

ANDREA DECKER

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Objective

Bioinorganic chemist with experience in electronic structure calculations and experimental spectroscopic methods seeking a research position on an interdisciplinary team understanding biologically important systems.

Education

- **Ph.D.** in Bio-Inorganic Chemistry, Stanford University, CA, anticipated Spring 2006
Thesis: "Oxygen Intermediates in Mononuclear Non-Heme Iron Systems: Spectroscopy and Electronic Structure Calculations"
Advisor: Professor Edward I. Solomon
- **Diplom** in Chemistry, Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen, Germany, 1999
Thesis: "Quantum Chemical Investigations into Antiferromagnetism"
Advisor: Professor Richard Dronskowski

Research Experience

2000 – present Graduate Research, Stanford University, CA; with Prof. E. I. Solomon

Studied structure-function correlation in metallo-enzymes

- Modeled the kinetics and thermodynamics of enzymatic reaction mechanisms and analyzed the electronic structures and bonding of oxygen intermediates in iron enzymes and biomimetic model complexes using density functional theory (DFT) (Gaussian and ADF program packages)
- Experimentally characterized the electronic structures of enzyme intermediates and model complexes using a variety of spectroscopic techniques: UV/Vis absorption, magnetic circular dichroism (MCD), electron paramagnetic resonance, and resonance raman; developed new MCD methodology for high-valent Fe(IV)-oxo systems
- Improved techniques for preparation of air- and temperature-sensitive biochemical samples

1999 Diplom Research, RWTH Aachen, Germany; with Prof. R. Dronskowski

- Developed a qualitative model for the origins of antiferromagnetism in crystalline solids using electronic band-structure calculations (YAeHMOP and LMTO program packages)

1997 – 1998 Undergraduate Research, RWTH Aachen, Germany

- Investigated the electronic structures of transition metal oxides (Theoretical solid state chemistry, with Prof. R. Dronskowski)
- Optimized process parameters for Syngas conversion on heterogeneous catalysts (Technical chemistry, with Prof. W. Keim)

1995 – 1996 Undergraduate Research, University of Leeds, UK; with Prof. K. Bartle

- Designed methods for essential oil fractionation using supercritical fluids

Teaching Experience

2000 – present Department of Chemistry, Stanford University

- Trained and supervised younger PhD students
- As Teaching Assistant taught small-group sessions, tutored students one-on-one, set up and supervised lab work, prepared and presented review sessions, wrote and supervised exams, and graded homework, lab reports and exams. Specific courses include: graduate-level physical inorganic chemistry (Winter 2004); undergraduate general and advanced inorganic chemistry (2000-2002); introductory organic chemistry laboratory (Spring 2001)

Language Skills

- German: Native speaker
- English: Written and oral fluency
- Spanish, French: Basic writing and conversational skills

Publications

12. **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**, accepted.
11. **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**, in press.
10. 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." *Biochem. Biophys. Res. Commun.* **2005**, 338, 206-214.
9. **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, 152-163.
8. **Decker, A.**; Solomon, E.I.: "Comparison of Fe(IV)=O Heme and Non-Heme Species: Electronic Structures, Bonding, and Reactivities." *Angew. Chem.* **2005**, 117, 2292-2295; *Angew. Chem. Int. Ed.* **2005**, 44, 2252-2255.
7. **Decker, A.**; Rohde, J.-U.; Que, L.; 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, 5378-5379.
6. Solomon, E.I.; **Decker, A.**; Lehnert, N.: "Non-heme iron enzymes: Contrasts to heme catalysis." *Proc. Natl. Acad. Sci. U. S. A.* **2003**, 100, 3589-3594.
5. 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 extradiol dioxygenases." *J. Am. Chem. Soc.* **2003**, 125, 11214-11227.
4. 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.: "Spectroscopic studies of the interaction of ferrous bleomycin with DNA." *J. Am. Chem. Soc.* **2003**, 125, 10810-10821.
3. **Decker, A.**; Landrum, G.A.; Dronskowski, R.: "Structural and electronic Peierls distortions in the elements (A): The crystal structure of tellurium." *Z. Anorg. Allg. Chem.* **2002**, 628, 295-302.
2. **Decker, A.**; Landrum, G.A.; Dronskowski, R.: "Structural and electronic Peierls distortions in the elements (B): The antiferromagnetism of chromium." *Z. Anorg. Allg. Chem.* **2002**, 628, 303-309.
1. Liu, X.H.; **Decker, A.**; Schmitz, D.; Dronskowski, R.: "Crystal structure refinement of lead cyanamide and the stiffness of the cyanamide anion." *Z. Anorg. Allg. Chem.* **2000**, 626, 103-105.

Oral and Poster Presentations

5. "Oxygen Intermediates in Mononuclear Non-Heme Iron Sites: Electronic Structures, Reactivities and Comparison to Heme Systems." Oral presentation at the 10th Gordon Graduate Research Seminar on Bioinorganic Chemistry, Ventura, CA, **2005**.
4. "Mononuclear Non-Heme Fe(IV)=O Systems: Electronic Structures and Comparison to Heme and Copper Species." Poster presentation at the 12th International Conference on Biological Inorganic Chemistry (ICBIC), Ann Arbor, MI, **2005**.
3. "Oxygen intermediates in mononuclear non-heme iron sites: Electronic structure and reactivity." Poster presentation at the 227th National Meeting of the American Chemical Society (ACS), Anaheim, CA, **2004**.
2. "Computational Bioinorganic Chemistry: Interaction of Non-Heme Iron Enzymes with Dioxygen." Poster presentation at the 4th Biomedical Computation@Stanford (BCATS) Symposium, Stanford, CA, **2003**.
1. "Interactions of mononuclear non-heme iron sites with dioxygen: Studies on electronic structure and reactivity." Poster presentation at the 11th International Conference on Biological Inorganic Chemistry (ICBIC), Cairns, Australia, **2003**.

References

Available upon request.