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## Publications

### PUBLICATIONS

- **Deciphering decomposition pathways of high explosives with cryogenic X-ray Raman spectroscopy.** *Proceedings of the National Academy of Sciences of the United States of America*
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- **Spectroscopy and crystallography define carotenoid oxygenases as a new subclass of mononuclear non-heme FeII enzymes.** *The Journal of biological chemistry*
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- **Determination of Thiol Protonation States by Sulfur X-ray Spectroscopy in Biological Systems** *JOURNAL OF PHYSICAL CHEMISTRY LETTERS*
  Ribson, R. D., Follmer, A. H., Babicz, J. T., Alfaro, V., Hadt, R. G., Hunter, M. S., Wilson, M. A., Sokaras, D., Alonso-Mori, R.
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- **Experimental electronic structures of the FeIV=O bond in S=1 heme vs. nonheme sites: Effect of the porphyrin ligand.** *Proceedings of the National Academy of Sciences of the United States of America*
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- **Quantifying d-d and Metal–Ligand Interactions across Distant Metal Sites as a Function of Ligand Architecture and Solvent** *ChemPhysChem*
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- **Application of X-Ray Spectroscopic Techniques in X-Ray Free Electron Laser Facilities** *Encyclopedia of Inorganic and Bioinorganic Chemistry*
  Alfaro, V., Schleissner, P., Babicz, J. T., Dehe, S., Ribson, R. D., Gee, L. B.
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- **The Liquid Jet Endstation for Hard X-ray Scattering and Spectroscopy at the Linac Coherent Light Source.** *Molecules (Basel, Switzerland)*
  Antolini, C., Sosa Alfaro, V., Reinhard, M., Chatterjee, G., Ribson, R., Sokaras, D., Gee, L., Sato, T., Kramer, P. L., Raj, S. L., Hayes, B., Schleissner, P., Garcia-Esparza, et al
  2024; 29 (10)

- **Nuclear Resonance Vibrational Spectroscopy Definition of Peroxy Intermediates in Catechol Dioxygenases: Factors that Determine Extra- versus Intradiol Cleavage.** *Journal of the American Chemical Society*
  Babicz, J. T., Rogers, M. S., DeWeese, D. E., Sutherlin, K. D., Banerjee, R., Bottger, L. H., Yoda, Y., Nagasawa, N., Saito, M., Kitao, S., Kurokuzu, M., Kobayashi, Y., Tamasaku, et al
  2023

- **Mechanisms of O2 Activation by Mononuclear Non-Heme Iron Enzymes.** *Biochemistry*
  Solomon, E. I., DeWeese, D. E., Babicz, J. T.
  2021

- **Direct coordination of pterin to FeII enables neurotransmitter biosynthesis in the pterin-dependent hydroxylases.** *Proceedings of the National Academy of Sciences of the United States of America*

Iyer, S. R., Tidemand, K. D., Babicz, J. T., Jacobs, A. B., Gee, L. B., Haahr, L. T., Yoda, Y., Kurokuzu, M., Kitao, S., Saito, M., Seto, M., Christensen, H. E., Peters, et al

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- **Nuclear Resonance Vibrational Spectroscopic Definition of the Fe(IV)2 Intermediate Q in Methane Monooxygenase and Its Reactivity.** *Journal of the American Chemical Society*

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- **Valence-Dependent Electrical Conductivity in a 3D Tetrahydroxyquinone-Based Metal-Organic Framework.** *Journal of the American Chemical Society*

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- **Evaluation of a concerted vs. sequential oxygen activation mechanism in α-ketoglutarate-dependent nonheme ferrous enzymes.** *Proceedings of the National Academy of Sciences of the United States of America*

  Goudarzi, S. n., Iyer, S. R., Babicz, J. T., Yan, J. J., Peters, G. H., Christensen, H. E., Hedman, B. n., Hodgson, K. O., Solomon, E. I.

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- **Mechanism of selective benzene hydroxylation catalyzed by iron-containing zeolites** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*

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- **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*

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- **Correlating the structures and activities of the resting oxidized and native intermediate states of a small laccase by paramagnetic NMR** *JOURNAL OF INORGANIC BIOCHEMISTRY*

  Machczynski, M. C., Babicz, J. T.

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