

Stanford



Britt Hedman

Professor of Photon Science
Photon Science Directorate

CONTACT INFORMATION

- **Administrative Contact**

Evelyn Castaneda

Email evelync@slac.stanford.edu

Tel (650) 926-4074

Bio

BIO

Hedman's research program is focused on the development and applications of x-ray absorption and emission spectroscopies using synchrotron radiation, with a scientific emphasis primarily on study of the electronic and structural aspects of metal ion active sites in bioinorganic and biological systems. A common theme is to investigate how structure at molecular and macromolecular levels relates to function.

A major long-term focus has been the active site of the enzyme nitrogenase, and the various nitrogenase metal clusters, including elucidating the electronic and geometric structure of those that are formed and changed along their biosynthetic pathways. Other systems of systematic studies include iron-sulfur cluster containing enzymes, blue and multi-copper proteins, heme-copper oxidases, and iron-containing oxidases. Methods developments include x-ray absorption spectroscopy (edge and extended fine structure - or EXAFS), including the application of multiple-scattering analysis in EXAFS studies of metal clusters relevant to bioinorganic systems, the development of methodology for polarized single crystal x-ray absorption spectroscopy, and methodology and instrumentation development for soft- through hard-energy XAS.

Hedman received her B.S and B.A. in Chemistry, M.Sc. in Inorganic Chemistry, and Ph.D. in Chemistry from the University of Umeå, Sweden. She was Assistant Professor (equivalent) in Inorganic Chemistry at the University of Umeå before coming to Stanford, initially as Senior Academic Scientific Staff, followed by appointed as Professor (Research) in 2002, and Professor of Photon Science in 2007.

ACADEMIC APPOINTMENTS

- Professor, Photon Science Directorate

ADMINISTRATIVE APPOINTMENTS

- Science Director, Stanford Synchrotron Radiation Lightsource, (2010- present)
- Vice Chair, Photon Science Faculty, (2007-2011)
- Deputy Director, Stanford Synchrotron Radiation Lightsource, (2005-2010)
- Assistant Director, Stanford Synchrotron Radiation Laboratory, (2001-2005)
- Co-Director, Structural Molecular Biology Program, Stanford Synchrotron Radiation Lightsource, (1998- present)

HONORS AND AWARDS

- International X-ray Absorption Society Contribution Trophy for Contribution to the Community, IXAS (2013)
- International X-ray Absorption Society Edward Stern Outstanding Achievement Award, IXAS (2009)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Member, Scientific Advisory Committee for Australian Synchrotron, ANSTO (2018 - present)
- Member, Scientific Advisory Committee, Advanced Photon Source, Argonne National Laboratory (2009 - 2015)
- Member, Scientific Advisory Committee, Canadian Light Source (2005 - 2007)
- Member & Sub-Group Chair, Committee of Visitors, Department of Energy, Biological and Environmental Research, Biological Systems Science Division (2017 - 2017)
- Member, International Union of Crystallography Commission on XAFS (2002 - 2011)
- Consultant, International Union of Crystallography Commission on XAFS (2011 - 2017)
- Member, BioCAT Advisory Committee, Advanced Photon Source, Argonne National Laboratory (2001 - 2008)
- Member, International XAFS Society Executive Committee (2000 - 2006)
- Member, International Union of Crystallography Commission on Synchrotron Radiation (1990 - 1996)

PROFESSIONAL EDUCATION

- Ph.D., University of Umeå, Sweden , Chemistry (1978)
- M.Sc., University of Umeå, Sweden , Inorganic Chemistry (1972)
- B.S., University of Umeå, Sweden , Chemistry (1971)

Teaching

STANFORD ADVISEES

Postdoctoral Faculty Sponsor

Marwa Atwa, Ozge Bozkurt, Melissa Cendejas, Weiying He, Anastassiya Khan, Chris Miller, Aruna Narayanan Nair, Lizzie Paulus, Anamika Poduval, Kewei Zhao

Publications

PUBLICATIONS

- **Methane Activation by a Mononuclear Copper Active Site in the Zeolite Mordenite: Effect of Metal Nuclearity on Reactivity.** *Journal of the American Chemical Society*
Heyer, A. J., Plessers, D., Braun, A., Rhoda, H. M., Bols, M. L., Hedman, B., Hodgson, K. O., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2022
- **Incorporation of an Asymmetric Mo-Fe-S Cluster as an Artificial Cofactor into Nitrogenase.** *Chembiochem : a European journal of chemical biology*
Tanifuji, K., Jasniewski, A., Lee, C. C., Solomon, J., Nagasawa, T., Ohki, Y., Tatsumi, K., Hedman, B., Hodgson, K., Hu, Y., Ribbe, M. W.
2022
- **Radical SAM-dependent formation of a nitrogenase cofactor core on NifB.** *Journal of inorganic biochemistry*
Liu, Y. A., Quechol, R., Solomon, J. B., Lee, C. C., Ribbe, M. W., Hu, Y., Hedman, B., Hodgson, K. O.
2022; 233: 111837
- **Characterization of a Nitrogenase Iron Protein Substituted with a Synthetic [Fe4Se4] Cluster.** *Angewandte Chemie (International ed. in English)*
Solomon, J., Tanifuji, K., Lee, C. C., Jasniewski, A., Hedman, B., Hodgson, K., Hu, Y., Ribbe, M.
2022
- **S K-edge XAS of CuII, CuI, and ZnII oxidized Dithiolene complexes: Covalent contributions to structure and the Jahn-Teller effect.** *Journal of inorganic biochemistry*

Ha, Y., Dille, S. A., Braun, A., Colston, K., Hedman, B., Hodgson, K. O., Basu, P., Solomon, E. I.
2022; 230: 111752

- **Tracing the incorporation of the "ninth sulfur" into the nitrogenase cofactor precursor with selenite and tellurite.** *Nature chemistry*
Tanifuji, K., Jasniewski, A. J., Villarreal, D., Stiebritz, M. T., Lee, C. C., Wilcoxen, J., Okhi, Y., Chatterjee, R., Bogacz, I., Yano, J., Kern, J., Hedman, B., Hodgson, et al
2021

- **Millisecond timescale reactions observed via X-ray spectroscopy in a 3D microfabricated fused silica mixer.** *Journal of synchrotron radiation*
Huyke, D. A., Ramachandran, A., Ramirez-Neri, O., Guerrero-Cruz, J. A., Gee, L. B., Braun, A., Sokaras, D., Garcia-Estrada, B., Solomon, E. I., Hedman, B., Delgado-Jaime, M. U., DePonte, D. P., Kroll, et al
2021; 28 (Pt 4): 1100-1113

- **Effect of 3d/4p Mixing on 1s2p Resonant Inelastic X-ray Scattering: Electronic Structure of Oxo-Bridged Iron Dimers.** *Journal of the American Chemical Society*
Kroll, T., Baker, M. L., Wilson, S. A., Lundberg, M., Juhin, A., Arrio, M., Yan, J. J., Gee, L. B., Braun, A., Weng, T., Sokaras, D., Hedman, B., Hodgson, et al
2021

- **A Thioether-Ligated Cupric Superoxide Model with Hydrogen Atom Abstraction Reactivity.** *Journal of the American Chemical Society*
Bhadra, M. n., Transue, W. J., Lim, H. n., Cowley, R. E., Lee, J. Y., Siegler, M. A., Josephs, P. n., Henkel, G. n., Lerch, M. n., Schindler, S. n., Neuba, A. n., Hodgson, K. O., Hedman, et al
2021

- **Short-lived metal-centered excited state initiates iron-methionine photodissociation in ferrous cytochrome c.** *Nature communications*
Reinhard, M. E., Mara, M. W., Kroll, T., Lim, H., Hadt, R. G., Alonso-Mori, R., Chollet, M., Glownia, J. M., Nelson, S., Sokaras, D., Kunus, K., Driel, T. B., Hartsock, et al
2021; 12 (1): 1086

- **Kbeta X-ray Emission Spectroscopy as a Probe of Cu(I) Sites: Application to the Cu(I) Site in Preprocessed Galactose Oxidase.** *Inorganic chemistry*
Lim, H., Baker, M. L., Cowley, R. E., Kim, S., Bhadra, M., Siegler, M. A., Kroll, T., Sokaras, D., Weng, T., Biswas, D. R., Dooley, D. M., Karlin, K. D., Hedman, et al
2020

- **Evaluation of a concerted vs. sequential oxygen activation mechanism in #-ketoglutarate-dependent nonheme ferrous enzymes.** *Proceedings of the National Academy of Sciences of the United States of America*
Goudarzi, S. n., Iyer, S. R., Babicz, J. T., Yan, J. J., Peters, G. H., Christensen, H. E., Hedman, B. n., Hodgson, K. O., Solomon, E. I.
2020

- **Biological sulfur in the blood cells of Ascidia ceratodes: XAS spectroscopy and a cellular-enzymatic hypothesis for vanadium reduction in the ascidians.** *Journal of inorganic biochemistry*
Frank, P. n., Carlson, R. M., Carlson, E. J., Hedman, B. n., Hodgson, K. O.
2020; 205: 110991

- **X-ray Absorption Spectroscopy as a Probe of Ligand Noninnocence in Metallocorroles: The Case of Copper Corroles** *INORGANIC CHEMISTRY*
Lim, H., Thomas, K. E., Hedman, B., Hodgson, K. O., Ghosh, A., Solomon, E. I.
2019; 58 (10): 6722–30

- **Formylglycine-generating enzyme binds substrate directly at a mononuclear Cu(I) center to initiate O-2 activation** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Appel, M. J., Meier, K. K., Lafrance-Vanassee, J., Lim, H., Tsai, C., Hedman, B., Hodgson, K. O., Tainer, J. A., Solomon, E. I., Bertozzi, C. R.
2019; 116 (12): 5370–75

- **Synchrotron X-radiolysis of L-cysteine at the sulfur K-edge: Sulfurous products, experimental surprises, and dioxygen as an oxidoreductant** *JOURNAL OF CHEMICAL PHYSICS*
Frank, P., Sarangi, R., Hedman, B., Hodgson, K. O.
2019; 150 (10)

- **Resonant inelastic X-ray scattering determination of the electronic structure of oxyhemoglobin and its model complex** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Yan, J. J., Kroll, T., Baker, M. L., Wilson, S. A., Decreau, R., Lundberg, M., Sokaras, D., Glatzel, P., Hedman, B., Hodgson, K. O., Solomon, E. I.
2019; 116 (8): 2854–59

- **Spectroscopic Characterization of an Eight-Iron Nitrogenase Cofactor Precursor that Lacks the "9th Sulfur".** *Angewandte Chemie (International ed. in English)*
Jasniewski, A. J., Wilcoxon, J. n., Tanifuji, K. n., Hedman, B. n., Hodgson, K. O., Britt, R. D., Hu, Y. n., Ribbe, M. W.
2019
- **The Electronic Structure of the Metal Active Site Determines the Geometric Structure and Function of the Metalloregulator NikR.** *Biochemistry*
Ha, Y. n., Hu, H. n., Higgins, K. n., Maroney, M. n., Hedman, B. n., Hodgson, K. n., Solomon, E. n.
2019
- **Tuning the Geometric and Electronic Structure of Synthetic High-Valent Heme Iron(IV)-Oxo Models in the Presence of a Lewis Acid and Various Axial Ligands.** *Journal of the American Chemical Society*
Ehudin, M. A., Gee, L. B., Sabuncu, S. n., Braun, A. n., Moënne-Loccoz, P. n., Hedman, B. n., Hodgson, K. O., Solomon, E. I., Karlin, K. D.
2019; 141 (14): 5942–60
- **Mechanism of selective benzene hydroxylation catalyzed by iron-containing zeolites** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Snyder, B. R., Bols, M. L., Rhoda, H. M., Vanelder, P., Bottger, L. H., Braun, A., Yan, J. J., Hadt, R. G., Babicz, J. T., Hu, M. Y., Zhao, J., Alp, E., Hedman, et al
2018; 115 (48): 12124–29
- **A mononuclear nonheme {FeNO}(6) complex: synthesis and structural and spectroscopic characterization** *CHEMICAL SCIENCE*
Hong, S., Yan, J. J., Karmalkar, D. G., Sutherlin, K. D., Kim, J., Lee, Y., Goo, Y., Mascharak, P. K., Hedman, B., Hodgson, K. O., Karlin, K. D., Solomon, E. I., Nam, et al
2018; 9 (34): 6952–60
- **Oxidation of Naphthalene with a Manganese(IV) Bis(hydroxo) Complex in the Presence of Acid** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Jeong, D., Yan, J. J., Noh, H., Hedman, B., Hodgson, K. O., Solomon, E. I., Cho, J.
2018; 57 (26): 7764–68
- **Structural characterization of a non-heme iron active site in zeolites that hydroxylates methane** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Snyder, B. R., Bottger, L. H., Bols, M. L., Yan, J. J., Rhoda, H. M., Jacobs, A. B., Hu, M. Y., Zhao, J., Alp, E., Hedman, B., Hodgson, K. O., Schoonheydt, R. A., Sels, et al
2018; 115 (18): 4565–70
- **A Six-Coordinate Peroxynitrite Low-Spin Iron(III) Porphyrinate Complex-The Product of the Reaction of Nitrogen Monoxide (center dot NO(g)) with a Ferric-Superoxide Species** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sharma, S. K., Schaefer, A. W., Lim, H., Matsumura, H., Moenue-Loccoz, P., Hedman, B., Hodgson, K. O., Solomon, E. I., Karlin, K. D.
2017; 139 (48): 17421–30
- **Sulfur K-Edge XAS Studies of the Effect of DNA Binding on the [Fe4S4] Site in EndoIII and MutY** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ha, Y., Arnold, A. R., Nunez, N. N., Bartels, P. L., Zhou, A., David, S. S., Barton, J. K., Hedman, B., Hodgson, K., Solomon, E. I.
2017; 139 (33): 11434–42
- **K- and L-edge X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) determination of differential orbital covalency (DOC) of transition metal sites** *COORDINATION CHEMISTRY REVIEWS*
Baker, M. L., Mara, M. W., Yan, J. J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2017; 345: 182–208
- **Metalloprotein entatic control of ligand-metal bonds quantified by ultrafast x-ray spectroscopy** *SCIENCE*
Mara, M. W., Hadt, R. G., Reinhard, M., Kroll, T., Lim, H., Hartsock, R. W., Alonso-Mori, R., Chollet, M., Glownia, J. M., Nelson, S., Sokaras, D., Kunnus, K., Hodgson, et al
2017; 356 (6344): 1276+
- **Spin-Polarization-Induced Preedge Transitions in the Sulfur K-Edge XAS Spectra of Open-Shell Transition-Metal Sulfates: Spectroscopic Validation of s-Bond Electron Transfer.** *Inorganic chemistry*
Frank, P., Szilagyi, R. K., Gramlich, V., Hsu, H., Hedman, B., Hodgson, K. O.
2017; 56 (3): 1080–1093
- **L-Edge X-ray Absorption Spectroscopic Investigation of {FeNO}(6): Delocalization vs Antiferromagnetic Coupling** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yan, J. J., Gonzales, M. A., Mascharak, P. K., Hedman, B., Hodgson, K. O., Solomon, E. I.

2017; 139 (3): 1215-1225

● **Activation in Cofactor Biogenesis.** *Journal of the American Chemical Society*

Cowley, R. E., Cirera, J., Qayyum, M. F., Rokhsana, D., Hedman, B., Hodgson, K. O., Dooley, D. M., Solomon, E. I.
2016; 138 (40): 13219-13229

● **Structure of the Reduced Copper Active Site in Preprocessed Galactose Oxidase: Ligand Tuning for One-Electron O-2 Activation in Cofactor Biogenesis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

Cowley, R. E., Cirera, J., Qayyum, M. F., Rokhsana, D., Hedman, B., Hodgson, K. O., Dooley, D. M., Solomon, E. I.
2016; 138 (40): 13219-13229

● **Assembly scaffold NifEN: A structural and functional homolog of the nitrogenase catalytic component.** *Proceedings of the National Academy of Sciences of the United States of America*

Fay, A. W., Blank, M. A., Rebelein, J. G., Lee, C. C., Ribbe, M. W., Hedman, B., Hodgson, K. O., Hu, Y.
2016; 113 (34): 9504-9508

● **Solvation structure of the halides from x-ray absorption spectroscopy.** *Journal of chemical physics*

Antalek, M., Pace, E., Hedman, B., Hodgson, K. O., Chillemi, G., Benfatto, M., Sarangi, R., Frank, P.
2016; 145 (4): 044318-?

● **Spectroscopic and Theoretical Study of Cu-I Binding to His111 in the Human Prion Protein Fragment 106-115** *INORGANIC CHEMISTRY*

Arcos-Lopez, T., Qayyum, M., Rivillas-Acevedo, L., Miotto, M. C., Grande-Aztatzi, R., Fernandez, C. O., Hedman, B., Hodgson, K. O., Vela, A., Solomon, E. I., Quintanar, L.
2016; 55 (6): 2909-2922

● **Spectroscopic and Theoretical Study of Cu(I) Binding to His111 in the Human Prion Protein Fragment 106-115.** *Inorganic chemistry*

Arcos-López, T., Qayyum, M., Rivillas-Acevedo, L., Miotto, M. C., Grande-Aztatzi, R., Fernández, C. O., Hedman, B., Hodgson, K. O., Vela, A., Solomon, E. I., Quintanar, L.
2016; 55 (6): 2909-2922

● **Uncoupling binding of substrate CO from turnover by vanadium nitrogenase** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Lee, C. C., Fay, A. W., Weng, T., Krest, C. M., Hedman, B., Hodgson, K. O., Hu, Y., Ribbe, M. W.
2015; 112 (45): 13845-13849

● **A high-resolution XAS study of aqueous Cu(II) in liquid and frozen solutions: Pyramidal, polymorphic, and non-centrosymmetric.** *Journal of chemical physics*

Frank, P., Benfatto, M., Qayyam, M., Hedman, B., Hodgson, K. O.
2015; 142 (8): 084310-?

● **Resonant Inelastic X-ray Scattering on Ferrous and Ferric Bis-imidazole Porphyrin and Cytochrome c: Nature and Role of the Axial Methionine-Fe Bond.** *Journal of the American Chemical Society*

Kroll, T., Hadt, R. G., Wilson, S. A., Lundberg, M., Yan, J. J., Weng, T., Sokaras, D., Alonso-Mori, R., Casa, D., Upton, M. H., Hedman, B., Hodgson, K. O., Solomon, et al
2014; 136 (52): 18087-18099

● **Goniometer-based femtosecond crystallography with X-ray free electron lasers** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

Cohen, A. E., Soltis, S. M., Gonzalez, A., Aguilera, L., Alonso-Mori, R., Barnes, C. O., Baxter, E. L., Brehmer, W., Brewster, A. S., Brunger, A. T., Calero, G., Chang, J. F., Chollet, et al
2014; 111 (48): 17122-17127

● **Sulfur K-Edge X-ray Absorption Spectroscopy and Density Functional Theory Calculations on Monooxo Mo-IV and Bisoxo Mo-VI Bis-dithiolenes: Insights into the Mechanism of Oxo Transfer in Sulfite Oxidase and Its Relation to the Mechanism of DMSO Reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

Ha, Y., Tenderholt, A. L., Holm, R. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
2014; 136 (25): 9094-9105

● **Sulfur K-edge X-ray absorption spectroscopy and density functional theory calculations on monooxo Mo(IV) and bisoxo Mo(VI) bis-dithiolenes: insights into the mechanism of oxo transfer in sulfite oxidase and its relation to the mechanism of DMSO reductase.** *Journal of the American Chemical Society*

Ha, Y., Tenderholt, A. L., Holm, R. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
2014; 136 (25): 9094-9105

- **Spectroscopic and computational insight into the activation of O₂ by the mononuclear Cu center in polysaccharide monooxygenases** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Kjaergaard, C. H., Qayyum, M. F., Wong, S. D., Xu, F., Hemsworth, G. R., Walton, D. J., Young, N. A., Davies, G. J., Walton, P. H., Johansen, K. S., Hodgson, K. O., Hedman, B., Solomon, et al
2014; 111 (24): 8797-8802
- **Spectroscopic and computational insight into the activation of O₂ by the mononuclear Cu center in polysaccharide monooxygenases.** *Proceedings of the National Academy of Sciences of the United States of America*
Kjaergaard, C. H., Qayyum, M. F., Wong, S. D., Xu, F., Hemsworth, G. R., Walton, D. J., Young, N. A., Davies, G. J., Walton, P. H., Johansen, K. S., Hodgson, K. O., Hedman, B., Solomon, et al
2014; 111 (24): 8797-8802
- **A Zinc Linchpin Motif in the MUTYH Glycosylase Interdomain Connector Is Required for Efficient Repair of DNA Damage** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Engstrom, L. M., Brinkmeyer, M. K., Ha, Y., Raetz, A. G., Hedman, B., Hodgson, K. O., Solomon, E. I., David, S. S.
2014; 136 (22): 7829-7832
- **Hydroxo-Bridged Dicopper(II,III) and -(III,III) Complexes: Models for Putative Intermediates in Oxidation Catalysis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Halvagar, M. R., Solntsev, P. V., Lim, H., Hedman, B., Hodgson, K. O., Solomon, E. I., Cramer, C. J., Tolman, W. B.
2014; 136 (20): 7269-7272
- **Biosynthesis of Nitrogenase Metalloclusters** *CHEMICAL REVIEWS*
Ribbe, M. W., Hu, Y., Hodgson, K. O., Hedman, B.
2014; 114 (8): 4063-4080
- **XAS spectroscopy, sulfur, and the brew within blood cells from *Ascidia ceratodes*.** *Journal of inorganic biochemistry*
Frank, P., Hedman, B., Hodgson, K. O.
2014; 131: 99-108
- **L-Edge X-ray Absorption Spectroscopy and DFT Calculations on Cu₂O₂ Species: Direct Electrophilic Aromatic Attack by Side-on Peroxo Bridged Dicopper(II) Complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Qayyum, M. F., Sarangi, R., Fujisawa, K., Stack, T. D., Karlin, K. D., Hodgson, K. O., Hedman, B., Solomon, E. I.
2013; 135 (46): 17417-17431
- **Metal-Ligand Covalency of Iron Complexes from High-Resolution Resonant Inelastic X-ray Scattering.** *Journal of the American Chemical Society*
Lundberg, M., Kroll, T., DeBeer, S., Bergmann, U., Wilson, S. A., Glatzel, P., Nordlund, D., Hedman, B., Hodgson, K. O., Solomon, E. I.
2013; 135 (45): 17121-17134
- **Stepwise Protonation and Electron-Transfer Reduction of a Primary Copper-Dioxygen Adduct** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Peterson, R. L., Ginsbach, J. W., Cowley, R. E., Qayyum, M. F., Himes, R. A., Siegler, M. A., Moore, C. D., Hedman, B., Hodgson, K. O., Fukuzumi, S., Solomon, E. I., Karlin, K. D.
2013; 135 (44): 16454-16467
- **X-ray absorption spectroscopic investigation of the electronic structure differences in solution and crystalline oxyhemoglobin** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Wilson, S. A., Green, E., Mathews, I. I., Benfatto, M., Hodgson, K. O., Hedman, B., Sarangi, R.
2013; 110 (41): 16333-16338
- **Preparation of Non-heme {FeNO}(7) Models of Cysteine Dioxygenase: Sulfur versus Nitrogen Ligation and Photorelease of Nitric Oxide** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
McQuilken, A. C., Ha, Y., Sutherlin, K. D., Siegler, M. A., Hodgson, K. O., Hedman, B., Solomon, E. I., Jameson, G. N., Goldberg, D. P.
2013; 135 (38): 14024-14027
- **Modified Reactivity toward O₂ in First Shell Variants of Fet3p: Geometric and Electronic Structure Requirements for a Functioning Trinuclear Copper Cluster** *BIOCHEMISTRY*
Kjaergaard, C. H., Qayyum, M. F., Augustine, A. J., Ziegler, L., Kosman, D. J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2013; 52 (21): 3702-3711
- **Modified reactivity toward O₂ in first shell variants of Fet3p: geometric and electronic structure requirements for a functioning trinuclear copper cluster.** *Biochemistry*

- Kjaergaard, C. H., Qayyum, M. F., Augustine, A. J., Ziegler, L., Kosman, D. J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2013; 52 (21): 3702-3711
- **AutoDrug: fully automated macromolecular crystallography workflows for fragment-based drug discovery.** *Acta crystallographica. Section D, Biological crystallography*
Tsai, Y., McPhillips, S. E., González, A., McPhillips, T. M., Zinn, D., Cohen, A. E., Feese, M. D., Bushnell, D., Tiefenbrunn, T., Stout, C. D., Ludaescher, B., Hedman, B., Hodgson, et al
2013; 69: 796-803
 - **Iron L-Edge X-ray Absorption Spectroscopy of Oxy-Picket Fence Porphyrin: Experimental Insight into Fe-O-2 Bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Wilson, S. A., Kroll, T., Decreau, R. A., Hocking, R. K., Lundberg, M., Hedman, B., Hodgson, K. O., Solomon, E. I.
2013; 135 (3): 1124-1136
 - **Geometric and electronic structures of the His-Fe(IV)=O and His-Fe(IV)-Tyr hemes of MauG** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Jensen, L. M., Meharennna, Y. T., Davidson, V. L., Poulos, T. L., Hedman, B., Wilmot, C. M., Sarangi, R.
2012; 17 (8): 1241-1255
 - **The x-ray absorption spectroscopy model of solvation about sulfur in aqueous L-cysteine** *JOURNAL OF CHEMICAL PHYSICS*
Sarangi, R., Frank, P., Benfatto, M., Morante, S., Minicozzi, V., Hedman, B., Hodgson, K. O.
2012; 137 (20)
 - **X-ray-induced photo-chemistry and X-ray absorption spectroscopy of biological samples** *JOURNAL OF SYNCHROTRON RADIATION*
George, G. N., Pickering, I. J., Pushie, M. J., Nienaber, K., Hackett, M. J., Ascone, I., Hedman, B., Hodgson, K. O., Aitken, J. B., Levina, A., Glover, C., Lay, P. A.
2012; 19: 875-886
 - **Spectroscopic and DFT Studies of Second-Sphere Variants of the Type 1 Copper Site in Azurin: Covalent and Nonlocal Electrostatic Contributions to Reduction Potentials** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hadz, R. G., Sun, N., Marshall, N. M., Hodgson, K. O., Hedman, B., Lu, Y., Solomon, E. I.
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