

317. Henson, M.J.; Solomon, E. I., review of *Crystal Structure of a Plant Catechol Oxidase Containing a Dicopper Center*, by Klabunde, T.; Eicken, C. J.; Sacchettini, J. C.; Krebs, B. *Chemtracts* **2000**, *13* (Basolo Issue), 97.
318. Henson, M.J.; Mukherjee, P.; Root, D. E.; Stack, T. D. P.; Solomon, E. I. Spectroscopic and Electronic Structural Studies of the Cu(III)₂ Bis-μ-oxo Core and Its Relation to the Side on Peroxo-Bridged Dimer. *J. Am. Chem. Soc.* **1999**, *121*, 10332.
319. DuBois, J. L.; Mukherjee, P.; Stack, T. D. P.; Hedman, B.; Solomon, E. I.; Hodgson, K. O. A Systematic K-edge X-ray Absorption Spectroscopic Study of Cu(III) Sites. *J. Am. Chem. Soc.* **2000**, *122*, 5775.
320. Solomon, E. I.; Brunold, T.; Davis, M. I.; Kemsley, J. N.; Lee S-K.; Lehnert, N.; Nesse, F.; Skulan, A. J.; Shan, Y-S.; Zhou, J. Geometric and Electronic Structure/Function Correlations in Non-Heme Iron Enzymes. *Chem. Rev.* **2000**, *100*, 235.
321. Solomon, E. I.; Randall, D. W.; Glaser, T. Electronic Structures of Active Sites in Electron Transfer Metalloproteins: Contributions to Reactivity. *Coord. Chem. Rev.* **2000**, *200*, 595.
322. Yang, Y.; Baldwin, J.; Ley, B. A.; Bollinger, J. M.; Solomon, E. I. Spectroscopic and Electronic Structure Description of the Reduced Binuclear Non-Heme Iron Active Site in Ribonucleotide Reductase From *E. coli*: Comparison to Reduced Δ⁹ Desaturase and Electronic Structure Contributions to Differences in O₂ Reactivity. *J. Am. Chem. Soc.* **2000**, *122*, 8495.
323. Brunold, T. C.; Gamelin, D.R.; Solomon, E. I. Excited-State Exchange Coupling in Bent Mn(III)O-Mn(III) Complexes: Dominance of the π/σ Superexchange Pathway and Its Possible Contributions to the Reactivities of Binuclear Metalloproteins. *J. Am. Chem. Soc.* **2000**, *122*, 8511.
324. Glaser, T.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Ligand K-edge X-ray Absorption Spectroscopy: A Direct Probe of Ligand-Metal Covalency. *Accounts of Chem. Res.* **2000**, *33*, 859.
325. DeBeer, S.; Randall, D. W.; Nersissian, A. M.; Valentine, J. S.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. X-ray Absorption Edge and EXAFS Studies of the Blue Copper Site in Stellacyanin: Effects of Axial Amide Coordination. *J. Phys. Chem. B* **2000**, *104*, 10814.
326. Randall, D. W.; DeBeer, S.; Hedman, B.; Hodgson, K. O.; Fujisawa, K.; Solomon, E. I. Spectroscopic and Electronic Structural Studies of Blue Copper Model Complexes. 1: Perturbation of the Thiolate – Cu Bond. *J. Am. Chem. Soc.* **2000**, *122*, 11620.
327. Randall, D. W.; DeBeer, S.; Holland, P. L.; Hodgson, K. O.; Tolman, W. B.; Solomon, E. I. Spectroscopic and Electronic Structural Studies of Blue Copper Model Complexes. 2: Comparison of 3- and 4- Coordinate Cu(II) Thiolate Complexes and Fungal Laccase. *J. Am. Chem. Soc.* **2000**, *122*, 11632.

328. Chen, P.; Fujisawa, K.; Solomon, E. I. Spectroscopic and Theoretical Studies of Mononuclear Copper(II) Alkyl- and Hydroperoxo Complexes: Electronic Structure contributions to Reactivity. *J. Am. Chem. Soc.* **2000**, *122*, 10177.
329. Neese, F.; Zaleski, J. M.; Loeb-Zaleski, K.; Solomon, E. I. Electronic Structure of Activated Bleomycin: Oxygen Intermediates in Heme Versus Non-Heme Iron. *J. Am. Chem. Soc.* **2000**, *122*, 11703.
330. McMaster, J.; Carducci, M. D.; Yang, Y-S.; Solomon, E. I. Enemark, J. H. Electronic Spectral Studies of Molybdenyl Complexes: 2. MCD Spectroscopy of [MoOS₄] Centers. *Inorg. Chem.* **2001**, *40*, 687.
331. Glaser, T.; Rose, K.; Shadle, S. E.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. S K- edge Xray Absorption Studies of Tetranuclear Iron-Sulfur Clusters: μ -Sulfide Bonding and Its Contribution to Electron Delocalization. *J. Am. Chem. Soc.* **2001**, *123*, 442.
332. Machonkin, T. E.; Solomon, E. I. The Thermodynamics, Kinetics, and Molecular Mechanism of Intramolecular Electron Transfer in Human Ceruloplasmin. *J. Am. Chem. Soc.* **2000**, *122*, 12547.
333. Hirsch, J.; DeBeer, S.; Solomon, E. I.; Hedman, B.; Hodgson K. O.; Burstyn, J. N. Raman and EXAFS Characterization of Sulfur-Ligand Cu(I) Ethylene Complex: A Model for the *Arabidopsis* Ethylene Receptor. *Inorg. Chem.* **2001**, *40*, 2439.
334. Wasinger, E. C.; Zaleski, K. L.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. X-ray Absorption Spectroscopic Investigation of Fe(II)-Peplomycin and Peplomycin Derivatives: The Effect of Axial Ligation on Fe-Pyrimidine Back-bonding. *J. Biol. Inorg. Chem.* **2002**, *7*, 157.
335. Mahadevan, V.; Henson, M.J.; Solomon, E. I.; Stack, T. D. P. Differential Reactivity Between Interconvertible Side-on Peroxo and Bis μ -oxo dicopper Isomers Using Peralkylated Diamine Ligands. *J. Am. Chem. Soc.* **2000**, *122*, 10249.
336. Lehnert, N.; DeBeer George, S.; Solomon, E. I. Recent Advances in Bioinorganic Spectroscopy. *Curr. Opin. Chem. Biol.* **2001**, *5*, 176.
337. Machonkin, T. E.; Quintanar, L.; Palmer, A. E.; Hassett, R.; Severance, S.; D. J. Kosman, Solomon, E. I. Spectroscopy and Reactivity of the Type 1 Copper Site in Fet3p from *Saccharomyces cerevisiae*: Correlation of Structure with Reactivity in the Multicopper Oxidases. *J. Am. Chem. Soc.* **2001**, *123*, 5507.
338. DeBeer George, S.; Metz, M.; Szilagyi, R. K.; Wang, H.; Cramer, S. P.; Y. Lu, Tolman, W. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2001**, *123*, 5757.

339. Glaser, T.; Bertini, I.; Moura, J.G.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Protein Effects on the Electronic Structure of the $[\text{Fe}_4\text{S}_4]^{2+}$ Cluster in Ferredoxin and HiPIP. *J. Am. Chem. Soc.* **2001**, *123*, 4859.
340. Zhou, J.; Kelly, W. L.; Bachmann, B. O.; Gunsior, M.; Townsend, C. A.; Solomon, E. I. Spectroscopic Studies of Substrate Interactions with Clavaminate Synthase 2, a Multifunctional α -KG-Dependent Non-Heme Iron Enzyme: Correlation with Mechanisms and Reactivities. *J. Am. Chem. Soc.* **2001**, *123*, 7388.
341. Metz, M.; Solomon, E. I. Dioxygen Binding to Deoxyhemocyanin: Electronic Structure and Mechanism of the Spin Forbidden Two-Electron Reduction of O_2 . *J. Am. Chem. Soc.* **2001**, *123*, 4938.
342. Tuzek, F.; Solomon, E. I. Excited Electronic States of Transition-Metal Dimers and the VBCI Model: An Overview. *Coord. Chem. Rev.* **2001**, (A.B.P Lever Special Issue) *219*, 1075.
343. Lehnert, N.; Ho, R. Y. N.; Que, L., Jr.; Solomon, E. I. Spectroscopic Properties and Electronic Structure of Low-spin Fe(III)-Alkylperoxo Complexes: Homolytic Cleavage of the O-O Bond. *J. Am. Chem. Soc.* **2001**, *123*, 8271.
344. Palmer, A.; Kyu Lee, S.; Solomon, E. I. Decay of the Peroxide Intermediate in Laccase: Reductive Cleavage of the O-O Bond. *J. Am. Chem. Soc.* **2001**, *123*, 6591.
345. Anxolabéhère-Mallart, E.; Glaser, T.; Frank, P.; Aliverti, A.; Zanetti, G.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Sulfur K-edge X-ray Absorption Spectroscopy of 2Fe- 2S Ferredoxin: Covalency of the Oxidized and Reduced 2Fe Forms and Comparison to Model Complexes. *J. Am. Chem. Soc.* **2001**, *123*, 5444.
346. Solomon, E. I. Geometric and Electronic Structure Contributions to Function in Bioinorganic Chemistry: Active Sites in Non-Heme Iron Enzymes. *Inorg. Chem.* **2001**, *40*, 3656.
347. Solomon, E. I.; Chen, P.; Metz, M.; Lee, S.; Palmer, A. E. Oxygen Binding, Activation and Reduction to Water by Copper Proteins. *Angew. Chem., Int. Ed* **2001**, *40*, 4570.
348. Chen, P.; Solomon, E. I. Frontier Molecular Orbital Analysis of Cu_n/O_2 Reactivity. (30th Anniversary Issue) *J. Inorg. Biochem.* **2002**, *88*, 368.
349. Henson, M.J.; Mahadevan, V.; Stack, T. D. P.; Solomon, E. I. A New Cu(II) Side On Peroxo Model Clarifies the Assignment of the Oxyhemocyanin Raman Spectrum. *Inorg. Chem.* **2001**, *40*, 5068.
350. Lehnert, N.; Ho, R. Y. N.; Que, L., Jr.; Solomon, E. I. Electronic Structure of High-Spin Iron(III)Alkylperoxo Complexes and Its Relation to Low-spin Analogues: Reaction Coordinate of O-O Bond Homolysis. *J. Am. Chem. Soc.* **2001**, *123*, 12802.

351. Lee, S.; DeBeer George, S.; Antholine, W. E.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Nature of the Intermediate Formed in the Reduction of O₂ to H₂O at the Trinuclear Copper Cluster Active Site in Native Laccase. *J. Am. Chem. Soc.* **2002**, *124*, 6180.
352. Solomon, E. I. Lever 65 – A Celebration of Contributions and Service to Inorganic Chemistry. (A.B.P. Lever Special Issue) *Coord. Chem. Rev.* **2001**, *219*, 1.
353. Liang, H.; Zhang, C. X.; Henson, M. J.; Sommer, R.; Hatwell, K. R.; Kaderli, S.; Zuberbühler, A.; Rheingold, A. L.; Solomon, E. I.; Karlin, K. D. Contrasting Copper- Dioxygen Chemistry Arising from Alike Tridentate Alkyltriamine Copper(I) Complexes. *J. Am. Chem. Soc.* **2002**, *124*, 4170.
354. Davis, M. I.; Orville, A.M.; Neese, F.; Zaleski, J. M.; Lipscomb, J. D.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of Protocatechuate 3,4-Dioxygenase: Nature of Tyrosinate-Fe(III) Bonds and Their Contribution to Reactivity. *J. Am. Chem. Soc.* **2002**, *124*, 602.
355. Chen, P.; DeBeer George, S.; Cabrito, I.; Antholine, W. E.; Moura, J.G.; Moura, I.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Electronic Structure Description of the μ_4 - Sulfide Bridged Tetranuclear Cu₄ Center in N₂O Reductase. *J. Am. Chem. Soc.* **2002**, *124*, 744.
356. Zhou, J.; Rocklin, A. M.; Lipscomb, J. D.; Que, L., Jr.; Solomon, E. I. Spectroscopic Studies of 1-Aminocyclopropane-1-Carboxylic Acid Oxidase: Molecular Mechanism and CO₂ Activation in the Biosynthesis of Ethylene. *J. Am. Chem. Soc.* **2002**, *124*, 4602.
357. Palmer, A. E.; Quintanar, L.; Severance, S.; Wang, T.-P.; Kosman, D.J.; Solomon, E. I. Spectroscopic Characterization and O₂ Reactivity of the Trinuclear Cu Cluster of Mutants of the Multicopper Oxidase Fet3p. *Biochemistry* **2002**, *41*, 6438.
358. Szilagyi, R. K.; Metz, M.; Solomon, E. I. Spectroscopic Calibration of Modern Density Functional Methods Using [CuCl₄]²⁻. *J. Phys. Chem. A.* **2002**, *106*, 2994
359. Solomon, E. I. Bioinorganic spectroscopy. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 14.
360. Enemark, J. H.; McMaster, J.; Yang, Y.; Solomon, E. I. DFT and spectroscopic studies of molybdenum thiolate centers. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 44.
361. Chen, P.; Cabrito, I.; Antholine, W. E.; Moura, I.; Moura, J. G.; Solomon, E. I. Spectroscopic studies of the Cu₂Z center of nitrous oxide reductase. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 177.
362. Lehnert, N.; Ho, R. Y. N.; Que, L., Jr.; Fujisawa, K.; Solomon, E. I. Activation of peroxide by high-spin and low-spin Fe(III) centers. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 313.
363. Palmer, A. E.; Quintanar, L.; Severance, S.; Wang, T.-P.; Kosman, D.; Solomon, E. I. The Activation of OB_{2B} by the Trinuclear Cu Cluster in Multicopper Oxidases. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 370.

364. Quintanar, L.; Palmer, A. E.; Machonkin, T.; Severance, S.; Wang, T.-P.; Kosman D. J.; Solomon, E. I. Spectroscopic characterization of the copper sites of Fet3p, a new member of the multicopper oxidases family. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 389.
365. Skulan, A. J.; Hanson, M. A.; Hsu, H.; Zheng, H.; Que, L., Jr.; Solomon, E. I. Electronic structure of high-valent oxo-bridged binuclear nonheme iron complexes and its contribution to reactivity. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 433.
366. Stack, D.P.; Mahadevan, V.; Henson, M. J.; DuBois, J.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Thermodynamic and reactivity studies of interconvertible μ - η^2 : η^2 peroxo and bis μ -oxo dicopper species. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 442.
367. Strand, K. R.; Yang, Y.; Andersson, K. K.; Solomon, E. I. Circular dichroism and magnetic circular dichroism studies of the diferrous form of the R2 subunit of ribonucleotide reductase from mouse. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 445.
368. Kemsley, J. N.; Zaleski, K. L.; Mitić, N.; Datta, S.; Acharya, T.; Caradonna, J. P.; Solomon, E. I. Interaction of non-heme ferrous active sites with substrates: structure/function correlations for phenylalanine hydroxylase and bleomycin. *J. Inorg. Biochem.* **2001**, *86* (ICBIC 10 Issue), 291.
369. Lehnert, N.; Ho, R. Y. N.; Neese, F.; Que, L., Jr.; Solomon, E. I. Electronic Structure and Reactivity of Low-spin Fe(III)-Hydroperoxo Complexes: Comparison to Activated Bleomycin. *J. Am. Chem. Soc.* **2002**, *124*, 10810.
370. Neese, F.; Solomon, E. I. Interpretation and Calculation of Spin-Hamiltonian Parameters in Transition Metal Complexes. In *Magnetism: Molecules to Materials IV*; Miller, J.S.; Drillon, M.; Eds.; WILEY-VCH Verlag GmbH & Co. KGaA: Weinheim, **2002**, *9*, 345.
371. Szilagyi, R. K.; Solomon, E. I. Electronic Structure and its Relation to Function in Copper Proteins. *Current Opinions in Biology* **2002**, *6*, 250.
372. Wasinger, E.; Mitić, N.; Hedman, B.; Caradonna, J.; Solomon, E. I.; Hodgson, K. X-ray Absorption Spectroscopic Investigation of the Resting Ferrous and Cosubstrate-Bound Active Sites of Phenylalanine Hydroxylase. *Biochemistry* **2002**, *41*, 6211.
373. Machonkin, T.; Mukherjee, P.; Henson, M. J.; Stack, T. D. P.; Solomon, E. I. The EPR Spectrum of a Cu(II/II/III) Cluster: Anisotropic Exchange in a Bent Cu(II)₂O₂ Core. *Inorg. Chim. Acta* (Special Raymond Issue), **2002**, *341*, 39.
374. Andersson, K. K.; Schmidt, P. P.; Strand, K. R.; Katterle, B.; Palmer, A. E.; Lee, S.; Solomon, E. I.; Gräslund, A.; Barra, A. Examples of High Frequency EPR Studies in Bioinorganic Chemistry. *J. Biol. Inorg. Chem.* **2003**, *8*, 235.

375. Basumallick, L.; DeBeer George, S.; Randall, D. W.; Hedman, B.; Hodgson, K. O.; Fujisawa, K.; Solomon, E. I. Spectroscopic comparison of the five-coordinate [Cu(SmeIm)(HB(3,5-*i*Pr₂pz)₃)] with the four-coordinate [Cu(SCPh₃)(HB(3,5-*i*Pr₂pz)₃)] effect of coordination number increase on a blue copper type site. *Inorg. Chim. Acta* (Special Weighardt Issue) **2002**, 337, 357.
376. Tuczek, F.; Solomon, E. I. The Valence Bond Configuration Interaction Model. In *Comp. Coord. Chem. II, Ed.* **2003**, Vol. 1, 541-557.
377. Lehnert, N.; Solomon, E. I. Density-functional investigation on the mechanism of H-atom abstraction by lipoxygenase. *J. Biol. Inorg. Chem.* **2003**, 8, 294.
378. Chen, P.; Cabrito, I.; Moura, I.; Moura, J. G.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of the μ_4 -Sulfide Bridged Tetranuclear Cu₄ Cluster in N₂O Reductase: Molecular Insight into the Catalytic Mechanism. *J. Am. Chem. Soc.* **2002**, 124, 10497.
379. Kennepohl, P.; Solomon, E. I. Spectroscopy and Electronic Structure of [FeX₄]ⁿ⁻ (X = Cl, SR) Complexes: Contributions to Electron Transfer in Bioinorganic Chemistry. *Comp. Coord. Chem. II* **2004**, Vol. 2, 691.
380. Kennepohl, P.; Solomon, E. I. Electronic Structure Contributions to Electron-Transfer Reactivity in Iron-Sulfur Active Sites: 1. Photoelectron Spectroscopic Determination of Electronic Relaxation. *Inorg. Chem.* **2003**, 42, 679.
381. Kennepohl, P.; Solomon, E. I. Electronic Structure Contributions to Electron-Transfer Reactivity in Iron-Sulfur Active Sites: 2. Reduction Potentials. *Inorg. Chem.* **2003**, 42, 689.
382. Kennepohl, P.; Solomon, E. I. Electronic Structure Contributions to Electron-Transfer Reactivity in Iron-Sulfur Active Sites: 3. Kinetics of Electronic Transfer. *Inorg. Chem.* **2003**, 42, 696.
383. Skulan, A. J.; Hanson, M. A.; Hua-fen Hsu, Yanhong Dong, Que, L., Jr.; Solomon, E. I. Spectroscopic Study of [Fe₂O₂(5-Et₃-TPA)₂]³⁺: Nature of the Fe₂O₂ Diamond Core and Its Possible Relevance to High-Valent Binuclear Non-Heme Enzyme Intermediates. *J. Am. Chem. Soc.* **2003**, 125, 7344.
384. Collman, J. P.; Katja E. Berg, Christopher J. Sunderland, Ally Aukauloo, Vance, M. A.; Solomon, E. I. Distal Metal Effects in Cobalt Porphyrins Related to CcO. *Inorg. Chem.* **2002**, 4, 6583.
385. Mirica, L. M.; Vance, M.; Jackson Rudd, D. A.; Hedman, B.; Hodgson, K. O.; Solomon, E. I.; Stack, T. D. P. A Stabilized μ - η^2 : η^2 Peroxodicopper(II) Complex with a Secondary Diamine Ligand and Its Tyrosinase-like Reactivity. *J. Am. Chem. Soc.* **2002**, 124, 9332.
386. Lehnert, N.; Fujisawa K.; Solomon, E. I. Electronic Structure and Reactivity of High- Spin IronAlkyl- and -Pterinperoxo Complexes. *Inorg. Chem.* **2003**, 42, 469.

387. Chen, P.; Root, D. E.; Campochiaro, C.; Fujisawa, K.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of the Diamagnetic Side-On Cu^{II}-Superoxo Complex Cu(O₂)[HB(3R-5- 'Prpz)₃]: Antiferromagnetic Coupling vs. Covalent Delocalization. *J. Am. Chem. Soc.* **2003**, *125*, 466.
388. Helton, M. E.; Chen, P.; Paul, P. P.; Tyeklár, Z.; Sommer, R.; Zhakarov, L.; Rheingold, A. L.; Solomon, E. I.; Karlin, K. D. Reaction of Elemental Sulfur with a Copper(I) Complex Forming a *trans*- μ -1,2 End-On Disulfide Complex: New Directions in Copper- Sulfur Chemistry. *J. Am. Chem. Soc.* **2003**, *125*, 1160.
389. Solomon, E. I.; Davis, M. I.; Neese, F.; Pau, M.Y. M. Variable-Temperature Variable- Field Magnetic Circular Dichroism (VTVH MCD) Combined with Electron Paramagnetic Resonance (EPR); Polarization of Electronic Transitions in Solution. In *Paramagnetic Resonance of Metallobiomolecules* in ACS Symposium series **2003**, 328.
390. Wasinger, E. C.; Davis, M.; Pau, M.; Orville, A. M.; Zaleski, J. M.; Hedman, B.; Lipscomb, J. D.; Hodgson, K. O.; Solomon, E. I. Spectroscopic Studies of the Effect of Ligand Donor Strength on the Fe-NO Bond in Intradiol Dioxygenases. *Inorg. Chem.* **2003**, *42*, 365.
391. Neidig, M. L.; Solomon, E. I., review of *Three-Dimensional Structure of a Purple Lipxygenase*. *Chemtracts-Inorg. Chem.* **2002**, Vol. 15, 417.
392. Henson, M. J.; Vance, M. A.; Zhang, C. X.; Liang, H. C.; Karlin, K. D.; Solomon, E. I. Resonance Raman Investigation of Equatorial Ligand Donor Effects on the Cu₂O₂²⁺ Core in End-on and Side-on μ -Peroxo-Dicopper(II) and Bis- μ -oxo-Dicopper(III) Complexes. *J. Am. Chem. Soc.* **2003**, *125*, 5186.
393. Skulan, A. J.; Hanson, M. A.; Hsu, H.; Dong, Y.; Que, L., Jr.; Solomon, E. I. EPR Spectroscopy of [Fe₂O₂(5-Et₃-TPA)₂]³⁺: Electronic Origin of the Unique Spin- Hamiltonian Parameters of the Fe₂^{III,IV}O₂ Diamond Core. *Inorg. Chem.* **2003**, *42*, 6489.
394. Davis, M. I.; Wasinger, E. C.; Decker, A.; Pau, M. Y. M.; Vaillancourt, F. H.; Bolin, J. T.; Eltis, L. D.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of 2,3-Dihydroxybiphenyl 1,2-Dioxygenase: O₂ Reactivity of the Non-Heme Ferrous Site in Extradial Dioxygenases. *J. Am. Chem. Soc.* **2003**, *125*, 11214.
395. Szilagyi, R. K.; Lim, B.S.; Glaser, T.; Holm, R. H.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Description of the Ground State Wave Function of Ni Dithiolenes using Sulfur K-edge X-ray Absorption Spectroscopy. *J. Am. Chem. Soc.* **2003**, *125*, 9158.
396. Palmer, A. E.; Szilagyi, R. K.; Cherry, J. R.; Jones, A.; Xu, F.; Solomon, E. I. 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. *Inorg. Chem.* **2003**, *42*, 4006.
397. Jackson, W. E.; Farges, F.; Yeager, M.; Mabrouk, P. A.; Rossano, S.; Waychunas, G. A.; Solomon, E. I. Brown, G. E., Jr. Multi-spectroscopic study of Fe(II) in silicate glasses:

Implications for the coordination environment of Fe(II) in silicate melts. *Geochimica et Cosmochimica Acta* **2005**, *69*, 4315.

398. Solomon, E. I. Structure/function correlations over non-heme iron enzymes. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 62.
399. Mitić, N.; Saleh, L.; Bollinger, J. M., Jr.; Solomon, E. I. First MCD characterization of intermediate X in ribonucleotide reductase: Insight into the geometric and electronic structure description of X. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 191.
400. Skulan, A. J.; Brunold, T.; Hanson, M. A.; Que, L., Jr.; Solomon, E. I. Electronic structure of the oxygen activating intermediates of ribonucleotide reductase: the peroxo intermediate and a model complex of the high-valent intermediate, X. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 231.
401. Wei, P.; Skulan, A. J.; Mitić, N.; Yang, Y.; Saleh, L.; Bollinger, J. M., Jr.; Solomon, E. I. Circular dichroism and magnetic circular dichroism studies of the reduced binuclear non-heme iron sites of D84E and D84E/W48F ribonucleotide reductase mutants. Comparison to reduced methane monooxygenase and contributions to O₂ reactivity. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 250.
402. Decker, A.; Lehnert, N.; Chow M. S.; Solomon E. I. Interactions of mononuclear non-heme iron sites with dioxygen: Studies on electronic structure and reactivity. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 124.
403. Schenk, G.; Neidig, M. L.; Zhou J.; Holman, T. R.; Solomon E. I. A. *J. Inorg. Biochem.* **2003**, *96* (ICBIC 11 Issue) 225.
404. Kemsley, J. N.; Wasinger, E. C.; Datta, S.; Mitić, N.; Acharya, T.; Hedman, B.; Caradonna, J. P.; Hodgson, K. O.; Solomon, E. I. Spectroscopic and Kinetic Studies of PKU-Inducing Mutants of Phenylalanine Hydroxylase: Arg158Gln and Glu280Lys. *J. Am. Chem. Soc.* **2003**, *125*, 5677.
405. Solomon, E. I.; Decker, A.; Lehnert, N. Perspective: Non-Heme Iron Enzymes: Contrasts to Heme Catalysis. (Thematic Issue on Bioinorganic Chemistry) *Proc. Natl. Acad. Sci. U.S.A.* **2003**, *100*, 3589.
406. Solomon, E. I.; Neidig, M. L.; Schenk, G.; Magnetic Circular Dichroism of Paramagnetic Species. *Comp. Coord. Chem. II Vol 2* **2003**, 339.
407. Solomon, E. I. Basumallick, L.; Dey, A.; Sarangi, R. Electron Transfer Sites in Bioinorganic Chemistry. (Special Issue on Bioinorganic Chemistry) *Proc. of Indian Natl. Sci. Acad.* **2004**, *70*, 267.
408. Wang, T.-P.; Quintanar, L.; Severance, S.; Solomon, E. I.; Kosman D. J. Targeted Suppression of the Ferroxidase and Iron Trafficking Activities of the Multicopper Oxidase, Fet3p, from *Saccharomyces cerevisiae*. *J. Biol. Inorg. Chem.* **2003**, *8*, 611.

409. Chen, P.; Fujisawa, K.; Helton, M. E.; Karlin, K. D. Solomon, E. I. Spectroscopy and Bonding in Side-On and End-On $\text{Cu}_2(\text{S}_2)$ Cores: Comparison to Peroxide Analogues. *J. Am. Chem. Soc.* **2003**, *125*, 6394.
410. Schenk, G.; Neidig, M. L.; Zhou, J.; Holman, T. R.; Solomon, E. I. Spectroscopic Characterization of Soybean Lipoxygenase-1 Mutants: The Role of Second Coordination Sphere Residues in the Regulation of Enzyme Activity. *Biochemistry* **2003**, *42*, 7294.
411. Wasinger, E. C.; DeGroot, M. F.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. L-edge X-ray Absorption Spectroscopy of Non-Heme Iron Sites I: Experimental Determination of Differential Orbital Covalency. *J. Am. Chem. Soc.* **2003**, *125*, 12894.
412. Kemsley, J. N.; Chow, M. S.; Loeb Zaleski, K.; Decker, A.; Shishova, E. Y.; Wasinger, E. C.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Spectroscopic Studies of the Interaction of Ferrous Bleomycin with DNA. *J. Am. Chem. Soc.* **2003**, *125*, 10810.
413. Collman, J. P.; Sunderland, C. J.; Berg, K. E.; Vance, M. A.; Solomon, E. I. Spectroscopic Evidence for a Heme-superoxide/Cu(I) Intermediate in a Functional Model of Cytochrome c Oxidase. *J. Am. Chem. Soc.* **2003**, *125*, 6648.
414. DeBeer George, S.; 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. Spectroscopic Investigation of Stellacyanin Mutants: Axial Ligand Interactions at the Blue Copper Site. *J. Am. Chem. Soc.* **2003**, *125*, 11314.
415. Solomon, E. I.; Szilagyi, R. K.; DeBeer George, S.; Basumallick, L. Electronic Structures of Metal Sites in Proteins and Models: Contributions to Function in Blue Copper Proteins. *Chem. Rev. (Editor's Choice Article for 2004)* **2004**, *104*, 419.
416. Strand, K. R.; Yang, Y.; Andersson, K. K.; Solomon, E. I. 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* **2003**, *42*, 12223.
417. Smolentsev, G.; Soldatov, A.V.; Wasinger, E.; Solomon, E.; Hodgson, K.; Hedman, B. Investigation of the Local Structure of Fe(II) Bleomycin and Peplomycins using Theoretical Analysis of Xanes. *Physica Scripta*. **2005**, Vol. T115, 862.
418. Mitić, N.; Saleh, L.; Schenk, G.; Bollinger, Jr. J. M.; Solomon, E. I. Rapid-Freeze- Quench Magnetic Circular Dichroism of Intermediate X in Ribonucleotide Reductase: New Structural Insight. *J. Am. Chem. Soc.* **2003**, *125*, 11200.
419. Jones, P. M.; May, J. A.; Reitz, J. B.; Solomon, E. I. Photoelectron Spectroscopic and Electronic Structure Studies of CH_2O Bonding and Reactivity on ZnO Surfaces: Steps in the Methanol Synthesis Reaction. *Inorg. Chem.* **2004**, *43*, 3349.

420. Schenk, G.; Pau, M. Y. M.; Solomon, E. I. Comparison between the Geometric and Electronic Structures and Reactivities of $\{\text{FeNO}\}^7$ and $\{\text{FeO}_2\}^8$ Complexes: A Density Functional Theory Study. *J. Am. Chem. Soc.* **2004**, *126*, 505.
421. Basumallick, L.; Szilagy, R. K.; Zhao, Y.; Shaphigh, J. P.; Sholes, L.P.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2003**, *125*, 14784.
422. E. I. Solomon, Basumallick, L.; Chen, P.; Kennepohl, P. Variable Energy Photoelectron Spectroscopy: Electronic Structure and Electronic Relaxation: Synchrotron Radiation in Inorganic and Bioinorganic Chemistry thematic issue. *Coord. Chem. Rev.* **2005**, *249*, 229.
423. Wei, P.; Skulan, A. J.; Mitić, N.; Yang, Y.; Saleh, L.; Bollinger, J. M., Jr.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2004**, *126*, 3777.
424. Ghosh, S.; Gorelsky, S. I.; Chen, P.; Cabrito, I.; Moura, J.G.; Moura, I.; Solomon, E. I. Activation of N_2O Reduction by the Fully Reduced μ_4 -Sulfide Bridged Tetranuclear Cu_z Cluster in Nitrous Oxide Reductase. *J. Am. Chem. Soc.* **2003**, *125*, 15708.
425. Solomon, E. I.; Hedman, B.; Hodgson, K. O.; Dey, A.; Szilagy, R. Ligand K-edge X-Ray Absorption Spectroscopy: Covalency of Ligand-Metal Bonds: Synchrotron Radiation in Inorganic and Bioinorganic Chemistry thematic issue. *Coord. Chem. Rev.* **2005**, *249*, 97.
426. Smolentsev, G.; Soldatov, A.V.; Wasinger, E.; Solomon, E.; Hodgson, K.; Hedman, B. Axial Ligation Fe(II)-Bleomycin Probed by XANES Spectroscopy. *Inorg. Chem.* **2004**, *43*, 1825.
427. Szilagy, R. K.; Bryngelson, P. A.; Maroney, M. J.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. S K-edge X-ray Absorption Spectroscopic Investigation of the Ni-Containing Superoxide Dismutase Active Site: New Structural Insight and Mechanism. *J. Am. Chem. Soc.* **2004**, *126*, 3018.
428. Chen, P.; Bell, J.; Eipper, B. A.; Solomon, E. I. Oxygen Activation by the Non-Coupled Binuclear Copper Active Site in Peptidylglycine α -Hydroxylating Monooxygenase. Spectroscopic Definition of the Resting Sites and the Putative $\text{Cu}^{\text{II}}_{\text{M}}\text{-OOH}$ Intermediate. *Biochemistry* **2004**, *43*, 5735.
429. Chen, P.; Gorelsky, S. I.; Ghosh, S.; Solomon, E. I. N_2O Reduction by the μ_4 -Sulfide Bridged Tetranuclear Cu_z Cluster Active Site. *Angew. Chem., Int. Ed.* **2004**, *43*, 4132.
430. Chen, P.; Solomon, E. I. Oxygen Activation by the Noncoupled Binuclear Copper Site in Peptidylglycine α -Hydroxylating Monooxygenase. Reaction Mechanism and Role of the Noncoupled Nature of the Active Site. *J. Am. Chem. Soc.* **2004**, *126*, 4991.

431. Neidig, M. L.; Kavana, M.; Moran, G. R.; Solomon, E. I. CD and MCD Studies of the NonHeme Ferrous Active Site in (4-Hydroxyphenyl) pyruvate Dioxygenase: Correlation Between Oxygen Activation in the Extradiol and α -KG Dependent Dioxygenases. *J. Am. Chem. Soc.* **2004**, *126*, 4486.
432. Decker, A.; Rohde, J.; Que, L., Jr.; Solomon, E. I. Spectroscopic and Quantum Chemical Characterization of the Electronic Structure and Bonding in a Non-Heme Fe(IV)=O Complex. *J. Am. Chem. Soc.* **2004**, *126*, 5378.
433. Holm, R. H.; Solomon, E. I. Preface: Biomimetic Inorganic Chemistry. *Chem. Rev.* **104**, **2004**, 347.
434. Solomon, E. I. Preface: Synchrotron Radiation in Inorganic and Bioinorganic Chemistry. *Coord. Chem. Rev.* **2005**, *249*, 1.
435. Liang, H. C.; Henson, M. J.; Hatcher, L. Q.; Vance, M. A.; Xin Zhang, C.; Lahti, D.; Kaderli, S.; Sommer, R. D.; Rheingold, A. L.; Zuberbuhler, A. D.; Solomon, E. I.; Karlin, K. D. Solvent Effects on the Conversion of Dicopper(II) μ - η^2 : η^2 -Peroxo to Bis- μ -oxo Dicopper(III) Complexes: Direct Probing of the Solvent Interaction. *Inorg. Chem.* **2004**, *43*, 4115.
436. Quintanar, L.; Gebhard, M. S.; Wang, T.-P.; Kosman D. J.; Solomon, E. I. Ferrous Binding to the Multicopper Oxidases *Saccharomyces cerevisiae* Fet3p and Human Ceruloplasmin: Contributions to Ferroxidase Activity. *J. Am. Chem. Soc.* **2004**, *126*, 6579.
437. Skulan, A. J.; Brunold, T. C.; Baldwin, J.; Saleh, L.; Bollinger, J. M., Jr.; Solomon, E. I. Nature of the Peroxo Intermediate of the W48F/D84E Ribonucleotide Reductase Variant: Implications for O₂ Activation by Binuclear Non-Heme Iron Enzymes. *J. Am. Chem. Soc.* **2004**, *126*, 8842.
438. Dey, A.; Glaser, T.; Couture, M. M. J.; Eltis, L. D.; Holm, R. H.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Ligand K-edge X-ray Absorption Spectroscopy of [Fe₄S₄]^{1+,2+,3+} Clusters: Changes in Bonding and Electronic Relaxation upon Redox. *J. Am. Chem. Soc.* **2004**, *126*, 8320.
439. Chen, P.; Solomon, E. I. O₂ activation by binuclear Cu sites: Noncoupled versus exchange coupled reaction mechanisms. *Proc. Natl. Acad. Sci. U.S.A.* **2004**, *101*, 13105.
440. Dey, A.; Glaser, T.; Moura, J. J. G.; Holm, R. H.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Ligand K-edge X-ray Absorption Spectroscopy and Density Functional Theory Calculations on [Fe₃S₄]^{0,+} Clusters: Effects of Bonding on Delocalization, Redox and its Perturbation by the Protein Environment. *J. Am. Chem. Soc.* **2004**, *126*, 16868.
441. Yoon, J.; Mirica, L. M.; Stack, T. D. P.; Solomon, E. I. Spectroscopic Demonstration of a Large Antisymmetric Exchange Contribution to the Spin-Frustrated Ground State of a DB_{3B} Symmetric Hydroxy-Bridged Trinuclear Cu(II) Complex: Ground-to-Excited State Superexchange Pathways. *J. Am. Chem. Soc.* **2004**, *126*, 12586.

442. DeBeer George, S.; Brant, P.; Solomon, E. I. Metal and Ligand K-edge XAS of Organotitanium Complexes: Metal 4p and 3d Contributions to Pre-edge Intensity and their Contributions to Bonding. *J. Am. Chem. Soc.* **2005**, *127*, 667.
443. Kennepohl, P.; Neese, F.; Schweitzer, D.; Jackson, H. L.; Kovacs, J. A.; Solomon, E. I. Spectroscopy of Non-Heme Iron Thiolate Complexes: insight into the electronic structure of the low spin active site of Nitrile Hydratase. *Inorg. Chem.* **2005**, *44*, 1826.
444. Basumallick, L.; Sarangi, R.; DeBeer George, S.; Elmore, B.; Hooper, A. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Spectroscopic and Density Functional Studies of the Red Copper Site in Nitrosocyanin: Role of the Protein in Determining Active Site Geometric and Electronic Structure. *J. Am. Chem. Soc.* **2005**, *127*, 3531.
445. Decker, A.; Solomon, E. I. Comparison of Fe(IV)=O Heme and Non-Heme Species: Electronic Structures, Bonding and Reactivities. *Angew. Chem., Int. Ed.* **2005**, *44*, 2252.
446. Salas, J.; Solomon, E. I. Dioxygen Binds End-On to Mononuclear Copper in a Precatalytic Enzyme Complex. *Chemtracts* **2004**, *17*, 351.
447. Aboelella, N. W.; Kryatov, S. V.; Gherman, B. F.; Brennessel, W. W.; Young, Jr. V. G.; Sarangi, R.; Rybak-Akimova, E. V.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.; Cramer, C. J.; Tolman, W. B.; Dioxygen Activation at a Single Copper Site: Structure, Bonding, and Mechanism of Formation of 1:1 Cu/O₂ Adducts. *J. Am. Chem. Soc.* **2004**, *126*, 16896.
448. Rulišek, L.; Solomon, E. I.; Ryde, U. A Combined Quantum and Molecular Mechanical Study of the O₂ Reductive Cleavage in the Catalytic Cycle of Multicopper Oxidases. *Inorg. Chem.* **2005**, *44*, 5612.
449. del Rio, D.; Sarangi, R.; Chufan, E. E.; Karlin, K. D.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Geometric and Electronic Structure of the Heme-Peroxo-Copper Complex [(F₈TPP)Fe^{III}-(O₂²⁻)-Cu^{II}(TMPA)](ClO₄). *J. Am. Chem. Soc.* **2005**, *127*, 11969.
450. Xiao, Y.; Dey, A.; Wang, H.; George, S. J.; Smith, M. C.; Adams, M. W. W.; Jenney, F. E., Jr.; Sturhahn, W.; Alp, E. E.; Zhao, J.; Yoda, Y.; Solomon, E. I.; Cramer, S. P. Normal Mode Analysis of *Pyrococcus furiosus* Rubredoxin via Nuclear Resonance Vibrational Spectroscopy (NRVS) and Resonance Raman Spectroscopy. *J. Am. Chem. Soc.* **2005**, *127*, 14596.
451. Decker, A.; Solomon, E. I. Dioxygen Activation by Copper, Heme and Non-Heme Iron Enzymes: Comparison of Electronic Structures and Reactivities. *Curr. Opin. Chem. Biol.* **2005**, *9*, 152.
452. Quintanar, L.; Stoj, C.; Wang, T.-P.; Kosman D. J.; Solomon, E. I. The Role of Aspartate 94 In The Decay of the Peroxide Intermediate in the Multicopper Oxidase Fet3p. *Biochemistry* **2005**, *44*, 6081.

453. Quintanar, L.; Yoon, J.; Aznar, C.; Palmer, A. E.; Andersson, K.; Britt, D.; Solomon, E.I. Spectroscopic and Electronic Structure Studies of the Trinuclear Cu Cluster Active Site of the Multicopper Oxidase Laccase: Nature of its Coordination Unsaturation. *J. Am. Chem. Soc.* **2005**, *127*, 13832.
454. Solomon, E. I. Preface Forum: Functional Insight from Physical Methods on Metalloenzymes. *Inorg. Chem.* **2005**, *44*, 723.
455. Gorelsky, S.; Basumallick, L.; Vura-Weis, J.; Sarangi, R.; Hodgson, K. O.; Hedman, B.; Fujisawa, K.; Solomon, E. I. Spectroscopic and DFT Investigation of $[M\{HB(3,5iPr_2pz)_3\}(SC_6F_5)]$ $\{M = Mn, Fe, Co, Ni, Cu, \text{ and } Zn\}$ Model Complexes: Periodic Trends in Metal-thiolate Bonding. *Inorg. Chem.* **2005**, *44*, 4947.
456. Mirica, L. M.; Vance, M.; Jackson Rudd, D.; Hedman, B.; Hodgson, K. O.; Solomon, E. I.; Stack, D. P. Tyrosinase Reactivity from a Model Complex: An Alternative Hydroxylation Mechanism. *Science* **2005**, *308*, 1890.
457. Dey, A.; Okamura, T.; Ueyama, N.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Sulfur K-Edge XAS and DFT Calculations on P450 Model Complexes: Effects of Hydrogen Bonding on Electronic Structure and Redox Potentials. *J. Am. Chem. Soc.* **2005**, *127*, 12046.
458. Yoon, J.; Mirica, L. M.; Stack, T. D. P.; Solomon, E. I. Variable-Temperature, Variable-Field Magnetic Circular Dichroism Studies of Tris-Hydroxy- and μ_3 -Oxo Bridged Trinuclear Cu(II) Complexes: Evaluation of Proposed Structures of the Native Intermediate of the Multicopper Oxidases. *J. Am. Chem. Soc.* **2005**, *127*, 13680.
459. Yoon, J.; Solomon, E. I. Ground State Electronic and Magnetic Properties of a μ_3 -Oxo Trinuclear Cu(II) Complex: Correlation to the Native Intermediate of the Multicopper Oxidases. *Inorg. Chem.* **2005**, *44*, 8076.
460. Wei, P.-p.; Skulan, A. J.; Wade, H.; DeGrado, W.F.; Solomon, E. I. Spectroscopic and Computational studies of the *de Novo* Designed Protein DF2t: Correlation to the Biferrous Active site of Ribonucleotide Reductase and Factors that Affect O_2 Reactivity. *J. Am. Chem. Soc.* **2005**, *127*, 16098.
461. Neidig, M. L.; Decker, A.; Kavana, M.; Moran, G. R.; Solomon, E. I. 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 Comm. (Special Issue in 50th Anniversary of the oxygenesis)* **2005**, *338*, 206.
462. Neidig, M. L.; Solomon, E. I. Structure-Function Correlations Over Oxygen Activating NonHeme Iron Enzymes. *Chem. Comm. (Featured Cover)* **2005**, 5843.
463. Li, L.; Narducci Sarjeant, A. A.; Vance, M. A.; Zakharov, L. N.; Rheingold, A. L.; Solomon, E. I.; Karlin, K. D. Exogenous Nitrile Substrate Hydroxylation by a New Dicopper-Hydroperoxide Complex. *J. Am. Chem. Soc.* **2005**, *127*, 15360.

464. Dey, A.; Roche, C. L.; Walters, M. A.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Sulfur KEdge XAS and DFT Calculations on $[\text{Fe}_4\text{S}_4]^{2+}$ Clusters: Effects of H-bonding and Structural Distortion on Covalency and Spin Topology. *Inorg. Chem.* **2005**, *44*, 8349.
465. Dey, A.; Chow, M. S.; Taniguchi, K.; Lugo-Mas, P.; Davin, S.; Maeda, M.; Kovacs, J. A.; Odaka, M.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Sulfur K-edge XAS and DFT Calculations on Nitrile Hydratase: Geometric and Electronic Structure of the Non-heme Iron Active Site. *J. Am. Chem. Soc.* **2006**, *128*, 533.
466. Hansen, D. F.; Gorelsky, S. I.; Sarangi, R.; Christensen, H. E. M.; Solomon, E. I.; Led, J. I. Reinvestigation of the Method to Map the Electronic Structure of Blue Copper Proteins by NMR Relaxation. *J. Biol. Inorg. Chem.* **2006**, *11*, 277.
467. Gorelsky, S. I.; Ghosh, S.; Solomon, E. I. Mechanism of N_2O Reduction by the μ_4 -S tetranuclear Cu₂ Cluster of Nitrous Oxide Reductase. *J. Am. Chem. Soc.* **2006**, *128*, 278.
468. Collman, J.; Yan, Y-L.; Eberspacher, T.; Xie, X.; Solomon, E. I. Oxygen Binding of WaterSoluble Cobalt Porphyrins in Aqueous Solution. *Inorg. Chem.* **2006**, *45*, 9628.
469. Hatcher, L.; Vance, M.; Sarjeant, A. N.; Solomon, E. I.; Karlin, K. D. Copper-Dioxygen Adducts and the Side-on Peroxo Dicopper(II)/Bis(μ -oxo) Dicopper(III) Equilibrium: Significant Ligand Electronic Effects. *Inorg. Chem.* **2006**, *45*, 3004.
470. Decker, A.; Chow, M. S.; Kemsley, J. N.; Lehnert, N.; Solomon, E. I. Direct Hydrogen-Atom Abstraction by Activated Bleomycin: An Experimental and Computational Study. *J. Am. Chem. Soc.* **2006**, *128*, 4719.
471. DeBeer George, S.; Huang, K-W.; Waymouth, R. M.; Solomon, E. I. Metal and Ligand K-edge XAS of Titanium-TEMPO Complexes: Determination of Oxidation States and Insights into TiO Bond Homolysis. *Inorg. Chem.* **2006**, *45*, 4468.
472. Mirica, L. M.; Jackson Rudd, D.; Vance, M.; Solomon, E. I.; Hodgson, K. O.; Hedman, B.; Stack, D. P. μ - $\eta^2\eta^2$ -Peroxodicopper(II) Complex with a Secondary Diamine Ligand: A Functional Model of Tyrosinase. *J. Am. Chem. Soc.* **2006**, *128*, 2654.
473. Yoon, J.; Solomon, E. I. Electronic Structures of Exchange Coupled Trigonal Trimeric Cu(II) Complexes: Spin Frustration, Antisymmetric Exchange and Pseudo-A terms and their Relation to O_2 Activation in the Multicopper Oxidases. *Coord. Chem. Rev.* **2007**, *251*, 379.
474. Decker, A.; Clay, M. D.; Solomon, E. I. Spectroscopy and Electronic Structures of Mono- and Binuclear High-Valent Non-Heme Iron-Oxo Systems. *J. Inorg. Biochem.* **2006**, *100*, 697.
475. Solomon, E. I.; Gorelsky, S. I.; Dey, A. Metal-Thiolate Bonds in Bioinorganic Chemistry. *Journal of Computational Chemistry* **2006**, *27*, 1415.
476. Sergraves, E. N.; Chruszcz, M.; Neidig, M. L.; Ruddat, V.; Zhou, J.; Weckler, A. T.; Minor, W.; Solomon, E. I.; Holman, T. R. Kinetic, Spectroscopic, and Structural Investigations of the

Soybean Lipoxygenase-1 First Coordination Sphere Mutant, Asn694Gly. *Biochemistry* **2006**, *45*, 10233.

477. Yoon, J.; Solomon, E. I. Unique spectroscopic features and electronic structures of copper proteins: relation to reactivity (Invited Review). In *Biological Magnetic Resonance*; G. R. Hanson, L. J. Berliner, Eds.; Springer Publishers: New York, **2009**; Vol 28.
478. Hatcher, L.Q.; Lee, D-H.; Vance, M. A.; Milligan, A. E.; Sarangi, R.; K. O. Hodgson, K. O.; Hedman, B.; Solomon, E. I.; Karlin, K. D. Dioxygen Reactivity of a Copper (I) Complex with a N₃S Thioether Chelate; Peroxo-Dicopper (II) Formation Including Sulfur-Ligation. *Inorg. Chem.* **2006**, *45*, 10055.
479. Ryde, U.; Hsiao, Y-W.; Rulisek, L.; Solomon, E. I. Identification of the peroxy adduct in multicopper oxidases by a combination of computational chemistry and EXAFS measurements. *J. Am. Chem. Soc.* **2007**, *129*, 726.
480. Dey, A.; Hocking, R. K.; Larsen, P.; Borovik, A. S.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. X-ray Absorption Spectroscopy and Density Functional Theory Studies of [(H₃buea)Fe^{III}-X]ⁿ⁻ (X= S²⁻, O²⁻, OH⁻): Comparison of Bonding and Hydrogen Bonding in Oxo and Sulfido Complexes. *J. Am. Chem. Soc.* **2006**, *128*, 9825.
481. Kitagawa, T.; Dey, A.; Lugo-Mas, P.; Benedict, J.; Kaminsky, W.; Solomon, E. I.; Kovacs, J. A. A Functional Model for the Cysteinate-Ligated Non-Heme Iron Enzyme Superoxide Reductase (SOR). *J. Am. Chem. Soc.* **2006**, *128*, 14448.
482. Lugo-Mas, P.; Dey, A.; Xu, L.; Davin, S. D.; Benedict, J.; Kaminsky, W.; Hedman, B.; Hodgson, K. O.; Solomon, E. I.; Kovacs, J. A. How Does Single Oxygen Atom Addition Affect the Properties of an Fe–Nitrile Hydratase Analogue? The Compensatory Role of the Unmodified Thiolate. *J. Am. Chem. Soc.* **2006**, *128*, 11211.
483. Hocking, R. K.; Wasinger, E. C.; DeGroot, M. F.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Fe L-edge XAS studies of K₄[Fe(CN)₆] and K₃[Fe(CN)₆]: a Direct Probe of Back-Bonding. *J. Am. Chem. Soc.* **2006**, *128*, 10442.
484. Neidig, M. L.; Decker, A.; Choroba, O. W.; Huang, F.; Kavana, M.; Moran, G. R.; Spencer, J. B.; Solomon, E. I. Spectroscopic and electronic structure studies of aromatic electrophilic attack and hydrogen-atom abstraction by non-heme iron enzymes. *Proc. Natl. Acad. Sci. U.S.A. (Inagural)* **2006**, *103*, 12966.
485. Sarangi, R.; Aboeella, N.; Fujisawa, K.; Tolman, W. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. X-Ray Absorption Edge Spectroscopy and Computational Studies on LCuO₂ Species: Superoxide-Cu^{II} versus Peroxide-Cu^{III} Bonding. *J. Am. Chem. Soc.* **2006**, *128*, 8286.
486. Sarangi, R.; Benfatto, M.; Hayakawa, K.; Bubacco, L.; Solomon, E. I.; Hodgson, K. O.; Hedman, B. MXAN analysis of the XANES energy region of a mononuclear copper complex: Applications to Bioinorganic Systems. *Inorg. Chem.* **2005**, *44*, 9652.

487. Solomon, E. I. Spectroscopic Methods in Bioinorganic Chemistry: Blue to Green to Red Copper Sites. *Inorg. Chem.* (Invited Award Paper) **2006**, *45*, 8012.
488. Stoj, C.; Augustine, A. J.; Zeigler, L.; Solomon, E. I.; Kosman D. J. Structural Basis of the Ferrous Iron Specificity of the Yeast Ferroxidase, Fet3p. *Biochemistry* **2006**, *45*, 12741.
489. Neidig, M. L.; Brown, C. D.; Kavana, M.; Choroba, O. W.; Spencer, J. B.; Moran G. R.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of the Role of Active Site Interactions in the Decarboxylation Reaction of α -keto Acid-dependent Dioxygenases. *J. Inorg. Biochem. 100th Anniversary Issue* **2006**, *12*, 2108.
490. Hocking, R. K.; Wasinger, E. C.; Yan, F. Y-L.; DeGroot, M. F.; Walker, F. A.; Hodgson, O.; Hedman, B.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2007**, *129*, 113.
491. Sarangi, R.; DeBeer George, S.; Rudd, D. J.; Szilagyi, R. K.; Ribas, X.; Rovira, C.; Almeida, M.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2007**, *129*, 2316.
492. Wei, P.-p.; Tomter, A. B.; Røhr, Å. K.; Andersson, K. K.; Solomon, E. I. 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* **2006**, *45*, 14043.
493. Chalupsky, J.; Neese, F.; Solomon, E. I.; Ryde, U.; Rulisek, L. Multireference *ab initio* Calculations on the Reaction Intermediates of the Multicopper Oxidases. *Inorg. Chem.* **2006**, *45*, 11051.
494. Ray, K.; DeBeer George, S.; Solomon, E. I.; Wieghardt, K.; Neese, F. Description of the Ground State Covalencies of the Bis(dithiolato) Transition Metal Complexes Using X-ray Absorption Spectroscopy and Time-Dependent-Density-Functional Calculations. *Chemistry European Journal* **2007**, *13*, 2783.
495. Song, W. J.; Seo, W. J.; DeBeer George, S.; Ohta, T.; Song, R.; Kang, M.-J.; Tosha, T.; Kitagawa, T.; Solomon, E. I.; Nam, W. Synthesis, Characterization, and Reactivities of Manganese(V)-Oxo Porphyrin Complexes. *J. Am. Chem. Soc.* **2007**, *129*, 1268.
496. Gorelsky, S. I.; Xie, X.; Chen, Y.; Fee, J. A.; Solomon, E. I. The Two State Issue in the Mixed Valence Binuclear Cu_A Center in Cytochrome *c* Oxidase and N₂O Reductase. *J. Am. Chem. Soc.* **2006**, *128*, 16452.
497. Pau, M.Y. M.; Davis, M. I.; Orville, A. M.; Lipscomb, J.; Solomon, E. I. Spectroscopic and Electronic Structure Study of the Enzyme-Substrate Complex of Intradiol Dioxygenases: Substrate Activation by a High Spin Ferric Non-Heme Iron Site. *J. Am. Chem. Soc.* **2007**, *129*, 1944.

498. Dey, A.; Jenney, F. E., Jr.; Adams, M. W. W.; Johnson, M. K.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. Sulfur K-edge X-ray Absorption Spectroscopy and Density Functional Theory Calculations on Superoxide Reductase: Role of the Axial Thiolate in Reactivity. *J. Am. Chem. Soc.* **2007**, *129*, 12418.
499. Quintanar, L.; Stoj, C.; Kosman D. J.; Solomon, E. I. Shall We Dance? How Multicopper Oxidase Chooses its Electron Transfer Partner. *Accounts of Chemical Research* **2007**, *40*, 445.
500. Ghiladi, R. A.; Chufan, E.; del Rio, D.; Solomon, E. I.; Krebs, C.; Huyhn, B. H.; Huang, H-w.; Moëne-Locco, P.; Kanderli, S.; Honecker, M.; Zuberhüeler, A. D.; Marzilli, L.; Cotter, R. J.; Karlin, K. D. Further Insights into the Spectroscopic Properties, Electronic Structure and Kinetics of Formation of the Heme-Peroxo-Copper Complex $[(F_8TPP)Fe^{III}-(O_2^{2-})Cu^{II}(TMPA)]^+$. *Inorg. Chem.* **2007**, *46*, 3889.
501. Ghosh, S.; Goreslsky, S.; George, S. D.; Chan, J. M.; Cabrito, I.; Dooley, D. M.; Moura, J. J. G.; Moura, I.; Solomon, E. I. Spectroscopic, Computational, and Kinetic Studies of the μ_4 -Sulfide Bridged Tetranuclear Cu_2 Cluster in N_2O Reductase: pH Effect on the Edge Ligand and Its Contribution to Reactivity. *J. Am. Chem. Soc.* **2007**, *129*, 3955.
502. Maiti, D.; Fry, H. C.; Woertink (Salas), J. S.; Vance, M. A.; Solomon, E. I.; Karlin, K. D. A 1:1 Copper-Dioxygen Adduct is an End-on Bound Superoxo Copper (II) Complex which Undergoes Oxygenation Reactions with Phenols. *J. Am. Chem. Soc.* **2007**, *129*, 264.
503. Maiti, D.; Woertink (Salas), J. S.; Vance, M. A.; Milligan, A. E.; Narducci Sarjeant, A. A.; Solomon, E. I.; Karlin, K. D. Copper (I)/ S_8 Reversible Reaction Leading to an End-on Bound Dicopper (II) Disulfide Complex: Nucleophilic Reactivity and Analogies to Copper-Dioxygen Chemistry. *J. Am. Chem. Soc.* **2007**, *129*, 8882.
504. Neidig, M.L.; Weckler, A. T.; Schenk, G.; Holman, T. R.; Solomon, E. I. Kinetic and Spectroscopic Studies of N694C Lipoyxygenase: A Probe of the Substrate Activation Mechanism of a Non-Heme Ferric Enzyme. *J. Am. Chem. Soc.* **2007**, *129*, 7531.
505. Stoj, C. S.; Augustine, A. J.; Solomon, E. I.; Kosman D. J. Structure-Function Analysis of the Cuprous Oxidase Activity in Fet3p from *Saccharomyces cerevisiae*. *J. Biol. Chem.* **2007**, *82*, 7862.
506. DeGroot, F. M. F.; Hocking, R.; Piamonteze, C.; Hedman, B.; Hodgson, K. O.; Solomon, E. I. New Developments in Charge Transfer Multiplet Calculations: Projection Operations, Mixedspin States, π -Bonding. *Am. Inst. Phys. 13th Int XAFS Conf. Proceedings* **2007**, 882, 123.
507. Goreslsky, S.; Solomon, E. I. Extended Charge Decomposition Analysis and Its Application for the Investigation of Electronic Relaxation. *Theoretical Chemistry Accounts* **2007**, *119*, 57.
508. Solomon, E. I.; Sarangi, R.; Woertink, J. S.; Augustine, A. J.; Yoon, J.; Ghosh, S. O_2 and N_2O Activation by Binuclear, Trinuclear and Tetranuclear Cu Clusters in Biology. *Accounts of Chemical Research* **2007**, *40*, 581.

509. Tenderholt, A.L.; Szilagy, R.; Holm, R.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. 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. *J. Inorg. Biochem.* (E.I. Stiefel Issue) **2007**, *101*, 1594.
- 510 Brown, C. D.; Neidig, M. L.; Neibergall, M. B.; Lipscomb, J. D.; Solomon, E. I. VTVH- MCD and DFT Studies of Thiolate Binding to $\{\text{FeNO}\}^7/\{\text{FeO}_2\}^8$ Complexes of Isopenicillin *N* synthase: Substrate Determination of Oxidase versus Oxygenase Activity in Non-Heme Fe Enzymes. *J. Am. Chem. Soc.* **2007**, *129*, 7427.
511. Lee, D-H ; Hatcher, L. Q.; Vance, M. A.; Sarangi, R.; Milligan, A. E.; Narducci Sarjeant, A.; Incarvito, C. D.; Rheingold, A. L.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Karlin, K. D. Copper(I) complex O₂-reactivity with a N3S thioether ligand: A copper- dioxygen adduct including sulfur-ligation, ligand oxygenation and comparisons with all nitrogen ligand analogues. *Inorg. Chem.* **2007**, *46*, 6056.
512. Mitic, N.; Clay, M. D.; Saleh, L.; Bollinger, J. M., Jr.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2007**, *129*, 9049.
513. Collman, J. P.; Decreau, R. A.; Yan, Y.; Yoon, J.; Solomon, E. I. Intramolecular Single- Turnover Reaction in a Cytochrome c Oxidase Model Bearing a Tyr244 Mimic. *J. Am. Chem. Soc.* **2007**, *129*, 5794.
514. Dey, A.; Green, K. N.; Jenkins, R. M.; Jeffrey, S. P.; Darensbourg, M. Y.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. S K-edge XAS and DFT calculations on square planar Ni(II)-thiolate complexes: Effects of Active and Passive H-bonding. *Inorg. Chem.* **2007**, *46*, 9655.
515. Dey, A.; Green, K. N.; Jenkins, R. M.; Jeffrey, S. P.; Darensbourg, M. Y.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. 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. *Inorg. Chem* **2007**, *46*, 4989.
516. Wei, P.-P.; Solomon, E. I. Advanced spectroscopic studies of RNR in Molecular Anatomy and Physiology of Proteins. In *Ribonucleotide Reductase*; Andersson, K. K., Ed.; Nova Science Publishers, Inc.: New York, **2008**; pp
517. Yano, J.; Robblee, J.; Pushkar, Y.; Marcus, M. A.; Bendix, J.; Collins, T. J.; Solomon, E. I. Yachandra, V.; D-B. George, S. Polarized X-ray Absorption Spectroscopy of Single-crystal Mn(V) Complexes Relevant to the Oxygen Evolving Complex of Photosystem II. *J. Am. Chem. Soc.* **2007**, *129*, 12989.
518. Yoon, J.; Liboiron, B. D.; Sarangi, R.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. The Two Oxidized Forms of the Trinuclear Cu Cluster in the Multicopper Oxidases and Mechanism for the Decay of the Native Intermediate. *Proc. Natl. Acad. Sci. U.S.A.* **2007**, *104* 13609.

519. Ghosh, S.; Dey, A.; Usov, O. M.; Sun, Y.; Grigoryants, V. M.; Scholes, C. P.; Solomon, E. I. Resolution of the Spectroscopy versus Crystallography Issue for NO Intermediates of Nitrite Reductase from *Rhodobacter sphaeroides*. *J. Am. Chem. Soc.* **2007**, *129*, 10310.
520. Pau, M.Y. M.; Lipscomb, J.; Solomon, E. I. Substrate Activation for O₂ Reactions by Oxidized Metal Centers in Biology. *PNAS (Invited Perspective)* **2007**, *104*, 18355.
521. Op't Holt, B.T.; Dustman, J.; Solomon, E. I. Structure/Function relationships in binuclear copper(II) dioxygen binding proteins. *ChemTracts: Inorganic Chemistry* **2006**, *19*, 435.
522. Decker, A.; Rohde, J-U; Klinker, E. J.; Wong, S. D.; Que, L. Jr.; Solomon, E. I. Spectroscopic and Quantum Chemical Studies on Low-Spin Fe(IV)=O Complexes: Fe-O bonding and Its Contributions to Reactivity. *J. Am. Chem. Soc.* **2007**, *129*, 15983.
523. Ohta, T.; Chakrabarty, S.; Lipscomb, J.; Solomon, E. I. Near-IR MCD of the Non-Heme Ferrous Active Site in Naphthalene 1,2-Dioxygenase: Correlation to Crystallography and Structural Insight into the Mechanism of Rieske Dioxygenases. *J. Am. Chem. Soc.* **2008**, *130*, 1601.
524. 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. CD and MCD of CytC3 and Taurine Dioxygenase: Role of the Facial Triad in alpha-KG-Dependent Oxygenases. *J. Am. Chem. Soc.* **2007**, *129*, 14224.
525. Yoon, J.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2007**, *129*, 13127.
526. Sarangi, R.; Gorelsky, S.; Basumallick, L.; Hwang, H. J.; Pratt, R.; Stack, D.; Lu, Y.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Spectroscopic and Density Functional Theory studies of the Blue Copper Site in M121SeM and C112SeC Azurin: Cu-Se vs Cu-S Bonding. *J. Am. Chem. Soc.* **2008**, *130*, 3866.
527. Sarangi, R.; York, J. T.; Helton, M. E.; Fujisawa, K.; Karlin, K. D.; Tolman, W. B.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. X-ray Absorption Spectroscopic and Theoretical Studies on (L)₂[Cu₂Sn]²⁺ Complexes: Disulfide Versus Disulfide(1-) Bonding. *J. Am. Chem. Soc.* *130*, **2008**, 676.
528. Augustine, A. J.; Quintanar, L.; Stoj, C. S.; Kosman, D. J.; Solomon, E. I. 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. *J. Am. Chem. Soc.* **2007**, *129*, 13118.
529. Dey, A.; Jenney, F. E., Jr.; Adams, M. W. W.; Babini, E.; Takahashi, Y.; Fukuyama, K.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Solvent Tuning of Electrochemical Potentials in the Active Sites of HiPIP vs Ferredoxin. *Science* **2007**, *318*, 1464.

530. Xie, X.; Gorelsky, S. I.; Sarangi, R.; Garner, D. K.; Hwang, H. J.; Hodgson, K. O.; Hedman, B.; Lu, Y.; Solomon, E. I. Perturbations to the Geometric and Electronic Structure of the CuA Site: Factors that Influence Delocalization and their Contributions to Electron Transfer. *J. Am. Chem. Soc.* **2008**, *130*, 5194.
531. Solomon, E. I.; Xie, X.; Dey, A. Mixed Valent Sites in Biological Electron Transfer. *Chemical Society Reviews* **2008**, *37*, 623.
532. 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. 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* **2008**, *47*, 2036.
533. Maiti, D.; Woertink, J. S.; Narducci Sarjeant, A. A.; Solomon, E. I.; Karlin, K. D. Copper Dioxygen Adducts: Formation of bis(μ -oxo)dicopper(III) versus (μ - 1,2)peroxodicopper(II) Complexes with Small Changes in One Pyridyl-Ligand Substituent. *Inorg. Chem.* **2008**, *47*, 3787.
534. Tenderholt, A.; Szilagyi, R.; Holm, R.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Electronic Control of the Bailar Twist in Formally d0-d2 Molybdenum tris(dithiolene) Complexes: A Sulfur K- edge X-ray Absorption Spectroscopy and Density Functional Theory Study. *Inorg. Chem.* **2008**, *47*, 6382.
535. Solomon, E. I.; Augustine, A. J.; Yoon, J. Reduction of O₂ to H₂O by the Multicopper Oxidases. *Dalt. Trans.* **2008**, *30*, 3921.
536. Maiti, D.; Lee, D.; Narducci Sarjeant, A. A.; Pau M. Y.; Solomon, E. I.; Gaoutchenova, K.; Sundermeyer J.; Karlin, K. D. Reaction of a Copper-Dioxygen Complex with Nitrogen Monoxide (\bullet NO) Leads to a Copper(II)-Peroxynitrite Species. *J. Am. Chem. Soc.* **2008**, *130*, 6700.
537. Schwartz, J. K.; Wei, P-P.; Mitchell, K. H.; Fox, B. G.; Solomon, E. I. Geometric and Electronic Studies of Toluene-4-monooxygenase and Component D Effector Protein: Elucidation of the Effector Interaction and Parallels with Methane Monooxygenase in O₂ Activation. *J. Am. Chem. Soc.* **2008**, *130*, 7098.
538. Schwartz, J. K.; Liu,.; Tosha, T.; Theil, E. C.; Solomon, E. I. Spectroscopic Definition of the Ferroxidase Site in M Ferritin: Comparison of Binuclear Substrate vs. Cofactor Active Sites. *J. Am. Chem. Soc.* **2008**, *130*, 9441.
539. Calhoun, J. R.; Bell, C. B., III; Smith, T. J.; Thamann, T. J.; DeGrado, W. F.; Solomon, E. I. Oxygen Reactivity of the Biferrous Site in the *de novo* Designed Four Helix Bundle Peptide DFsc: Nature of the "Intermediate" and Reaction Mechanism. *J. Am. Chem. Soc.* **2008**, *130*, 9188.
540. Mitic, N.; Schwartz, J. K.; Brazeau, B.; Lipscomb, J.; Solomon, E. I. CD and MCD Studies of the Effects of Component B Variant Binding on the Biferrous Active Site of Methane Monooxygenase. *Biochemistry* **2008**, *47*, 8386.

541. Ghosh, S.; Cirera, J.; Vance, M. A.; Ono, T.; Fujisawa, K.; Solomon, E. I. Spectroscopic and Electronic Structure Studies of Phenolate Cu(II) Complexes: Phenolate ring Orientation and Activation related to Cofactor Biogenesis. *J. Am. Chem. Soc.* **2008**, *130*, 16262.
542. Collman, J. P.; Dey, A.; Decreau, R. A.; Yang, Y.; Hosseini, A.; Solomon, E. I.; Eberspacher, T.
A. Interaction of nitric oxide with a functional model of cytochrome c oxidase. *Proc. Natl. Acad. Sci. U.S.A.* **2008**, *105*, 9892.
543. Sarangi, R.; Hocking, R. K.; Neidig, M.L.; Benfatto, M.; Holman, T.R.; Solomon, E. I.; Hodgson, K. O.; Hedman, B. Geometric Structure Determination of N694C Lipoxygenase: A Comparative Near-Edge X-Ray Absorption Spectroscopy and Extended X-Ray Absorption Fine Structure Study. *Inorg. Chem.* **2008**, *47*, 11543.
544. Bell, C. B., III; Wong, S. D.; Xiao, Y.; Klinker, E.; Tenderholt, A. L.; Smith, M.; Rohde, J.; Que, L., Jr.; Cramer, S.; Solomon, E. I. A Combined NRVs and DFT Study of Fe(IV)=O Model Complexes: a Diagnostic Method for the Elucidation of non-Heme Iron Enzyme Intermediates. *Angew. Chem., Int. Ed.* **2008**, *47*, 9071.
545. Tomter, A.B.; Bell, C. B., III; Røehr, Å. K.; Andersson, K. K.; Solomon, E. I. Circular dichroism and magnetic circular dichroism studies of the biferrous site of the class Ib ribonucleotide reductase from *Bacillus cereus*: Comparison to the class 1a enzymes. *Biochemistry* **2008**, *47*, 11300.
546. Collman, J. P.; Yang, Y.; Dey, A.; Decreau, R. A.; Ghosh, S.; Ohta, T.; Solomon, E.I. A Functional Nitric Oxide Reductase Model. *Proc. Natl. Acad. Sci. U.S.A.* **2008**, *105*, 15660.
547. Chow, M. S.; Liu, L. V.; Solomon, E. I. New Insights into the Mechanism of the Reaction of Activated Bleomycin with DNA. *Proc. Natl. Acad. Sci. U.S.A.* **2008**, *105*, 13241.
548. Collman, J. P.; Dey, A.; Yang, Y.; Decreau, R. A.; Ohta, T.; Solomon, E. I. Intermediates Involved in the Two Electron Reduction of NO to N₂O by a Functional Synthetic Model of Heme Containing Bacterial NO Reductase. *J. Am. Chem. Soc.* **2008**, *130*, 16498.
549. Hocking, R. K.; DeBeer George, S.; Gross, Z.; Walker, F. A.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. Fe L- and K-edge XAS of Low-Spin Ferric Corrole: Bonding and Reactivity Relative to Low-Spin Ferric Porphyrin. *Inorg. Chem.* **2009**, *48*, 1678.
550. 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. Reactive Intermediates in Oxygenation Reactions with Mononuclear Non-Heme Iron Catalysts. *Angew. Chem., Int. Ed.* **2009**, *48*, 1257.
551. Ghosh, S.; Dey, A.; Sun, Y; Scholes, C. P.; Solomon, E.I. Spectroscopic and Computational Studies of Nitrite Reductase: Proton Induced Electron Transfer and Backbonding Contributions to Reactivity. *J. Am. Chem. Soc.* **2009**, *131*, 277.

552. Solomon, E.I.; Hocking R.K.; Pau, M.Y. M. Nature of the Catecholate-Fe(III) bond: High affinity binding and substrate activation in bioinorganic chemistry. *Computational Inorganic and Bioinorganic Chemistry, Encyclopedia Inorganic Chemistry Monograph*, John Wiley & Sons, Inc.: New York, **2009**.
553. Solomon, E. I.; Bell, C. B., III. Chapter 1: Bioinorganic and Inorganic Spectroscopy. In *Physical Inorganic Chemistry*; Bakac, A., Ed.; John Wiley & Sons, Inc.: New York, **2010**; pp 1-37.
554. Bell, C. B., III.; Calhoun, J. R.; Bobyr, E.; Wei, P-P.; Hedman, B.; Hodgson, K. O.; DeGrado, W.
F.; Solomon, E. I. Spectroscopic definition of the biferrous and biferric sites of de novo designed 4-helix bundle DFsc peptides: Implications for O₂ reactivity of binuclear non-heme iron enzymes. *Biochemistry* **2009**, *48*, 59.
555. Ghosh, S.; Xie, X.; Dey, A.; Sun, Y.; Scholes, C. P.; Solomon, E. I. Thermodynamic equilibrium between blue and green copper sites and the role of the protein in controlling function. *Proc. Natl. Acad. Sci. U.S.A.* **2009**, *106*, 4969.
556. Solomon, E.I.; Wong, S.D.; Liu, L.V.; Decker, A.; Chow, M.S. Peroxo and Oxo Intermediates in Mononuclear Non-heme Iron Enzymes and Related Active Sites. *Curr. Opin. Chem. Biol.* **2009**, *13*, 99.
557. Op't Holt, B.T.; Vance, M.A.; Mirica, L M.; Heppner, D.; Stack, T.D.P.; Solomon E.I. Reaction Coordinate of a Functional Model of Tyrosinase: Spectroscopic and Computational Characterization. *J. Am. Chem. Soc.* **2009**, *131*, 6421.
558. Xie, X.; Hadt, R.G.; Pauleta, S.R.; González, P.J.; Sun, U.; Moura, I.; Solomon, E. I. A variable temperature spectroscopic study on p. pantotrophus pseudoazurin: protein constraints on the blue Cu site. *J. Inorg. Biochem. (Invited Latin American Issue)* **2009**, *103*, 1307.
559. Chow, M. S.; Eser, B. E.; Wilson, S. A.; Hedman, B.; Hodgson, K. O.; Fitzpatrick, P. F.; Solomon, E. I. Spectroscopy and Kinetics of Wild-Type and Mutant Tyrosine Hydroxylase: Mechanistic Insight into O₂ Activation. *J. Am. Chem. Soc.* **2009**, *131*, 7685.
560. Yoon, J.; Fujii, S.; Solomon, E. I. Geometric and Electronic Structure Differences Between the Type 3 Copper Sites of the Multicopper Oxidases and Hemocyanin/Tyrosinase. *Proc. Natl. Acad. Sci. U.S.A.* **2009**, *106*, 6585.
561. Jensen, K.; Clay, M.; Bell, C. B., III; Solomon, E. I. Peroxo-Type Intermediates in Class I Ribonucleotide Reductase and Related Binuclear non-Heme Iron Enzymes. *J. Am. Chem. Soc.* **2009**, *131*, 12155.
562. Lucas, H. R.; Li, L.; Narducci Sarjeant, A. A.; Vance, M. A.; Solomon, E. I.; Karlin, K. D. Toluene and Ethylbenzene Aliphatic C-H Bond Oxidations Initiated by a Dicopper(II)- μ -1,2Peroxo Complex. *J. Am. Chem. Soc.* **2009**, *131*, 3230.

563. Dey, A.; Jiang, Y.; Ortiz de Montellano, P.; Hodgson, K. O.; Hedman, B.; Solomon, E. I. S Kedge XAS and DFT Calculations on Cytochrome P450: Covalent and Ionic Contributions to the Cysteine-Fe Bond and Their Contribution to Reactivity. *J. Am. Chem. Soc.* **2009**, *131*, 7869.
564. Maiti, D.; Woertink, J. S.; Ghiladi, R. A.; Solomon, E. I.; Karlin, K. D. Molecular oxygen and sulfur reactivity of a cyclotrimeratrylene derived trinuclear copper(I) complex. *Inorg. Chem.* **2009**, *48*, 8342.
565. Straganz, G. D.; Diebold, A. R.; Egger, S.; Nidetzky, B.; Solomon, E. I. Kinetic and CD/MCD Spectroscopic Studies of the Atypical, 3-His Ligated, Non-heme Fe²⁺ Center in Diketone Dioxygenase: The Role of Hydrophilic Outer Shell Residues in Catalysis. *Biochemistry* **2010**, *49*, 996.
566. Cho, J.; Annaraj, J.; Kim, S. Y.; Ogura, T.; Solomon, E. I.; Nam, W. Geometric and Electronic Structure and Reactivity of a Mononuclear "Side-On" Nickel(III)-Peroxo Complex. *Nature Chemistry* **2009**, *1*, 568.
567. Woertink, J.S.; Smeets, P.J.; Groothaert, M.H.; Vance, M.A.; Sels, B.F.; Schoonheydt, R.A.; Solomon, E. I. A [Cu₂O]²⁺ core in Cu-ZSM-5, the active site in the oxidation of methane to methanol. *Proc. Natl. Acad. Sci. U.S.A.* **2009**, *106*, 18908.
568. Park, G-Y.; Deepalatha, S.; Puiu, S. C.; Lee, D.H.; Mondal, B.; Narducci Sarjeant, A.A.; del Rio, D.; Pau, M.Y.M.; Solomon, E. I.; Karlin, K. D. A peroxy nitrite complex of copper; formation from a copper-nitrosyl complex, transformation to nitrite and exogeneous phenol oxidative coupling or nitration. *J. Biol. Inorg. Chem.* **2009**, *14*, 1301.
569. Ribeiro, S.J.L.; Ferreira, M.d.C.; Solomon, E.I.; Farrell, N.P. Preface for Latin American Bioinorganic Chemistry 2008 Special issue. *J. Inorg. Biochem.* **2009**, *103*, 125.