



Keith Hodgson

David Mulvane Ehrsam and Edward Curtis Franklin Professor of Chemistry and
Professor of Photon Science at SLAC
Photon Science Directorate

CONTACT INFORMATION

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Bio

BIO

Combining inorganic, biophysical and structural chemistry, Professor Keith Hodgson investigates how structure at molecular and macromolecular levels relates to function. Studies in the Hodgson lab have pioneered the use of synchrotron x-radiation to probe the electronic and structural environment of biomolecules. Recent efforts focus on the applications of x-ray diffraction, scattering and absorption spectroscopy to examine metalloproteins that are important in Earth's biosphere, such as those that convert nitrogen to ammonia or methane to methanol.

Keith O. Hodgson was born in Virginia in 1947. He studied chemistry at the University of Virginia (B.S. 1969) and University of California, Berkeley (Ph.D. 1972), with a postdoctoral year at the ETH in Zurich. He joined the Stanford Chemistry Department faculty in 1973, starting up a program of fundamental research into the use of x-rays to study chemical and biological structure that made use of the unique capabilities of the Stanford Synchrotron Radiation Lightsource (SSRL). His lab carried out pioneering x-ray absorption and x-ray crystallographic studies of proteins, laying the foundation for a new field now in broad use worldwide. In the early eighties, he began development of one of the world's first synchrotron-based structural molecular biology research and user programs, centered at SSRL. He served as SSRL Director from 1998 to 2005, and SLAC National Accelerator Laboratory (SLAC) Deputy Director (2005-2007) and Associate Laboratory Director for Photon Science (2007-2011).

Today the Hodgson research group investigates how molecular structure at different organizational levels relates to biological and chemical function, using a variety of x-ray absorption, diffraction and scattering techniques. Typical of these molecular structural studies are investigations of metal ions as active sites of biomolecules. His research group develops and utilizes techniques such as x-ray absorption and emission spectroscopy (XAS and XES) to study the electronic and metrical details of a given metal ion in the biomolecule under a variety of natural conditions.

A major area of focus over many years, the active site of the enzyme nitrogenase is responsible for conversion of atmospheric di-nitrogen to ammonia. Using XAS studies at the S, Fe and Mo edge, the Hodgson group has worked to understand the electronic structure as a function of redox in this cluster. They have developed new methods to study long distances in the cluster within and outside the protein. Studies are ongoing to learn how this cluster functions during catalysis and interacts with substrates and inhibitors. Other components of the protein are also under active study.

Additional projects include the study of iron in dioxygen activation and oxidation within the binuclear iron-containing enzyme methane monooxygenase and in cytochrome oxidase. Lab members are also investigating the role of copper in electron transport and in dioxygen activation. Other studies include the electronic structure of iron-sulfur clusters in models and enzymes.

The research group is also focusing on using the next generation of x-ray light sources, the free electron laser. Such a light source, called the LCLS, is also located at SLAC. They are also developing new approaches using x-ray free electron laser radiation to image noncrystalline biomolecules and study chemical reactivity on ultrafast time scales.

ACADEMIC APPOINTMENTS

- Professor, Photon Science Directorate
- Professor, Chemistry
- Member, Bio-X
- Faculty Fellow, Sarafan ChEM-H

ADMINISTRATIVE APPOINTMENTS

- Chair, Department of Chemistry, Stanford University, (2014-2020)

HONORS AND AWARDS

- Member, National Academy of Sciences (2011)
- E.O. Lawrence Award, U.S. Department of Energy (2002)
- World Bank Lecturer, World Bank (1984)
- Robert A. Welch Foundation Lecturer, Robert A. Welch Foundation (1981)
- Sidhu Award for Contributions to X-ray Diffraction, Pittsburgh Diffraction Society (1978)
- Alfred P. Sloan Fellow, Alfred P. Sloan Foundation (1976-78)
- NATO Postdoctoral Fellowship, Eidgenössische Technische Hochschule, Zürich, Switzerland (1972-73)

PROFESSIONAL EDUCATION

- NATO Postdoctoral Fellow, Eidgenössische Technische Hochschule, Zürich, Switzerland , Chemistry (1973)
- PhD, University of California at Berkeley , Chemistry (1972)
- BS, University of Virginia , Chemistry (1969)

Teaching

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biophysics (Phd Program)

Publications

PUBLICATIONS

- **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
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- **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., Aguila, 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
- **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
- **Structure and reactivity of a mononuclear non-haem iron(III)-peroxo complex** *NATURE*
Cho, J., Jeon, S., Wilson, S. A., Liu, L. V., Kang, E. A., Braymer, J. J., Lim, M. H., Hedman, B., Hodgson, K. O., Valentine, J. S., Solomon, E. I., Nam, W.
2011; 478 (7370): 502-505
- **Solvent tuning of electrochemical potentials in the active sites of HiPIP versus ferredoxin** *SCIENCE*
Dey, A., Jenney, F. E., Adams, M. W., Babini, E., Takahashi, Y., Fukuyama, K., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 318 (5855): 1464-1468
- **Sulfur K-edge X-ray absorption spectroscopy as a probe of ligand-metal bond covalency: Metal vs ligand oxidation in copper and nickel dithiolene complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sarangi, R., George, S. D., Rudd, D. J., Szilagy, R. K., Ribas, X., Rovira, C., Almeida, M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 129 (8): 2316-2326
- **Femtosecond diffractive imaging with a soft-X-ray free-electron laser** *NATURE PHYSICS*
Chapman, H. N., Barty, A., Bogan, M. J., Boutet, S., Frank, M., Hau-Riege, S. P., Marchesini, S., Woods, B. W., Bajt, S., Benner, H., London, R. A., Ploenjes, E., Kuhlmann, et al
2006; 2 (12): 839-843
- **Structural genomics of the *Thermotoga maritima* proteome implemented in a high-throughput structure determination pipeline** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Lesley, S. A., Kuhn, P., Godzik, A., Deacon, A. M., Mathews, I., Kreuzsch, A., Spraggon, G., Klock, H. E., McMullan, D., Shin, T., VINCENT, J., Robb, A., Brinen, et al
2002; 99 (18): 11664-11669
- **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
- **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.
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- **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.
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- **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.
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- **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*
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- **Modified Reactivity toward O-2 in First Shell Variants of Fet3p: Geometric and Electronic Structure Requirements for a Functioning Trinuclear Copper Cluster** *BIOCHEMISTRY*
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- **AutoDrug: fully automated macromolecular crystallography workflows for fragment-based drug discovery.** *Acta crystallographica. Section D, Biological crystallography*
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- **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.
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- **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*
Hadt, R. G., Sun, N., Marshall, N. M., Hodgson, K. O., Hedman, B., Lu, Y., Solomon, E. I.
2012; 134 (40): 16701-16716
- **(Fe-IV=O)(TBC)(CH₃CN)](2+): Comparative Reactivity of Iron(IV)-Oxo Species with Constrained Equatorial Cyclam Ligation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Wilson, S. A., Chen, J., Hong, S., Lee, Y., Clemancey, M., Garcia-Serres, R., Nomura, T., Ogura, T., Latour, J., Hedman, B., Hodgson, K. O., Nam, W., Solomon, et al
2012; 134 (28): 11791-11806
- **Revisiting the Polyoxometalate-Based Late-Transition-Metal-Oxo Complexes: The "Oxo Wall" Stands** *INORGANIC CHEMISTRY*
O'Halloran, K. P., Zhao, C., Ando, N. S., Schultz, A. J., Koetzle, T. F., Piccoli, P. M., Hedman, B., Hodgson, K. O., Boby, E., Kirk, M. L., Knottenbelt, S., Depperman, E. C., Stein, et al
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- **Fractal morphology, imaging and mass spectrometry of single aerosol particles in flight** *NATURE*
Loh, N. D., Hampton, C. Y., Martin, A. V., Starodub, D., Sierra, R. G., Barty, A., Aquila, A., Schulz, J., Lomb, L., Steinbrener, J., Shoeman, R. L., Kassemeyer, S., Bostedt, et al
2012; 486 (7404): 513-517
- **Geometric and Electronic Structure of [Cu(MeAN)](2)(mu-eta(2):eta(2)(O-2(2-)))](2+) with an Unusually Long O-O Bond: O-O Bond Weakening vs Activation for Reductive Cleavage** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Spectroscopic and Crystallographic Characterization of "Alternative Resting" and "Resting Oxidized" Enzyme Forms of Bilirubin Oxidase: Implications for Activity and Electrochemical Behavior of Multicopper Oxidases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Substrate and Metal Control of Barrier Heights for Oxo Transfer to Mo and W Bis-dithiolene Sites** *INORGANIC CHEMISTRY*
Tenderholt, A. L., Hodgson, K. O., Hedman, B., Holm, R. H., Solomon, E. I.
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- **The X-ray Absorption Spectroscopic Model of the Copper(II) Imidazole Complex Ion in Liquid Aqueous Solution: A Strongly Solvated Square Pyramid** *INORGANIC CHEMISTRY*
Frank, P., Benfatto, M., Hedman, B., Hodgson, K. O.
2012; 51 (4): 2086-2096
- **High-Resolution Analysis of Zn²⁺ Coordination in the Alkaline Phosphatase Superfamily by EXAFS and X-ray Crystallography** *JOURNAL OF MOLECULAR BIOLOGY*
Boby, E., Lassila, J. K., Wiersma-Koch, H. I., Fenn, T. D., Lee, J. J., Nikolic-Hughes, I., Hodgson, K. O., Rees, D. C., Hedman, B., Herschlag, D.
2012; 415 (1): 102-117
- **Spectroscopic Elucidation of a New Heme/Copper Dioxygen Structure Type: Implications for O center dot center dot center dot O Bond Rupture in Cytochrome c Oxidase** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Kieber-Emmons, M. T., Qayyum, M. F., Li, Y., Halime, Z., Hodgson, K. O., Hedman, B., Karlin, K. D., Solomon, E. I.
2012; 51 (1): 168-172
- **Profiling structured beams using injected aerosols** *Conference on X-Ray Free-Electron Lasers - Beam Diagnostics, Beamline Instrumentation, and Applications*
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- **S K-edge XAS and DFT Calculations on SAM Dependent Pyruvate Formate-Lyase Activating Enzyme: Nature of Interaction between the Fe₄S₄ Cluster and SAM and its Role in Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Structural Models of the [Fe₄S₄] Clusters of Homologous Nitrogenase Fe Proteins** *INORGANIC CHEMISTRY*

- Blank, M. A., Lee, C. C., Hu, Y., Hodgson, K. O., Hedman, B., Ribbe, M. W.
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- **A Codeposition Route to CuI-Pyridine Coordination Complexes for Organic Light-Emitting Diodes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Liu, Z., Qayyum, M. F., Wu, C., Whited, M. T., Djurovich, P. I., Hodgson, K. O., Hedman, B., Solomon, E. I., Thompson, M. E.
2011; 133 (11): 3700-3703
 - **S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}(7) Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}(7) and {FeO2}(8)** *INORGANIC CHEMISTRY*
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 - **Spectroscopic Characterization of the Isolated Iron-Molybdenum Cofactor (FeMoco) Precursor from the Protein NifEN** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
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 - **Definition of the intermediates and mechanism of the anticancer drug bleomycin using nuclear resonance vibrational spectroscopy and related methods** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
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 - **S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}(7) Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}(7) and {FeO(2)}(8).** *Inorganic chemistry*
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 - **Characterization of Isolated Nitrogenase FeVco** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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 - **Systematic Perturbation of the Trinuclear Copper Cluster in the Multicopper Oxidases: The Role of Active Site Asymmetry in Its Reduction of O-2 to H2O** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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 - **Heme-Copper-Dioxygen Complexes: Toward Understanding Ligand-Environmental Effects on the Coordination Geometry, Electronic Structure, and Reactivity** *INORGANIC CHEMISTRY*
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- **Fe L-Edge X-ray Absorption Spectroscopy Determination of Differential Orbital Covalency of Siderophore Model Compounds: Electronic Structure Contributions to High Stability Constants** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
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- **Formation of a homocitrate-free iron-molybdenum cluster on NifEN: Implications for the role of homocitrate in nitrogenase assembly** *DALTON TRANSACTIONS*
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- **Crystal Structure of Histidine Phosphotransfer Protein ShpA, an Essential Regulator of Stalk Biogenesis in *Caulobacter crescentus*** *JOURNAL OF MOLECULAR BIOLOGY*
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