016**, 22 (26), 8796.

- (4) Chung, L.W.; Sameera, W.M.C.; Ramozzi, R.; Page, A.J.; Hatanaka, M.; Petrova, G.P.; Harris, T.V.; Li, X.; Ke, Z.; Liu, F.; Li, H.B.; Ding, L.; Morokuma, K. The ONIOM Method and Its Applications. *Chem. Rev.* **2015**, *115*, 5678.
- (5) Harris, T.V.; Szilagyi, R.K. Iron-Sulfur Bond Covalency from Electronic Structure Calculations for Classical Iron-Sulfur Clusters. *J. Comput. Chem.* **2014**, *35* (7), 540.
- (6) Harris, T.V.; Kurashige, Y.; Yanai, T.; Morokuma, K. *Ab Initio* Density Matrix Renormalization Group Study of Magnetic Coupling in Dinuclear Iron and Chromium Complexes. *J. Chem. Phys.* **2014**, *140* (5), 054303.
- (7) Harris, T.V.; Morokuma, K. QM/MM Structural and Spectroscopic Analysis of the Di-iron(II) and Di-iron(III) Ferroxidase Site in M Ferritin. *Inorg. Chem.* **2013**, *52* (15), 8551.
- (8) Harris, T.V.; Szilagyi, R.K. Comparative Assessment of the Composition and Charge State of Nitrogenase FeMo-Cofactor. *Inorg. Chem.* **2011**, *50* (11), 4811.
- (9) Harris, T.V.; Szilagyi, R.K.; McFarlane Holman, K. L. Electronic Structural Investigations of Ruthenium Compounds and Anticancer Prodrugs. *J. Biol. Inorg. Chem.* **2009**, *14* (6), 891.
- (10) Pool, V.L.; Klem, M.T.; Holroyd, J.; Harris, T.; Arenholz, E.; Young, M.; Douglas, T.; Idzerda, Y.U. Site Determination of Zn Doping in Protein Encapsulated $Zn_xFe_{3-x}O_4$ Nanoparticles. *J. Appl. Phys.* **2009**, *105* (7), 07B515.
- (11) Pandey, A.S.; Harris, T.V.; Giles, L.J.; Peters, J.W.; Szilagyi, R.K. Dithiomethylether as a Ligand in the Hydrogenase H-Cluster. *J. Am. Chem. Soc.* **2008**, *130* (13), 4533.

Book Chapter

Harris, T.V.; Szilagyi, R.K. Nitrogenase Structure and Function Relationships by Density Functional Theory. In *Nitrogen Fixation: Methods and Protocols*; Ribbe, M.W. Ed.; Humana Press: New York, 2011; pp 267-292.

CONFERENCE PRESENTATIONS

<i>11th FIFC Symposium</i> , Kyoto, Japan	1/23/2014
<i>10th FIFC Symposium</i> , Kyoto, Japan	11/30/2012
<i>CPMD Meeting</i> , Barcelona, Spain	9/5/2011
<i>50th Sanibel Symposium</i> , St. Simon's Island, GA	2/24/2010
<i>MT ACS Spring Meeting-in-Miniature</i> , Butte, MT (oral)	2/20/2010
<i>14th International Conference on Biological Chemistry</i> , Nagoya, Japan	7/25/2009
<i>ACS Montana Section Meeting</i> , Bozeman, MT (oral)	4/18/2009
<i>ACS National Meeting</i> , Salt Lake City, UT (oral)	3/22/2009
<i>Gordon Research Conference on Iron-Sulfur Enzymes</i> , New London, NH	6/8/2008
<i>ACS Montana Section Meeting</i> , Butte, MT (oral)	4/14/2007
<i>ACS National Meeting</i> , Chicago, IL	3/25/2007

AWARDS AND HONORS

Japan Society for the Promotion of Science (JSPS) Postdoctoral Fellowship	2012
NSF Materials Computation Center Travel Grant	2011
Kopriva Graduate Student Fellowship	2009
Molecular Biosciences Fellowship	2007–2011
ACS Montana Travel Grant	2007
Summa cum laude, Willamette University	2006
ACS Portland Harold Zeh Award	2005
Hatfield Library Research Award	2005
Phi Beta Kappa (junior year)	2005

REFERENCES

- (1) John Hanson (Professor)
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Phone: 253-879-2693
Email: hanson@pugetsound.edu
- (2) Dan Burgard (Professor)
Department of Chemistry
University of Puget Sound
Phone: 253-879-1570
Email: dburgard@pugetsound.edu
- (3) Stacia Rink (Visiting Assistant Professor)
Department of Chemistry
University of Puget Sound
Phone: 253-879-5993
Email: srink@pugetsound.edu