



Edward I. Solomon

Monroe E. Spaght Professor in the School of Humanities and Sciences and Professor of Photon Science
Chemistry

CONTACT INFORMATION

- **Alternate Contact**

Sippy Baniya - Administrative Associate

Email sbaniy@stanford.edu

Tel (650) 723-4313

Bio

BIO

Professor Edward Solomon's research spans the fields of physical-inorganic, bioinorganic, and theoretical-inorganic chemistry. His work focuses on spectroscopic elucidation of the electronic structure of transition metal complexes and its contribution to reactivity. He has developed new spectroscopic and electronic structure methods and applied these to active sites in catalysis. He has made significant contributions to our understanding of metal sites involved in electron and oxo transfer, copper sites involved in O₂ binding, activation and reduction to water, in structure/function correlations over non-heme iron enzymes, and in the correlation of biological to heterogeneous catalysis.

Edward I. Solomon grew up in North Miami Beach, Florida, received his Ph.D. at Princeton (1972) and was a postdoctoral fellow at The Ørsted Institute in Denmark and at Caltech. He started his career at MIT in late 1975, became a full professor in 1981, and joined the faculty at Stanford in 1982 where he is now the Monroe E. Spaght Professor of Humanities and Sciences and Professor of Photon Science at SLAC National Accelerator Laboratory. He has been a visiting professor in France, Argentina, Japan, China, India, Australia and Brazil. He has received ACS National Awards in Inorganic Chemistry, Distinguished Service in the Advancement of Inorganic Chemistry, the Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, the Ira Remsen Award, and the Kosolapoff Award, the Centenary Medal from the Royal Society of Chemistry (UK), the Wheland Medal from the University of Chicago, the Bailar Medal from the University of Illinois, the Frontiers in Biological Chemistry Award from the Max-Planck- Institute (Mülheim), the Chakravorty Award from the Chemical Research Society of India and the Dean's Award for Distinguished Teaching at Stanford among others. He is a member of the National Academy of Sciences, the American Academy of Arts and Sciences and a Fellow in American Association for the Advancement of Science and in the American Chemical Society.

The Solomon lab uses both experimental and theoretical techniques to define the electronic and geometric structures of biologically- and catalytically-relevant transition metal sites, with the goal of applying insights into electronic structure to obtain a detailed understanding of reactivity and function. This research utilizes a wide range of spectroscopic, theoretical, and chemical techniques to probe structure/function relationships, gain mechanistic insight, and address fundamental questions of relevance to chemistry and biology. The systems under study can be divided into five general areas:

– Electron Transfer Sites

- Copper Active Sites in Biology
- Mononuclear Non-Heme Iron Enzymes: Structure/Function Correlation
- Binuclear Non-Heme Iron Enzymes: Dioxygen Binding and Activation
- Correlations from Biological to Heterogenous Catalysis

ACADEMIC APPOINTMENTS

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

ADMINISTRATIVE APPOINTMENTS

- Affiliated Faculty Member and Researcher, Stanford Precourt Institute for Energy, (2013- present)
- Member, Digestive Disease Center, Stanford Medical School, (2005- present)
- Professor of Photon Science, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, (2005- present)
- Affiliated Faculty Member, Stanford-NIH Graduate Training Program in Biotechnology, (1993-2010)
- Faculty Member, Stanford Biophysics Program, (1990- present)

HONORS AND AWARDS

- Member, National Academy of Sciences (2005)
- Fellow, American Academy of Arts and Sciences (1998)
- Fellow, inaugural class, American Chemical Society (2009)
- Fellow, American Association for the Advancement of Science (1981)
- Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, American Chemical Society (2016)
- ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, American Chemical Society (2006)
- ACS Award in Inorganic Chemistry, American Chemical Society (2001)
- Centenary Medal and Lectureship, Royal Society of Chemistry, UK (2003)
- Dean's Award for Distinguished Teaching, Stanford University (1990)
- Chakravorty Award & Lectureship, Chemical Research Society of India (2008)
- Fellow, Stanford ChEM-H Institute (2015)
- Honorary Member, Israel Chemical Society (2015)
- Kosolapoff Award, Auburn Section, American Chemical Society (2015)
- Issue dedicated to EIS, Coordination Chemistry Review (2012)
- Prof. Edward I. Solomon Award, ScienceJet (2011)
- Voice of Inorganic Chemistry, American Chemical Society (2011)
- Fellow, Japan Society of the Promotion of Science (2009, 2002, 1995)
- Visiting Scholar, National Science Council, Taiwan (2009)
- Issue dedicated to EIS, Inorganica Chimica Acta (2008)
- Bailar Medal, University of Illinois (2007)
- Thomas Chemistry Scholar, University of Missouri - Columbia (2007)
- Highly Cited Researcher, Institute for Scientific Information (2005)

- NIH MERIT Award, National Institutes of Health (2002, 1995)
- Frontiers in Biological Chemistry Award and Lectureship, MPI, Mülheim (2001)
- G. W. Wheland Medal, University of Chicago (2000)
- Invited Professor, Tata Institute, Bombay, India (2000)
- Golden Jubilee Invited Professor, TATA Institute, Mumbai, India (1996)
- Remsen Award, Maryland ACS and Johns Hopkins University (1994)
- Invited Professor, Tokyo Institute of Technology (1992)
- First Monroe E. Spaght Professor of Chemistry, Stanford University (1991)
- Invited Professor, Universite de Paris, Orsay (1987)
- Creativity Extension, National Science Foundation (1985-7)
- Young Faculty Award, General Electric (1979-80)
- Young Faculty Award, Dupont (1979-80)
- Fellow, Alfred P. Sloan Foundation (1976-79)
- Young Faculty Award, General Electric (1976-77)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Editorial Board Member, Chemical Reviews (1990 - present)
- Editorial Advisory Board Member, Biochemistry (2008 - present)
- Editorial Board Member, Inorganica Chimica Acta (1980 - present)
- Editorial Board Member, Journal of Inorganic Biochemistry (1991 - present)
- Editorial Board Member, Coordination Chemistry Reviews (1996 - present)
- Editorial Board Member, Indian Journal of Chemistry (2001 - present)
- Editorial Board Member, Encyclopedia of Inorganic and Bioinorganic Chemistry (2012 - present)
- Editorial Board Member, International Journal of Inorganic Chemistry (2008 - present)
- Editorial Board Member, Central European Journal of Chemistry/Open Chemistry (2003 - present)
- Editorial Board Member, Chemistry Central Journal (2006 - present)
- Editorial Board Member, Open Access Books Versita (2012 - present)
- Editorial Board Member, Journal of Thermodynamics & Catalysis (2011 - present)
- Editorial Board Member, Current Inorganic Chemistry (2010 - present)
- Editorial Board Member, Open Inorganic Chemistry Journal (2007 - present)
- Editorial Board Member, Metal Based Drugs (2006 - 2011)
- Member, Society of Biological Inorganic Chemistry (1996 - present)
- Member, International EPR Society (1996 - present)
- Editorial Board Member, Journal of Biological Inorganic Chemistry (1995 - 2003)
- Editorial Board Member, Chemistry & Biology (1993 - 2004)
- Editorial Board Member, Chemtracts Inorganic Chemistry (1992 - 2009)
- Associate Editor, Inorganic Chemistry (1985 - 2015)

PROFESSIONAL EDUCATION

- Postdoc, California Inst. of Technology, Pasadena, CA , Bioinorganic (H. Gray) (1975)

- Postdoc, University of Copenhagen (H.C. Ørsted Inst.), Denmark , Phys. Inorg. (C.Ballhausen) (1974)
- Postdoc, Princeton University, Princeton, N.J. , Chem. Phys. (D. McClure) (1973)
- PhD, Princeton University, Princeton, N.J. , Phys. Chem (1972)
- M.S., Princeton University, Princeton, N.J. , Phys. Chem (1970)
- B.S., Rensselaer Polytechnic Institute, Troy, NY , Chemistry (1968)

LINKS

- The Solomon Laboratory: <http://www.stanford.edu/group/solomon/home.html>

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

Professor Solomon's research spans the fields of physical-inorganic and bioinorganic chemistry, emphasizing the application of a wide variety of spectroscopic and computational methods to determine the electronic structure of transition metal complexes. Research is directed toward both high symmetry small molecule complexes to define in detail electronic structure contributions to chemical and physical properties, and metal ion active sites in catalysis to understand their unusual spectral features in terms of electronic and geometric structure and to evaluate these structural contributions to reactivity. Many studies focus on fundamental problems in bioinorganic chemistry. Areas of present interest include: 1) Electronic structure contributions to electron transfer in copper, iron-sulfur and heme sites; 2) O₂ binding, activation, and reduction by Cu cluster active sites; 3) Structure/function correlations over non-heme iron enzymes; 4) Development of new spectroscopic and electronic structure methods in bioinorganic chemistry; and 5) Correlation of biological to heterogeneous catalysis.

Teaching

COURSES

2018-19

- Bio-Inorganic Chemistry: BIOPHYS 297, CHEM 297 (Win)
- Inorganic Chemistry II: CHEM 153 (Spr)
- Inorganic Chemistry Seminar: CHEM 259 (Aut, Win, Spr)
- Research Progress in Inorganic Chemistry: CHEM 258A (Win)
- Research Progress in Inorganic Chemistry: CHEM 258B (Spr)
- Research Progress in Inorganic Chemistry: CHEM 258C (Aut, Win)

2017-18

- Inorganic Chemistry II: CHEM 153 (Spr)
- Inorganic Chemistry Seminar: CHEM 259 (Aut, Win, Spr)
- Research Progress in Inorganic Chemistry: CHEM 258A (Win)
- Research Progress in Inorganic Chemistry: CHEM 258B (Spr)
- Research Progress in Inorganic Chemistry: CHEM 258C (Aut, Win)

2016-17

- Advanced Inorganic Chemistry: CHEM 253 (Win)
- Inorganic Chemistry II: CHEM 153 (Spr)
- Inorganic Chemistry Seminar: CHEM 259 (Aut, Win, Spr)
- Research Progress in Inorganic Chemistry: CHEM 258A (Win)
- Research Progress in Inorganic Chemistry: CHEM 258B (Spr)

- Research Progress in Inorganic Chemistry: CHEM 258C (Aut, Win)

2015-16

- Bio-Inorganic Chemistry: BIOPHYS 297, CHEM 297 (Win)
- Inorganic Chemistry II: CHEM 153 (Spr)
- Inorganic Chemistry Seminar: CHEM 259 (Aut, Win, Spr)
- Research Progress in Inorganic Chemistry: CHEM 258A (Win)
- Research Progress in Inorganic Chemistry: CHEM 258B (Spr)
- Research Progress in Inorganic Chemistry: CHEM 258C (Aut, Win)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Bridget Connor, Ethan Crace, Will Keown, Sam Schneider

Postdoctoral Faculty Sponsor

Leland Gee, Katlyn Meier, Shiliang Tian, Wesley Transue

Doctoral Dissertation Advisor (AC)

Jeffrey Babicz, Augustin Braun, Shyam Iyer, Ariel Jacobs, Stephen Jones, Ioannis Kipouros, Hannah Rhoda

Doctoral Dissertation Co-Advisor (AC)

Hyeongtaek Lim

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biophysics (Phd Program)

Publications

PUBLICATIONS

- **O₂ Reduction to Water by High Potential Multicopper Oxidases: Contributions of the T1 Copper Site Potential and the Local Environment of the Trinuclear Copper Cluster.** *Journal of the American Chemical Society*
Sekretaryova, A., Jones, S. M., Solomon, E. I.
2019
- **Chloride Control of the Mechanism of Human Serum Ceruloplasmin (Cp) Catalysis.** *Journal of the American Chemical Society*
Tian, S., Jones, S. M., Jose, A., Solomon, E. I.
2019
- **X-ray Absorption Spectroscopy as a Probe of Ligand Noninnocence in Metalloporphyrins: The Case of Copper Porphyrins** *INORGANIC CHEMISTRY*
Lim, H., Thomas, K. E., Hedman, B., Hodgson, K. O., Ghosh, A., Solomon, E. I.
2019; 58 (10): 6722–30
- **Spin Interconversion of Heme-Peroxo-Copper Complexes Facilitated by Intramolecular Hydrogen-Bonding Interactions** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Schaefer, A. W., Ehdin, M. A., Quist, D. A., Tang, J. A., Karlin, K. D., Solomon, E. I.
2019; 141 (12): 4936–51
- **Spin Interconversion of Heme-Peroxo-Copper Complexes Facilitated by Intramolecular Hydrogen-Bonding Interactions.** *Journal of the American Chemical Society*
Schaefer, A. W., Ehdin, M. A., Quist, D. A., Tang, J. A., Karlin, K. D., Solomon, E. I.
2019

- **Influence of intramolecular secondary sphere hydrogen-bonding interactions on cytochrome c oxidase inspired low-spin heme-peroxo-copper complexes** *CHEMICAL SCIENCE*
Ehudin, M. A., Schaefer, A. W., Adam, S. M., Quist, D. A., Diaz, D. E., Tang, J. A., Solomon, E. I., Karlin, K. D.
2019; 10 (10): 2893–2905
- **Formylglycine-generating enzyme binds substrate directly at a mononuclear Cu(I) center to initiate O₂ activation.** *Proceedings of the National Academy of Sciences of the United States of America*
Appel, M. J., Meier, K. K., Lafrance-Vanasse, J., Lim, H., Tsai, C., Hedman, B., Hodgson, K. O., Tainer, J. A., Solomon, E. I., Bertozzi, C. R.
2019
- **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
- **X-ray Absorption Spectroscopy as a Probe of Ligand Noninnocence in Metalloporphyrins: The Case of Copper Porphyrins.** *Inorganic chemistry*
Lim, H., Thomas, K. E., Hedman, B., Hodgson, K. O., Ghosh, A., Solomon, E. I.
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., Braun, A., Moëne-Loccoz, P., Hedman, B., Hodgson, K. O., Solomon, E. I., Karlin, K. D.
2019; 141 (14): 5942–60
- **Influence of intramolecular secondary sphere hydrogen-bonding interactions on cytochrome c oxidase inspired low-spin heme-peroxo-copper complexes.** *Chemical science*
Ehudin, M. A., Schaefer, A. W., Adam, S. M., Quist, D. A., Diaz, D. E., Tang, J. A., Solomon, E. I., Karlin, K. D.
2019; 10 (10): 2893–2905
- **Characterization of the Preprocessed Copper Site Equilibrium in Amine Oxidase and Assignment of the Reactive Copper Site in Topaquinone Biogenesis.** *Journal of the American Chemical Society*
Adelson, C. N., Johnston, E. M., Hilmer, K. M., Watts, H., Dey, S. G., Brown, D. E., Broderick, J. B., Shepard, E. M., Dooley, D. M., Solomon, E. I.
2019
- **Geometric and Electronic Structure Contributions to O-O Cleavage and the Resultant Intermediate Generated in Heme-Copper Oxidases.** *Journal of the American Chemical Society*
Schaefer, A. W., Roveda, A. C., Jose, A., Solomon, E. I.
2019; 141 (25): 10068–81
- **Nuclear Resonance Vibrational Spectroscopy Definition of O₂ Intermediates in an Extradioxygenase: Correlation to Crystallography and Reactivity.** *Journal of the American Chemical Society*
Sutherlin, K. D., Wasada-Tsutsui, Y., Mbughuni, M. M., Rogers, M. S., Park, K., Liu, L. V., Kwak, Y., Srncic, M., Bottger, L. H., Frenette, M., Yoda, Y., Kobayashi, Y., Kurokuzu, et al
2018
- **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. E., Bols, M. L., Rhoda, H. M., Vanelderen, P., Bottger, L. H., Braun, A., Yan, J. J., Hadt, R. G., Babicz, J. T., Hu, M. Y., Zhao, J., Alp, E. E., Hedman, et al
2018
- **Spectroscopic and Electronic Structure Study of ETHE1: Elucidating the Factors Influencing Sulfur Oxidation and Oxygenation in Mononuclear Nonheme Iron Enzymes.** *Journal of the American Chemical Society*
Goudarzi, S., Babicz, J. T., Kabil, O., Banerjee, R., Solomon, E. I.
2018
- **Spectroscopic Identification of the alpha-Fe/alpha-O Active Site in Fe-CHA Zeolite for the Low-Temperature Activation of the Methane C-H Bond** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Bols, M. L., Hallaert, S. D., Snyder, B. R., Devos, J., Plessers, D., Rhoda, H. M., Dusselier, M., Schoonheydt, R. A., Pierloot, K., Solomon, E., Sels, B. F.
2018; 140 (38): 12021–32

- **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
- **O₂ Activation by Nonheme FeII alpha-Ketoglutarate-Dependent Enzyme Variants: Elucidating the Role of the Facial Triad Carboxylate in FIIH.** *Journal of the American Chemical Society*
Iyer, S. R., Chaplin, V. D., Knapp, M. J., Solomon, E. I.
2018
- **An intravascular magnetic wire for the high-throughput retrieval of circulating tumour cells in vivo** *NATURE BIOMEDICAL ENGINEERING*
Vermesh, O., Aalipour, A., Ge, T., Saenz, Y., Guo, Y., Alam, I. S., Park, S., Adelson, C. N., Mitsutake, Y., Vilches-Moure, J., Godoy, E., Bachmann, M. H., Ooi, et al
2018; 2 (9): 696–705
- **Activating metal sites for biological electron transfer**
Solomon, E.
AMER CHEMICAL SOC.2018
- **Kinetic and spectroscopic investigation of oxygen activation at a single iron center via Gibbs free energy coupling: Generation of an active alkane oxidation catalyst**
Cunningham, L., Babicz, J., Tucker, W., McCracken, J., Rybak-Akimova, E., Solomon, E., Caradonna, J.
AMER CHEMICAL SOC.2018
- **Second-Sphere Effects on Methane Hydroxylation in Cu-Zeolites** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Snyder, B. R., Vanelderden, P., Schoonheydt, R. A., Sels, B. F., Solomon, E.
2018; 140 (29): 9236–43
- **Intramolecular Hydrogen Bonding Enhances Stability and Reactivity of Mononuclear Cupric Superoxide Complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Bhadra, M., Lee, J. C., Cowley, R. E., Kim, S., Siegler, M. A., Solomon, E., Karlin, K. D.
2018; 140 (29): 9042–45
- **Second-Sphere Effects on Methane Hydroxylation in Cu-Zeolites.** *Journal of the American Chemical Society*
Snyder, B. E., Vanelderden, P., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2018
- **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
- **NRVS Studies of the Peroxide Shunt Intermediate in a Rieske Dioxygenase and Its Relation to the Native Fe-II O-2 Reaction** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sutherlin, K. D., Rivard, B. S., Bottger, L. H., Liu, L. V., Rogers, M. S., Srncic, M., Park, K., Yoda, Y., Kitao, S., Kobayashi, Y., Saito, M., Seto, M., Hu, et al
2018; 140 (16): 5544–59
- **Iron and Copper Active Sites in Zeolites and Their Correlation to Metalloenzymes** *CHEMICAL REVIEWS*
Snyder, B. R., Bols, M. L., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2018; 118 (5): 2718–68
- **Oxygen Activation by Cu LPMOs in Recalcitrant Carbohydrate Polysaccharide Conversion to Monomer Sugars** *CHEMICAL REVIEWS*
Meier, K. K., Jones, S. M., Kaper, T., Hansson, H., Koetsier, M. J., Karkehabadi, S., Solomon, E. I., Sandgren, M., Kelemen, B.
2018; 118 (5): 2593–2635
- **Introduction: Oxygen Reduction and Activation in Catalysis** *CHEMICAL REVIEWS*

Solomon, E. L., Stahl, S. S.

2018; 118 (5): 2299–2301

- **An intravascular magnetic wire for the high-throughput retrieval of circulating tumour cells in vivo.** *Nature biomedical engineering*
Vermesh, O., Aalipour, A., Ge, T. J., Saenz, Y., Guo, Y., Alam, I. S., Park, S. M., Adelson, C. N., Mitsutake, Y., Vilches-Moure, J., Godoy, E., Bachmann, M. H., Ooi, et al
2018; 2 (9): 696–705
- **An intravascular magnetic wire for the high-throughput retrieval of circulating tumour cells in vivo.** *Nature biomedical engineering*
Vermesh, O., Aalipour, A., Ge, T. J., Saenz, Y., Guo, Y., Alam, I. S., Park, S., Adelson, C. N., Mitsutake, Y., Vilches-Moure, J., Godoy, E., Bachmann, M., Ooi, et al
2018; 2: 696–705
- **L-edge spectroscopy of dilute, radiation-sensitive systems using a transition-edge-sensor array** *JOURNAL OF CHEMICAL PHYSICS*
Titus, C. J., Baker, M. L., Lee, S., Cho, H., Doriese, W. B., Fowler, J. W., Gaffney, K., Gard, J. D., Hilton, G. C., Kenney, C., Knight, J., Li, D., Marks, et al
2017; 147 (21): 214201
- **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., Moenne-Loccoz, P., Hedman, B., Hodgson, K. O., Solomon, E. I., Karlin, K. D.
2017; 139 (48): 17421–30
- **High-resolution structure of a lytic polysaccharide monoxygenase from *Hypocrea jecorina* reveals a predicted linker as an integral part of the catalytic domain** *JOURNAL OF BIOLOGICAL CHEMISTRY*
Hansson, H., Karkehabadi, S., Mikkelsen, N., Douglas, N. R., Kim, S., Lam, A., Kaper, T., Kelemen, B., Meier, K. K., Jones, S. M., Solomon, E. I., Sandgren, M.
2017; 292 (46): 19099–109
- **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
- **Investigation of the 4 H+/4 e- reduction of oxygen performed by heme-copper oxidases**
Schaefer, A., Adam, S., Kieber-Emmons, M., Karlin, K., Solomon, E.
AMER CHEMICAL SOC.2017
- **New insight into the reaction mechanism of the formylglycine generating enzyme: A spectroscopic perspective**
Meier, K., Appel, M., Solomon, E.
AMER CHEMICAL SOC.2017
- **Oxygen activation by Cu sites**
Solomon, E.
AMER CHEMICAL SOC.2017
- **Insight into the electronic structure of transition metal ion complexes from resonant inelastic X-ray scattering**
Kroll, T., Hadt, R., Wilson, S., Baker, M., Lundberg, M., Yan, J., Weng, T., Sokaras, D., Alonso-Mori, R., Casa, D., Upton, M., Hedman, B., Hodgson, et al
AMER CHEMICAL SOC.2017
- **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
- **A Mononuclear Nonheme Iron(V)-Imido Complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hong, S., Sutherlin, K. D., Vardhaman, A., Yan, J. J., Park, S., Lee, Y., Jang, S., Lu, X., Ohta, T., Ogura, T., Solomon, E. I., Nam, W.
2017; 139 (26): 8800–8803
- **Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine)(2)(CN)(2)]** *STRUCTURAL DYNAMICS*
Kjaer, K. S., Zhang, W., Alonso-Mori, R., Bergmann, U., Chollet, M., Hadt, R. G., Hartssock, R. W., Harlang, T., Kroll, T., Kubicek, K., Lemke, H. T., Liang, H. W., Liu, et al
2017; 4 (4): 044030

- **Geometric and Electronic Structural Contributions to Fe/O-2 Reactivity**
Solomon, E. I.
SPRINGER.2017: S163
- **RIBONUCLEOTIDE REDUCTASE, AND A COMPARISON OF THE DIMANGANESE ACTIVE SITES OF MANGANESE CATALASE**
Lofstad, M., Bottger, L. H., Hammerstad, M., Rohr, A., Hersleth, H., Zaltariov, M. F., Arion, V. B., Solomon, E. I., Andersson, K.
SPRINGER.2017: S157
- **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., Hartssock, R. W., Alonso-Mori, R., Chollet, M., Glowonia, J. M., Nelson, S., Sokaras, D., Kunnus, K., Hodgson, et al
2017; 356 (6344): 1276-+
- **Reduction in Heme-Copper Oxidases.** *Journal of the American Chemical Society*
Schaefer, A. W., Kieber-Emmons, M. T., Adam, S. M., Karlin, K. D., Solomon, E. I.
2017
- **Peroxide Activation for Electrophilic Reactivity by the Binuclear Non-heme Iron Enzyme AurF.** *Journal of the American Chemical Society*
Park, K., Li, N., Kwak, Y., Srnc, M., Bell, C. B., Liu, L. V., Wong, S. D., Yoda, Y., Kitao, S., Seto, M., Hu, M., Zhao, J., Krebs, et al
2017; 139 (20): 7062-7070
- **Intermediate in Turnover of Nitrous Oxide Reductase and Molecular Insight into the Catalytic Mechanism.** *Journal of the American Chemical Society*
Johnston, E. M., Carreira, C., Dell'Acqua, S., Dey, S. G., Pauleta, S. R., Moura, I., Solomon, E. I.
2017; 139 (12): 4462-4476
- **Spectroscopic Definition of the Cu-Z degrees Intermediate in Turnover of Nitrous Oxide Reductase and Molecular Insight into the Catalytic Mechanism** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Johnston, E. M., Carreira, C., Dell'Acqua, S., Dey, S. G., Pauleta, S. R., Moura, I., Solomon, E. I.
2017; 139 (12): 4462-4476
- **Cores with Enhanced Oxidative Reactivity.** *Journal of the American Chemical Society*
Garcia-Bosch, I., Cowley, R. E., Díaz, D. E., Peterson, R. L., Solomon, E. I., Karlin, K. D.
2017; 139 (8): 3186-3195
- **Substrate and Lewis Acid Coordination Promote O-O Bond Cleavage of an Unreactive L(2)Cu(II)2(O-2(2-)) Species to Form L2Cu2III(O)(2) Cores with Enhanced Oxidative Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Garcia-Bosch, I., Cowley, R. E., Diaz, D. E., Peterson, R. L., Solomon, E. I., Karlin, K. D.
2017; 139 (8): 3186-3195
- **Frontier Molecular Orbital Contributions to Chlorination versus Hydroxylation Selectivity in the Non-Heme Iron Halogenase SyrB2.** *Journal of the American Chemical Society*
Srnc, M., Solomon, E. I.
2017; 139 (6): 2396-2407
- **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
- **: 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
- **Critical Aspects of Heme-Peroxo-Cu Complex Structure and Nature of Proton Source Dictate Metal-O-peroxo Breakage versus Reductive O-O Cleavage Chemistry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Adam, S. M., Garcia-Bosch, I., Schaefer, A. W., Sharma, S. K., Siegler, M. A., Solomon, E. I., Karlin, K. D.
2017; 139 (1): 472-481
- **Breakage versus Reductive O-O Cleavage Chemistry.** *Journal of the American Chemical Society*
Adam, S. M., Garcia-Bosch, I., Schaefer, A. W., Sharma, S. K., Siegler, M. A., Solomon, E. I., Karlin, K. D.

2017; 139 (1): 472-481

- **Mechanism of chloride inhibition of bilirubin oxidases and its dependence on potential and pH.** *ACS catalysis*
de Poulpiquet, A., Kjaergaard, C. H., Rouhana, J., Mazurenko, I., Infossi, P., Gounel, S., Gadiou, R., Giudici-Ortoni, M. T., Solomon, E. I., Mano, N., Lojou, E.
2017; 7 (6): 3916-23
- **Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution.** *Chemical science*
Zhang, W., Kjaer, K. S., Alonso-Mori, R., Bergmann, U., Chollet, M., Fredin, L. A., Hadt, R. G., Hartsock, R. W., Harlang, T., Kroll, T., Kubicek, K., Lemke, H. T., Liang, et al
2017; 8 (1): 515-23
- **Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution** *CHEMICAL SCIENCE*
Zhang, W., Kjaer, K. S., Alonso-Mori, R., Bergmann, U., Chollet, M., Fredin, L. A., Hadt, R. G., Hartsock, R. W., Harlang, T., Kroll, T., Kubicek, K., Lemke, H. T., Liang, et al
2017; 8 (1): 515-523
- **Reactivity of a Cobalt(III)-Hydroperoxo Complex in Electrophilic Reactions** *INORGANIC CHEMISTRY*
Shin, B., Sutherlin, K. D., Ohta, T., Ogura, T., Solomon, E. I., Cho, J.
2016; 55 (23): 12391-12399
- **O-2 Activation by Non-Heme Iron Enzymes** *BIOCHEMISTRY*
Solomon, E. I., Goudarzi, S., Sutherlin, K. D.
2016; 55 (46): 6363-6374
- **Nuclear Resonance Vibrational Spectroscopic Definition of Peroxy Intermediates in Nonheme Iron Sites.** *Journal of the American Chemical Society*
Sutherlin, K. D., Liu, L. V., Lee, Y., Kwak, Y., Yoda, Y., Saito, M., Kurokuzu, M., Kobayashi, Y., Seto, M., Que, L., Nam, W., Solomon, E. I.
2016; 138 (43): 14294-14302
- **Mechanism of O2 activation and substrate hydroxylation in noncoupled binuclear copper monooxygenases.** *Proceedings of the National Academy of Sciences of the United States of America*
Cowley, R. E., Tian, L., Solomon, E. I.
2016; 113 (43): 12035-12040
- **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
- **Activating Metal Sites for Biological Electron Transfer** *ISRAEL JOURNAL OF CHEMISTRY*
Solomon, E. I., Hadt, R. G., Snyder, B. E.
2016; 56 (9-10): 649-659
- **Structure/function correlations over binuclear non-heme iron active sites.** *Journal of biological inorganic chemistry*
Solomon, E. I., Park, K.
2016; 21 (5-6): 575-588
- **The active site of low-temperature methane hydroxylation in iron-containing zeolites.** *Nature*
Snyder, B. E., Vanelderden, P., Bols, M. L., Hallaert, S. D., Böttger, L. H., Ungur, L., Pierloot, K., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2016; 536 (7616): 317-321
- **Reversible S-nitrosylation in an engineered azurin** *NATURE CHEMISTRY*
Tian, S., Liu, J., Cowley, R. E., Hosseinzadeh, P., Marshall, N. M., Yu, Y., Robinson, H., Nilges, M. J., Blackburn, N. J., Solomon, E. I., Lu, Y.
2016; 8 (7): 670-677
- **Peroxo and Superoxo Moieties Bound to Copper Ion: Electron-Transfer Equilibrium with a Small Reorganization Energy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cao, R., Saracini, C., Ginsbach, J. W., Kieber-Emmons, M. T., Siegler, M. A., Solomon, E. I., Fukuzumi, S., Karlin, K. D.

2016; 138 (22): 7055-7066

- **Electronic Structure of the Ferryl Intermediate in the alpha-Ketoglutarate Dependent Non-Heme Iron Halogenase SyrB2: Contributions to H Atom Abstraction Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Srncic, M., Wong, S. D., Matthews, M. L., Krebs, C., Bollinger, J. M., Solomon, E. I.
2016; 138 (15): 5110-5122
- **Dioxygen Activation by a Macrocyclic Copper Complex Leads to a Cu2O2 Core with Unexpected Structure and Reactivity** *CHEMISTRY-A EUROPEAN JOURNAL*
Garcia-Bosch, I., Cowley, R. E., Diaz, D. E., Siegler, M. A., Nam, W., Solomon, E. I., Karlin, K. D.
2016; 22 (15): 5133-5137
- **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
- **Dioxygen Binding, Activation, and Reduction to H2O by Cu Enzymes.** *Inorganic chemistry*
Solomon, E. I.
2016; 55 (13): 6364-75
- **Activating Metal Sites for Biological Electron Transfer.** *Israel journal of chemistry*
Solomon, E. I., Hadt, R. G., Snyder, B. E.
2016; 56 (9-10): 649-59
- **CD/MCD/VTMCD Studies of Escherichia coli Bacterioferritin Support a Binuclear Iron Cofactor Site** *BIOCHEMISTRY*
Kwak, Y., Schwartz, J. K., Huang, V. W., Boice, E., Kurtz, D. M., Solomon, E. I.
2015; 54 (47): 7010-7018
- **Final-State Projection Method in Charge-Transfer Multiplet Calculations: An Analysis of Ti L-Edge Absorption Spectra** *JOURNAL OF PHYSICAL CHEMISTRY B*
Kroll, T., Solomon, E. I., de Groot, F. M.
2015; 119 (43): 13852-13858
- **Systematic Perturbations of Binuclear Non-heme Iron Sites: Structure and Dioxygen Reactivity of de Novo Due Ferri Proteins** *BIOCHEMISTRY*
Snyder, R. A., Betzu, J., Butch, S. E., Reig, A. J., DeGrado, W. F., Solomon, E. I.
2015; 54 (30): 4637-4651
- **Molecular-Level Insight into the Differential Oxidase and Oxygenase Reactivities of de Novo Due Ferri Proteins.** *Journal of the American Chemical Society*
Snyder, R. A., Butch, S. E., Reig, A. J., DeGrado, W. F., Solomon, E. I.
2015; 137 (29): 9302-9314
- **Two-Electron Reduction versus One-Electron Oxidation of the Type 3 Pair in the Multicopper Oxidases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kjaergaard, C. H., Jones, S. M., Gounel, S., Mano, N., Solomon, E. I.
2015; 137 (27): 8783-8794
- **Spectroscopic Definition of the Copper Active Sites in Mordenite: Selective Methane Oxidation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Vanelderden, P., Snyder, B. E., Tsai, M., Hadt, R. G., Vancauwenbergh, J., Coussens, O., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2015; 137 (19): 6383-6392
- **Amine Oxidative N-Dealkylation via Cupric Hydroperoxide Cu-OOH Homolytic Cleavage Followed by Site-Specific Fenton Chemistry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kim, S., Ginsbach, J. W., Lee, J. Y., Peterson, R. L., Liu, J. J., Siegler, M. A., Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2015; 137 (8): 2867-2874

- **New Insights into Structure and Luminescence of Eu-III and Sm-III Complexes of the 3,4,3-L1(1,2-HOPO) Ligand** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Daumann, L. J., Tatum, D. S., Snyder, B. E., Ni, C., Law, G., Solomon, E. I., Raymond, K. N.
2015; 137 (8): 2816-2819
- **A N3S(thioether)-ligated Cu(II)-superoxo with enhanced reactivity.** *Journal of the American Chemical Society*
Kim, S., Lee, J. Y., Cowley, R. E., Ginsbach, J. W., Siegler, M. A., Solomon, E. I., Karlin, K. D.
2015; 137 (8): 2796-2799
- **Electron transfer and reaction mechanism of laccases.** *Cellular and molecular life sciences*
Jones, S. M., Solomon, E. I.
2015; 72 (5): 869-883
- **A "Naked" Fe-III-(O-2(2-))-Cu-II Species Allows for Structural and Spectroscopic Tuning of Low-Spin Heme-Peroxo-Cu Complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Garcia-Bosch, I., Adam, S. M., Schaefer, A. W., Sharma, S. K., Peterson, R. L., Solomon, E. I., Karlin, K. D.
2015; 137 (3): 1032-1035
- **Spectroscopic and Computational Studies of Nitrile Hydratase: Insights into Geometric and Electronic Structure and the Mechanism of Amide Synthesis.** *Chemical science*
Light, K. M., Yamanaka, Y., Odaka, M., Solomon, E. I.
2015; 6 (11): 6280-94
- **Two-Electron Reduction versus One-Electron Oxidation of the Type 3 Pair in the Multicopper Oxidases.** *Journal of the American Chemical Society*
Kjaergaard, C. H., Jones, S. M., Gounel, S., Mano, N., Solomon, E. I.
2015; 137 (27): 8783-94
- **Protonation state of the Cu4S2 Cu-Z site in nitrous oxide reductase: redox dependence and insight into reactivity** *CHEMICAL SCIENCE*
Johnston, E. M., Dell'Acqua, S., Pauleta, S. R., Moura, I., Solomon, E. I.
2015; 6 (10): 5670-5679
- **Spectroscopic and computational studies of nitrile hydratase: insights into geometric and electronic structure and the mechanism of amide synthesis** *CHEMICAL SCIENCE*
Light, K. M., Yamanaka, Y., Odaka, M., Solomon, E. I.
2015; 6 (11): 6280-6294
- **Protonation state of the Cu4S2 CuZ site in nitrous oxide reductase: redox dependence and insight into reactivity.** *Chemical science*
Johnston, E. M., Dell'Acqua, S., Pauleta, S. R., Moura, I., Solomon, E. I.
2015; 6 (10): 5670-79
- **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
- **Mechanism of the Reduction of the Native Intermediate in the Multicopper Oxidases: Insights into Rapid Intramolecular Electron Transfer in Turnover** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Heppner, D. E., Kjaergaard, C. H., Solomon, E. I.
2014; 136 (51): 17788-17801
- **Reactivity of the binuclear non-heme iron active site of ?? desaturase studied by large-scale multireference ab initio calculations.** *Journal of the American Chemical Society*
Chalupský, J., Rokob, T. A., Kurashige, Y., Yanai, T., Solomon, E. I., Rulíšek, L., Srnc, M.
2014; 136 (45): 15977-15991
- **Anisotropic Covalency Contributions to Superexchange Pathways in Type One Copper Active Sites** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hadt, R. G., Gorelsky, S. I., Solomon, E. I.
2014; 136 (42): 15034-15045
- **Anisotropic covalency contributions to superexchange pathways in type one copper active sites.** *Journal of the American Chemical Society*

- Hadt, R. G., Gorelsky, S. I., Solomon, E. I.
2014; 136 (42): 15034-15045
- **Modeling nuclear resonance vibrational spectroscopic data of binuclear nonheme iron enzymes using density functional theory** *CANADIAN JOURNAL OF CHEMISTRY*
Park, K., Solomon, E. I.
2014; 92 (10): 975-978
 - **Mechanistic Insights into the Oxidation of Substituted Phenols via Hydrogen Atom Abstraction by a Cupric-Superoxo Complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lee, J. Y., Peterson, R. L., Ohkubo, K., Garcia-Bosch, I., Himes, R. A., Woertink, J., Moore, C. D., Solomon, E. I., Fukuzumi, S., Karlin, K. D.
2014; 136 (28): 9925-9937
 - **Preface for the forum on insights into spectroscopy and reactivity from electronic structure theory.** *Inorganic chemistry*
Gagliardi, L., Solomon, E. I.
2014; 53 (13): 6357-6360
 - **The Role of Chloride in the Mechanism of O₂ Activation at the Mononuclear Nonheme Fe(II) Center of the Halogenase HctB** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pratter, S. M., Light, K. M., Solomon, E. I., Straganz, G. D.
2014; 136 (26): 9385-9395
 - **Sulfur K-Edge X-ray Absorption Spectroscopy and Density Functional Theory Calculations on Mono-oxo Mo(IV) and Bis-oxo 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 mono-oxo Mo(IV) and bis-oxo 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
 - **Tuning of the copper-thioether bond in tetradentate N3S(thioether) ligands; O-O bond reductive cleavage via a [Cu(II)2(μ-1,2-peroxo)]²⁺/[Cu(III)2(μ-oxo)2]²⁺ equilibrium.** *Journal of the American Chemical Society*
Kim, S., Ginsbach, J. W., Billah, A. I., Siegler, M. A., Moore, C. D., Solomon, E. I., Karlin, K. D.
2014; 136 (22): 8063-8071
 - **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
 - **Tuning of the Copper-Thioether Bond in Tetradentate N3S(thioether) Ligands; O-O Bond Reductive Cleavage via a [Cu-2(II)(μ-1,2-peroxo)]²⁺/[Cu-2(III)(μ-oxo)(2)]²⁺ Equilibrium** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Kim, S., Ginsbach, J. W., Billah, A. I., Siegler, M. A., Moore, C. D., Solomon, E. I., Karlin, K. D.
2014; 136 (22): 8063-8071
- **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
 - **Tracking excited-state charge and spin dynamics in iron coordination complexes.** *Nature*
Zhang, W., Alonso-Mori, R., Bergmann, U., Bressler, C., Chollet, M., Galler, A., Gawelda, W., Hadt, R. G., Hartsock, R. W., Kroll, T., Kjær, K. S., Kubicek, K., Lemke, et al
2014; 509 (7500): 345-348
 - **Tracking excited-state charge and spin dynamics in iron coordination complexes.** *Nature*
Zhang, W., Alonso-Mori, R., Bergmann, U., Bressler, C., Chollet, M., Galler, A., Gawelda, W., Hadt, R. G., Hartsock, R. W., Kroll, T., Kjær, K. S., Kubicek, K., Lemke, et al
2014; 509 (7500): 345-348
 - **Observation of a Cu-2(II)(μ -1,2-peroxo)/Cu-2(III)(μ -oxo)(2) Equilibrium and its Implications for Copper-Dioxygen Reactivity** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Kieber-Emmons, M. T., Ginsbach, J. W., Wick, P. K., Lucas, H. R., Helton, M. E., Lucchese, B., Suzuki, M., Zuberbuehler, A. D., Karlin, K. D., Solomon, E. I.
2014; 53 (19): 4935-4939
 - **Evolution of Iron(II)-Finger Peptides by Using a Bipyridyl Amino Acid** *CHEMBIOCHEM*
Kang, M., Light, K., Ai, H., Shen, W., Kim, C. H., Chen, P. R., Lee, H. S., Solomon, E. I., Schultz, P. G.
2014; 15 (6): 822-825
 - **Copper active sites in biology.** *Chemical reviews*
Solomon, E. I., Heppner, D. E., Johnston, E. M., Ginsbach, J. W., Cirera, J., Qayyum, M., Kieber-Emmons, M. T., Kjaergaard, C. H., Hadt, R. G., Tian, L.
2014; 114 (7): 3659-3853
 - **[Cu₂O](2+) Active Site Formation in Cu-ZSM-5: Geometric and Electronic Structure Requirements for N₂O Activation.** *Journal of the American Chemical Society*
Tsai, M., Hadt, R. G., Vanelderden, P., Sels, B. F., Schoonheydt, R. A., Solomon, E. I.
2014; 136 (9): 3522-3529
 - **Spectroscopic Studies of Single and Double Variants of M Ferritin: Lack of Conversion of a Biferrous Substrate Site into a Cofactor Site for O-2 Activation** *BIOCHEMISTRY*
Kwak, Y., Schwartz, J. K., Haldar, S., Behera, R. K., Tosha, T., Theil, E. C., Solomon, E. I.
2014; 53 (3): 473-482
 - **First- and second-sphere contributions to Fe(II) site activation by cosubstrate binding in non-heme Fe enzymes.** *Dalton transactions*
Light, K. M., Hangasky, J. A., Knapp, M. J., Solomon, E. I.
2014; 43 (4): 1505-1508
 - **Copper-sulfenate complex from oxidation of a cavity mutant of Pseudomonas aeruginosa azurin** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Sieracki, N. A., Tian, S., Hadt, R. G., Zhang, J., Woertink, J. S., Nilges, M. J., Sun, F., Solomon, E. I., Lu, Y.
2014; 111 (3): 924-929
 - **Determination of the Active Form of the Tetranuclear Copper Sulfur Cluster in Nitrous Oxide Reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Johnston, E. M., Dell'Acqua, S., Ramos, S., Pauleta, S. R., Moura, I., Solomon, E. I.
2014; 136 (2): 614-617
 - **Spectroscopy and Redox Chemistry of Copper in Mordenite** *CHEMPHYSICHEM*
Vanelderden, P., Vancauwenbergh, J., Tsai, M., Hadt, R. G., Solomon, E. I., Schoonheydt, R. A., Sels, B. F.
2014; 15 (1): 91-99
 - **Efficient C-H Bond Activations via O₂ Cleavage by a Dianionic Cobalt(II) Complex.** *Chemical science*
Nguyen, A. I., Hadt, R. G., Solomon, E. I., Tilley, T. D.

2014; 5 (7): 2874–78

- **Modeling nuclear resonance vibrational spectroscopic data of binuclear non-heme iron enzymes using density functional theory.** *Canadian journal of chemistry*
Park, K., Solomon, E. I.
2014; 92 (10): 975–78
- **First- and second-sphere contributions to Fe(II) site activation by cosubstrate binding in non-heme Fe enzymes** *DALTON TRANSACTIONS*
Light, K. M., Hangasky, J. A., Knapp, M. J., Solomon, E. I.
2014; 43 (4): 1505-1508
- **Efficient C-H bond activations via O-2 cleavage by a dianionic cobalt(II) complex** *CHEMICAL SCIENCE*
Nguyen, A. I., Hadt, R. G., Solomon, E. I., Tilley, T. D.
2014; 5 (7): 2874-2878
- **Crystallographic and spectroscopic characterization and reactivities of a mononuclear non-haem iron(III)-superoxo complex.** *Nature communications*
Hong, S., Sutherlin, K. D., Park, J., Kwon, E., Siegler, M. A., Solomon, E. I., Nam, W.
2014; 5: 5440-?
- **Excited state potential energy surfaces and their interactions in Fe-IV=O active sites** *DALTON TRANSACTIONS*
Srncic, M., Wong, S. D., Solomon, E. I.
2014; 43 (47): 17567-17577
- **Geometric and Electronic Structure of the Mn(IV)Fe(III) Cofactor in Class Ic Ribonucleotide Reductase: Correlation to the Class Ia Binuclear Non-Heme Iron Enzyme.** *Journal of the American Chemical Society*
Kwak, Y., Jiang, W., Dassama, L. M., Park, K., Bell, C. B., Liu, L. V., Wong, S. D., Saito, M., Kobayashi, Y., Kitao, S., Seto, M., Yoda, Y., Alp, et al
2013; 135 (46): 17573-17584
- **Geometric and electronic structure of the Mn(IV)Fe(III) cofactor in class Ic ribonucleotide reductase: correlation to the class Ia binuclear non-heme iron enzyme.** *Journal of the American Chemical Society*
Kwak, Y., Jiang, W., Dassama, L. M., Park, K., Bell, C. B., Liu, L. V., Wong, S. D., Saito, M., Kobayashi, Y., Kitao, S., Seto, M., Yoda, Y., Alp, et al
2013; 135 (46): 17573-17584
- **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
- **Geometric and Electronic Structure Contributions to Function in Non-heme Iron Enzymes** *ACCOUNTS OF CHEMICAL RESEARCH*
Solomon, E. I., Light, K. M., Liu, L. V., Srncic, M., Wong, S. D.
2013; 46 (11): 2725-2739
- **Correlation of the Electronic and Geometric Structures in Mononuclear Copper(II) Superoxide Complexes.** *Inorganic chemistry*
Ginsbach, J. W., Peterson, R. L., Cowley, R. E., Karlin, K. D., Solomon, E. I.
2013; 52 (22): 12872-12874
- **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
- **Circular Dichroism, Magnetic Circular Dichroism, and Variable Temperature Variable Field Magnetic Circular Dichroism Studies of Biferrous and Mixed-Valent myo-Inositol Oxygenase: Insights into Substrate Activation of O₂ Reactivity.** *Journal of the American Chemical Society*
Snyder, R. A., Bell, C. B., Diao, Y., Krebs, C., Bollinger, J. M., Solomon, E. I.
2013; 135 (42): 15851-15863
- **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
- **Axial interactions in the mixed-valent CuA active site and role of the axial methionine in electron transfer.** *Proceedings of the National Academy of Sciences of the United States of America*
Tsai, M., Hadt, R. G., Marshall, N. M., Wilson, T. D., Lu, Y., Solomon, E. I.
2013; 110 (36): 14658-14663
 - **Molecular Origin of Rapid versus Slow Intramolecular Electron Transfer in the Catalytic Cycle of the Multicopper Oxidases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Heppner, D. E., Kjaergaard, C. H., Solomon, E. I.
2013; 135 (33): 12212-12215
 - **Elucidation of the Fe(IV)=O intermediate in the catalytic cycle of the halogenase SyrB2.** *Nature*
Wong, S. D., Srnec, M., Matthews, M. L., Liu, L. V., Kwak, Y., Park, K., Bell, C. B., Alp, E. E., Zhao, J., Yoda, Y., Kitao, S., Seto, M., Krebs, et al
2013; 499 (7458): 320-323
 - **Elucidation of the Fe(IV)=O intermediate in the catalytic cycle of the halogenase SyrB2** *NATURE*
Wong, S. D., Srnec, M., Matthews, M. L., Liu, L. V., Kwak, Y., Park, K., Bell, C. B., Alp, E. E., Zhao, J., Yoda, Y., Kitao, S., Seto, M., Krebs, et al
2013; 499 (7458): 320-?
 - **Spectroscopic Studies of the Mononuclear Non-Heme Fe-II Enzyme FIIH: Second-Sphere Contributions to Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Light, K. M., Hangasky, J. A., Knapp, M. J., Solomon, E. I.
2013; 135 (26): 9665-9674
 - **Modified Reactivity toward O-2 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
 - **Characterization of Metastable Intermediates Formed in the Reaction between a Mn(II) Complex and Dioxygen, Including a Crystallographic Structure of a Binuclear Mn(III)-Peroxo Species** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Coggins, M. K., Sun, X., Kwak, Y., Solomon, E. I., Rybak-Akimova, E., Kovacs, J. A.
2013; 135 (15): 5631-5640
 - **Nuclear resonance vibrational spectroscopic and computational study of high-valent diiron complexes relevant to enzyme intermediates.** *Proceedings of the National Academy of Sciences of the United States of America*
Park, K., Bell, C. B., Liu, L. V., Wang, D., Xue, G., Kwak, Y., Wong, S. D., Light, K. M., Zhao, J., Alp, E. E., Yoda, Y., Saito, M., Kobayashi, et al
2013; 110 (16): 6275-6280
 - **Nuclear resonance vibrational spectroscopic and computational study of high-valent diiron complexes relevant to enzyme intermediates** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Park, K., Bell, C. B., Liu, L. V., Wang, D., Xue, G., Kwak, Y., Wong, S. D., Light, K. M., Zhao, J., Alp, E. E., Yoda, Y., Saito, M., Kobayashi, et al
2013; 110 (16): 6269-6280
 - **Comparison of High-Spin and Low-Spin Nonheme Fe-III-OOH Complexes in O-O Bond Homolysis and H-Atom Abstraction Reactivities** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Liu, L. V., Hong, S., Cho, J., Nam, W., Solomon, E. I.
2013; 135 (8): 3286-3299
 - **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

- **Nuclear Resonance Vibrational Spectroscopy and DFT study of Peroxo-Bridged Biferric Complexes: Structural Insight into Peroxo Intermediates of Binuclear Non-heme Iron Enzymes** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Park, K., Tsugawa, T., Furutachi, H., Kwak, Y., Liu, L. V., Wong, S. D., Yoda, Y., Kobayashi, Y., Saito, M., Kurokuzu, M., Seto, M., Suzuki, M., Solomon, et al
2013; 52 (4): 1294-1298
- **Mononuclear nickel(II)-superoxo and nickel(III)-peroxo complexes bearing a common macrocyclic TMC ligand** *CHEMICAL SCIENCE*
Cho, J., Kang, H. Y., Liu, L. V., Sarangi, R., Solomon, E. I., Nam, W.
2013; 4 (4): 1502-1508
- **Ribonucleotide reductase class I with different radical generating clusters** *COORDINATION CHEMISTRY REVIEWS*
Tomter, A. B., Zoppellaro, G., Andersen, N. H., Hersleth, H., Hammerstad, M., Rohr, A. K., Sandvik, G. K., Strand, K. R., Nilsson, G. E., Bell, C. B., Barra, A., Blasco, E., Le Pape, et al
2013; 257 (1): 3-26
- **Bilirubin oxidase from *Magnaporthe oryzae*: an attractive new enzyme for biotechnological applications** *APPLIED MICROBIOLOGY AND BIOTECHNOLOGY*
Durand, F., Gounel, S., Kjaergaard, C. H., Solomon, E. I., Mano, N.
2012; 96 (6): 1489-1498
- **Alteration of the oxygen-dependent reactivity of de novo Due Ferri proteins** *NATURE CHEMISTRY*
Reig, A. J., Pires, M. M., Snyder, R. A., Wu, Y., Jo, H., Kulp, D. W., Butch, S. E., Calhoun, J. R., Szyperski, T. G., Solomon, E. I., DeGrado, W. F.
2012; 4 (11): 900-906
- **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
- **Analysis of resonance Raman data on the blue copper site in pseudoazurin: Excited state pi and sigma charge transfer distortions and their relation to ground state reorganization energy** *JOURNAL OF INORGANIC BIOCHEMISTRY*
Hadt, R. G., Xie, X., Pauleta, S. R., Moura, I., Solomon, E. I.
2012; 115: 155-162
- **pi-Frontier molecular orbitals in S=2 ferryl species and elucidation of their contributions to reactivity** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Srncic, M., Wong, S. D., England, J., Que, L., Solomon, E. I.
2012; 109 (36): 14326-14331
- **(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
- **Structure/function correlations among coupled binuclear copper proteins through spectroscopic and reactivity studies of NspF** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Ginsbach, J. W., Kieber-Emmons, M. T., Nomoto, R., Noguchi, A., Ohnishi, Y., Solomon, E. I.
2012; 109 (27): 10793-10797
- **Geometric and Electronic Structure of [Cu(MeAN)]₂(μ-η²:η²(O₂(2-)))](2+) with an Unusually Long O-O Bond: O-O Bond Weakening vs Activation for Reductive Cleavage** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Park, G. Y., Qayyum, M. F., Woertink, J., Hodgson, K. O., Hedman, B., Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2012; 134 (20): 8513-8524
- **Geometric and electronic structure of [Cu(MeAN)]₂(μ-η²:η²(O₂(2-)))](2+) with an unusually long O-O bond: O-O bond weakening vs activation for reductive cleavage.** *Journal of the American Chemical Society*
Park, G. Y., Qayyum, M. F., Woertink, J., Hodgson, K. O., Hedman, B., Narducci Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2012; 134 (20): 8513-8524
- **Bilirubin oxidase from *Bacillus pumilus*: A promising enzyme for the elaboration of efficient cathodes in biofuel cells** *BIOSENSORS & BIOELECTRONICS*
Durand, F., Kjaergaard, C. H., Suraniti, E., Gounel, S., Hadt, R. G., Solomon, E. I., Mano, N.

2012; 35 (1): 140-146

- **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*
Kjaergaard, C. H., Durand, F., Tasca, F., Qayyum, M. F., Kauffmann, B., Gounel, S., Suraniti, E., Hodgson, K. O., Hedman, B., Mano, N., Solomon, E. I.
2012; 134 (12): 5548-5551
- **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.
2012; 51 (6): 3436-3442
- **Spectroscopic Studies of the Iron and Manganese Reconstituted Tyrosyl Radical in Bacillus Cereus Ribonucleotide Reductase R2 Protein** *PLOS ONE*
Tomter, A. B., Zoppellaro, G., Bell, C. B., Barra, A., Andersen, N. H., Solomon, E. I., Andersson, K. K.
2012; 7 (3)
- **Structural and Spectroscopic Properties of the Peroxidoferric Intermediate of Ricinus communis Soluble Delta(9) Desaturase** *INORGANIC CHEMISTRY*
Srnc, M., Rokob, T. A., Schwartz, J. K., Kwak, Y., Rulisek, L., Solomon, E. I.
2012; 51 (5): 2806-2820
- **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
- **Ligand Field and Molecular Orbital Theories of Transition Metal X-ray Absorption Edge Transitions** *MOLECULAR ELECTRONIC STRUCTURES OF TRANSITION METAL COMPLEXES I*
Hocking, R. K., Solomon, E. I.
2012; 142: 155-184
- **Cu-ZSM-5: A biomimetic inorganic model for methane oxidation** *JOURNAL OF CATALYSIS*
Vanelderden, P., Hadt, R. G., Smeets, P. J., Solomon, E. I., Schoonheydt, R. A., Sels, B. F.
2011; 284 (2): 157-164
- **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*
Dey, A., Peng, Y., Broderick, W. E., Hedman, B., Hodgson, K. O., Broderick, J. B., Solomon, E. I.
2011; 133 (46): 18656-18662
- **Electronic Structure of a Low-Spin Heme/Cu Peroxide Complex: Spin-State and Spin-Topology Contributions to Reactivity** *INORGANIC CHEMISTRY*
Kieber-Emmons, M. T., Li, Y., Halime, Z., Karlin, K. D., Solomon, E. I.
2011; 50 (22): 11777-11786
- **Activation of alpha-Keto Acid-Dependent Dioxygenases: Application of an {FeNO}(7)/{FeO2}(8) Methodology for Characterizing the Initial Steps of O-2 Activation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Diebold, A. R., Brown-Marshall, C. D., Neidig, M. L., Brownlee, J. M., Moran, G. R., Solomon, E. I.
2011; 133 (45): 18148-18160
- **Rapid C-H Bond Activation by a Monocopper(III)-Hydroxide Complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Donoghue, P. J., Tehranchi, J., Cramer, C. J., Sarangi, R., Solomon, E. I., Tolman, W. B.
2011; 133 (44): 17602-17605
- **X-ray Absorption Spectroscopic and Computational Investigation of a Possible S center dot center dot center dot S Interaction in the [Cu3S2](3+) Core** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sarangi, R., Yang, L., Winikoff, S. G., Gagliardi, L., Cramer, C. J., Tolman, W. B., Solomon, E. I.
2011; 133 (43): 17180-17191
- **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
- **Spectroscopic and Computational Studies of alpha-Keto Acid Binding to Dke1: Understanding the Role of the Facial Triad and the Reactivity of beta-Diketones** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Diebold, A. R., Straganz, G. D., Solomon, E. I.
2011; 133 (40): 15979-15991
- **Hybrid Genetic Algorithm with an Adaptive Penalty Function for Fitting Multimodal Experimental Data: Application to Exchange-Coupled Non-Kramers Binuclear Iron Active Sites** *JOURNAL OF CHEMICAL INFORMATION AND MODELING*
Beaser, E., Schwartz, J. K., Bell, C. B., Solomon, E. I.
2011; 51 (9): 2164-2173
 - **Comparative molecular chemistry of molybdenum and tungsten and its relation to hydroxylase and oxotransferase enzymes** *COORDINATION CHEMISTRY REVIEWS*
Holm, R. H., Solomon, E. I., Majumdar, A., Tenderholt, A.
2011; 255 (9-10): 993-1015
 - **Recent advances in understanding blue copper proteins** *COORDINATION CHEMISTRY REVIEWS*
Solomon, E. I., Hadt, R. G.
2011; 255 (7-8): 774-789
 - **Covalent and electrostatic tuning of the reduction potential of a type 1 blue copper site through second coordination sphere interactions** *241st National Meeting and Exposition of the American-Chemical-Society (ACS)*
Hadt, R. G., Sun, N., Marshall, N. M., Lu, Y., Hodgson, K. O., Hedman, B., Solomon, E. I.
AMER CHEMICAL SOC.2011
 - **Variable-temperature variable-field magnetic circular dichroism (VTVH MCD) and nuclear resonance vibrational spectroscopy (NRVS) studies on Fe-IV=O intermediates: Electronic and geometric structural insight into reactivity** *241st National Meeting and Exposition of the American-Chemical-Society (ACS)*
Wong, S. D., Bell, C. B., Liu, L. V., Kwak, Y., England, J., Zhao, J., Que, L., Solomon, E. I.
AMER CHEMICAL SOC.2011
 - **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
 - **Cupric Superoxo-Mediated Intermolecular C-H Activation Chemistry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Peterson, R. L., Himes, R. A., Kotani, H., Suenobu, T., Tian, L., Siegler, M. A., Solomon, E. I., Fukuzumi, S., Karlin, K. D.
2011; 133 (6): 1702-1705
 - **XAS and DFT Investigation of Mononuclear Cobalt(III) Peroxo Complexes: Electronic Control of the Geometric Structure in CoO₂ versus NiO₂ Systems** *INORGANIC CHEMISTRY*
Sarangi, R., Cho, J., Nam, W., Solomon, E. I.
2011; 50 (2): 614-620
 - **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*
Sun, N., Liu, L. V., Dey, A., Villar-Acevedo, G., Kovacs, J. A., Darensbourg, M. Y., Hodgson, K. O., Hedman, B., Solomon, E. I.
2011; 50 (2): 427-436
 - **Copper dioxygen (bio) inorganic chemistry** *FARADAY DISCUSSIONS*
Solomon, E. I., Ginsbach, J. W., Heppner, D. E., Kieber-Emmons, M. T., Kjaergaard, C. H., Smeets, P. J., Tian, L., Woertink, J. S.
2011; 148: 11-39
 - **Nuclear Resonance Vibrational Spectroscopy on the Fe-IV=O S=2 Non-Heme Site in TMG(3)tren: Experimentally Calibrated Insights into Reactivity** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Wong, S. D., Bell, C. B., Liu, L. V., Kwak, Y., England, J., Alp, E. E., Zhao, J., Que, L., Solomon, E. I.
2011; 50 (14): 3215-3218
 - **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*
Liu, L. V., Bell, C. B., Wong, S. D., Wilson, S. A., Kwak, Y., Chow, M. S., Zhao, J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010; 107 (52): 22419-22424
 - **CD and MCD Spectroscopic Studies of the Two Dps Miniferritin Proteins from Bacillus anthracis: Role of O₂ and H₂O₂ Substrates in Reactivity of the Diiron Catalytic Centers** *BIOCHEMISTRY*

- Schwartz, J. K., Liu, X. S., Tosha, T., Diebold, A., Theil, E. C., Solomon, E. I.
2010; 49 (49): 10516-10525
- **Bis(mu-oxo) Dicopper(III) Species of the Simplest Peralkylated Diamine: Enhanced Reactivity toward Exogenous Substrates** *INORGANIC CHEMISTRY*
Kang, P., Bobyr, E., Dustman, J., Hodgson, K. O., Hedman, B., Solomon, E. I., Stack, T. D.
2010; 49 (23): 11030-11038
 - **Synthesis, Structural, and Spectroscopic Characterization and Reactivities of Mononuclear Cobalt(III)-Peroxo Complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cho, J., Sarangi, R., Kang, H. Y., Lee, J. Y., Kubo, M., Ogura, T., Solomon, E. I., Nam, W.
2010; 132 (47): 16977-16986
 - **Oxygen Precursor to the Reactive Intermediate in Methanol Synthesis by Cu-ZSM-5** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Smeets, P. J., Hadt, R. G., Woertink, J. S., Vanelderen, P., Schoonheydt, R. A., Sels, B. F., Solomon, E. I.
2010; 132 (42): 14736-14738
 - **Spectroscopic and Computational Studies of an End-on Bound Superoxo-Cu(II) Complex: Geometric and Electronic Factors That Determine the Ground State** *INORGANIC CHEMISTRY*
Woertink, J. S., Tian, L., Maiti, D., Lucas, H. R., Himes, R. A., Karlin, K. D., Neese, F., Wuertele, C., Holthausen, M. C., Bill, E., Sundermeyer, J., Schindler, S., Solomon, et al
2010; 49 (20): 9450-9459
 - **Density functional theory calculations on Fe-O and O-O cleavage of ferric hydroperoxide species: Role of axial ligand and spin state** *INORGANICA CHIMICA ACTA*
Dey, A., Solomon, E. I.
2010; 363 (12): 2762-2767
 - **Sulfur Donor Atom Effects on Copper(I)/O-2 Chemistry with Thioanisole Containing Tetradentate N3S Ligand Leading to mu-1,2-Peroxo-Dicopper(II) Species** *INORGANIC CHEMISTRY*
Lee, Y., Lee, D., Park, G. Y., Lucas, H. R., Sarjeant, A. A., Kieber-Emmons, M. T., Vance, M. A., Milligan, A. E., Solomon, E. I., Karlin, K. D.
2010; 49 (19): 8873-8885
 - **Solvation Effects on S K-Edge XAS Spectra of Fe-S Proteins: Normal and Inverse Effects on WT and Mutant Rubredoxin** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sun, N., Dey, A., Xiao, Z., Wedd, A. G., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010; 132 (36): 12639-12647
 - **The Three-His Triad in Dke1: Comparisons to the Classical Facial Triad** *BIOCHEMISTRY*
Diebold, A. R., Neidig, M. L., Moran, G. R., Straganz, G. D., Solomon, E. I.
2010; 49 (32): 6945-6952
 - **Sulfur K-Edge X-ray Absorption Spectroscopy and Density Functional Calculations on Mo(IV) and Mo(VI)=O Bis-dithiolenes: Insights into the Mechanism of Oxo Transfer in DMSO Reductase and Related Functional Analogues** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Tenderholt, A. L., Wang, J., Szilagy, R. K., Holm, R. H., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010; 132 (24): 8359-8371
 - **Multireference Ab Initio Calculations of g tensors for Trinuclear Copper Clusters in Multicopper Oxidases** *JOURNAL OF PHYSICAL CHEMISTRY B*
Vancoillie, S., Chalupsky, J., Ryde, U., Solomon, E. I., Pierloot, K., Neese, F., Rulisek, L.
2010; 114 (22): 7692-7702
 - **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*
Augustine, A. J., Kjaergaard, C., Qayyum, M., Ziegler, L., Kosman, D. J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010; 132 (17): 6057-6067
 - **Transition-Metal Ions in Zeolites: Coordination and Activation of Oxygen** *INORGANIC CHEMISTRY*
Smeets, P. J., Woertink, J. S., Sels, B. F., Solomon, E. I., Schoonheydt, R. A.
2010; 49 (8): 3573-3583
 - **Heme-Copper-Dioxygen Complexes: Toward Understanding Ligand-Environmental Effects on the Coordination Geometry, Electronic Structure, and Reactivity** *INORGANIC CHEMISTRY*

- Halime, Z., Kieber-Emmons, M. T., Qayyum, M. F., Mondal, B., Gandhi, T., Puiu, S. C., Chufan, E. E., Sarjeant, A. A., Hodgson, K. O., Hedman, B., Solomon, E. I., Karlin, K. D.
2010; 49 (8): 3629-3645
- **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*
Hocking, R. K., George, S. D., Raymond, K. N., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010; 132 (11): 4006-4015
 - **Spectroscopic and DFT studies of activated bleomycin and its reactivity**
Liu, L. V., Chow, M. S., Bell, C. B., Wong, S. D., Zhao, J., Solomon, E. I.
AMER CHEMICAL SOC.2010
 - **Spectroscopic and computational studies on cytochrome oxidase model complexes: Role of the copper ligand denticity on geometric and electronic structure**
Kieber-Emmons, M. T., Halime, Z., Qayyum, M. F., Hodgson, K. O., Hedman, B., Karlin, K. D., Solomon, E. I.
AMER CHEMICAL SOC.2010
 - **Phenolate stabilized bis(mu-oxo)dicopper(III) species: An intermediate prior to the phenolate hydroxylation**
Kang, P., Woertink, J., Wasinger, E., Solomon, E. I., Stack, T. D.
AMER CHEMICAL SOC.2010
 - **Reaction Coordinate of Isopenicillin N Synthase: Oxidase versus Oxygenase Activity** *BIOCHEMISTRY*
Brown-Marshall, C. D., Diebold, A. R., Solomon, E. I.
2010; 49 (6): 1176-1182
 - **Kinetic and CD/MCD Spectroscopic Studies of the Atypical, Three-His-Ligated, Non-Heme Fe²⁺ Center in Diketone Dioxygenase: The Role of Hydrophilic Outer Shell Residues in Catalysis** *BIOCHEMISTRY*
Straganz, G. D., Diebold, A. R., Egger, S., Nidetzky, B., Solomon, E. I.
2010; 49 (5): 996-1004
 - **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*
Sun, N., Liu, L. V., Dey, A., Villar-Acevedo, G., Kovacs, J. A., Darensbourg, M. Y., Hodgson, K. O., Hedman, B., Solomon, E. I.
2010
 - **Thioether S-ligation in a side-on mu-eta(2):eta(2)-peroxodicopper(II) complex** *CHEMICAL COMMUNICATIONS*
Park, G. Y., Lee, Y., Lee, D., Woertink, J. S., Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2010; 46 (1): 91-93
 - **Copper(I)/O(2)Chemistry with Imidazole Containing Tripodal Tetradentate Ligands Leading to mu-1,2-Peroxo-Dicopper(II) Species** *INORGANIC CHEMISTRY*
Lee, Y., Park, G. Y., Lucas, H. R., Vajda, P. L., Kamaraj, K., Vance, M. A., Milligan, A. E., Woertink, J. S., Siegler, M. A., Sarjeant, A. A., Zakharov, L. N., Rheingold, A. L., Solomon, et al
2009; 48 (23): 11297-11309
 - **A [Cu₂O](2+) core in Cu-ZSM-5, the active site in the oxidation of methane to methanol** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Woertink, J. S., Smeets, P. J., Groothaert, M. H., Vance, M. A., Sels, B. F., Schoonheydt, R. A., Solomon, E. I.
2009; 106 (45): 18908-18913
 - **A peroxynitrite complex of copper: formation from a copper-nitrosyl complex, transformation to nitrite and exogenous phenol oxidative coupling or nitration** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Park, G. Y., Deepalatha, S., Puiu, S. C., Lee, D., Mondal, B., Sarjeant, A. A., del Rio, D., Pau, M. Y., Solomon, E. I., Karlin, K. D.
2009; 14 (8): 1301-1311
 - **A variable temperature spectroscopic study on Paracoccus pantotrophus pseudoazurin: Protein constraints on the blue Cu site** *1st Latin American Meeting on Biological Inorganic Chemistry (LABIC2008)*
Xie, X., Hadt, R. G., Pauleta, S. R., Gonzalez, P. J., Un, S., Moura, I., Solomon, E. I.
ELSEVIER SCIENCE INC.2009: 1307-13

- **Geometric and electronic structure and reactivity of a mononuclear 'side-on' nickel(III)-peroxo complex** *NATURE CHEMISTRY*
Cho, J., Sarangi, R., Annaraj, J., Kim, S. Y., Kubo, M., Ogura, T., Solomon, E. I., Nam, W.
2009; 1 (7): 568-572
- **Molecular Oxygen and Sulfur Reactivity of a Cyclotrimeratrylene Derived Trinuclear Copper(I) Complex** *INORGANIC CHEMISTRY*
Maiti, D., Woertink, J. S., Ghiladi, R. A., Solomon, E. I., Karlin, K. D.
2009; 48 (17): 8342-8356
- **Peroxo-Type Intermediates in Class I Ribonucleotide Reductase and Related Binuclear Non-Heme Iron Enzymes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Jensen, K. P., Bell, C. B., Clay, M. D., Solomon, E. I.
2009; 131 (34): 12155-12171
- **Spectroscopy and Kinetics of Wild-Type and Mutant Tyrosine Hydroxylase: Mechanistic Insight into O₂ Activation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chow, M. S., Eser, B. E., Wilson, S. A., Hodgson, K. O., Hedman, B., Fitzpatrick, P. F., Solomon, E. I.
2009; 131 (22): 7685-7698
- **S K-edge XAS and DFT Calculations on Cytochrome P450: Covalent and Ionic Contributions to the Cysteine-Fe Bond and Their Contribution to Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Jiang, Y., de Montellano, P. O., Hodgson, K. O., Hedman, B., Solomon, E. I.
2009; 131 (22): 7869-7878
- **Reaction Coordinate of a Functional Model of Tyrosinase: Spectroscopic and Computational Characterization** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
't Holt, B. T., Vance, M. A., Mirica, L. M., Heppner, D. E., Stack, T. D., Solomon, E. I.
2009; 131 (18): 6421-6438
- **Geometric and electronic structure differences between the type 3 copper sites of the multicopper oxidases and hemocyanin/tyrosinase** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Yoon, J., Fujii, S., Solomon, E. I.
2009; 106 (16): 6585-6590
- **Thermodynamic equilibrium between blue and green copper sites and the role of the protein in controlling function** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Ghosh, S., Xie, X., Dey, A., Sun, Y., Scholes, C. P., Solomon, E. I.
2009; 106 (13): 4969-4974
- **Copper dioxygen chemistry with diamines at low temperatures**
Verma, P., Kang, P., Mirica, L. M., Vance, M., Solomon, E. I., Stack, T. D.
AMER CHEMICAL SOC.2009
- **A functional nitric oxide reductase model**
Decreau, R., Yang, Y., Dey, A., Ohta, T., Dey, S. G., Solomon, E. I., Collman, J. P.
AMER CHEMICAL SOC.2009
- **Toluene and Ethylbenzene Aliphatic C-H Bond Oxidations Initiated by a Dicopper(II)-mu-1,2-Peroxo Complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lucas, H. R., Li, L., Sarjeant, A. A., Vance, M. A., Solomon, E. I., Karlin, K. D.
2009; 131 (9): 3230-3245
- **Fe L- and K-edge XAS of Low-Spin Ferric Corrole: Bonding and Reactivity Relative to Low-Spin Ferric Porphyrin** *INORGANIC CHEMISTRY*
Hocking, R. K., George, S. D., Gross, Z., Walker, F. A., Hodgson, K. O., Hedman, B., Solomon, E. I.
2009; 48 (4): 1678-1688
- **Peroxo and oxo intermediates in mononuclear nonheme iron enzymes and related active sites** *CURRENT OPINION IN CHEMICAL BIOLOGY*
Solomon, E. I., Wong, S. D., Liu, L. V., Decker, A., Chow, M. S.
2009; 13 (1): 99-113
- **Spectroscopic and Computational Studies of Nitrite Reductase: Proton Induced Electron Transfer and Backbonding Contributions to Reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Ghosh, S., Dey, A., Sun, Y., Scholes, C. P., Solomon, E. I.
2009; 131 (1): 277-288
- **Spectroscopic Definition of the Biferrous and Biferic Sites in de Novo Designed Four-Helix Bundle DFsc Peptides: Implications for O-2 Reactivity of Binuclear Non-Heme Iron Enzymes** *BIOCHEMISTRY*
Bell, C. B., Calhoun, J. R., Bobyr, E., Wei, P., Hedman, B., Hodgson, K. O., DeGrado, W. F., Solomon, E. T.
2009; 48 (1): 59-73
 - **Reactive Intermediates in Oxygenation Reactions with Mononuclear Nonheme Iron Catalysts** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Yoon, J., Wilson, S. A., Jang, Y. K., Seo, M. S., Nehru, K., Hedman, B., Hodgson, K. O., Bill, E., Solomon, E. I., Nam, W.
2009; 48 (7): 1257-1260
 - **Geometric Structure Determination of N694C Lipoxygenase: A Comparative Near-Edge X-Ray Absorption Spectroscopy and Extended X-Ray Absorption Fine Structure Study** *INORGANIC CHEMISTRY*
Sarangi, R., Hocking, R. K., Neidig, M. L., Benfatto, M., Holman, T. R., Solomon, E. I., Hodgson, K. O., Hedman, B.
2008; 47 (24): 11543-11550
 - **Intermediates Involved in the Two Electron Reduction of NO to N2O by a Functional Synthetic Model of Heme Containing Bacterial NO Reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Collman, J. P., Dey, A., Yang, Y., Decreau, R. A., Ohta, T., Solomon, E. I.
2008; 130 (49): 16498-?
 - **Spectroscopic and Electronic Structure Studies of Phenolate Cu(II) Complexes: Phenolate Ring Orientation and Activation Related to Cofactor Biogenesis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ghosh, S., Cirera, J., Vance, M. A., Ono, T., Fujisawa, K., Solomon, E. I.
2008; 130 (48): 16262-16273
 - **Circular Dichroism and Magnetic Circular Dichroism Studies of the Biferrous Site of the Class Ib Ribonucleotide Reductase from Bacillus cereus: Comparison to the Class Ia Enzymes** *BIOCHEMISTRY*
Tomter, A. B., Bell, C. B., Rohr, A. K., Andersson, K. K., Solomon, E. I.
2008; 47 (43): 11300-11309
 - **A functional nitric oxide reductase model** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Collman, J. P., Yang, Y., Dey, A., Decreau, R. A., Ghosh, S., Ohta, T., Solomon, E. I.
2008; 105 (41): 15660-15665
 - **Further insights into the mechanism of the reaction of activated bleomycin with DNA** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chow, M. S., Liu, L. V., Solomon, E. I.
2008; 105 (36): 13241-13245
 - **INOR 37-Role of second coordination sphere carboxylate residues in the reduction of dioxygen by the multicopper oxidases** *236th National Meeting of the American-Chemical-Society*
Augustine, A. J., Yoon, J., Stoj, C. S., Kosman, D., Solomon, E. I.
AMER CHEMICAL SOC.2008
 - **INOR 566-Sulfur K-edge X-ray absorption spectroscopic and density functional theory studies of metal bis- and tris-dithiolene complexes** *236th National Meeting of the American-Chemical-Society*
Tenderholt, A. L., Szilagy, R. K., Holm, R. H., Hodgson, K. O., Hedman, B., Solomon, E. I.
AMER CHEMICAL SOC.2008
 - **CD and MCD studies of the effects of component B variant binding on the biferrous active site of methane monooxygenase** *BIOCHEMISTRY*
Mitic, N., Schwartz, J. K., Brazeau, B. J., Lipscomb, J. D., Solomon, E. I.
2008; 47 (32): 8386-8397
 - **Oxygen reactivity of the biferrous site in the de novo designed four helix bundle peptide DFsc: Nature of the "intermediate" and reaction mechanism** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Calhoun, J. R., Bell, C. B., Smith, T. J., Thamann, T. J., DeGrado, W. F., Solomon, E. I.
2008; 130 (29): 9188-?
 - **Spectroscopic definition of the ferroxidase site in M ferritin: Comparison of binuclear substrate vs cofactor active sites** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Schwartz, J. K., Liu, X. S., Tosha, T., Theil, E. C., Solomon, E. I.
2008; 130 (29): 9441-9450
- **Interaction of nitric oxide with a functional model of cytochrome c oxidase** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Collman, J. P., Dey, A., Decreau, R. A., Yang, Y., Hosseini, A., Solomon, E. I., Eberspacher, T. A.
2008; 105 (29): 9892-9896
 - **Electronic control of the "Bailar Twist" in formally d(0)-d(2) molybdenum tris(dithiolene) complexes: A sulfur K-edge X-ray absorption spectroscopy and density functional theory study** *INORGANIC CHEMISTRY*
Tenderholt, A. L., Szilagy, R. K., Holm, R. H., Hodgson, K. O., Hedman, B., Solomon, E. I.
2008; 47 (14): 6382-6392
 - **Geometric and electronic structure studies of the binuclear nonheme ferrous active site of Toluene-4-monooxygenase: Parallels with methane monooxygenase and insight into the role of the effector proteins in O-2 activation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Schwartz, J. K., Wei, P., Mitchell, K. H., Fox, B. G., Solomon, E. I.
2008; 130 (22): 7098-7109
 - **Reaction of a copper-dioxygen complex with nitrogen Monoxide(center dot NO) leads to a copper(II) - Peroxynitrite species** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Maiti, D., Lee, D., Sarjeant, A. A., Pau, M. Y., Solomon, E. I., Gaoutchenova, K., Sundermeyer, J., Karlin, K. D.
2008; 130 (21): 6700-?
 - **Copper dioxygen adducts: Formation of bis(mu-oxo)dicopper(III) versus (mu-1,2)peroxodicopper(II) complexes with small changes in one pyridyl-ligand substituent** *INORGANIC CHEMISTRY*
Maiti, D., Woertink, J. S., Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2008; 47 (9): 3787-3800
 - **Perturbations to the geometric and electronic structure of the CUA site: Factors that influence delocalization and their contributions to electron transfer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Xie, X., Gorelsky, S. I., Sarangi, R., Garner, D. K., Hwang, H. J., Hodgson, K. O., Hedman, B., Lu, Y., Solornon, E. I.
2008; 130 (15): 5194-5205
 - **Spectroscopic and density functional theory studies of the blue-copper site in M121SeM and C112SeC azurin: Cu-Se versus Cu-S bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sarangi, R., Gorelsky, S. I., Basumallick, L., Hwang, H. J., Pratt, R. C., Stack, T. D., Lu, Y., Hodgson, K. O., Hedman, B., Solomon, E. I.
2008; 130 (12): 3866-3877
 - **Spectroscopic studies of perturbed T1 Cu sites in the multicopper oxidases Saccharomyces cerevisiae Fet3p and Rhus vernicifera laccase: Allosteric coupling between the T1 and trinuclear Cu sites** *BIOCHEMISTRY*
Augustine, A. J., Kragh, M. E., Sarangi, R., Fujii, S., Liboiron, B. D., Stoj, C. S., Kosman, D. J., Hodgson, K. O., Hedman, B., Solomon, E. I.
2008; 47 (7): 2036-2045
 - **Near-IR MCD of the nonheme ferrous active site in naphthalene 1,2-dioxygenase: Correlation to crystallography and structural insight into the mechanism of Rieske dioxygenases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ohta, T., Chakrabarty, S., Lipscomb, J. D., Solomon, E. I.
2008; 130 (5): 1601-1610
 - **X-ray absorption spectroscopic and theoretical studies on (L)(2)[Cu-2(S-2)n](2+) complexes: Disulfide versus disulfide(center dot 1-) bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sarangi, R., York, J. T., Helton, M. E., Fujisawa, K., Karlin, K. D., Tolman, W. B., Hodgson, K. O., Hedman, B., Solomon, E. I.
2008; 130 (2): 676-686
 - **Mixed valent sites in biological electron transfer** *CHEMICAL SOCIETY REVIEWS*
Solomon, E. I., Xie, X., Dey, A.
2008; 37 (4): 623-638
 - **Extended charge decomposition analysis and its application for the investigation of electronic relaxation** *THEORETICAL CHEMISTRY ACCOUNTS*
Gorelsky, S. I., Solomon, E. I.
2008; 119 (1-3): 57-67

- **A Combined NRVs and DFT Study of Fe-IV=O Model Complexes: A Diagnostic Method for the Elucidation of Non-Heme Iron Enzyme Intermediates** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Bell, C. B., Wong, S. D., Xiao, Y., Klinker, E. J., Tenderholt, A. L., Smith, M. C., Rohde, J., Que, L., Cramer, S. P., Solomon, E. I.
2008; 47 (47): 9071-9074
- **O-2 Reduction to H2O by the multicopper oxidases** *DALTON TRANSACTIONS*
Solomon, E. I., Augustine, A. J., Yoon, J.
2008: 3921-3932
- **Spectroscopic and quantum chemical studies on low-spin Fe-IV=O complexes: Fe-O bonding and its contributions to reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Decker, A., Rohde, J., Klinker, E. J., Wong, S. D., Que, L., Solomon, E. I.
2007; 129 (51): 15983-15996
- **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
- **CD and MCD of CytC3 and taurine dioxygenase: Role of the facial triad in alpha-KG-dependent oxygenases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Neidig, M. L., Brown, C. D., Light, K. M., Fujimori, D. G., Nolan, E. M., Price, J. C., Barr, E. W., Bollinger, J. M., Krebs, C., Walsh, C. T., Solomon, E. I.
2007; 129 (46): 14224-14231
- **Substrate activation for O-2 reactions by oxidized metal centers in biology** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Pau, M. Y., Lipscomb, J. D., Solomon, E.
2007; 104 (47): 18355-18362
- **SK-Edge XAS and DFT calculations on square-planar NiII-thiolate complexes: Effects of active and passive H-bonding** *INORGANIC CHEMISTRY*
Dey, A., Green, K. N., Jenkins, R. M., Jeffrey, S. P., Darensbourg, M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 46 (23): 9655-9660
- **Sulfur K-edge XAS of W-V=O vs. Mo-V=O bis(dithiolene) complexes: Contributions of relativistic effects to electronic structure and reactivity of tungsten enzymes** *JOURNAL OF INORGANIC BIOCHEMISTRY*
Tenderholt, A. L., Szilagy, R. K., Holm, R. H., Hodgson, K., Hedman, B., Solomon, E.
2007; 101 (11-12): 1594-1600
- **Polarized X-ray absorption spectroscopy of single-crystal Mn(V) complexes relevant to the oxygen-evolving complex of photosystem II** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yano, J., Robblee, J., Pushkar, Y., Marcus, M. A., Bendix, J., Workman, J. M., Collins, T. J., Solomon, E. I., George, S. D., Yachandra, V. K.
2007; 129 (43): 12989-13000
- **Spectroscopic and kinetic studies of perturbed trinuclear copper clusters: The role of protons in reductive cleavage of the O-O bond in the multicopper oxidase Fet3p** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Augustine, A. J., Quintanar, L., Stoj, C. S., Kosman, D. J., Solomon, E. I.
2007; 129 (43): 13118-13126
- **Electronic structure of the peroxy intermediate and its correlation to the native intermediate in the multicopper oxidases: Insights into the reductive cleavage of the O-O bond** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yoon, J., Solomon, E. I.
2007; 129 (43): 13127-13136
- **Sulfur K-edge X-ray absorption Spectroscopy and density functional theory calculations on superoxide reductase: Role of the axial thiolate in reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Jenney, F. E., Adams, M. W., Johnson, M. K., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 129 (41): 12418-12431
- **Resolution of the spectroscopy versus crystallography issue for NO intermediates of nitrite reductase from Rhodobacter sphaeroides** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ghosh, S., Dey, A., Usov, O. M., Sun, Y., Grigoryants, V. M., Scholes, C. P., Solomon, E. I.
2007; 129 (34): 10310-?

- **The two oxidized forms of the trinuclear Cu cluster in the multicopper oxidases and mechanism for the decay of the native intermediate** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Yoon, J., Liboiron, B. D., Sarangi, R., Hodgson, K. O., Hedman, B., Solomona, E. I.
2007; 104 (34): 13609-13614
- **Spectroscopic and electronic structure studies of intermediate X in ribonucleotide reductase R2 and two variants: A description of the Fe-IV-Oxo bond in the Fe-III-O-Fe-IV dimer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mitic, N., Clay, M. D., Saleh, L., Bollinger, J. M., Solomon, E. I.
2007; 129 (29): 9049-9065
- **Copper(I) complex O-2-reactivity with a N3S thioether ligand: A copper-dioxygen adduct including sulfur ligation, ligand oxygenation, and comparisons with all nitrogen ligand analogues** *INORGANIC CHEMISTRY*
Lee, D., Hatcher, L. Q., Vance, M. A., Sarangi, R., Milligan, A. E., Sarjeant, A. A., Incarvito, C. D., Rheingold, A. L., Hodgson, K. O., Hedman, B., Solomon, E. I., Karlin, K. D.
2007; 46 (15): 6056-6068
- **Copper(I)/S-8 reversible reactions leading to an end-on bound dicopper(II) disulfide complex: Nucleophilic reactivity and analogies to copper-dioxygen chemistry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Maiti, D., Woertink, J. S., Vance, M. A., Milligan, A. E., Sarjeant, A. A., Solomon, E. I., Karlin, K. D.
2007; 129 (28): 8882-8892
- **O-2 and N2O activation by bi-, tri-, and tetranuclear Cu clusters in biology** *ACCOUNTS OF CHEMICAL RESEARCH*
Solomon, E. I., Sarangi, R., Woertink, J. S., Augustine, A. J., Yoon, J., Ghosh, S.
2007; 40 (7): 581-591
- **Kinetic and spectroscopic studies of N694C lipoxygenase: A probe of the substrate activation mechanism of a nonheme ferric enzyme** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Neidig, M. L., Weckler, A. T., Schenk, G., Holman, T. R., Solomon, E. I.
2007; 129 (24): 7531-7537
- **VTVH-MCD and DFT studies of thiolate bonding to {FeNO}(7)/{FeO2}(8) complexes of isopenicillin N synthase: Substrate determination of oxidase versus oxygenase activity in nonheme Fe enzymes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brown, C. D., Neidig, M. L., Neibergall, M. B., Lipscomb, J. D., Solomon, E. I.
2007; 129 (23): 7427-7438
- **Sulfur K-edge XAS and DFT studies on Ni-II complexes with oxidized thiolate ligands: Implications for the roles of oxidized thiolates in the active sites of Fe and Co nitrile hydratase** *INORGANIC CHEMISTRY*
Dey, A., Jeffrey, S. P., Darensbourg, M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 46 (12): 4989-4996
- **Further insights into the spectroscopic properties, electronic structure, and kinetics of formation of the heme-peroxo-copper complex [(F8TPP)Fe-III-(O-2(2-))-Cu-II(TMPA)](+)** *INORGANIC CHEMISTRY*
Ghiladi, R. A., Chufan, E. E., del Rio, D., Solomon, E. I., Krebs, C., Huynh, B. H., Huang, H., Moenne-Loccoz, P., Kaderli, S., Honecker, M., Zuberbuehler, A. D., Marzilli, L., Cotter, et al
2007; 46 (10): 3889-3902
- **Intramolecular single-turnover reaction in a cytochrome c oxidase model bearing a Tyr244 mimic** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Collman, J. P., Decreau, R. A., Yan, Y., Yoon, J., Solomon, E. I.
2007; 129 (18): 5794-?
- **Spectroscopic, computational, and kinetic studies of the mu(4)-sulfide-bridged tetranuclear Cu-Z cluster in N2O reductase: pH effect on the edge ligand and its contribution to reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ghosh, S., Gorelsky, S. I., George, S. D., Chan, J. M., Cabrito, I., Dooley, D. M., Moura, J. J., Moura, I., Solomon, E. I.
2007; 129 (13): 3955-3965
- **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., Szilagyi, R. K., Ribas, X., Rovira, C., Almeida, M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 129 (8): 2316-2326
- **Spectroscopic and electronic structure study of the enzyme-substrate complex of intradiol dioxygenases: Substrate activation by a high-spin ferric non-heme iron site** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Pau, M. Y., Davis, M. I., Orville, A. M., Lipscomb, J. D., Solomon, E. I.
2007; 129 (7): 1944-1958
- **Synthesis, characterization, and reactivities of manganese(V)-oxo porphyrin complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Song, W. J., Seo, M. S., George, S. D., Ohta, T., Song, R., Kang, M., Tosha, T., Kitagawa, T., Solomon, E. I., Nam, W.
2007; 129 (5): 1268-1277
 - **Identification of the peroxy adduct in multicopper oxidases by a combination of computational chemistry and extended X-ray absorption fine-structure measurements** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ryde, U., Hsiao, Y., Rulisek, L., Solomon, E. I.
2007; 129 (4): 726-727
 - **Fe L-edge x-ray absorption spectroscopy of low-spin heme relative to non-heme Fe complexes: Delocalization of Fe d-electrons into the porphyrin ligand** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hocking, R. K., Wasinger, E. C., Yan, Y., deGroot, F. M., Walker, F. A., Hodgson, K. O., Hedman, B., Solomon, E. I.
2007; 129 (1): 113-125
 - **Description of the ground-state covalencies of the bis(dithiolato) transition-metal complexes from X-ray absorption spectroscopy and time-dependent density-functional calculations** *CHEMISTRY-A EUROPEAN JOURNAL*
Ray, K., George, S. D., Solomon, E. I., Wieghardt, K., Neese, F.
2007; 13 (10): 2783-2797
 - **The two-state issue in the mixed-valence binuclear Cu-A center in cytochrome c oxidase and N2O reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gorelsky, S. I., Xie, X., Chen, Y., Fee, J. A., Solomon, E. I.
2006; 128 (51): 16452-16453
 - **Multireference ab initio calculations on reaction intermediates of the multicopper oxidases** *INORGANIC CHEMISTRY*
Chalupsky, J., Neese, F., Solomon, E. I., Ryde, U., Rulisek, L.
2006; 45 (26): 11051-11059
 - **Spectroscopic and electronic structure studies of the role of active site interactions in the decarboxylation reaction of alpha-keto acid-dependent dioxygenases** *JOURNAL OF INORGANIC BIOCHEMISTRY*
Neidig, M. L., Brown, C. D., Kavana, M., Choroba, O. W., Spencer, J. B., Moran, G. R., Solomon, E. I.
2006; 100 (12): 2108-2116
 - **Circular dichroism and magnetic circular dichroism studies of the active site of p53R2 from human and mouse: Iron binding and nature of the biferrous site relative to other ribonucleotide reductases** *BIOCHEMISTRY*
Wei, P., Tomter, A. B., Rohr, A. K., Andersson, K. K., Solomon, E. I.
2006; 45 (47): 14043-14051
 - **A functional model for the cysteinylated non-heme iron enzyme superoxide reductase (SOR)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kitagawa, T., Dey, A., Lugo-Mas, P., Benedict, J. B., Kaminsky, W., Solomon, E., Kovacs, J. A.
2006; 128 (45): 14448-14449
 - **Spectroscopic methods in bioinorganic chemistry: Blue to green to red copper sites** *INORGANIC CHEMISTRY*
Solomon, E. I.
2006; 45 (20): 8012-8025
 - **Metal-thiolate bonds in bioinorganic chemistry** *JOURNAL OF COMPUTATIONAL CHEMISTRY*
Solomon, E. I., Gorelsky, S. I., Dey, A.
2006; 27 (12): 1415-1428
 - **How does single oxygen atom addition affect the properties of an Fe-nitrile hydratase analogue? The compensatory role of the unmodified thiolate** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lugo-Mas, P., Dey, A., Xu, L., Davin, S. D., Benedict, J., Kaminsky, W., Hodgson, K. O., Hedman, B., Solomon, E. I., Kovacs, J. A.
2006; 128 (34): 11211-11221
 - **Spectroscopic and electronic structure studies of aromatic electrophilic attack and hydrogen-atom abstraction by non-heme iron enzymes** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Neidig, M. L., Decker, A., Choroba, O. W., Huang, F., Kavana, M., Moran, G. R., Spencer, J. B., Solomon, E. I.

2006; 103 (35): 12966-12973

- **Fe L-edge XAS studies of K-4[Fe(CN)(6)] and K-3[Fe(CN)(6)]: A direct probe of back-bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hocking, R. K., Wasinger, E. C., de Groot, F. M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2006; 128 (32): 10442-10451
- **X-ray absorption spectroscopy and density functional theory studies of [(H(3)buea)Fe-III-X](n-) (X = S²⁻, O²⁻, OH⁻): Comparison of bonding and hydrogen bonding in oxo and sulfido complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Hocking, R. K., Larsen, P., Borovik, A. S., Hodgson, K. O., Hedman, B., Solomon, E. I.
2006; 128 (30): 9825-9833
- **X-ray absorption edge spectroscopy and computational studies on LCuO₂ species: Superoxide-Cu-II versus peroxide-Cu-III bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sarangi, R., Aboeella, N., Fujisawa, K., Tolman, W. B., Hedman, B., Hodgson, K. O., Solomon, E. I.
2006; 128 (25): 8286-8296
- **Metal and ligand K-edge XAS of titanium-TEMPO complexes: Determination of oxidation states and insights into Ti-O bond homolysis** *INORGANIC CHEMISTRY*
George, S. D., Huang, K., Waymouth, R. M., Solomon, E. I.
2006; 45 (11): 4468-4477
- **Direct hydrogen-atom abstraction by activated bleomycin: An experimental and computational study** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Decker, A., Chow, M. S., Kemsley, J. N., Lehnert, N., Solomon, E. I.
2006; 128 (14): 4719-4733
- **Spectroscopy and electronic structures of mono- and binuclear high-valent non-heme iron-oxo systems** *JOURNAL OF INORGANIC BIOCHEMISTRY*
Decker, A., Clay, M. D., Solomon, E. I.
2006; 100 (4): 697-706
- **Reinvestigation of the method used to map the electronic structure of blue copper proteins by NMR relaxation** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Hansen, D. F., Gorelsky, S. I., Sarangi, R., Hodgson, K. O., Hedman, B., Christensen, H. E., SOLOMON, E. I., Led, J. J.
2006; 11 (3): 277-285
- **mu-eta(2):eta(2)-Peroxicopper(II) complex with a secondary diamine ligand: A functional model of tyrosinase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mirica, L. M., Rudd, D. J., Vance, M. A., SOLOMON, E. I., Hodgson, K. O., Hedman, B., Stack, T. D.
2006; 128 (8): 2654-2665
- **Sulfur K-Edge XAS and DFT calculations on nitrile hydratase: Geometric and electronic structure of the non-heme iron active site** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., CHOW, M., Taniguchi, K., Lugo-Mas, P., Davin, S., Maeda, M., Kovacs, J. A., Odaka, M., Hodgson, K. O., Hedman, B., Solomon, E. I.
2006; 128 (2): 533-541
- **Mechanism of N₂O reduction by the mu(4)-S tetranuclear Cu-z cluster of nitrous oxide reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gorelsky, S. I., Ghosh, S., Solomon, E. I.
2006; 128 (1): 278-290
- **Oxygen binding of water-soluble cobalt porphyrins in aqueous solution** *INORGANIC CHEMISTRY*
Collman, J. P., Yan, Y. L., Eberspacher, T., Xie, X. J., SOLOMON, E. I.
2005; 44 (26): 9628-9630
- **MXAN analysis of the XANES energy region of a mononuclear copper complex: Applications to bioinorganic systems** *INORGANIC CHEMISTRY*
Sarangi, R., Benfatto, M., Hayakawa, K., Bubacco, L., SOLOMON, E. I., Hodgson, K. O., Hedman, B.
2005; 44 (26): 9652-9659
- **Spectroscopic and computational studies of NTBC bound to the non-heme iron enzyme (4-hydroxyphenyl)pyruvate dioxygenase: Active site contributions to drug inhibition** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Neidig, M. L., Decker, A., Kavana, M., Moran, G. R., Solomon, E. I.
2005; 338 (1): 206-214

- **Spectroscopic and computational studies of the de novo designed protein DF2t: Correlation to the biferrrous active site of ribonucleotide reductase and factors that affect O-2 reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Wei, P. P., Skulan, A. J., Wade, H., DeGrado, W. F., Solomon, E. I.
2005; 127 (46): 16098-16106
- **Sulfur K-edge XAS and DFT calculations on [Fe4S4](2+) clusters: Effects of H-bonding and structural distortion on covalency and spin topology** *INORGANIC CHEMISTRY*
Dey, A., Roche, C. L., Walters, M. A., Hodgson, K. O., Hedman, B., Solomon, E. I.
2005; 44 (23): 8349-8354
- **Ground-state electronic and magnetic properties of a mu(3)-Oxo-bridged trinuclear Cu(II) complex: Correlation to the native intermediate of the multicopper oxidases** *INORGANIC CHEMISTRY*
Yoon, J., Solomon, E. I.
2005; 44 (22): 8076-8086
- **Normal mode analysis of Pyrococcus furiosus rubredoxin via nuclear resonance vibrational spectroscopy (NRVS) and resonance Raman spectroscopy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Xiao, Y. M., Wang, H. X., George, S. J., Smith, M. C., Adams, M. W., Jenney, F. E., Sturhahn, W., Alp, E. E., Zhao, J. O., Yoda, Y., Dey, A., SOLOMON, E. I., Cramer, et al
2005; 127 (42): 14596-14606
- **Spectroscopic and electronic structure studies of the trinuclear Cu cluster active site of the multicopper oxidase laccase: Nature of its coordination unsaturation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Quintanar, L., Yoon, J. J., Aznar, C. P., Palmer, A. E., Andersson, K. K., Britt, R. D., Solomon, E. I.
2005; 127 (40): 13832-13845
- **Variable-temperature, variable-field magnetic circular dichroism studies of tris-hydroxy- and mu(3)-oxo-bridged trinuclear Cu(II) complexes: Evaluation of proposed structures of the native intermediate of the multicopper oxidases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yoon, J., Mirica, L. M., Stack, T. D., Solomon, E. I.
2005; 127 (39): 13680-13693
- **Geometric and electronic structure of the heme-peroxo-copper complex [(F8TPP)Fe-III-(O-2(2-))-Cu-II(TMPA)](ClO4)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
del Rio, D., Sarangi, R., Chufan, E. E., Karlin, K. D., Hedman, B., Hodgson, K. O., Solomon, E. I.
2005; 127 (34): 11969-11978
- **Sulfur K-edge XAS and DFT calculations on P450 model complexes: Effects of hydrogen bonding on electronic structure and redox potentials** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Okamura, T., Ueyama, N., Hedman, B., Hodgson, K. O., Solomon, E. I.
2005; 127 (34): 12046-12053
- **A combined quantum and molecular mechanical study of the O-2 reductive cleavage in the catalytic cycle of multicopper oxidases** *INORGANIC CHEMISTRY*
Rulisek, L., SOLOMON, E. I., Ryde, U.
2005; 44 (16): 5612-5628
- **Spectroscopic and DFT investigation of [M{HB(3,5-(i)Pr(2)pz)(3)}(SC6F5)] (M = Mn, Fe, Co, Ni, Cu, and Zn) model complexes: Periodic trends in metal-thiolate bonding** *INORGANIC CHEMISTRY*
Gorelsky, S. I., Basumallick, L., Vura-Weis, J., Sarangi, R., Hodgson, K. O., Hedman, B., Fujisawa, K., Solomon, E. I.
2005; 44 (14): 4947-4960
- **Tyrosinase reactivity in a model complex: An alternative hydroxylation mechanism** *SCIENCE*
Mirica, L. M., Vance, M., Rudd, D. J., Hedman, B., Hodgson, K. O., Solomon, E. I., Stack, T. D.
2005; 308 (5730): 1890-1892
- **Role of aspartate 94 in the decay of the peroxide intermediate in the multicopper oxidase Fet3p** *BIOCHEMISTRY*
Quintanar, L., Stoj, C., Wang, T. P., Kosman, D. J., Solomon, E. J.
2005; 44 (16): 6081-6091
- **Dioxygen activation by copper, heme and non-heme iron enzymes: comparison of electronic structures and reactivities** *CURRENT OPINION IN CHEMICAL BIOLOGY*

- Decker, A., Solomon, E. I.
2005; 9 (2): 152-163
- **Spectroscopy of non-heme iron thiolate complexes: Insight into the electronic structure of the low-spin active site of nitrile hydratase** *INORGANIC CHEMISTRY*
Kennepohl, P., Neese, F., Schweitzer, D., Jackson, H. L., Kovacs, J. A., Solomon, E. I.
2005; 44 (6): 1826-1836
 - **Spectroscopic and density functional studies of the red copper site in nitrosocyanin: Role of the protein in determining active site geometric and electronic structure** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Basumallick, L., Sarangi, R., George, S. D., Elmore, B., Hooper, A. B., Hedman, B., Hodgson, K. O., Solomon, E. I.
2005; 127 (10): 3531-3544
 - **Preface forum: "Functional insight from physical methods on metalloenzymes"** *INORGANIC CHEMISTRY*
SOLOMON, E. I.
2005; 44 (4): 723-726
 - **Metal and ligand K-Edge XAS of organotitanium complexes: Metal 4p and 3d contributions to pre-edge intensity and their contributions to bonding** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
George, S. D., Brant, P., Solomon, E. I.
2005; 127 (2): 667-674
 - **Structure-function correlations in oxygen activating non-heme iron enzymes** *CHEMICAL COMMUNICATIONS*
Neidig, M. L., Solomon, E. I.
2005: 5843-5863
 - **Investigation of the local structure of Fe(II) bleomycin and peplomycins using theoretical analysis of XANES** *PHYSICA SCRIPTA*
Smolentsev, G., Soldatov, A. V., Wasinger, E., Solomon, E., Hodgson, K., Hedman, B.
2005; T115: 862-863
 - **Comparison of Fe-IV = O heme and non-heme species: Electronic structures, bonding, and reactivities** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Decker, A., Solomon, E. I.
2005; 44 (15): 2252-2255
 - **Ligand K-edge X-ray absorption spectroscopy and DFT calculations on [Fe3S4](0,+) clusters: Delocalization, redox, and effect of the protein environment** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Glaser, T., Moura, J. J., HOLM, R. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
2004; 126 (51): 16868-16878
 - **Spectroscopic demonstration of a large antisymmetric exchange contribution to the spin-frustrated ground state of a D-3 symmetric hydroxy-bridged trinuclear Cu(II) complex: Ground-to-excited state superexchange pathways** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yoon, J., Mirica, L. M., Stack, T. D., Solomon, E. I.
2004; 126 (39): 12586-12595
 - **O-2 activation by binuclear Cu sites: Noncoupled versus exchange coupled reaction mechanisms** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chen, P., Solomon, E. I.
2004; 101 (36): 13105-13110
 - **Nature of the peroxo intermediate of the W48F/D84E ribonucleotide reductase variant: Implications for O-2 activation by binuclear non-heme iron enzymes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Skulan, A. J., Brunold, T. C., Baldwin, J., Saleh, L., Bollinger, J. M., SOLOMON, E. I.
2004; 126 (28): 8842-8855
 - **Solvent effects on the conversion of dicopper(II) mu-eta(2):eta(2)-peroxo to bis-mu-oxo dicopper(III) complexes: Direct probing of the solvent interaction** *INORGANIC CHEMISTRY*
Liang, H. C., Henson, M. J., Hatcher, L. Q., Vance, M. A., Zhang, C. X., Lahti, D., Kaderli, S., Sommer, R. D., Rheingold, A. L., Zuberbuhler, A. D., SOLOMON, E. I., Karlin, K. D.
2004; 43 (14): 4115-4117

- **Ligand K-Edge X-ray absorption spectroscopy of [Fe₄S₄](1+,2+,3+) clusters: Changes in bonding and electronic relaxation upon redox** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dey, A., Glaser, T., Couture, M. M., Eltis, L. D., HOLM, R. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
2004; 126 (26): 8320-8328
- **Ferrous binding to the multicopper oxidases *Saccharomyces cerevisiae* Fet3p and human ceruloplasmin: Contributions to ferroxidase activity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Quintanar, L., Gebhard, M., Wang, T. P., Kosman, D. J., Solomon, E. I.
2004; 126 (21): 6579-6589
- **Photoelectron spectroscopic and electronic structure studies of CH₂O bonding and reactivity on ZnO surfaces: Steps in the methanol synthesis reaction** *INORGANIC CHEMISTRY*
Jones, P. M., May, J. A., Reitz, J. B., Solomon, E. I.
2004; 43 (11): 3349-3370
- **Oxygen activation by the noncoupled binuclear copper site in peptidylglycine alpha-hydroxylating monooxygenase. Spectroscopic definition of the resting sites and the putative Cu-M(II)-OOH intermediate** *BIOCHEMISTRY*
Chen, P., Bell, J., EIPPER, B. A., Solomon, E. I.
2004; 43 (19): 5735-5747
- **Spectroscopic and quantum chemical characterization of the electronic structure and bonding in a non-heme FeIV[double bond]O complex.** *Journal of the American Chemical Society*
Decker, A., Rohde, J., Que, L., Solomon, E. I.
2004; 126 (17): 5378-5379
- **Spectroscopic and quantum chemical characterization of the electronic structure and bonding in a non-heme Fe-IV=O complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Decker, A., Rohde, J. U., Que, L., Solomon, E. I.
2004; 126 (17): 5378-5379
- **Oxygen activation by the noncoupled binuclear copper site in peptidylglycine alpha-hydroxylating monooxygenase. Reaction mechanism and role of the noncoupled nature of the active site** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chen, P., Solomon, E. I.
2004; 126 (15): 4991-5000
- **CD and MCD studies of the non-heme ferrous active site in (4-hydroxyphenyl)pyruvate dioxygenase: Correlation between oxygen activation in the extradiol and alpha-KG-dependent dioxygenases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Neidig, M. L., Kavana, M., Moran, G. R., Solomon, E. I.
2004; 126 (14): 4486-4487
- **Electronic and spectroscopic studies of the non-heme reduced binuclear iron sites of two ribonucleotide reductase variants: Comparison to reduced methane monooxygenase and contributions to O-2 reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Wei, P. P., Skulan, A. J., Mitic, N., Yang, Y. S., Saleh, L., Bollinger, J. M., Solomon, E. I.
2004; 126 (12): 3777-3788
- **Axial ligation of Fe(II)-bleomycin probed by XANES spectroscopy** *INORGANIC CHEMISTRY*
Smolentsev, G., Soldatov, A. V., Wasinger, E. C., SOLOMON, E. I.
2004; 43 (6): 1825-1827
- **S K-edge X-ray absorption spectroscopic investigation of the Ni-containing superoxide dismutase active site: New structural insight into the mechanism** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Szilagy, R. K., Bryngelson, P. A., Maroney, M. J., Hedman, B., Hodgson, K. O., Solomon, E. I.
2004; 126 (10): 3018-3019
- **Electronic structures of metal sites in proteins and models: Contributions to function in blue copper proteins** *CHEMICAL REVIEWS*
SOLOMON, E. I., Szilagy, R. K., George, S. D., Basumallick, L.
2004; 104 (2): 419-458
- **Comparison between the geometric and electronic structures and reactivities of {FeNO}(7) and {FeO₂}(8) complexes: A density functional theory study** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Schenk, G., Pau, M. Y., Solomon, E. I.

2004; 126 (2): 505-515

- **N₂O reduction by the $\mu(4)$ -sulfide-bridged tetranuclear Cu-Z cluster active site** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Chen, P., Gorelsky, S. I., Ghosh, S., Solomon, E. I.
2004; 43 (32): 4132-4140
- **Activation of N₂O reduction by the fully reduced $\mu(4)$ -sulfide bridged tetranuclear Cu-Z cluster in nitrous oxide reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Ghosh, S., Gorelsky, S. I., Chen, P., Cabrito, I., Moura, J. J., Moura, I., Solomon, E. I.
2003; 125 (51): 15708-15709
- **Spectroscopic studies of the Met182Thr mutant of nitrite reductase: Role of the axial ligand in the geometric and electronic structure of blue and green copper sites** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Basumallick, L., Szilagyi, R. K., Zhao, Y. W., Shapleigh, J. P., Scholes, C. P., SOLOMON, E. I.
2003; 125 (48): 14784-14792
- **Circular dichroism and magnetic circular dichroism studies of the biferrous form of the R2 subunit of ribonucleotide reductase from mouse: Comparison to the R2 from Escherichia coli and other binuclear ferrous enzymes** *BIOCHEMISTRY*
Strand, K. R., Yang, Y. S., Andersson, K. K., SOLOMON, E. I.
2003; 42 (42): 12223-12234
- **L-edge X-ray absorption spectroscopy of non-heme iron sites: Experimental determination of differential orbital covalency** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Wasinger, E. C., de Groot, F. M., Hedman, B., Hodgson, K. O., Solomon, E. I.
2003; 125 (42): 12894-12906
- **EPR spectroscopy of [Fe₂O₂(5-Et-3-TPA)₂](3+): Electronic origin of the unique spin-hamiltonian parameters of the (Fe₂O₂)-O-III,IV diamond core** *INORGANIC CHEMISTRY*
Skulan, A. J., Hanson, M. A., Hsu, H. F., Dong, Y. H., Que, L., SOLOMON, E. I.
2003; 42 (20): 6489-6496
- **Spectroscopic investigation of stellacyanin mutants: Axial ligand interactions at the blue copper site** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
George, S. D., Basumallick, L., Szilagyi, R. K., Randall, D. W., Hill, M. G., Nersissian, A. M., Valentine, J. S., Hedman, B., Hodgson, K. O., Solomon, E. I.
2003; 125 (37): 11314-11328
- **Spectroscopic and electronic structure studies of 2,3-dihydroxybiphenyl 1,2-dioxygenase: O-2 reactivity of the non-heme ferrous site in extradiol dioxygenases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Davis, M. I., Wasinger, E. C., Decker, A., Pau, M. Y., Vaillancourt, F. H., Bolin, J. T., Eltis, L. D., Hedman, B., Hodgson, K. O., Solomon, E. I.
2003; 125 (37): 11214-11227
- **Rapid-freeze-quench magnetic circular dichroism of intermediate X in ribonucleotide reductase: New structural insight** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mitic, N., Saleh, L., Schenk, G., Bollinger, J. M., Solomon, E. I.
2003; 125 (37): 11200-11201
- **Spectroscopic studies of the interaction of ferrous bleomycin with DNA** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kemsley, J. N., Zaleski, K. L., Chow, M. S., Decker, A., Shishova, E. Y., Wasinger, E. C., Hedman, B., Hodgson, K. O., Solomon, E. I.
2003; 125 (36): 10810-10821
- **Description of the ground state wave functions of Ni dithiolenes using sulfur K-edge X-ray absorption spectroscopy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Szilagyi, R. K., Lim, B. S., Glaser, T., Holm, R. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
2003; 125 (30): 9158-9169
- **Spectroscopic characterization of the Leu513His variant of fungal laccase: Effect of increased axial ligand interaction on the geometric and electronic structure of the type 1 Cu site** *INORGANIC CHEMISTRY*
Palmer, A. E., Szilagyi, R. K., Cherry, J. R., Jones, A., Xu, F., Solomon, E. I.
2003; 42 (13): 4006-4017
- **Spectroscopic characterization of soybean lipoxygenase-1 mutants: the role of second coordination sphere residues in the regulation of enzyme activity** *BIOCHEMISTRY*
Schenk, G., Neidig, M. L., Zhou, J., Holman, T. R., SOLOMON, E. I.

2003; 42 (24): 7294-7302

- **Spectroscopic study of [Fe₂O₂(5-Et-3-TPA)(2)](3+): Nature of the Fe₂O₂ diamond core and its possible relevance to high-valent binuclear non-heme enzyme intermediates** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Skulan, A. J., Hanson, M. A., Hsu, H. F., Que, L., Solomon, E. I.
2003; 125 (24): 7344-7356
- **Spectroscopic evidence for a heme-superoxide/Cu(I) intermediate in a functional model of cytochrome C oxidase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Collman, J. P., Sunderland, C. J., Berg, K. E., Vance, M. A., SOLOMON, E. I.
2003; 125 (22): 6648-6649
- **Spectroscopy and bonding in side-on and end-on Cu-2(S-2) cores: Comparison to peroxide analogues** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chen, P., Fujisawa, K., Helton, M. E., Karlin, K. D., SOLOMON, E. I.
2003; 125 (21): 6394-6408
- **Spectroscopic and kinetic studies of PKU-inducing mutants of phenylalanine hydroxylase: Arg158Gln and Glu280Lys** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kemsley, J. N., Wasinger, E. C., Datta, S., Mitic, N., Acharya, T., Hedman, B., Caradonna, J. P., Hodgson, K. O., SOLOMON, E. I.
2003; 125 (19): 5677-5686
- **Resonance Raman investigation of equatorial ligand donor effects on the Cu₂O₂²⁺ core in end-on and side-on mu-peroxo-dicopper(II) and bis-mu-oxo-dicopper(III) complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Henson, M. J., Vance, M. A., Zhang, C. X., Liang, H. C., Karlin, K. D., SOLOMON, E. I.
2003; 125 (17): 5186-5192
- **Non-heme iron enzymes: Contrasts to heme catalysis** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
SOLOMON, E. I., Decker, A., Lehnert, N.
2003; 100 (7): 3589-3594
- **Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 3. Kinetics of electron transfer** *INORGANIC CHEMISTRY*
Kennepohl, P., SOLOMON, E. I.
2003; 42 (3): 696-708
- **Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 1. Photoelectron spectroscopic determination of electronic relaxation** *INORGANIC CHEMISTRY*
Kennepohl, P., SOLOMON, E. I.
2003; 42 (3): 679-688
- **Electronic structure contributions to electron-transfer reactivity in iron-sulfur active sites: 2. Reduction potentials** *INORGANIC CHEMISTRY*
Kennepohl, P., SOLOMON, E. I.
2003; 42 (3): 689-695
- **Reaction of elemental sulfur with a copper(I) complex forming a trans-mu-1,2 end-on disulfide complex: New directions in copper-sulfur chemistry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Helton, M. E., Chen, P., Paul, P. P., Tyeklar, Z., Sommer, R. D., Zakharov, L. N., Rheingold, A. L., SOLOMON, E. I., Karlin, K. D.
2003; 125 (5): 1160-1161
- **Density-functional investigation on the mechanism of H-atom abstraction by lipoxygenase** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Lehnert, N., Solomon, E. I.
2003; 8 (3): 294-305
- **Examples of high-frequency EPR studies in bioinorganic chemistry** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Andersson, K. K., Schmidt, P. P., Katterle, B., Strand, K. R., Palmer, A. E., Lee, S. K., SOLOMON, E. I., Graslund, A., Barra, A. L.
2003; 8 (3): 235-247
- **Spectroscopic studies of the effect of ligand donor strength on the Fe-NO bond in intradiol dioxygenases** *INORGANIC CHEMISTRY*
Wasinger, E. C., Davis, M. I., Pau, M. Y., Orville, A. M., Zaleski, J. M., Hedman, B., Lipscomb, J. D., Hodgson, K. O., SOLOMON, E. I.
2003; 42 (2): 365-376

- **Electronic structure and reactivity of high-spin iron-alkyl- and -pterinperoxo complexes** *INORGANIC CHEMISTRY*
Lehnert, N., Fujisawa, K., SOLOMON, E. I.
2003; 42 (2): 469-481
- **Spectroscopic and electronic structure studies of the diamagnetic side-on Cu-II-superoxo complex Cu(O-2)[HB(3-R-5-(i)Prpz)(3)]: Antiferromagnetic coupling versus covalent delocalization** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chen, P., Root, D. E., Campochiaro, C., Fujisawa, K., SOLOMON, E. I.
2003; 125 (2): 466-474
- **Distal metal effects in cobalt porphyrins related to CcO** *INORGANIC CHEMISTRY*
Collman, J. P., Berg, K. E., Sunderland, C. J., Aukauloo, A., Vance, M. A., SOLOMON, E. I.
2002; 41 (25): 6583-6596
- **The EPR spectrum of a Cu(II/II/III) cluster: anisotropic exchange in a bent Cu(II)(2)O-2 core** *INORGANICA CHIMICA ACTA*
Machonkin, T. E., Mukherjee, P., Henson, M. J., Stack, T. D., SOLOMON, E. I.
2002; 341: 39-44
- **Electronic structure and reactivity of low-spin Fe(III)-hydroperoxo complexes: Comparison to activated bleomycin** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lehnert, N., Neese, F., Ho, R. Y., Que, L., Solomon, E. I.
2002; 124 (36): 10810-10822
- **Spectroscopic and electronic structure studies of the mu(4)-sulfide bridged tetranuclear Cu-z cluster in N2O reductase: Molecular insight into the catalytic mechanism** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chen, P., Cabrito, I., Moura, J. J., Moura, I., Solomon, E. I.
2002; 124 (35): 10497-10507
- **A stabilized mu-eta(2):eta(2) peroxodicopper(II) complex with a secondary diamine ligand and its tyrosinase-like reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mirica, L. M., Vance, M., Rudd, D. J., Hedman, B., Hodgson, K. O., SOLOMON, E. I., Stack, T. D.
2002; 124 (32): 9332-9333
- **Nature of the intermediate formed in the reduction of O-2 to H2O at the trinuclear copper cluster active site in native laccase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lee, S. K., George, S. D., Antholine, W. E., Hedman, B., Hodgson, K. O., Solomon, E. I.
2002; 124 (21): 6180-6193
- **Spectroscopic characterization and O-2 reactivity of the trinuclear Cu cluster of mutants of the multicopper oxidase Fet3p** *BIOCHEMISTRY*
Palmer, A. E., Quintanar, L., Severance, S., Wang, T. P., Kosman, D. J., Solomon, E. I.
2002; 41 (20): 6438-6448
- **X-ray absorption spectroscopic investigation of the resting ferrous and cosubstrate-bound active sites of phenylalanine hydroxylase** *BIOCHEMISTRY*
Wasinger, E. C., Mitic, N., Hedman, B., Caradonna, J., SOLOMON, E. I., Hodgson, K. O.
2002; 41 (20): 6211-6217
- **Spectroscopic studies of 1-aminocyclopropane-1-carboxylic acid oxidase: Molecular mechanism and CO2 activation in the biosynthesis of ethylene** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhou, J., Rocklin, A. M., Lipscomb, J. D., Que, L., Solomon, E. I.
2002; 124 (17): 4602-4609
- **Contrasting copper-dioxygen chemistry arising from alike tridentate alkyltriamine copper(I) complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Liang, H. C., Zhang, C. X., Henson, M. J., Sommer, R. D., Hatwell, K. R., Kaderli, S., Zuberbuhler, A. D., Rheingold, A. L., SOLOMON, E. I., Karlin, K. D.
2002; 124 (16): 4170-4171
- **Electronic structure and its relation to function in copper proteins** *CURRENT OPINION IN CHEMICAL BIOLOGY*
Szilagy, R. K., Solomon, E. I.
2002; 6 (2): 250-258
- **Electronic structure description of the mu(4)-sulfide bridged tetranuclear Cu-z center in N2O reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Chen, P., George, S. D., Cabrito, I., Antholine, W. E., Moura, J. J., Moura, I., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2002; 124 (5): 744-745
- **Frontier molecular orbital analysis of Cu-n-O-2 reactivity** *JOURNAL OF INORGANIC BIOCHEMISTRY*
Chen, P., Solomon, E. I.
2002; 88 (3-4): 368-374
 - **Spectroscopic and electronic structure studies of protocatechuate 3,4-dioxygenase: Nature of tyrosinate-Fe(III) bonds and their contribution to reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Davis, M. I., Orville, A. M., Neese, F., Zaleski, J. M., Lipscomb, J. D., SOLOMON, E. I.
2002; 124 (4): 602-614
 - **X-ray absorption spectroscopic investigation of Fe(II)-peplomycin and peplomycin derivatives: the effect of axial ligation on Fe-pyrimidine back-bonding** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Wasinger, E. C., Zaleski, K. L., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2002; 7 (1-2): 157-164
 - **Electronic structure of high-spin iron(III)-alkylperoxo complexes and its relation to low-spin analogues: Reaction coordinate of O-O bond homolysis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lehnert, N., Ho, R. Y., Que, L., SOLOMON, E. I.
2001; 123 (51): 12802-12816
 - **A new Cu(II) side-on peroxo model clarifies the assignment of the oxyhemocyanin Raman spectrum** *INORGANIC CHEMISTRY*
Henson, M. J., Mahadevan, V., Stack, T. D., SOLOMON, E. I.
2001; 40 (20): 5068-?
 - **Excited electronic states of transition-metal dimers and the VBCI model: an overview** *COORDINATION CHEMISTRY REVIEWS*
Tuczek, F., SOLOMON, E. I.
2001; 219: 1075-1112
 - **Spectroscopic properties and electronic structure of low-spin Fe(III)-alkylperoxo complexes: Homolytic cleavage of the O-O bond** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lehnert, N., Ho, R. Y., Que, L., SOLOMON, E. I.
2001; 123 (34): 8271-8290
 - **Spectroscopic studies of substrate interactions with clavaminic synthase 2, a multifunctional alpha-KG-dependent non-heme iron enzyme: Correlation with mechanisms and reactivities** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhou, J., Kelly, W. L., Bachmann, B. O., Gunsior, M., TOWNSEND, C. A., SOLOMON, E. I.
2001; 123 (30): 7388-7398
 - **Invited award contribution for ACS Award in Inorganic Chemistry. Geometric and electronic structure contributions to function in bioinorganic chemistry: active sites in non-heme iron enzymes.** *Inorganic chemistry*
SOLOMON, E. I.
2001; 40 (15): 3656-3669
 - **Decay of the peroxide intermediate in laccase: Reductive cleavage of the O-O bond** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Palmer, A. E., Lee, S. K., SOLOMON, E. I.
2001; 123 (27): 6591-6599
 - **A quantitative description of the ground-state wave function of Cu-A by X-ray absorption spectroscopy: Comparison to plastocyanin and relevance to electron transfer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
George, S. D., Metz, M., Szilagyi, R. K., Wang, H. X., Cramer, S. P., Lu, Y., Tolman, W. B., Hedman, B., Hodgson, K. O., Solomon, E. I.
2001; 123 (24): 5757-5767
 - **Spectroscopy and reactivity of the type 1 copper site in Fet3p from *Saccharomyces cerevisiae*: Correlation of structure with reactivity in the multicopper oxidases** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Machonkin, T. E., Quintanar, L., Palmer, A. E., Hassett, R., Severance, S., Kosman, D. J., SOLOMON, E. I.
2001; 123 (23): 5507-5517
 - **Sulfur K-edge X-ray absorption spectroscopy of 2Fe-2S ferredoxin: Covalency of the oxidized and reduced 2Fe forms and comparison to model complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Anxolabehere-Mallart, E., Glaser, T., Frank, P., Aliverti, A., Zanetti, G., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2001; 123 (23): 5444-5452
- **Dioxygen binding to deoxyhemocyanin: Electronic structure and mechanism of the spin-forbidden two-electron reduction of O₂** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Metz, M., SOLOMON, E. I.
2001; 123 (21): 4938-4950
 - **Protein effects on the electronic structure of the [Fe₄S₄](2+) cluster in ferredoxin and HiPIP** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Glaser, T., Bertini, I., Moura, J. J., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2001; 123 (20): 4859-4860
 - **Raman and extended X-ray absorption fine structure characterization of a sulfur-ligated Cu(I) ethylene complex: Modeling the proposed ethylene binding site of Arabidopsis thaliana ETR1** *INORGANIC CHEMISTRY*
Hirsch, J., George, S. D., SOLOMON, E. I., Hedman, B., Hodgson, K. O., Burstyn, J. N.
2001; 40 (10): 2439-?
 - **Recent advances in bioinorganic spectroscopy** *CURRENT OPINION IN CHEMICAL BIOLOGY*
Lehnert, N., George, S. D., Solomon, E. I.
2001; 5 (2): 176-187
 - **Electronic spectral studies of molybdenyl complexes. 2. MCD spectroscopy of [MoOS₄]⁽⁻⁾ centers** *INORGANIC CHEMISTRY*
McMaster, J., Carducci, M. D., Yang, Y. S., SOLOMON, E. I., ENEMARK, J. H.
2001; 40 (4): 687-702
 - **SK-edge X-ray absorption studies of tetranuclear iron-sulfur clusters: mu-sulfide bonding and its contribution to electron delocalization** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Glaser, T., Rose, K., Shadle, S. E., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2001; 123 (3): 442-454
 - **Oxygen Binding, Activation, and Reduction to Water by Copper Proteins.** *Angewandte Chemie (International ed. in English)*
Solomon, E. I., Chen, P., Metz, M., Lee, S. K., Palmer, A. E.
2001; 40 (24): 4570-90
 - **The thermodynamics, kinetics, and molecular mechanism of intramolecular electron transfer in human ceruloplasmin** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Machonkin, T. E., SOLOMON, E. I.
2000; 122 (50): 12547-12560
 - **Ligand K-edge X-ray absorption spectroscopy: A direct probe of ligand-metal covalency** *ACCOUNTS OF CHEMICAL RESEARCH*
Glaser, T., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
2000; 33 (12): 859-868
 - **Electronic structure of activated bleomycin: Oxygen intermediates in heme versus non-heme iron** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Neese, F., Zaleski, J. M., Zaleski, K. L., SOLOMON, E. I.
2000; 122 (47): 11703-11724
 - **Spectroscopic and electronic structural studies of blue copper model complexes. 1. Perturbation of the thiolate-Cu bond** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Randall, D. W., George, S. D., Hedman, B., Hodgson, K. O., Fujisawa, K., SOLOMON, E. I.
2000; 122 (47): 11620-11631
 - **Spectroscopic and theoretical studies of mononuclear copper(II) alkyl- and hydroperoxo complexes: Electronic structure contributions to reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Chen, P., Fujisawa, K., SOLOMON, E. I.
2000; 122 (41): 10177-10193
 - **Differential reactivity between interconvertible side-on peroxo and bis-mu-oxodicopper isomers using peralkylated diamine ligands** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mahadevan, V., Henson, M. J., SOLOMON, E. I., Stack, T. D.
2000; 122 (41): 10249-10250

- **Excited-state exchange coupling in bent Mn(III)-O-Mn(III) complexes: Dominance of the pi/sigma superexchange pathway and its possible contributions to the reactivities of binuclear metalloproteins** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brunold, T. C., Gamelin, D. R., SOLOMON, E. I.
2000; 122 (35): 8511-8523
- **Spectroscopic and electronic structure description of the reduced binuclear non-heme iron active site in ribonucleotide reductase from E. coli: Comparison to reduced Delta(9) desaturase and electronic structure contributions to differences in O-2 reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yang, Y. S., Baldwin, J., Ley, B. A., Bollinger, J. M., SOLOMON, E. I.
2000; 122 (35): 8495-8510
- **A systematic K-edge X-ray absorption spectroscopic study of Cu(III) sites** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dubois, J. L., Mukherjee, P., Stack, T. D., Hedman, B., SOLOMON, E. I., Hodgson, K. O.
2000; 122 (24): 5775-5787
- **Electronic structure contributions to electron transfer in blue Cu and Cu-A** *JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY*
Randall, D. W., Gamelin, D. R., LaCroix, L. B., Solomon, E. I.
2000; 5 (1): 16-29
- **Geometric and electronic structure/function correlations in non-heme iron enzymes.** *Chemical reviews*
Solomon, E. I., Brunold, T. C., Davis, M. I., Kemsley, J. N., Lee, S. K., Lehnert, N., Neese, F., Skulan, A. J., Yang, Y. S., Zhou, J.
2000; 100 (1): 235-350
- **X-ray absorption spectroscopy of folded and unfolded copper(I) azurin** *INORGANICA CHIMICA ACTA*
DeBeer, S., Wittung-Stafshede, P., Leckner, J., Karlsson, G., Winkler, J. R., Gray, H. B., MALMSTROM, B. G., SOLOMON, E. I., Hedman, B., Hodgson, K. O.
2000; 297 (1-2): 278-282
- **Geometric and electronic structure/function correlations in non-heme iron enzymes** *CHEMICAL REVIEWS*
SOLOMON, E. I., Brunold, T. C., Davis, M. I., Kemsley, J. N., Lee, S. K., Lehnert, N., Neese, F., Skulan, A. J., Yang, Y. S., Zhou, J.
2000; 100 (1): 235-349
- **Spectroscopic and electronic structural studies of the Cu(III)(2) bis-mu-oxo core and its relation to the side-on peroxo-bridged dimer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Henson, M. J., Mukherjee, P., Root, D. E., Stack, T. D., SOLOMON, E. I.
1999; 121 (44): 10332-10345
- **Ligand K-edge and metal L-edge X-ray absorption spectroscopy and density functional calculations of oxomolybdenum complexes with thiolate and related ligands: Implications for sulfite oxidase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Izumi, Y., Glaser, T., Rose, K., McMaster, J., Basu, P., ENEMARK, J. H., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1999; 121 (43): 10035-10046
- **Relationship between the dipole strength of ligand pre-edge transitions and metal-ligand covalency** *INORGANIC CHEMISTRY*
Neese, F., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1999; 38 (21): 4854-4860
- **Reversible dioxygen binding to hemerythrin. 1. Electronic structures of deoxy- and oxyhemerythrin** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brunold, T. C., SOLOMON, E. I.
1999; 121 (36): 8277-8287
- **Reversible dioxygen binding to hemerythrin. 2. Mechanism of the proton-coupled two-electron transfer to O-2 at a single iron center** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brunold, T. C., SOLOMON, E. I.
1999; 121 (36): 8288-8295
- **Investigation of the anomalous spectroscopic features of the copper sites in chicken ceruloplasmin: Comparison to human ceruloplasmin** *BIOCHEMISTRY*
Machonkin, T. E., Musci, G., Zhang, H. H., di Patti, M. C., Calabrese, L., Hedman, B., Hodgson, K. O., Solomon, E. I.
1999; 38 (34): 11093-11102
- **Spectroscopic investigation of reduced protocatechuate 3,4-dioxygenase: Charge-induced alterations in the active site iron coordination environment** *INORGANIC CHEMISTRY*
Davis, M. I., Wasinger, E. C., Westre, T. E., Zaleski, J. M., Orville, A. M., Lipscomb, J. D., Hedman, B., Hodgson, K. O., SOLOMON, E. I.

1999; 38 (16): 3676-3683

- **Spectroscopic studies and electronic structure description of the high potential type 1 copper site in fungal laccase: Insight into the effect of the axial ligand** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Palmer, A. E., Randall, D. W., Xu, F., SOLOMON, E. I.
1999; 121 (30): 7138-7149
- **Resonance Raman evidence for a hydrogen-bonded oxo bridge in the R2 protein of ribonucleotide reductase from mouse** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hanson, M. A., Schmidt, P. P., Strand, K. R., Graslund, A., SOLOMON, E. I., Andersson, K. K.
1999; 121 (28): 6755-6756
- **Targeted mutations in a *Trametes villosa* laccase - Axial perturbations of the T1 copper** *JOURNAL OF BIOLOGICAL CHEMISTRY*
Xu, F., Palmer, A. E., Yaver, D. S., Berka, R. M., Gambetta, G. A., Brown, S. H., SOLOMON, E. I.
1999; 274 (18): 12372-12375
- **MCD C-term signs, saturation behavior, and determination of band polarizations in randomly oriented systems with spin $S \geq 1/2$. Applications to $S = 1/2$ and $S = 5/2$** *INORGANIC CHEMISTRY*
Neese, F., SOLOMON, E. I.
1999; 38 (8): 1847-1865
- **Circular dichroism and magnetic circular dichroism studies of the reduced binuclear non-heme iron site of stearyl-ACP Delta(9)-desaturase: Substrate binding and comparison to ribonucleotide reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yang, Y. S., Broadwater, J. A., Pulver, S. C., Fox, B. G., SOLOMON, E. I.
1999; 121 (12): 2770-2783
- **Investigation of the electronic structure of 2Fe-2S model complexes and the Rieske protein using ligand K-edge X-ray absorption spectroscopy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Rose, K., Shadle, S. E., Glaser, T., de Vries, S., Cherepanov, A., Canters, G. W., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1999; 121 (11): 2353-2363
- **Circular dichroism and magnetic circular dichroism spectroscopy of the catalytically competent ferrous active site of phenylalanine hydroxylase and its interaction with pterin cofactor** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kemsley, J. N., Mitic, N., Zaleski, K. L., Caradonna, J. P., SOLOMON, E. I.
1999; 121 (7): 1528-1536
- **X-ray absorption spectra of the oxidized and reduced forms of C112D azurin from *Pseudomonas aeruginosa*** *INORGANIC CHEMISTRY*
DeBeer, S., Kiser, C. N., Mines, G. A., Richards, J. H., Gray, H. B., SOLOMON, E. I., Hedman, B., Hodgson, K. O.
1999; 38 (3): 433-438
- **MCD C-Term Signs, Saturation Behavior, and Determination of Band Polarizations in Randomly Oriented Systems with Spin $S \geq (1)/(2)$. Applications to $S = (1)/(2)$ and $S = (5)/(2)$.** *Inorganic chemistry*
Neese, F., Solomon, E. I.
1999; 38 (8): 1847-65
- **X-ray Absorption Spectra of the Oxidized and Reduced Forms of C112D Azurin from *Pseudomonas aeruginosa*.** *Inorganic chemistry*
DeBeer, S., Kiser, C. N., Mines, G. A., Richards, J. H., Gray, H. B., Solomon, E. I., Hedman, B., Hodgson, K. O.
1999; 38 (3): 433-38
- **Spectroscopic Investigation of Reduced Protocatechuate 3,4-Dioxygenase: Charge-Induced Alterations in the Active Site Iron Coordination Environment.** *Inorganic chemistry*
Davis, M. I., Wasinger, E. C., Westre, T. E., Zaleski, J. M., Orville, A. M., Lipscomb, J. D., Hedman, B., Hodgson, K. O., Solomon, E. I.
1999; 38 (16): 3676-83
- **Relationship between the Dipole Strength of Ligand Pre-Edge Transitions and Metal-Ligand Covalency.** *Inorganic chemistry*
Neese, F., Hedman, B., Hodgson, K. O., Solomon, E. I.
1999; 38 (21): 4854-60
- **Substrate binding to the alpha-ketoglutarate-dependent non-heme iron enzyme clavaminic synthase 2: Coupling mechanism of oxidative decarboxylation and hydroxylation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhou, J., Gunsior, M., Bachmann, B. O., TOWNSEND, C. A., SOLOMON, E. I.

1998; 120 (51): 13539-13540

- **Calculation of zero-field splittings, g-values, and the relativistic nephelauxetic effect in transition metal complexes. Application to high-spin ferric complexes** *INORGANIC CHEMISTRY*
Neese, F., SOLOMON, E. I.
1998; 37 (26): 6568-6582
- **Peroxo-, oxo-, and hydroxo-bridged dicopper complexes: Observation of exogenous hydrocarbon substrate oxidation** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Obias, H. V., Lin, Y., Murthy, N. N., Pidcock, E., SOLOMON, E. I., Ralle, M., Blackburn, N. J., Neuhold, Y. M., Zuberbuhler, A. D., Karlin, K. D.
1998; 120 (49): 12960-12961
- **Detailed spectroscopic and theoretical studies on [Fe(EDTA)(O-2)](3-): Electronic structure of the side-on ferric-peroxide bond and its relevance to reactivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Neese, F., SOLOMON, E. I.
1998; 120 (49): 12829-12848
- **Spectroscopic and functional characterization of a ligand coordination mutant of soybean lipoxygenase-1: First coordination sphere analogue of human 15-lipoxygenase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Holman, T. R., Zhou, J., SOLOMON, E. I.
1998; 120 (48): 12564-12572
- **Propylene oxidation on copper oxide surfaces: Electronic and geometric contributions to reactivity and selectivity** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Reitz, J. B., SOLOMON, E. I.
1998; 120 (44): 11467-11478
- **Investigation of iron-sulfur covalency in rubredoxins and a model system using sulfur K-edge X-ray absorption spectroscopy** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Rose, K., Shadle, S. E., Eidsness, M. K., Kurtz, D. M., Scott, R. A., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1998; 120 (41): 10743-10747
- **Spectroscopic and geometric variations in perturbed blue copper centers: Electronic structures of stellacyanin and cucumber basic protein** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
LaCroix, L. B., Randall, D. W., Nersissian, A. M., Hoitink, C. W., Canters, G. W., Valentine, J. S., SOLOMON, E. I.
1998; 120 (37): 9621-9631
- **Effect of protonation on peroxo-copper bonding: Spectroscopic and electronic structure study of [Cu-2((UN-O)-(OOH)](2+)** *INORGANIC CHEMISTRY*
Root, D. E., Mahroof-Tahir, M., Karlin, K. D., SOLOMON, E. I.
1998; 37 (19): 4838-4848
- **Spectroscopic studies of oxidized manganese catalase and mu-oxo-bridged dimanganese(III) model complexes: Electronic structure of the active site and its relation to catalysis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brunold, T. C., Gamelin, D. R., Stemmler, T. L., Mandal, S. K., Armstrong, W. H., Penner-Hahn, J. E., SOLOMON, E. I.
1998; 120 (34): 8724-8738
- **Site-directed mutations in fungal laccase: effect on redox potential, activity and pH profile** *BIOCHEMICAL JOURNAL*
Xu, F., Berka, R. M., Wahleithner, J. A., Nelson, B. A., Shuster, J. R., Brown, S. H., Palmer, A. E., SOLOMON, E. I.
1998; 334: 63-70
- **Investigation of the reactive oxygen intermediate in an arene hydroxylation reaction performed by xylyl-bridged binuclear copper complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pidcock, E., Obias, H. V., Zhang, C. X., Karlin, K. D., SOLOMON, E. I.
1998; 120 (31): 7841-7847
- **Spectroscopic and magnetic studies of human ceruloplasmin: Identification of a redox-inactive reduced Type 1 copper site** *BIOCHEMISTRY*
Machonkin, T. E., Zhang, H. H., Hedman, B., Hodgson, K. O., Solomon, E. I.
1998; 37 (26): 9570-9578
- **Spectroscopic study of [Fe-2(O-2)(OBz)(2){HB(pz')3}(2)]: Nature of the mu-1,2 peroxide-Fe(III) bond and its possible relevance to O-2 activation by non-heme iron enzymes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brunold, T. C., Tamura, N., Kitajima, N., Moro-oka, Y., SOLOMON, E. I.

1998; 120 (23): 5674-5690

- **Spectroscopy of mixed-valence Cu-A-type centers: Ligand-field control of ground-state properties related to electron transfer** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gamelin, D. R., Randall, D. W., Hay, M. T., Houser, R. P., Mulder, T. C., Canters, G. W., de Vries, S., Tolman, W. B., Lu, Y., SOLOMON, E. I.
1998; 120 (21): 5246-5263
- **Electronic and geometric structure of a trinuclear mixed-valence copper(II,II,III) cluster** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Root, D. E., Henson, M. J., Machonkin, T., Mukherjee, P., Stack, T. D., SOLOMON, E. I.
1998; 120 (20): 4982-4990
- **Magnetic circular dichroism spectroscopic studies of mononuclear non-heme ferrous model complexes. Correlation of excited- and ground-state electronic structure with geometry** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pavel, E. G., Kitajima, N., SOLOMON, E. I.
1998; 120 (16): 3949-3962
- **Electron spectroscopic studies of CH₃OH chemisorption on Cu₂O and ZnO single-crystal surfaces: Methoxide bonding and reactivity related to methanol synthesis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Jones, P. M., May, J. A., Reitz, J. B., SOLOMON, E. I.
1998; 120 (7): 1506-1516
- **Spectroscopic investigation of the metal ligation and reactivity of the ferrous active sites of bleomycin and bleomycin derivatives** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Loeb, K. E., Zaleski, J. M., Hess, C. D., Hecht, S. M., SOLOMON, E. I.
1998; 120 (6): 1249-1259
- **Circular dichroism and magnetic circular dichroism spectroscopic studies of the non-heme ferrous active site in clavamate synthase and its interaction with alpha-ketoglutarate cosubstrate** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pavel, E. G., Zhou, J., Busby, R. W., Gunsior, M., TOWNSEND, C. A., SOLOMON, E. I.
1998; 120 (4): 743-753
- **Spectroscopic characterization of an engineered purple Cu-A center in azurin** *INORGANIC CHEMISTRY*
Hay, M. T., Ang, M. C., Gamelin, D. R., SOLOMON, E. I., Antholine, W. E., Ralle, M., Blackburn, N. J., Massey, P. D., Wang, X. T., Kwon, A. H., Lu, Y.
1998; 37 (2): 191-198
- **Calculation of Zero-Field Splittings, g-Values, and the Relativistic Nephelauxetic Effect in Transition Metal Complexes. Application to High-Spin Ferric Complexes.** *Inorganic chemistry*
Neese, F., Solomon, E. I.
1998; 37 (26): 6568-82
- **Effect of Protonation on Peroxo-Copper Bonding: Spectroscopic and Electronic Structure Study of [Cu(2)((UN-O)-(OOH)](2+).** *Inorganic chemistry*
Root, D. E., Mahroof-Tahir, M., Karlin, K. D., Solomon, E. I.
1998; 37 (19): 4838-48
- **Spectroscopic investigation of peroxide binding to the trinuclear copper cluster site in laccase: Correlation with the peroxy-level intermediate and relevance to catalysis** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Sundaram, U. M., Zhang, H. H., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1997; 119 (51): 12525-12540
- **Circular dichroism and magnetic circular dichroism studies of the mixed-valence binuclear non-heme iron active site in uteroferrin and its anion complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Yang, Y. S., McCormick, J. M., SOLOMON, E. I.
1997; 119 (49): 11832-11842
- **Irreversible reduction of dioxygen by simple peralkylated diamine-copper(I) complexes: Characterization and thermal stability of a [Cu-2(mu-O)(2)](2+) core** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mahadevan, V., Hou, Z. G., Cole, A. P., Root, D. E., Lal, T. K., SOLOMON, E. I., Stack, T. D.
1997; 119 (49): 11996-11997
- **New insights from spectroscopy into the structure/function relationships of lipoxygenases** *CHEMISTRY & BIOLOGY*
SOLOMON, E. I., Zhou, J., Neese, F., Pavel, E. G.

1997; 4 (11): 795-808

- **Ligand K-edge X-ray absorption spectroscopic studies: metal-ligand covalency in transition metal tetrathiolates** *INORGANICA CHIMICA ACTA*
Williams, K. R., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1997; 263 (1-2): 315-321
- **Cu K-edge XAS study of the [Cu-2(μ -O)(2)] core: Direct experimental evidence for the presence of Cu(III)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Dubois, J. L., Mukherjee, P., Collier, A. M., Mayer, J. M., SOLOMON, E. I., Hedman, B., Stack, T. D., Hodgson, K. O.
1997; 119 (36): 8578-8579
- **A multiplet analysis of Fe K-edge 1s \rightarrow 3d pre-edge features of iron complexes** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Westre, T. E., Kennepohl, P., DeWitt, J. G., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1997; 119 (27): 6297-6314
- **Spectroscopic characterization of the catalytically competent ferrous site of the resting, activated, and substrate-bound forms of phenylalanine hydroxylase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Loeb, K. E., Westre, T. E., Kappock, T. J., Mitic, N., Glasfeld, E., Caradonna, J. P., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1997; 119 (8): 1901-1915
- **Influence of copper-sulfur covalency and copper-copper bonding on valence delocalization and electron transfer in the Cu-A site of cytochrome c oxidase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Williams, K. R., Gamelin, D. R., LaCroix, L. B., Houser, R. P., Tolman, W. B., Mulder, T. C., DeVries, S., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1997; 119 (3): 613-614
- **Ligand field circular dichroism and magnetic circular dichroism studies of component B and substrate binding to the hydroxylase component of methane monooxygenase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pulver, S. C., Froland, W. A., Lipscomb, J. D., SOLOMON, E. I.
1997; 119 (2): 387-395
- **Multicopper oxidases and oxygenases** *CHEMICAL REVIEWS*
SOLOMON, E. I., Sundaram, U. M., Machonkin, T. E.
1996; 96 (7): 2563-2605
- **Structural and functional aspects of metal sites in biology** *CHEMICAL REVIEWS*
HOLM, R. H., Kennepohl, P., SOLOMON, E. I.
1996; 96 (7): 2239-2314
- **Trinuclear intermediate in the copper-mediated reduction of O-2: Four electrons from three coppers** *SCIENCE*
Cole, A. P., Root, D. E., Mukherjee, P., SOLOMON, E. I., Stack, T. D.
1996; 273 (5283): 1848-1850
- **Excited-state contributions to ground-state properties of mixed-valence dimers: Spectral and electronic-structural studies of [Fe-2(OH)(3)(tmtacn)(2)](2+) related to the [Fe2S2](+) active sites of plant-type ferredoxins** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gamelin, D. R., Bominaar, E. L., Kirk, M. L., Wieghardt, K., SOLOMON, E. I.
1996; 118 (34): 8085-8097
- **Electronic structure of the perturbed blue copper site in nitrite reductase: Spectroscopic properties, bonding, and implications for the entatic/rack state** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
LaCroix, L. B., Shadle, S. E., Wang, Y. N., Averill, B. A., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1996; 118 (33): 7755-7768
- **Excited-state distortions and electron delocalization in mixed-valence dimers: Vibronic analysis of the near-IR absorption and resonance Raman profiles of [Fe-2(OH)(3)(tmtacn)(2)](2+)** *INORGANIC CHEMISTRY*
Gamelin, D. R., Bominaar, E. L., Mathoniere, C., Kirk, M. L., Wieghardt, K., Girerd, J. J., SOLOMON, E. I.
1996; 35 (15): 4323-4335
- **Chemical and spectroscopic definition of the peroxide-level intermediate in the multicopper oxidases: Relevance to the catalytic mechanism of dioxygen reduction to water** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Shin, W., Sundaram, U. M., Cole, J. L., Zhang, H. H., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1996; 118 (13): 3202-3215

- **Electronic structure of the oxidized and reduced blue copper sites: Contributions to the electron transfer pathway, reduction potential, and geometry** *INORGANICA CHIMICA ACTA*
SOLOMON, E. I., Penfield, K. W., Gewirth, A. A., LOWERY, M. D., Shadle, S. E., GUCKERT, J. A., LaCroix, L. B.
1996; 243 (1-2): 67-78
- **X-Ray magnetic circular dichroism at temperatures <1K: Demonstration with the blue copper site in plastocyanin** *INORGANICA CHIMICA ACTA*
Christiansen, J., Peng, G., Young, A. T., LaCroix, L. B., SOLOMON, E. I., Cramer, S. P.
1996; 243 (1-2): 229-232
- **A study of a series of recombinant fungal laccases and bilirubin oxidase that exhibit significant differences in redox potential, substrate specificity, and stability** *BIOCHIMICA ET BIOPHYSICA ACTA-PROTEIN STRUCTURE AND MOLECULAR ENZYMOLOGY*
Xu, F., Shin, W. S., Brown, S. H., Wahleithner, J. A., Sundaram, U. M., SOLOMON, E. I.
1996; 1292 (2): 303-311
- **Structural and Functional Aspects of Metal Sites in Biology.** *Chemical reviews*
Holm, R. H., Kennepohl, P., Solomon, E. I.
1996; 96 (7): 2239-2314
- **Multicopper Oxidases and Oxygenases.** *Chemical reviews*
Solomon, E. I., Sundaram, U. M., Machonkin, T. E.
1996; 96 (7): 2563-2606
- **Excited-State Distortions and Electron Delocalization in Mixed-Valence Dimers: Vibronic Analysis of the Near-IR Absorption and Resonance Raman Profiles of [Fe(2)(OH)(3)(tmtacn)(2)](2+).** *Inorganic chemistry*
Gamelin, D. R., Bominaar, E. L., Mathonière, C., Kirk, M. L., Wieghardt, K., Girerd, J. J., Solomon, E. I.
1996; 35 (15): 4323-35
- **Circular dichroism and magnetic circular dichroism studies of the fully reduced binuclear non-heme iron active site in the Escherichia coli R2 subunit of ribonucleoside diphosphate reductase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pulver, S. C., Tong, W. H., Bollinger, J. M., Stubbe, J., SOLOMON, E. I.
1995; 117 (51): 12664-12678
- **MAGNETIC CIRCULAR-DICHROISM SPECTROSCOPY AS A PROBE OF THE GEOMETRIC AND ELECTRONIC-STRUCTURE OF NONHEME FERROUS ENZYMES** *COORDINATION CHEMISTRY REVIEWS*
SOLOMON, E. I., Pavel, E. G., Loeb, K. E., Campochiaro, C.
1995; 144: 369-460
- **SINGLE-CRYSTAL MORPHOLOGY OF THE COPPER-ACETATE DIMERS CU-2(CH3COO)(4)CENTER-DOT-2H(2)O AND CU-2(CH3COO)(4)PZ** *JOURNAL OF CRYSTAL GROWTH*
Bell, S. J., Jennings, K. L., DANIELSON, E. D., SOLOMON, E. I., Musselman, R. L.
1995; 154 (1-2): 108-112
- **SATURATION MAGNETIZATION MAGNETIC CIRCULAR-DICHROISM SPECTROSCOPY OF SYSTEMS WITH POSITIVE ZERO-FIELD SPLITTINGS - APPLICATION TO FESIF6-CENTER-DOT-6H(2)O** *INORGANIC CHEMISTRY*
Campochiaro, C., Pavel, E. G., SOLOMON, E. I.
1995; 34 (18): 4669-4675
- **EPR DEFINITION OF THE NONHEME FERRIC ACTIVE-SITES OF MAMMALIAN 15-LIPOXYGENASE - MAJOR SPECTRAL DIFFERENCE RELATIVE TO HUMAN 5-LIPOXYGENASES AND PLANT LIPOXYGENASES AND THEIR LIGAND-FIELD ORIGIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhang, Y., Gan, Q. F., Pavel, E. G., Sigal, E., SOLOMON, E. I.
1995; 117 (28): 7422-7427
- **SPECTROSCOPIC DEFINITION OF THE GEOMETRIC AND ELECTRONIC-STRUCTURE OF THE NONHEME IRON ACTIVE-SITE IN IRON(II) BLEOMYCIN - CORRELATION WITH OXYGEN REACTIVITY** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Loeb, K. E., Zaleski, J. M., Westre, T. E., GUJARDO, R. J., Mascharak, P. K., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1995; 117 (16): 4545-4561
- **NEAR-INFRARED CIRCULAR-DICHROISM, MAGNETIC CIRCULAR-DICHROISM, AND X-RAY-ABSORPTION SPECTRAL COMPARISON OF THE NONHEME FERROUS ACTIVE-SITES OF PLANT AND MAMMALIAN 15-LIPOXYGENASES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*

- Pavlosky, M. A., Zhang, Y., Westre, T. E., Gan, Q. F., Pavel, E. G., Campochiaro, C., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1995; 117 (15): 4316-4327
- **ELECTRONIC-STRUCTURE OF THE REDUCED BLUE COPPER ACTIVE-SITE - CONTRIBUTIONS TO REDUCTION POTENTIALS AND GEOMETRY** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
GUCKERT, J. A., LOWERY, M. D., SOLOMON, E. I.
1995; 117 (10): 2817-2844
 - **LIGAND K-EDGE X-RAY-ABSORPTION SPECTROSCOPIC STUDIES - METAL-LIGAND COVALENCY IN A SERIES OF TRANSITION-METAL TETRACHLORIDES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Shadle, S. E., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1995; 117 (8): 2259-2272
 - **GNXAS, A MULTIPLE-SCATTERING APPROACH TO EXAFS ANALYSIS - METHODOLOGY AND APPLICATIONS TO IRON COMPLEXES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Westre, T. E., DICICCO, A., Filipponi, A., Natoli, C. R., Hedman, B., SOLOMON, E. I., Hodgson, K. O.
1995; 117 (5): 1566-1583
 - **SPECTROSCOPIC AND ELECTRONIC-STRUCTURE STUDIES OF MET-HEMERYTHRIN MODEL COMPLEXES - A DESCRIPTION OF THE FERRIC-OXO DIMER BOND** *INORGANIC CHEMISTRY*
Brown, C. A., REMAR, G. J., Musselman, R. L., SOLOMON, E. I.
1995; 34 (3): 688-717
 - **DETERMINATION OF THE GEOMETRIC AND ELECTRONIC-STRUCTURE OF ACTIVATED BLEOMYCIN USING X-RAY-ABSORPTION SPECTROSCOPY** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Westre, T. E., Loeb, K. E., Zaleski, J. M., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1995; 117 (4): 1309-1313
 - **SPECTROSCOPIC AND THEORETICAL DESCRIPTION OF THE ELECTRONIC-STRUCTURE OF S=3/2 IRON-NITROSYL COMPLEXES AND THEIR RELATION TO O-2 ACTIVATION BY NONHEME IRON ENZYME ACTIVE-SITES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Brown, C. A., Pavlosky, M. A., Westre, T. E., Zhang, Y., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1995; 117 (2): 715-732
 - **BIOINORGANIC SPECTROSCOPY** *BIOCHEMICAL SPECTROSCOPY*
SOLOMON, E. I., Kirk, M. L., Gamelin, D. R., PULVER, S.
1995; 246: 71-110
 - **ELECTRONIC SPECTRAL STUDIES OF MOLYBDENYL COMPLEXES - IMPLICATIONS FOR OXOMOLYBDENUM ENZYMES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Carducci, M. D., Brown, C., SOLOMON, E. I., ENEMARK, J. H.
1994; 116 (26): 11856-11868
 - **Magnetic circular dichroism studies of exogenous ligand and substrate binding to the non-heme ferrous active site in phthalate dioxygenase.** *Chemistry & biology*
Pavel, E. G., Martins, L. J., ELLIS, W. R., SOLOMON, E. I.
1994; 1 (3): 173-183
 - **LIGAND K-EDGE X-RAY-ABSORPTION SPECTROSCOPY AS A PROBE OF LIGAND-METAL BONDING - CHARGE DONATION AND COVALENCY IN COPPER-CHLORIDE SYSTEMS** *INORGANIC CHEMISTRY*
Shadle, S. E., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1994; 33 (19): 4235-4244
 - **DETERMINATION OF THE FE-N-O ANGLE IN (FENO)(7) COMPLEXES USING MULTIPLE-SCATTERING EXAFS ANALYSIS BY GNXAS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Westre, T. E., DICICCO, A., Filipponi, A., Natoli, C. R., Hedman, B., SOLOMON, E. I., Hodgson, K. O.
1994; 116 (15): 6757-6768
 - **CHARGE-TRANSFER STATES AND ANTIFERROMAGNETISM OF BRIDGED CU DIMERS - APPLICATION TO OXYHEMOCYANIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Tuczek, F., SOLOMON, E. I.
1994; 116 (15): 6916-6924

- **SPECTROSCOPY OF BINUCLEAR DIOXYGEN COMPLEXES** *CHEMICAL REVIEWS*
SOLOMON, E. I., Tucek, F., Root, D. E., Brown, C. A.
1994; 94 (3): 827-856
- **ELECTRONIC-STRUCTURE AND SPECTROSCOPY OF MANGANESE CATALASE AND DI-MU-OXO [MN(III)MN(IV)] MODEL COMPLEXES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gamelin, D. R., Kirk, M. L., Stemmler, T. L., Pal, S., Armstrong, W. H., PENNERHAHN, J. E., SOLOMON, E. I.
1994; 116 (6): 2392-2399
- **SPECTROSCOPIC STUDIES OF THE COUPLED BINUCLEAR NONHEME IRON ACTIVE-SITE IN THE FULLY REDUCED HYDROXYLASE COMPONENT OF METHANE MONOOXYGENASE - COMPARISON TO DEOXY AND DEOXY-AZIDE HEMERYTHRIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
PULVER, S., Froland, W. A., Fox, B. G., Lipscomb, J. D., SOLOMON, E. I.
1993; 115 (26): 12409-12422
- **ELECTRONIC-STRUCTURES OF ACTIVE-SITES ON METAL-OXIDE SURFACES - DEFINITION OF THE CU/ZNO METHANOL SYNTHESIS CATALYST BY PHOTOELECTRON-SPECTROSCOPY** *CHEMICAL REVIEWS*
SOLOMON, E. I., Jones, P. M., May, J. A.
1993; 93 (8): 2623-2644
- **CONSTRUCTION OF A BLUE COPPER SITE AT THE NATIVE ZINC SITE OF YEAST COPPER-ZINC SUPEROXIDE-DISMUTASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lu, Y., LaCroix, L. B., LOWERY, M. D., SOLOMON, E. I., Bender, C. J., Peisach, J., Roe, J. A., Gralla, E. B., Valentine, J. S.
1993; 115 (14): 5907-5918
- **CHARGE-TRANSFER STATES OF BRIDGED TRANSITION-METAL DIMERS - MONOCLEAR VS BINUCLEAR COPPER AZIDE SYSTEMS WITH RELEVANCE TO OXY-HEMOCYANIN** *INORGANIC CHEMISTRY*
Tucek, F., SOLOMON, E. I.
1993; 32 (13): 2850-2862
- **ELECTRONIC-STRUCTURE CONTRIBUTIONS TO FUNCTION IN BIOINORGANIC CHEMISTRY** *SCIENCE*
SOLOMON, E. I., LOWERY, M. D.
1993; 259 (5101): 1575-1581
- **X-RAY ABSORPTION SPECTROSCOPIC STUDIES OF THE BLUE COPPER SITE - METAL AND LIGAND K-EDGE STUDIES TO PROBE THE ORIGIN OF THE EPR HYPERFINE SPLITTING IN PLASTOCYANIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Shadle, S. E., PENNERHAHN, J. E., Schugar, H. J., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1993; 115 (2): 767-776
- **ELECTRONIC ABSORPTION-SPECTROSCOPY OF COPPER PROTEINS** *METALLOBIOCHEMISTRY, PART C*
SOLOMON, E. I., LOWERY, M. D., LaCroix, L. B., Root, D. E.
1993; 226: 1-33
- **GROUND-STATE ELECTRONIC-STRUCTURE OF THE DIMER-OF-DIMERS COMPLEX [(MN₂O₂)₂(TPHPN)₂]⁴⁺ - POTENTIAL RELEVANCE TO THE PHOTOSYSTEM-II WATER OXIDATION CATALYST** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Kirk, M. L., Chan, M. K., Armstrong, W. H., SOLOMON, E. I.
1992; 114 (26): 10432-10440
- **SPECTROSCOPIC STUDIES OF SIDE-ON PEROXIDE-BRIDGED BINUCLEAR COPPER(II) MODEL COMPLEXES OF RELEVANCE TO OXYHEMOCYANIN AND OXYTYROSINASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Baldwin, M. J., Root, D. E., Pate, J. E., Fujisawa, K., Kitajima, N., SOLOMON, E. I.
1992; 114 (26): 10421-10431
- **SPECTROSCOPIC AND THEORETICAL DESCRIPTION OF THE ELECTRONIC-STRUCTURE OF THE S = 3/2 NITROSYL COMPLEX OF NONHEME IRON ENZYMES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhang, Y., Pavlosky, M. A., Brown, C. A., Westre, T. E., Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1992; 114 (23): 9189-9191
- **AXIAL LIGAND BONDING IN BLUE COPPER PROTEINS** *INORGANICA CHIMICA ACTA*
LOWERY, M. D., SOLOMON, E. I.
1992; 198: 233-243

- **VARIABLE-ENERGY PHOTOELECTRON SPECTROSCOPIC STUDIES OF H₂S CHEMISORPTION ON CU₂O AND ZNO SINGLE-CRYSTAL SURFACES - HS- BONDING TO COPPER(I) AND ZINC(II) SITES RELATED TO CATALYTIC POISONING** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lin, J. Y., May, J. A., Didziulis, S. V., SOLOMON, E. I.
1992; 114 (12): 4718-4727
- **ELECTRONIC-STRUCTURES OF ACTIVE-SITES IN COPPER PROTEINS - CONTRIBUTIONS TO REACTIVITY** *CHEMICAL REVIEWS*
SOLOMON, E. I., Baldwin, M. J., LOWERY, M. D.
1992; 92 (4): 521-542
- **SINGLE-CRYSTAL POLARIZED ABSORPTION SPECTROSCOPIC STUDY OF THE ELECTRONIC-STRUCTURE OF MU-1,2-PEROXO BINUCLEAR COBALT COMPLEXES** *INORGANIC CHEMISTRY*
Tuczek, F., SOLOMON, E. I.
1992; 31 (6): 944-953
- **COORDINATION CHEMISTRY OF NH₃ ON ZNO(0001) AND CUCL(111) SURFACES - SIGMA-BONDING INTERACTIONS WITH D-10 METAL-ION SITES** *INORGANIC CHEMISTRY*
Lin, J. Y., Jones, P. M., LOWERY, M. D., Gay, R. R., Cohen, S. L., SOLOMON, E. I.
1992; 31 (4): 686-695
- **CHEMICAL AND SPECTROSCOPIC STUDIES OF THE MIXED-VALENT DERIVATIVES OF THE NONHEME IRON PROTEIN HEMERYTHRIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
McCormick, J. M., REEM, R. C., SOLOMON, E. I.
1991; 113 (24): 9066-9079
- **SPECTROSCOPIC AND CHEMICAL STUDIES OF THE ASCORBATE OXIDASE TRINUCLEAR COPPER ACTIVE-SITE - COMPARISON TO LACCASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cole, J. L., Avigliano, L., Morpurgo, L., SOLOMON, E. I.
1991; 113 (24): 9080-9089
- **SPECTROSCOPIC AND THEORETICAL-STUDIES OF AN END-ON PEROXIDE-BRIDGED COUPLED BINUCLEAR COPPER(II) MODEL COMPLEX OF RELEVANCE TO THE ACTIVE-SITES IN HEMOCYANIN AND TYROSINASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Baldwin, M. J., ROSS, P. K., Pate, J. E., Tyeklar, Z., Karlin, K. D., SOLOMON, E. I.
1991; 113 (23): 8671-8679
- **VARIABLE PHOTON ENERGY PHOTOELECTRON SPECTROSCOPIC STUDY OF CO ADSORPTION TO COORDINATIVELY UNSATURATED TETRAHEDRON CU(I) AND ZN(II) SITES ON CUCL(111) AND ZNO(1010) SURFACES - D10 CONTRIBUTIONS TO CO BONDING AND ACTIVATION** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Lin, J. Y., Jones, P., GUCKERT, J., SOLOMON, E. I.
1991; 113 (22): 8312-8326
- **SPECTROSCOPIC CHARACTERIZATION OF THE PEROXIDE INTERMEDIATE IN THE REDUCTION OF DIOXYGEN CATALYZED BY THE MULTICOPPER OXIDASES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cole, J. L., Ballou, D. P., SOLOMON, E. I.
1991; 113 (22): 8544-8546
- **SPECTROSCOPIC STUDIES OF THE NONHEME FERRIC ACTIVE-SITE IN SOYBEAN LIPOXYGENASE - MAGNETIC CIRCULAR-DICHROISM AS A PROBE OF ELECTRONIC AND GEOMETRIC STRUCTURE - LIGAND-FIELD ORIGIN OF ZERO-FIELD SPLITTING** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Zhang, Y., Gebhard, M. S., SOLOMON, E. I.
1991; 113 (14): 5162-5175
- **EXCITED-STATE SPECTRAL FEATURES OF THE RADICAL REDUCED, NATIVE AND FULLY REDUCED FORMS OF THE COUPLED BINUCLEAR NONHEME IRON CENTER IN RIBONUCLEOTIDE REDUCTASE - ACTIVE-SITE DIFFERENCES RELATIVE TO HEMERYTHRIN** *NEW JOURNAL OF CHEMISTRY*
McCormick, J. M., REEM, R. C., FOROUGH, J., Bollinger, J. M., Jensen, G. M., Stephens, P. J., Stubbe, J., SOLOMON, E. I.
1991; 15 (6): 439-444
- **VARIABLE-TEMPERATURE VARIABLE-FIELD MAGNETIC CIRCULAR-DICHROISM STUDIES OF THE FE(II) ACTIVE-SITE IN METAPYROCATECHASE - IMPLICATIONS FOR THE MOLECULAR MECHANISM OF EXTRADIOL DIOXYGENASES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Mabrouk, P. A., Orville, A. M., Lipscomb, J. D., SOLOMON, E. I.

1991; 113 (11): 4053-4061

- **AN ELECTRONIC STRUCTURAL COMPARISON OF COPPER PEROXIDE COMPLEXES OF RELEVANCE TO HEMOCYANIN AND TYROSINASE ACTIVE-SITES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
ROSS, P. K., SOLOMON, E. I.
1991; 113 (9): 3246-3259
- **SPECTROSCOPIC STUDIES OF THE ELECTRONIC-STRUCTURE OF IRON(III) TRIS(CATECHOLATES)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Karpishin, T. B., Gebhard, M. S., SOLOMON, E. I., Raymond, K. N.
1991; 113 (8): 2977-2984
- **SINGLE-CRYSTAL SPECTROSCOPIC STUDIES OF FE(SC₆H₄PH-2)₄(2-) ELECTRONIC-STRUCTURE OF THE FERROUS SITE IN RUBREDOXIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gebhard, M. S., Koch, S. A., Millar, M., Devlin, F. J., Stephens, P. J., SOLOMON, E. I.
1991; 113 (5): 1640-1649
- **SPECTROSCOPIC AND CHEMICAL STUDIES OF THE LACCASE TRINUCLEAR COPPER ACTIVE-SITE - GEOMETRIC AND ELECTRONIC-STRUCTURE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cole, J. L., Clark, P. A., SOLOMON, E. I.
1990; 112 (26): 9534-9548
- **STRUCTURE-FUNCTION CORRELATIONS IN COPPER CLUSTERS IN PROTEINS** *27TH INTERNATIONAL CONF ON COORDINATION CHEMISTRY*
SOLOMON, E. I., Cole, J. L., Baldwin, M. J.
INT UNION PURE APPLIED CHEMISTRY.1990: 1063-66
- **VARIABLE-ENERGY PHOTOELECTRON SPECTROSCOPIC COMPARISON OF THE BONDING IN FERRIC SULFIDE AND FERRIC-CHLORIDE - AN ALTERNATIVE DESCRIPTION OF THE NEAR-IR VISIBLE SPIN-FORBIDDEN TRANSITIONS IN HIGH-SPIN D₅ COMPLEXES** *INORGANIC CHEMISTRY*
Butcher, K. D., Gebhard, M. S., SOLOMON, E. I.
1990; 29 (11): 2067-2074
- **VARIABLE-PHOTON-ENERGY PHOTOELECTRON SPECTROSCOPIC STUDIES OF HIGH-SPIN-D₆ TETRAHEDRAL FECL₄(2-) - ELECTRONIC RELAXATION EFFECTS ON IONIZATION** *INORGANIC CHEMISTRY*
Butcher, K. D., Didziulis, S. V., Briat, B., SOLOMON, E. I.
1990; 29 (9): 1626-1637
- **REACTIVITY OF THE LACCASE TRINUCLEAR COPPER ACTIVE-SITE WITH DIOXYGEN - AN X-RAY ABSORPTION-EDGE STUDY** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Cole, J. L., TAN, G. O., Yang, E. K., Hodgson, K. O., SOLOMON, E. I.
1990; 112 (6): 2243-2249
- **VARIABLE PHOTON ENERGY PHOTOELECTRON-SPECTROSCOPY ON FECL₄ - AN UNUSUAL ELECTRONIC-STRUCTURE FOR HIGH-SPIN D₅ COMPLEXES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Butcher, K. D., Didziulis, S. V., Briat, B., SOLOMON, E. I.
1990; 112 (6): 2231-2242
- **SINGLE-CRYSTAL SPECTRAL STUDIES OF FE(S₂,3,5,6-(ME)₄C₆H)₄ - THE ELECTRONIC-STRUCTURE OF THE FERRIC TETRATHIOLATE ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gebhard, M. S., Deaton, J. C., Koch, S. A., Millar, M., SOLOMON, E. I.
1990; 112 (6): 2217-2231
- **X-RAY ABSORPTION-EDGE SPECTROSCOPY OF LIGANDS BOUND TO OPEN-SHELL METAL-IONS - CHLORINE K-EDGE STUDIES OF COVALENCY IN CUCL₄2-** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hedman, B., Hodgson, K. O., SOLOMON, E. I.
1990; 112 (4): 1643-1645
- **X-RAY ABSORPTION-EDGE AND EXAFS STUDY OF THE COPPER SITES IN ZNO METHANOL SYNTHESIS CATALYSTS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
KAU, L. S., Hodgson, K. O., SOLOMON, E. I.
1989; 111 (18): 7103-7109

- **CHEMISTRY OF COPPER OVERLAYERS ON ZINC-OXIDE SINGLE-CRYSTAL SURFACES - MODEL ACTIVE-SITES FOR CU/ZNO METHANOL SYNTHESIS CATALYSTS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Didziulis, S. V., Butcher, K. D., Cohen, S. L., SOLOMON, E. I.
1989; 111 (18): 7110-7123
- **DETAILED SPECTROSCOPIC ANALYSIS OF HALF-MET HEMOCYANINS - MIXED-VALENT CONTRIBUTIONS TO ELECTRONIC-PROPERTIES AND STRUCTURE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Westmoreland, T. D., WILCOX, D. E., Baldwin, M. J., MIMS, W. B., SOLOMON, E. I.
1989; 111 (16): 6106-6123
- **SPECTROSCOPIC STUDIES OF THE CHARGE-TRANSFER AND VIBRATIONAL FEATURES OF BINUCLEAR COPPER(II) AZIDE COMPLEXES - COMPARISON TO THE COUPLED BINUCLEAR COPPER ACTIVE-SITE IN MET AZIDE HEMOCYANIN AND TYROSINASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pate, J. E., ROSS, P. K., Thamann, T. J., Reed, C. A., Karlin, K. D., Sorrell, T. N., SOLOMON, E. I.
1989; 111 (14): 5198-5209
- **SPECTROSCOPIC STUDIES OF THE COUPLED BINUCLEAR FERRIC ACTIVE-SITE IN METHEMERYTHRINS AND OXYHEMERYTHRIN - THE ELECTRONIC-STRUCTURE OF EACH IRON CENTER AND THE IRON-OXO AND IRON PEROXIDE BONDS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
REEM, R. C., McCormick, J. M., Richardson, D. E., Devlin, F. J., Stephens, P. J., Musselman, R. L., SOLOMON, E. I.
1989; 111 (13): 4688-4704
- **EDGE AND EXAFS STUDIES OF CU COORDINATION IN DEOXY HEMOCYANIN** *PHYSICA B-CONDENSED MATTER*
Tan, G., KAU, L. S., Hodgson, K. O., SOLOMON, E. I.
1989; 158 (1-3): 110-111
- **LOW-ENERGY X-RAY ABSORPTION-EDGE SPECTROSCOPY - APPLICATIONS TO THE NITROGENASE COFACTOR AND ELECTRONIC-STRUCTURE OF S AND CL IN INORGANIC SOLIDS** *PHYSICA B-CONDENSED MATTER*
Hedman, B., Frank, P., GHELLER, S. F., Newton, W. E., SOLOMON, E. I., Hodgson, K. O.
1989; 158 (1-3): 71-73
- **DETAILED SPECTRAL STUDIES OF COPPER-ACETATE - EXCITED-STATE INTERACTIONS IN COPPER DIMERS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
ROSS, P. K., Allendorf, M. D., SOLOMON, E. I.
1989; 111 (11): 4009-4021
- **TRANSVERSE AND LONGITUDINAL ZEEMAN EFFECT ON [PPH4][FECL4] - ASSIGNMENT OF THE LIGAND-FIELD TRANSITIONS AND THE ORIGIN OF THE A-6(1) GROUND-STATE ZERO-FIELD SPLITTING** *INORGANIC CHEMISTRY*
Deaton, J. C., Gebhard, M. S., SOLOMON, E. I.
1989; 28 (5): 877-889
- **VARIABLE PHOTON ENERGY PHOTOELECTRON SPECTROSCOPIC STUDIES OF COVALENT BONDING IN 3D10 TRANSITION-METAL COMPOUNDS** *INORGANIC CHEMISTRY*
Didziulis, S. V., Cohen, S. L., Butcher, K. D., SOLOMON, E. I.
1988; 27 (13): 2238-2250
- **ELECTRONIC-STRUCTURE OF PLASTOCYANIN - EXCITED-STATE SPECTRAL FEATURES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gewirth, A. A., SOLOMON, E. I.
1988; 110 (12): 3811-3819
- **VARIABLE PHOTON ENERGY PHOTOELECTRON SPECTROSCOPIC STUDIES OF COPPER CHLORIDES - AN EXPERIMENTAL PROBE OF METAL-LIGAND BONDING AND CHANGES IN ELECTRONIC-STRUCTURE ON IONIZATION** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Didziulis, S. V., Cohen, S. L., Gewirth, A. A., SOLOMON, E. I.
1988; 110 (1): 250-268
- **Coupled binuclear copper proteins: catalytic mechanisms and structure-reactivity correlations.** *Progress in clinical and biological research*
SOLOMON, E. I.
1988; 274: 309-329

- **ELECTRON-PARAMAGNETIC RESONANCE STUDIES OF THE TUNGSTEN-CONTAINING FORMATE DEHYDROGENASE FROM CLOSTRIDIUM-THERMOACETICUM** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Deaton, J. C., SOLOMON, E. I., Watt, G. D., WETHERBEE, P. J., DURFOR, C. N.
1987; 149 (2): 424-430
- **X-RAY ABSORPTION-EDGE DETERMINATION OF THE OXIDATION-STATE AND COORDINATION-NUMBER OF COPPER - APPLICATION TO THE TYPE-3 SITE IN RHUS-VERNICIFERA LACCASE AND ITS REACTION WITH OXYGEN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
KAU, L. S., SPIRASOLOMON, D. J., PENNERHAHN, J. E., Hodgson, K. O., SOLOMON, E. I.
1987; 109 (21): 6433-6442
- **CHEMICAL AND SPECTROSCOPIC STUDIES OF THE COUPLED BINUCLEAR COPPER SITE IN TYPE-2 DEPLETED RHUS LACCASE - COMPARISON TO THE HEMOCYANINS AND TYROSINASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
SPIRASOLOMON, D. J., SOLOMON, E. I.
1987; 109 (21): 6421-6432
- **VIBRATIONAL, ELECTRONIC, AND RESONANCE RAMAN SPECTRAL STUDIES OF [CU₂(XYL-O)₂]⁺, A COPPER(II) PEROXIDE MODEL COMPLEX OF OXYHEMOCYANIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Pate, J. E., CRUSE, R. W., Karlin, K. D., SOLOMON, E. I.
1987; 109 (9): 2624-2630
- **SPECTROSCOPIC AND THEORETICAL-STUDIES OF THE UNUSUAL ELECTRON-PARAMAGNETIC-RES PARAMETERS OF DISTORTED TETRAHEDRAL CUPRIC SITES - CORRELATIONS TO X-RAY SPECTRAL FEATURES OF CORE LEVELS** *INORGANIC CHEMISTRY*
Gewirth, A. A., Cohen, S. L., Schugar, H. J., SOLOMON, E. I.
1987; 26 (7): 1133-1146
- **ALLOSTERIC INTERACTIONS IN SIPUNCULID AND BRACHIOPOD HEMERYTHRINS** *BIOCHEMISTRY*
Richardson, D. E., Emad, M., REEM, R. C., SOLOMON, E. I.
1987; 26 (4): 1003-1013
- **SPECTROSCOPIC STUDIES OF THE BINUCLEAR FERROUS ACTIVE-SITE OF DEOXYHEMERYTHRIN - COORDINATION-NUMBER AND PROBABLE BRIDGING LIGANDS FOR THE NATIVE AND LIGAND BOUND FORMS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
REEM, R. C., SOLOMON, E. I.
1987; 109 (4): 1216-1226
- **POLARIZED, SINGLE-CRYSTAL, ELECTRONIC SPECTRAL STUDIES OF CU₂CL₆²⁻ - EXCITED-STATE EFFECTS OF THE BINUCLEAR INTERACTION** *INORGANIC CHEMISTRY*
DESJARDINS, S. R., WILCOX, D. E., Musselman, R. L., SOLOMON, E. I.
1987; 26 (2): 288-300
- **XANES EXAFS STUDY OF THE COPPER ACTIVE-SITE IN METHANOL SYNTHESIS CATALYST** *JOURNAL DE PHYSIQUE*
KAU, L. S., SOLOMON, E. I., Hodgson, K. O.
1986; 47 (C-8): 289-292
- **LOW-TEMPERATURE MAGNETIC CIRCULAR-DICHROISM STUDIES OF NATIVE LACCASE - CONFIRMATION OF A TRINUCLEAR COPPER ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
SPIRASOLOMON, D. J., Allendorf, M. D., SOLOMON, E. I.
1986; 108 (17): 5318-5328
- **RESONANCE RAMAN STUDIES OF THE COUPLED BINUCLEAR COPPER ACTIVE-SITE IN MET AZIDE HEMOCYANIN** *SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY*
Pate, J. E., Thamann, T. J., SOLOMON, E. I.
1986; 42 (2-3): 313-318
- **SPECTROSCOPIC STUDIES OF ACTIVE-SITES - BLUE COPPER AND ELECTRONIC STRUCTURAL ANALOGS** *ACS SYMPOSIUM SERIES*
SOLOMON, E. I., Gewirth, A. A., Cohen, S. L.
1986; 307: 236-266
- **ELECTRONIC-STRUCTURE AND BONDING OF THE BLUE COPPER SITE IN PLASTOCYANIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Penfield, K. W., Gewirth, A. A., SOLOMON, E. I.

1985; 107 (15): 4519-4529

- **LOW-TEMPERATURE MAGNETIC CIRCULAR-DICHROISM STUDIES OF NATIVE LACCASE - SPECTROSCOPIC EVIDENCE FOR EXOGENOUS LIGAND BRIDGING AT A TRINUCLEAR COPPER ACTIVE-SITE** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Allendorf, M. D., SPIRA, D. J., SOLOMON, E. I.
1985; 82 (10): 3063-3067
- **SUBSTRATE-ANALOG BINDING TO THE COUPLED BINUCLEAR COPPER ACTIVE-SITE IN TYROSINASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
WILCOX, D. E., Porras, A. G., Hwang, Y. T., Lerch, K., Winkler, M. E., SOLOMON, E. I.
1985; 107 (13): 4015-4027
- **ACTIVATION OF NIT-1 NITRATE REDUCTASE BY W-FORMATE DEHYDROGENASE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Deaton, J. C., SOLOMON, E. I., DURFOR, C. N., WETHERBEE, P. J., Burgess, B. K., Jacobs, D. B.
1984; 121 (3): 1042-1047
- **RESONANT FLUORESCENCE STUDY OF THE EU-3+-SUBSTITUTED CA-2+ SITE IN BUSYCON HEMOCYANIN - STRUCTURAL COUPLING BETWEEN THE HETEROTROPIC ALLOSTERIC EFFECTOR AND THE COUPLED BINUCLEAR COPPER ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hwang, Y. T., Andrews, L. J., SOLOMON, E. I.
1984; 106 (13): 3832-3838
- **EXTENDED X-RAY ABSORPTION FINE-STRUCTURE STUDY OF THE COUPLED BINUCLEAR COPPER ACTIVE-SITE OF TYROSINASE FROM NEUROSPORA-CRASSA** *BIOCHIMICA ET BIOPHYSICA ACTA*
WOOLERY, G. L., Powers, L., WINKLER, M., SOLOMON, E. I., Lerch, K., SPIRO, T. G.
1984; 788 (2): 155-161
- **EXAFS STUDIES OF BINUCLEAR COPPER SITE OF OXYZIDOHEMOCYANIN, DEOXYZIDOHEMOCYANIN, METAQUOZIDOHEMOCYANIN, METFLUOROZIDOHEMOCYANIN, AND METAZIDOHEMOCYANIN FROM ARTHROPODS AND MOLLUSKS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
WOOLERY, G. L., Powers, L., WINKLER, M., SOLOMON, E. I., SPIRO, T. G.
1984; 106 (1): 86-92
- **ELECTRON-PARAMAGNETIC-RES STUDIES OF THE ELECTRON-PARAMAGNETIC-RES NONDETECTABLE MET DERIVATIVE OF HEMOCYANIN - PERTURBATIONS AND DISPLACEMENT OF THE ENDOGENOUS BRIDGE IN THE COUPLED BINUCLEAR COPPER ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
WILCOX, D. E., Long, J. R., SOLOMON, E. I.
1984; 106 (7): 2186-2194
- **ON THE SPECTRAL FEATURES ASSOCIATED WITH PEROXIDE REACTIVITY OF THE COUPLED BINUCLEAR COPPER ACTIVE-SITE IN TYPE-2 DEPLETED AND NATIVE RHUS LACCASE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
PENNERHAHN, J. E., Hedman, B., Hodgson, K. O., SPIRA, D. J., SOLOMON, E. I.
1984; 119 (2): 567-574
- **QUANTITATIVE CU(I) DETERMINATION USING X-RAY ABSORPTION-EDGE SPECTROSCOPY - OXIDATION OF THE REDUCED BINUCLEAR COPPER SITE IN TYPE-2 DEPLETED RHUS LACCASE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Hahn, J. E., Co, M. S., SPIRA, D. J., Hodgson, K. O., SOLOMON, E. I.
1983; 112 (2): 737-745
- **HIGH-RESOLUTION ELECTRON-ENERGY LOSS VIBRATIONAL STUDIES OF CO COORDINATION TO THE (1010) SURFACE OF ZNO** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
DAMICO, K. L., McFeely, F. R., SOLOMON, E. I.
1983; 105 (21): 6380-6383
- **ACTIVE-SITES IN COPPER PROTEINS AN ELECTRONIC-STRUCTURE OVERVIEW** *STRUCTURE AND BONDING*
SOLOMON, E. I., Penfield, K. W., WILCOX, D. E.
1983; 53: 2-57

- **NITRITE REACTIVITY OF THE BINUCLEAR COPPER SITE IN T2D RHUS LACCASE - PREPARATION OF HALF MET-NO₂- T2D LACCASE AND ITS CORRELATION TO HALF MET-NO₂- HEMOCYANIN AND TYROSINASE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
SPIRA, D. J., SOLOMON, E. I.
1983; 112 (2): 729-736
- **DETAILED ABSORPTION, REFLECTANCE, AND UV PHOTOELECTRON SPECTROSCOPIC AND THEORETICAL-STUDIES OF THE CHARGE-TRANSFER TRANSITIONS OF CUCL₄²⁻ - CORRELATION OF THE SQUARE-PLANAR AND THE TETRAHEDRAL LIMITS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
DESJARDINS, S. R., Penfield, K. W., Cohen, S. L., Musselman, R. L., SOLOMON, E. I.
1983; 105 (14): 4590-4603
- **EXAFS INVESTIGATION OF THE BINUCLEAR CUPRIC SITE IN MET T2D RHUS LACCASE AND ITS AZIDE BOUND DERIVATIVE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
SPIRA, D. J., Co, M. S., SOLOMON, E. I., Hodgson, K. O.
1983; 112 (2): 746-753
- **OBSERVATION OF AN ELECTRIC QUADRUPOLE TRANSITION IN THE X-RAY ABSORPTION-SPECTRUM OF A CU(II) COMPLEX** *CHEMICAL PHYSICS LETTERS*
Hahn, J. E., Scott, R. A., Hodgson, K. O., Doniach, S., DESJARDINS, S. R., SOLOMON, E. I.
1982; 88 (6): 595-598
- **The nature of the binuclear copper site in Limulus and other hemocyanins.** *Progress in clinical and biological research*
SOLOMON, E. I., EICKMAN, N. C., HIMMELWRIGHT, R. S., Hwang, Y. T., Plon, S. E., WILCOX, D. E.
1982; 81: 189-230
- **PREPARATION OF A SPECTRAL PROBE DERIVATIVE OF THE HEMOCYANIN BIO-POLYMER - EFFECTS OF ALLOSTERIC INTERACTIONS ON THE COUPLED BINUCLEAR COPPER ACTIVE-SITE** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA-BIOLOGICAL SCIENCES*
Hwang, Y. T., SOLOMON, E. I.
1982; 79 (8): 2564-2568
- **PREPARATION AND CHARACTERIZATION OF A STABLE HALF MET DERIVATIVE OF TYPE-2 DEPLETED RHUS LACCASE - EXOGENOUS LIGAND-BINDING TO THE TYPE-3 SITE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
SPIRA, D. J., Winkler, M. E., SOLOMON, E. I.
1982; 107 (2): 721-726
- **ANGLE-RESOLVED ULTRAVIOLET PHOTO-ELECTRON SPECTROSCOPIC STUDIES OF CO BINDING TO 3 CHEMICALLY DIFFERENT SURFACES OF ZNO - CONFIRMATION OF STEP-BINDING SITES ON (0001BAR)** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
DAMICO, K. L., Trenary, M., Shinn, N. D., SOLOMON, E. I., McFeely, F. R.
1982; 104 (19): 5102-5105
- **ANION BINDING TO OXIDIZED TYPE-2 DEPLETED AND NATIVE LACCASE - A SPECTROSCOPICALLY EFFECTIVE MODEL FOR EXOGENOUS LIGAND-BINDING TO THE TYPE-3 TYPE-2 ACTIVE-SITE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Winkler, M. E., SPIRA, D. J., LUBIEN, C. D., Thamann, T. J., SOLOMON, E. I.
1982; 107 (2): 727-734
- **SPECTROSCOPIC STUDIES ON PLASTOCYANIN SINGLE-CRYSTALS - A DETAILED ELECTRONIC-STRUCTURE DETERMINATION OF THE BLUE COPPER ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Penfield, K. W., Gay, R. R., HIMMELWRIGHT, R. S., EICKMAN, N. C., Norris, V. A., Freeman, H. C., SOLOMON, E. I.
1981; 103 (15): 4382-4388
- **AN ANGLE RESOLVED PHOTOEMISSION DETERMINATION OF THE COORDINATION OF CO ON THE ZNO(0001) SURFACE** *JOURNAL OF CHEMICAL PHYSICS*
MCCLELLAN, M. R., Trenary, M., Shinn, N. D., SAYERS, M. J., DAMICO, K. L., SOLOMON, E. I., McFeely, F. R.
1981; 74 (8): 4726-4731
- **SPECTROSCOPIC STUDIES OF STELLACYANIN, PLASTOCYANIN, AND AZURIN - ELECTRONIC-STRUCTURE OF THE BLUE COPPER SITES** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
SOLOMON, E. I., Hare, J. W., Dooley, D. M., Dawson, J. H., Stephens, P. J., Gray, H. B.
1980; 102 (1): 168-178

- **ULTRAVIOLET PHOTOEMISSION-STUDIES OF THE BONDING OF CO TO THE ZNO(1010) SURFACE AND ITS INTERACTION WITH ATOMIC-HYDROGEN** *JOURNAL OF VACUUM SCIENCE & TECHNOLOGY*
DAMICO, K. L., MCCLELLAN, M. R., SAYERS, M. J., Gay, R. R., McFeely, F. R., SOLOMON, E. I.
1980; 17 (5): 1080-1084
- **CHEMICAL AND SPECTROSCOPIC COMPARISON OF THE BINUCLEAR COPPER ACTIVE-SITE OF MOLLUSK AND ARTHROPOD HEMOCYANINS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
HIMMELWRIGHT, R. S., EICKMAN, N. C., LUBIEN, C. D., SOLOMON, E. I.
1980; 102 (16): 5378-5388
- **ANGLE-RESOLVED PHOTOEMISSION INVESTIGATION OF THE BONDING GEOMETRY OF CO TO ZNO (1010)** *CHEMICAL PHYSICS LETTERS*
SAYERS, M. J., MCCLELLAN, M. R., Gay, R. R., SOLOMON, E. I., McFeely, F. R.
1980; 75 (3): 575-578
- **PHOTOELECTRON STUDY OF THE INTERACTION OF CO WITH ZNO** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Gay, R. R., Nodine, M. H., Henrich, V. E., Zeiger, H. J., SOLOMON, E. I.
1980; 102 (22): 6752-6761
- **CHEMICAL AND SPECTROSCOPIC STUDIES OF THE BINUCLEAR COPPER ACTIVE-SITE OF NEUROSPORA TYROSINASE - COMPARISON TO HEMOCYANINS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
HIMMELWRIGHT, R. S., EICKMAN, N. C., LUBIEN, C. D., Lerch, K., SOLOMON, E. I.
1980; 102 (24): 7339-7344
- **SPECTROSCOPIC AND THEORETICAL-ANALYSIS OF THE INTENSE T-1(1U) J-A-1(1G) TRANSITIONS IN MO(CO)6 AND W(CO)6** *INORGANIC CHEMISTRY*
TROGLER, W. C., DESJARDINS, S. R., SOLOMON, E. I.
1979; 18 (8): 2131-2136
- **COMPARISON OF HALF-MET AND MET APO HEMOCYANIN - LIGAND BRIDGING AT THE BINUCLEAR COPPER ACTIVE-SITE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1979; 101 (6): 1576-1586
- **LIGAND DISPLACEMENT-REACTIONS OF OXYHEMOCYANIN - COMPARISON OF REACTIVITIES OF ARTHROPODS AND MOLLUSKS** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
Hepp, A. F., HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1979; 89 (4): 1050-1057
- **GEOMETRIC AND ELECTRONIC-STRUCTURE OF OXYHEMOCYANIN - SPECTRAL AND CHEMICAL CORRELATIONS TO MET APO, HALF MET, MET, AND DIMER ACTIVE-SITES** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
EICKMAN, N. C., HIMMELWRIGHT, R. S., SOLOMON, E. I.
1979; 76 (5): 2094-2098
- **REACTIONS AND INTERCONVERSION OF MET AND DIMER HEMOCYANIN** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1979; 86 (3): 628-634
- **MAGNETIC-SUSCEPTIBILITY STUDIES OF LACCASE AND OXYHEMOCYANIN** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Dooley, D. M., Scott, R. A., ELLINGHAUS, J., SOLOMON, E. I., Gray, H. B.
1978; 75 (7): 3019-3022
- **PREPARATION AND CHARACTERIZATION OF MET APO HEMOCYANIN - SINGLE COPPER(II) ACTIVE-SITE** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1978; 81 (1): 243-247
- **SPECTROSCOPIC STUDIES OF LIGAND PERTURBATION EFFECTS ON HALF OXIDIZED ACTIVE-SITE OF BUSYCON-CANALICULATUM HEMOCYANIN** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*

- HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1978; 81 (1): 237-242
- **CHEMICAL AND SPECTROSCOPIC CONFORMATION OF AN EXOGENOUS LIGAND BRIDGE IN HALF MET HEMOCYANIN** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
HIMMELWRIGHT, R. S., EICKMAN, N. C., SOLOMON, E. I.
1978; 84 (2): 300-305
 - **PRODUCTION OF HYDROGEN BY UV IRRADIATION OF MO₂(SO₄)₄·4H₂O IN AQUEOUS SULFURIC-ACID - ELECTRONIC ABSORPTION-SPECTRUM OF K₃MO₂(SO₄)₄·3.5H₂O AT 15 K** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
ERWIN, D. K., GEOFFROY, G. L., Gray, H. B., HAMMOND, G. S., SOLOMON, E. I., TROGLER, W. C., ZAGARS, A. A.
1977; 99 (11): 3620-3621
 - **STUDIES OF POLARIZATION BEHAVIOR, TEMPERATURE-DEPENDENCE, AND VIBRONIC STRUCTURE OF 23000-CM⁻¹ ABSORPTION SYSTEM IN ELECTRONIC-SPECTRA OF MO₂(O₂CCH₃)₄ AND RELATED COMPOUNDS - EMISSION-SPECTRUM OF MO₂(O₂CCF₃)₄ AT 1.3K** *INORGANIC CHEMISTRY*
TROGLER, W. C., SOLOMON, E. I., TRAJBERG, I. B., BALLHAUSEN, C. J., Gray, H. B.
1977; 16 (4): 828-836
 - **EMISSION-SPECTRA AND LIFETIMES OF RE₂CL₈·2H₂O, RE₂BR₈·2H₂O, AND MO₂CL₈·4H₂O AT 1.3K UPON EXCITATION OF DELTA-]DELTA] TRANSITION** *INORGANIC CHEMISTRY*
TROGLER, W. C., SOLOMON, E. I., Gray, H. B.
1977; 16 (12): 3031-3033
 - **SUSCEPTIBILITY STUDIES OF LACCASE AND OXYHEMOCYANIN USING AN ULTRASENSITIVE MAGNETOMETER - ANTIFERROMAGNETIC BEHAVIOR OF TYPE-3 COPPER IN RHUS LACCASE** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
SOLOMON, E. I., Dooley, D. M., Wang, R. H., Gray, H. B., Cerdonio, M., MOGNO, F., Romani, G. L.
1976; 98 (4): 1029-1031
 - **SPECTROSCOPIC STUDIES AND A STRUCTURAL MODEL FOR BLUE COPPER CENTERS IN PROTEINS** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
SOLOMON, E. I., Hare, J. W., Gray, H. B.
1976; 73 (5): 1389-1393
 - **TEMPERATURE-DEPENDENCE OF MAGNETIC-SUSCEPTIBILITY OF COBALT(II) STELLACYANIN** *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*
SOLOMON, E. I., Wang, R. H., McMillin, D. R., Gray, H. B.
1976; 69 (4): 1039-1042
 - **INFRARED SPECTRAL STUDIES OF METAL-BINDING EFFECTS ON SECONDARY STRUCTURE OF BEAN PLASTOCYANIN** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Hare, J. W., SOLOMON, E. I., Gray, H. B.
1976; 98 (11): 3205-3209
 - **INFRARED AND VISIBLE CIRCULAR-DICHROISM AND MAGNETIC CIRCULAR-DICHROISM STUDIES ON COBALT(II)-SUBSTITUTED BLUE COPPER PROTEINS** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
SOLOMON, E. I., Rawlings, J., McMillin, D. R., Stephens, P. J., Gray, H. B.
1976; 98 (25): 8046-8048
 - **SIMULTANEOUS PAIR ELECTRONIC-TRANSITIONS IN YB₂O₃** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
Schugar, H. J., SOLOMON, E. I., CLEVELAND, W. L., Goodman, L.
1975; 97 (22): 6442-6450
 - **IDENTIFICATION OF STRUCTURE OF T-31G(I)-A-32G BAND IN NI(H₂O)₆⁺⁺ COMPLEX** *MOLECULAR PHYSICS*
SOLOMON, E. I., BALLHAUSEN, C. J.
1975; 29 (1): 279-299

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- ACS Voices of Inorganic Chemistry: Edward I. Solomon (2011)