Stanford



Daniel Stack

Associate Professor of Chemistry

CONTACT INFORMATION

- **Administrative Contact**

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Bio

BIO

Research in the Stack group focuses on the mechanism of dioxygen activation and the subsequent oxidative reactivity with primarily copper complexes ligated by imidazoles or histamines. Specifically, the group is interested in substrate hydroxylations and full dioxygen reduction. The remarkable specificity and energy efficiency of metalloenzymes provide the inspiration for the work. Trapping and characterizing immediate species, primarily at low temperatures, provide key mechanistic insights especially through substrate reactivity along with spectroscopic and metrical correlation to DFT calculations. Our objective is to move these efficient enzymatic mechanisms into small synthetic complexes, not only to reproduce biological reactivity, but more importantly to move the oxidative mechanism beyond that possible in the protein matrix.

Daniel Stack was born, raised and attended college in Portland Oregon. He received his B.A. from Reed College in 1982 (Phi Beta Kappa), working with Professor Tom Dunne on weak nickel-pyrazine complexes. In Boston, he pursued his doctoral study in synthetic inorganic chemistry at Harvard University (Ph.D., 1988) with Professor R. H. Holm, investigating site-differentiated synthetic analogues of biological Fe4S4 cubanes. As an NSF Postdoctoral Fellow with Professor K. N. Raymond at the University of California at Berkeley, he worked on synthesizing new, higher iron affinity ligands similar to enterobactin, a bacterial iron sequestering agent. He started his independent career in 1991 at Stanford University primarily working on oxidation catalysis and dioxygen activation, and was promoted to an Associate Professor in 1998. His contributions to undergraduate education have been recognized at the University level on several occasions, including the Dinkelspiel Award for Outstanding Contribution to Undergraduate Education in 2003.

Areas of current focus include:

Copper Dioxygen Chemistry

Our current interests focus on stabilizing species formed in the reaction of dioxygen with Cu(I) complexes formed with biologically relevant imidazole or histamine ligation. Many multi-copper enzymes ligated in this manner are capable of impressive hydroxylation reactions, including oxidative depolymerization of cellulose, methane oxidation, and energy-efficient reduction of dioxygen to water. Oxygenation of such complexes at extreme

solution temperatures (-125°C) yield transient Cu(III) containing complexes. As Cu(III) is currently uncharacterized in any biological enzyme, developing connections between the synthetic and biological realms is a major focus.

ACADEMIC APPOINTMENTS

- Associate Professor, Chemistry

HONORS AND AWARDS

- Dinkelspiel Award for Outstanding Contribution to Undergraduate Education, Stanford University (2003)
- Hoefer Teaching Award, Stanford University (1997)
- Bing Foundation Teaching Award, Stanford University (1995-98)
- Shell Foundation New Faculty Award, Shell Foundation (1993-95)
- Harvard Danforth Distinguished Teaching Award, Harvard University (1983, 1984)

PROFESSIONAL EDUCATION

- NSF Postdoctoral Fellow, University of California at Berkeley , Inorganic Chemistry (1988)
- PhD, Harvard University , Inorganic Chemistry (1988)
- BA, Reed College , Chemistry (1982)

LINKS

- Stack Research Group: http://stacklab.stanford.edu/

Teaching

COURSES

2026-27

- Inorganic Chemistry I: CHEM 151 (Win)

2025-26

- Inorganic Chemistry I: CHEM 151 (Win)

2024-25

- Inorganic Chemistry I: CHEM 151 (Win)

2023-24

- Inorganic Chemistry I: CHEM 151 (Win)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Ben Charnay, Emma Choy, Jason Misleh

Doctoral Dissertation Advisor (AC)

Ricky Hage, Viet Tran

Publications

PUBLICATIONS

- **Imidazolate-Stabilized Cu(III): Dioxygen to Oxides at Type 3 Copper Sites.** *Angewandte Chemie (International ed. in English)*
  Large, T. A., Keown, W., Gary, J. B., Chiang, L., Stack, T. D.

2024: e202416967

- **Fast and Versatile Functionalization of Glassy Carbon.** *Langmuir : the ACS journal of surfaces and colloids*
  Ainsworth, J., Cook, T. C., Stack, T. D.
  2022
- **Phenolate-bonded bis(μ-oxido)-bis-copper(III) intermediates: hydroxylation and dehalogenation reactivities.** *Faraday discussions*
  Kang, P., Lin, B. L., Large, T. A., Ainsworth, J., Wasinger, E. C., Stack, T. D.
  2022
- **Electrocatalytic alcohol oxidation by covalently immobilized ruthenium complex on carbon.** *Journal of inorganic biochemistry*
  Cook, T. C., Stenehjem, E. D., Ainsworth, J., Stack, T. D.
  2022; 231: 111784
- **Selective Oxidation of Exogenous Substrates by a Bis-Cu(III) Bis-Oxide Complex: Mechanism and Scope.** *Inorganica chimica acta*
  Large, T. A., Mahadevan, V., Keown, W., Stack, T. D.
  2019; 486: 782-792
- **Exclusive imidazole ligation to CuO2 and CuIIICuO2 cores.** *Chemical communications (Cambridge, England)*
  Keown, W. n., Large, T. A., Chiang, L. n., Wasinger, E. C., Stack, T. D.
  2019
- **Electronic Structure and Reactivity Studies of a Nonsymmetric One-Electron Oxidized CuII Bis-phenoxide Complex.** *Inorganica chimica acta*
  Chiang, L., Wasinger, E. C., Shimazaki, Y., Young, V., Storr, T., Stack, T. D.
  2018; 481: 151-158
- **Simplest Monodentate Imidazole Stabilization of the oxy-Tyrosinase Cu2 O2 Core: Phenolate Hydroxylation through a Cu(III) Intermediate.** *Angewandte Chemie (International ed. in English)*
  Chiang, L., Keown, W., Citek, C., Wasinger, E. C., Stack, T. D.
  2016; 55 (35): 10453-10457
- **Direct Copper(III) Formation from O2 and Copper(I) with Histamine Ligation.** *Journal of the American Chemical Society*
  Gary, J. B., Citek, C., Brown, T. A., Zare, R. N., Wasinger, E. C., Stack, T. D.
  2016; 138 (31): 9986-9995
- **Manganese(II)/Picolinic Acid Catalyst System for Epoxidation of Olefins** *ORGANIC LETTERS*
  Moretti, R. A., Du Bois, J., Stack, T. D.
  2016; 18 (11): 2528-2531
- **Metal complex assembly controlled by surface ligand distribution on mesoporous silica: Quantification using refractive index matching and impact on catalysis** *JOURNAL OF CATALYSIS*
  Smith, B. J., Gallegos, P. A., Butsch, K., Stack, T. D.
  2016; 335: 197-203
- **Formation of hybrid guanidine-stabilized bis(μ-oxo)dicopper cores in solution: Electronic and steric perturbations.** *European journal of inorganic chemistry*
  Herres-Pawlis, S., Haase, R., Verma, P., Hoffmann, A., Kang, P., Stack, T. D.
  2015; 2015 (32): 5426-5436
- **Sequential "click" functionalization of mesoporous titania for energy-relay dye enhanced dye-sensitized solar cells** *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*
  Unger, E. L., Fretz, S. J., Lim, B., Margulis, G. Y., McGehee, M. D., Stack, T. D.
  2015; 17 (9): 6565-6571
- **Primary amine stabilization of a dicopper(III) bis(μ-oxo) species: modeling the ligation in pMMO.** *Journal of the American Chemical Society*
  Citek, C., Lin, B. L., Phelps, T. E., Wasinger, E. C., Stack, T. D.
  2014; 136 (41): 14405-8
- **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

- **Squish and CuAAC: Additive-Free Covalent Mono layers of Discrete Molecules in Seconds** *LANGMUIR*
  Pellow, M. A., Stack, T. D., Chidsey, C. E.
  2013; 29 (18): 5383-5387
- **Gas-Phase Azide Functionalization of Carbon** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Stenehjem, E. D., Ziatdinov, V. R., Stack, T. D., Chidsey, C. E.
  2013; 135 (3): 1110-1116
- **Recent advances in phenoxyl radical complexes of salen-type ligands as mixed-valent galactose oxidase models.** *Coordination chemistry reviews*
  Lyons, C. T., Stack, T. D.
  2013; 257 (2): 528-540
- **Catalytic Phenol Hydroxylation with Dioxygen: Extension of the Tyrosinase Mechanism beyond the Protein Matrix** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
  Hoffmann, A., Citek, C., Binder, S., Goos, A., Ruebhausen, M., Troeppner, O., Ivanovic-Burmazovic, I., Wasinger, E. C., Stack, T. D., Herres-Pawlis, S.
  2013; 52 (20): 5398-5401
- **Self-assembly of the oxy-tyrosinase core and the fundamental components of phenolic hydroxylation** *NATURE CHEMISTRY*
  Citek, C., Lyons, C. T., Wasinger, E. C., Stack, T. D.
  2012; 4 (4): 317-322
- **Deposition of Dense Siloxane Monolayers from Water and Trimethoxyorganosilane Vapor** *LANGMUIR*
  Lowe, R. D., Pellow, M. A., Stack, T. D., Chidsey, C. E.
  2011; 27 (16): 9928-9935
- **Unexpected C(carbene)-X (X: I, Br, Cl) Reductive Elimination From N-Heterocyclic Carbene Copper Halide Complexes Under Oxidative Conditions.** *Organometallics*
  Lin, B. L., Kang, P., Stack, T. D.
  2010; 29 (17): 3683-3685
- **Detailed Evaluation of the Geometric and Electronic Structures of One-Electron Oxidized Group 10 (Ni, Pd, and Pt) Metal(II)-(Disalicylidene)diamine Complexes** *INORGANIC CHEMISTRY*
  Shimazaki, Y., Stack, T. P., Storr, T.
  2009; 48 (17): 8383–92
- **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
- **Structure and spectroscopy of copper-dioxygen complexes** *CHEMICAL REVIEWS*
  Mirica, L. M., Ottenwaelder, X., Stack, T. D.
  2004; 104 (2): 1013-1045
- **Efficient epoxidation of electron-deficient olefins with a cationic manganese complex** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Murphy, A., Dubois, G., Stack, T. D.
  2003; 125 (18): 5250-5251
- **C-H bond activation by a ferric methoxide complex: Modeling the rate-determining step in the mechanism of lipoxygenase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Goldsmith, C. R., Jonas, R. T., Stack, T. D.
  2002; 124 (1): 83-96
- **Aryl C-H activation by Cu-II to form an organometallic Aryl-Cu-III species: A novel twist on copper disproportionation** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
  Ribas, X., JACKSON, D. A., Donnadieu, B., Mahia, J., Parella, T., Xifra, R., Hedman, B., Hodgson, K. O., Llobet, A., Stack, T. D.
  2002; 41 (16): 2991-2994

- **Stereospecificity and self-selectivity in the generation of a chiral molecular tetrahedron by metal-assisted self-assembly** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
  Enemark, E. J., Stack, T. D.
  1998; 37 (7): 932-935

- **Ligand Self-Recognition in the Self-Assembly of a [{Cu(L)}2]2+ Complex: The Role of Chirality.** *Angewandte Chemie (International ed. in English)*
  Masood, M. A., Enemark, E. J., Stack, T. D.
  1998; 37 (7): 928-932

- **Stereospecificity and Self-Selectivity in the Generation of a Chiral Molecular Tetrahedron by Metal-Assisted Self-Assembly.** *Angewandte Chemie (International ed. in English)*
  Enemark, E. J., Stack, T. D.
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- **Catalytic galactose oxidase models: Biomimetic Cu(II)-phenoxyl-radical reactivity** *SCIENCE*
  Wang, Y. D., Dubois, J. L., Hedman, B., Hodgson, K. O., Stack, T. D.
  1998; 279 (5350): 537-540

- **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

- **C-H bond activation by a ferric methoxide complex: A model for the rate-determining step in the mechanism of lipoxygenase** *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*
  Jonas, R. T., Stack, T. D.
  1997; 119 (36): 8566-8567

- **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