

## Jeffrey Babicz

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### Publications

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#### 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*  
Paredes Mellone, O. A., Nielsen, M. H., Babicz, J. T., Vinson, J., Willey, T. M., Sokaras, D.  
2025; 122 (23): e2426320122
- **Spectroscopy and crystallography define carotenoid oxygenases as a new subclass of mononuclear non-heme FeII enzymes.** *The Journal of biological chemistry*  
DeWeese, D. E., Everett, M. P., Babicz, J. T., Daruwalla, A., Solomon, E. I., Kiser, P. D.  
2025: 108444
- **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.  
2025; 16 (9): 2401-2408
- **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*  
Braun, A., Gee, L. B., Waters, M. D., Jose, A., Baker, M. L., Mara, M. W., Babicz, J. T., Ehudin, M. A., Quist, D. A., Zhou, A., Kroll, T., Titus, C. J., Lee, et al  
2025; 122 (8): e2420205122
- **Quantifying d-d and Metal–Ligand Interactions across Distant Metal Sites as a Function of Ligand Architecture and Solvent** *ChemPhysChem*  
Yang, Z., et al  
2025
- **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.  
2025
- **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 Extraversus 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 O<sub>2</sub> 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  
2021; 118 (15)
- **Nuclear Resonance Vibrational Spectroscopic Definition of the Fe(IV)2 Intermediate Q in Methane Monooxygenase and Its Reactivity.** *Journal of the American Chemical Society*  
Jacobs, A. B., Banerjee, R., Deweese, D. E., Braun, A., Babicz, J. T., Gee, L. B., Sutherlin, K. D., Böttger, L. H., Yoda, Y., Saito, M., Kitao, S., Kobayashi, Y., Seto, et al  
2021
  - **Valence-Dependent Electrical Conductivity in a 3D Tetrahydroxyquinone-Based Metal-Organic Framework.** *Journal of the American Chemical Society*  
Chen, G., Gee, L. B., Xu, W., Zhu, Y., Lezama-Pacheco, J. S., Huang, Z., Li, Z., Babicz, J. T., Choudhury, S., Chang, T., Reed, E., Solomon, E. I., Bao, et al  
2020
  - **Evaluation of a concerted vs. sequential oxygen activation mechanism in  $\alpha$ -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.  
2020
  - **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. R., 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., Hedman, et al  
2018; 115 (48): 12124–29
  - **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.  
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  - **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
  - **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.  
2016; 159: 62-69