

**KATHERINE M. DAVIS**

DEPARTMENT OF CHEMISTRY • 1515 DICKEY DR • ATLANTA, GA 30322

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**EDUCATION**

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- 2014**            **Ph.D. Physics**  
Purdue University, West Lafayette, IN
- 2011**            **M.S. Physics**  
Purdue University, West Lafayette, IN
- 2009**            **B.S. Physics & Mathematics** (Summa Cum Laude)  
Minor in French  
University of Louisville, Louisville, KY

**ACADEMIC POSITIONS**

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- 2020 –**            **Emory University**, Atlanta, GA  
Assistant Professor, Department of Chemistry  
*Affiliated Member:* Department of Physics Graduate Program
- 2016 – 2019**    **Princeton University**, Princeton, NJ  
Postdoctoral Fellow, Department of Chemistry  
Advisor: Prof. John T. Groves
- The Pennsylvania State University**, State College, PA  
Postdoctoral Fellow, Department of Chemistry  
Co-advisor: Prof. Amie Boal
- Project: Structure and mechanism of iron-containing enzymes and biomimetic complexes
- 2014 – 2016**    **Princeton University**, Princeton, NJ  
Postdoctoral Fellow, Department of Chemistry  
Advisor: Prof. Nozomi Ando
- Project: X-ray structural methods to study radical SAM enzymes
- 2009 – 2014**    **Purdue University**, West Lafayette, IN  
Graduate Student, Department of Physics and Astronomy  
Advisor: Prof. Yulia Pushkar
- Thesis: Oxidation state and local structure of the photosynthetic Mn<sub>4</sub>Ca catalytic cluster revealed via time-resolved x-ray spectroscopy
- 2008 – 2009**    **University of California Irvine**, Irvine, CA  
Undergraduate Research Assistant through NSF REU program  
Department of Earth System Science  
Advisor: Prof. Todd K. Dupont
- Undergraduate Thesis (completed at the University of Louisville): Control methods and inversion techniques to determine ice stream basal friction fields
- 2007**            **University of Louisville**, Louisville, KY  
Undergraduate Research Assistant, Department of Physics and Astronomy  
Advisors: Dr. Lutz G Haberzettl, and Prof. Gerard M. Williger
- Project: Data reduction of near-IR images in the Clowes-Campusano large quasar group

## FELLOWSHIPS AND AWARDS

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<b>2022</b>	ESI MIRA Award (R35)
<b>2021</b>	Beckman Young Investigator Award
<b>2018</b>	NIH Pathway to Independence Award (K99/R00)
<b>2015 – 2018</b>	Arnold O. Beckman Postdoctoral Fellowship
<b>2014</b>	Humboldt Postdoctoral Research Fellowship (awarded, but declined)
<b>2012</b>	Lijuan Wang Memorial Award – outstanding female graduate student (Purdue)
<b>2011 – 2014</b>	National Science Foundation Graduate Research Fellowship
<b>2009 – 2011</b>	Purdue Doctoral Fellowship
<b>2009</b>	Bennett Award in Physics – awarded to an outstanding senior in physics (U of L)
<b>2008</b>	Sigma Pi Sigma Physics Honors Society (U of L)
<b>2007</b>	Bullitt Award in Mathematics – awarded to the most promising math major (U of L)
<b>2007</b>	Pi Mu Epsilon Mathematics Honors Society (U of L)
<b>2005 – 2009</b>	Grawemeyer Scholarship (U of L)

## GRANTS

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### PI, Co-PI, and Co-I

#### Ongoing

<b>NIH R35 GM147557</b>	(ESI MIRA)	09/2022 – 08/2027
<i>Unraveling the dynamics that enable unusual heme enzyme reactivity</i>		
Role: PI	\$250,000/year direct costs	\$1.66 million total
<b>Supplement (to NIH R35) for equipment</b>		06/2024 – 05/2025
Role: PI	\$113,260 one time direct	\$113,260 total
<b>Beckman Young Investigator Award</b>		09/2021 – 08/2025
<i>X-rays shine light on the synergy between metalloenzyme structure and electronics</i>		
Role: PI	\$150,000/year direct costs	\$600,000 total

#### Completed

<b>Supplement (to NIH R35) for equipment</b>		06/2023 – 05/2024
Role: PI	\$85,000 one time direct	\$85,000 total
<b>Supplement (to NIH R35) for undergrad summer research</b>		06/2023 – 05/2024
Role: PI	\$6,959 one time direct	\$10,891 total
<b>NIH K99/R00 GM129460</b> (Pathway to Independence Award)		09/2018 – 05/2023
<i>Learning the Steps to Metalloenzyme Choreography</i>		
Role: PI	\$249,000/year total costs (R00)	\$747,000 total

#### Pending

<b>Sloan Research Fellowship</b>		09/2025 – 08/2027
Role: PI	\$75,000 one time direct	\$75,000 total

#### Not funded

<b>Halle Institute Collaborative Partnership Research Grant</b>		09/2024 – 08/2026
Role: PI	\$5,000/year direct costs	\$10,000 total
<b>Camille-Dreyfus Teacher Scholar Award</b>		09/2024 – 09/2029
<i>Investigating the structural and mechanistic features that enable atypical metalloenzyme reactivities.</i>		
Role: PI	\$100,000 one time direct	\$100,000 total
<b>Cottrell Scholars Program</b>		09/2024 – 09/2027
Role: PI	\$40,000/year direct costs	\$120,000 total

<b>ACS Petroleum Research Fund</b> (declined on technicality)	01/2024 – 12/2025
Role: Co-PI                      \$31,250/year direct costs	\$62,500 total
<b>HHMI Freeman Hrabowski Scholars Program</b>	09/2023 – 08/2028
Role: PI                              \$400,000/year direct costs	\$2 million total
<b>NIH R01</b>	07/2023 – 06/2028
Role: Co-I                              \$250,000/year direct costs	\$1,956,250 total
<b>Pew Biomedical Scholars Program</b>	08/2021 – 07/2025
Role: PI                              \$75,000/year total costs	\$300,000 total
<b>Searle Scholars Program</b>	07/2021 – 06/2024
Role: PI                              \$100,000/year total costs	\$300,000 total

Other*Ongoing*

<b>NIH IMSD T32</b>	09/2022 – 08/2027
Role: Faculty Preceptor	
<b>NIH BDCI T32</b>	09/2023 – 08/2028
Role: Faculty Preceptor	
<b>NSF REU Site Application</b>	05/2025 – 04/2028
Role: Key Personnel	

*Completed*

<b>NIH ORIP S10 Instrumentation Grant</b> (for the APS)	01/2023 – 12/2023
Role: Key Personnel	

*Pending*

n/a

*Not funded*

<b>NIH MARC T34</b>	06/2023 – 05/2028
Role: Faculty Preceptor	
<b>NSF REU Site Application</b>	05/2023 – 04/2026 & 05/2022 – 04/2025
Role: Key Personnel	
<b>DOE EFRC</b>	12/2022 – 11/2026
Role: Key Personnel	
<b>Beckman Scholars Institutional Application</b>	06/2022 – 05/2025
Role: Key Personnel	
<b>NIH R24</b>	06/2021 – 05/2022
Role: Key Personnel	

**PUBLICATIONS**

**Journal Impact Factors (2023):** *Nature* (50.5), *Nat. Chem.* (19.2), *J. Am. Chem. Soc.* (14.4), *Nat. Chem. Bio.* (12.9), *Phys. Rev. X* (11.6), *Redox Biol.* (10.7), *P. Natl. Acad. Sci. USA* (9.4), *eLife* (6.4), *J. Thromb. Haemost.* (5.5), *J. Phys. Chem. Lett.* (4.8), *Structure* (4.4), *RSC Chem. Biol.* (4.2), *Molecules* (4.2), *Sci. Rep.* (3.8), *ACS Chem. Biol.* (3.5), *J. Phys. Chem. C* (3.3), *Biochemistry* (2.9), *J. Phys. Chem. B* (2.8), *Methods Enzymol.* (1.7)

*Corresponding authorship is indicated with an asterisk. Members of my group are underlined. Authors marked with a † contributed equally. All publications are peer-reviewed unless otherwise specified in the comments.*

1. McWhorter, K. L.; Ambarian, J. A.; Purohit, V.; Jhunjunwala, R.; **Davis, K. M.\*** Common chemical logic via alkylperoxy intermediates in mononuclear iron systems. (**in preparation – invited submission due October**).
2. Wu, K.; McWhorter, K. L.; Wan, Y.; Ford, A.; Phillips, E.; Tan, L.; Waidmann, L.; Vazquez Hernandez, J.; **Davis, K. M.\***; Li, G.\* Streamlined Synthesis of  $\alpha$ -Amino Esters via Co-Catalyzed Carbene Insertion into N–H Bonds. (**in preparation – anticipated submission October**).
3. Ireland, K. A.<sup>†</sup>; Kayrouz, C. M.<sup>†</sup>; Abbott, M. L.; Seyedsayamdost, M. R.; **Davis, K. M.\*** Comparative Analysis of SAM-Dependent N-Methyltransferases in Ovoselenol and Ovothiol Biosynthesis: Structural and Phylogenetic Perspectives (**in preparation – anticipated submission October**).
4. Blue, T. C.; Jones, S. K.; **Davis, K. M.\*** Bioinformatic and biochemical analysis of OYEBi uncovers novel N-methyl-proline demethylase activity in the OYE 2-ER Family (**in preparation – anticipated submission October**).

1. York, E. S.; Dratch, B. D.; Ito, J.; Horwitz, S. M.; Ambarian, J. A.; Emamian, S.; Gill, S.; Jones, J.; Chonat, S.; Lollar, P.; Meeks, S. L.; **Davis, K. M.\***; Batsuli, G.\* Persistent polyclonal splenic-derived Factor VIII-specific IgM recognize C2 domain epitopes and mediate inhibitor development. (**in revision at J. Thromb. Haemost.**).

*Contribution:* My group was responsible for molecular docking analyses to predict differences in the binding modes of thirteen unique IgM antibodies to FVIII. Our results were complementary to assays performed by the Batsuli Lab and provided crucial support for their less conclusive fluid-phase ELISA data critical for the conclusions of the manuscript.

2. Sharma, M.; Pascoe, C. A.; Jones, S. K.; **Davis, K. M.\***; Biegasiwicz, K. F.\* Intermolecular Heterocycle Synthesis Enabled by Enzymatic Halide Recycling with Vanadium-Dependent Haloperoxidases (**in revision**).

*Contribution:* My group was responsible for molecular docking simulations important for rationalizing observed differences in reactivity between substrates and provide support for the proposed mechanism. A preprint of this manuscript can be found at <https://doi.org/10.26434/chemrxiv-2024-jptl>.

3. Marques Netto, C. G. C.\*; Bell, S.; Castro, C. B.; Machado, P. H.; Purohit, V.; **Davis, K. M.**; Batista, A P. L.; Dyer, R. B.\* Photo-controlled release of urea enables the detection of urea-urease intermediates by cryo-FTIR. (**submitted**).

*Contribution:* My group provided supporting data confirming additionally validating the utility of caged urea for initiating catalysis within urease, as well as assistance with manuscript preparation.

4. Nguy, A. K. L.<sup>†</sup>; Ireland, K. A.<sup>†</sup>; Kayrouz, C. M.<sup>†</sup>; Cáceres, J. C.; Greene, B. L.; **Davis, K. M.**; Seyedsayamdost, M. R.\* Non-Canonical Cytochrome P450 Enzymes in Nature. (**submitted**).

*Contribution:* My group was responsible for all structural characterization of the enzymes, without which there would be no direct evidence for non-canonical features. These contributions are complementary to the Seyedsayamdost lab's bioinformatic identification of these unusual P450s, and were critical to the conclusions of the manuscript.

1. Zhang, Y.; McWhorter, K. L.; Rosen, Paul C.; Klaus, Jennifer R.; Gallant, Étienne; Amayz Lopez, C.; Jhunjunwala, R.; Chandler, Josephine, R.; **Davis, K. M.\***; Seyedsayamdost, M. R.\* Combatting Melioidosis with Chemical Synthetic Lethality. (**accepted at PNAS**).

*Contribution:* My group was responsible for all structural characterization of FolE2 without which, there would be no direct evidence for covalent inhibition of the enzyme by DHL. These contributions are complementary to the Seyedsayamdost lab's identification of both the enzyme as a drug target and DHL as an inhibitor, and were critical for the conclusions of the manuscript.

2. Ireland, K. A.<sup>†</sup>; Kayrouz, C. M.<sup>†</sup>; Abbott, M. L.; Seyedsayamdost, M. R.; **Davis, K. M.**\* Structural insights into the convergent evolution of type IV sulfoxide synthase EgtB, an ergothioneine-biosynthetic homolog of ovothiol synthase OvoA. *Structure* **2024**, Article ASAP. <https://doi.org/10.1016/j.str.2024.08.006>.

*Contribution:* All aspects of this publication were completed by my group, excluding protein purification and simple activity assays in support of our conclusions, which were provided by the Seyedsayamdost lab. We solved five structures of two representative EgtB-IV enzymes, analyzed the associated data, and drafted the manuscript.

3. Kayrouz, C. M.<sup>†</sup>; Ireland, K. A.<sup>†</sup>; Ying, V.; **Davis, K. M.**; Seyedsayamdost, M. R.\* Ovoselenol, a Selenium-containing Antioxidant Derived from Convergent Evolution. *Nature Chem.* **2024**, Article ASAP. <https://doi.org/10.1038/s41557-024-01600-2>.

*Contribution:* My group was responsible for all structural biology experiments included in this publication critical for understanding substrate specificity and regioselectivity. We solved two structures of wild-type OvsA and one structure of an engineered OvsA variant, analyzed all associated data, and helped draft the manuscript.

Note: A previous version of this manuscript was posted (April 10<sup>th</sup>, 2024) without peer-review on the pre-print server BioRxiv: <https://www.biorxiv.org/content/10.1101/2024.04.10.588772v1>.

4. Chioti, V.<sup>†</sup>; McWhorter, K. L.<sup>†</sup>; Blue, T. C.; Li, Y.; Xu, F.; Jeffrey, P.; **Davis, K. M.**\*; Seyedsayamdost, M. R.\* Potent and Specific Antibiotic Combination Therapy Against *Clostridioides difficile*. *Nature Chem. Biol.* **2024**, *20*, 924-933.

*Contribution:* My group performed all structural characterization of the natural products, as well as computational docking, DFT and MD simulations essential for demonstrating how these molecules bind to differing targets despite sharing the same privileged scaffold. This is an essential and equal contribution to that of the Seyedsayamdost Lab.

Note: A previous version of this manuscript containing our initial results was posted without peer-review on the pre-print server ChemRxiv in 2021 (below).

Chioti, V. T.<sup>†</sup>; McWhorter, K. L.<sup>†</sup>; Blue, T. C.; Xu, F.; Jeffrey, P. D.; **Davis, K. M.**\*; Seyedsayamdost, M. R.\* Structural and Functional Analysis of Keratinicyclin Reveals Synergistic Antibiosis with Vancomycin against *Clostridium difficile*. *ChemRxiv.* **2021**. Preprint. <https://doi.org/10.26434/chemrxiv.14668545>.

5. Maximova, O.; Allen, W.; Yee, G.; Israel, C.; Leshchev, D.; Stavitski, E.; Ding, Y.; **Davis, K. M.**; Wessells, C.; Friebel, D.; Pushkar, Y. Spectroscopic characterization of Mn<sup>1+</sup> low oxidation state in Prussian Blue based battery anodes. *J. Phys. Chem. Lett.* **2024**, *15*, 1521–1528.

*Contribution:* Collected, analyzed and prepared resonant inelastic scattering data and figures of manganese standards important for comparison to battery data.

6. Ireland, K. A.; Kayrouz, C. M.; Huang, J.; Seyedsayamdost, M. R.; **Davis, K. M.**\* Structural Characterization and Ligand-Induced Conformational Changes of SenB, a Se-Glycosyltransferase Involved in Selenoneine Biosynthesis. *Biochemistry.* **2023**, *62*, 3337-3342.

*Contribution:* All aspects of this publication were completed by my group, excluding protein purification and simple activity assays in support of our conclusions, which were provided by the Seyedsayamdost lab. We solved the structure of SenB, collected small angle x-ray scattering data to assess conformational changes, performed ligand-docking simulations, analyzed all associated data, and drafted the manuscript.

7. Dratch, B. D.; McWhorter, K. L.; Blue, T. C.<sup>†</sup>; Jones, S. K.<sup>†</sup>; Horwitz, S. M.; **Davis, K. M.**\* Insights into substrate recognition by the unusual nitrating enzyme RufO. *ACS Chem. Biol.* **2023**, *18*, 1713-1718.

*Contribution:* All aspects of this publication were completed by my group.

8. Hauser, N.; Ireland, K. A.; Chioti, V.; **Davis, K. M.**\*; Seyedsayamdost, M. R.\* Robust Chemoenzymatic Synthesis of the Keratinimicin Aglycone Facilitated by the Structure and Selectivity of OxyB. *ACS Chem. Biol.* **2023**, *18*, 1472-1479.

*Contribution:* My group solved the crystal structure of the relevant OxyB enzyme and identified key features important for understanding its utility in chemoenzymatic syntheses. This is an essential and equal contribution to that of the Seyedsayamdost Lab.

9. Emamian, S.; Ireland, K. A.<sup>†</sup>; Purohit, V.<sup>†</sup>; Maximova, O.; Allen, W.; McWhorter, K. L.; Jensen, S.; Casa, D. M.; Bury, G.; Pushkar, Y. N.\*; **Davis, K. M.**\* X-ray Emission Spectroscopy of Single Protein Crystals Yields Insights into Heme Enzyme Intermediates. *J. Phys. Chem. Lett.* **2023**, 1, 41-48.

*Contribution:* All aspects of this publication were completed by my group, excluding design and production of the spectrometer provided by the Pushkar group.

10. Braffman, N. R.<sup>†</sup>; Ruskoski, T. B.<sup>†</sup>; **Davis, K. M.**; Glasser, N.; Johnsona, C.; Okaforb, C. D.; Boal, A. K.; Balskus, E. P. Structural Basis for an Unprecedented Enzymatic Alkylation in Cylindrocyclophane Biosynthesis. *eLife*. **2022**, 11:e75761.

*Contribution:* This work is a continuation of a project I started as a postdoc in which I determined initial crystallization conditions for the enzyme CylK and designed key experiments required to phase the diffraction data and solve the structure.

11. Horwitz, S. M.; Blue, T. C.; Ambarian, J. A.; Hoshino, S.; Seyedsayamdost, M. R.; **Davis, K. M.**\* Structural Insights into Inhibition of the Drug Target Dihydroorotate Dehydrogenase by Bacterial Hydroxyalkylquinolines. *RSC Chem. Biol.* **2022**, 3, 420-425.

*Contribution:* All aspects of this publication were completed by my group, excluding purification of the natural product HMNQ provided by the Seyedsayamdost group.

*Note:* Nominated for the *RSC Chem. Biol.* 2022 Outstanding Paper Award.

12. Lau, S. H.; Chen, L.; Kevlishvili, I.; **Davis, K. M.**; Liu, P.; Carrow, B. P. Capturing the Most Active State of a Palladium(0) Cross-Coupling Catalyst. *ChemRxiv*. **2021**. Preprint. <https://doi.org/10.26434/chemrxiv-2021-477kn>.

*Contribution:* I designed, performed, and analyzed data from X-ray spectroscopy experiments in support of hypotheses developed by the Carrow lab.

*Note:* This publication has not yet been peer-reviewed. It currently resides on the ChemRxiv pre-print server.

13. Blue, T. C. & **Davis, K. M.**\* Computational Approaches: An Underutilized Tool in the Quest to Elucidate Radical SAM Dynamics. *Molecules*. **2021**, 26, 2590.

*Contribution:* All aspects of this publication were completed by my group.

14. Copeland, R. A.; **Davis, K. M.**; Shoda, T. K. C.; Blaesi, E. J.; Boal, A. K.; Krebs, C.; Bollinger, Jr., J. M. An Iron(IV)-oxo Intermediate Initiating L-Arginine Oxidation but not Ethylene Production by the 2-Oxoglutarate-Dependent Ethylene-Forming Enzyme (EFE). *J. Am. Chem. Soc.* **2021**, 143, 2293–2303.

*Contribution:* This work is a continuation of a project I started as a postdoc in which I assisted with crystallization, as well as solved and analyzed structures of EFE important for understanding the basis of the enzyme's ambifunctionality.

15. Gallant, E.; Li, A.; **Davis, K. M.**; Syedsayamdost, M. R. *Burkholderia*-Derived Natural Products: From Discovery to Target Identification Toward Chemical Ecology. *Invited Book Chapter Submission: "Comprehensive Natural Products III"* Edited by Tadhg Begley and Ben Liu. *Elsevier*, pg. 121–141 (**2020**).

*Contribution:* Provided structural context and figures for the review.

16. Seyedsayamdost, M. R.; Caruso, A.; **Davis, K. M.** The Chemistry and Structural Enzymology of RiPP-Modifying Radical SAM Metalloenzymes. *Invited Book Chapter Submission: "Comprehensive Natural Products III"* Edited by Tadhg Begley and Ben Liu. *Elsevier*, pg. 49–64 (**2020**).

*Contribution:* Provided structural context and figures for the review.

Before Emory

17. Zhou, S.; Pan, J.; **Davis, K. M.**; Schaperdoth, I.; Boal, A. K.; Krebs, C.; Bollinger, Jr., J. M. Steric Enforcement of Cis-Epoxy Formation in the Radical C–O Coupling Reaction by which (S)-2-Hydroxypropylphosphonate Epoxidase (HppE) Produces Fosfomycin. *J. Am. Chem. Soc.* **2019**, *141*, 20397-20406.
18. **Davis K. M.**; Altmyer M.; Martinie, R. J.; Schaperdoth, I.; Krebs, C.; Bollinger Jr., M. J.; Boal, A. K. Structure of a Ferryl Mimic in the Archetypal Iron(II)- and 2-(Oxo)-glutarate-Dependent Dioxygenase, TauD. *Biochemistry.* **2019**, *58*, 4218-4223.
19. Nelp, M. T.; Zhang, V.; **Davis, K. M.**; Stiefel, K.; Groves, J. T. Potent Activation of Indoleamine 2,3-Dioxygenase by Polysulfides. *J. Am. Chem. Soc.* **2019**, *141*, 15288-15300.
20. Rose, H. R.; Maggiolo, A. O.; McBride, M.; Palowitch, G. M.; Pandelia, M. E.; **Davis, K. M.**; Yennawar, N. H.; Boal, A. K. Structures of Class Id Ribonucleotide Reductase Catalytic Subunits Reveal a Minimal Architecture for Deoxynucleotide Biosynthesis. *Biochemistry.* **2019**, *58*, 1845-1860.
21. Xu, F.; Wu, Y.; Zhang, C.; **Davis, K. M.**; Moon K.; Bushin, L. B.; Seyedsayamdost, M. R. A Genetics-Free Method for High-Throughput Discovery of Cryptic Microbial Metabolites. *Nat. Chem. Bio.* **2019**, *15*, 161-168.
  - Highlighted in “Hijacked Bacteria Reveal New Compounds, New Drug Candidates” (Discover Magazine – Jan. 14, 2019)
22. **Davis, K. M.**; Sullivan, B.T.; Palenik, M. C.; Yan, L.; Purohit, V.; Robison G.; Kosheleva, I.; Henning R. W.; Seidler, G. T.; Pushkar, Y. N. Rapid Evolution of the Photosystem II Electronic Structure During Water Splitting. *Phys. Rev. X* **2018**, *8*, 041014.
  - Highlighted in “Pinning down the Chemistry of Photosynthetic Water Splitting.” (APS Physics – October 23, 2018)
23. Pushkar, Y.; **Davis, K. M.**; Palenik, M. C. Model of the Oxygen Evolving Complex Which is Highly Predisposed to O–O Bond Formation. *J. Phys. Chem. Lett.* **2018**, *9*, 3525-3531.
24. **Davis, K. M.**; Schramma, K. R.; Hansen, W. A.; Bacik, J. P.; Khare, S. D.; Seyedsayamdost, M. R.; Ando, N. Structures of the Peptide-Modifying Radical SAM Enzyme SuiB Elucidate the Basis of Substrate Recognition, *P. Natl. Acad. Sci. USA.* **2017**, *114*, 10420-10425.
25. **Davis, K. M.** & Boal, A. K. Chapter Eleven - Mechanism-Based Strategies for Structural Characterization of Radical SAM Reaction Intermediates, In *Methods Enzymol.* (David, S. S., Ed.), **2017**, pp 331-359, Academic Press.
26. Jensen, S. C.; **Davis, K. M.**; Sullivan, B.; Hartzler, D. A.; Seidler, G. T.; Casa, D. M.; Kasman, E.; Colmer, H. E.; Massie, A. A.; Jackson, T. A.; Pushkar, Y. X-ray Emission Spectroscopy of Biomimetic Mn Coordination Complexes. *J. Phys. Chem. Lett.* **2017**, *8*, 2584-2589.
27. Sullivan, B.; Robison, G.; Osborn, J.; Kay, M.; Thompson, P.; **Davis, K. M.**; Zakharova, T.; Antipova, O.; Pushkar, Y. On the Nature of the Cu-Rich Aggregates in Brain Astrocytes. *Redox Biol.* **2017**, *11*, 231-239.
28. Rustiguel, J. K.; Soares, R. O. S.; Meisburger, S. P.; **Davis, K. M.**; Malzbender, K. L.; Ando, N.; Dias-Baruffi, M.; Nonato, M. C. Full-Length Model of the Human Galectin-4 and Insights into Dynamics of Inter-Domain Communication. *Sci. Rep.* **2016**, *6*, 33633.
29. **Davis, K. M.**; Palenik, M.; Yan, L.; Smith, P. F.; Seidler, G. T.; Dismukes, G. C.; Pushkar, Y. N. X-ray Emission Spectroscopy of Mn Coordination Complexes Toward Interpreting the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II. *J. Phys. Chem. C* **2016**, *120*, 3326-3333.
30. **Davis, K. M.** & Pushkar, Y. Structure of the Oxygen Evolving Complex of Photosystem II at Room Temperature. *J. Phys. Chem. B.* **2015**, *119*, 3492-3498.
31. Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.;...**Davis, K. M.** et al. Serial Time-Resolved Crystallography of Photosystem II Using a Femtosecond X-ray Laser. *Nature.* **2014**, *513*, 261-265.

- Highlighted in “Researchers Capture Images of Photosynthesis in Action.” (Nature World News – July 10, 2014)
  - Highlighted in “Scientists Capture Snapshots of Water Splitting in Photosynthesis for the First Time Ever.” (Science World Report – July 10, 2014)
32. **Davis, K. M.**; Kosheleva, I.; Henning, R. W.; Seidler, G. T.; Pushkar, Y. Kinetic Modeling of the X-Ray-Induced Damage to a Metalloprotein. *J. Phys. Chem. B* **2013**, *117*, 9161-9169.
  33. Chen, J.; Lee, Y.-M.; **Davis, K. M.**; Wu, X.; Seo, M. S.; Cho, K.-B.; Yoon, H.; Park, Y. J.; Fukuzumi, S.; Pushkar, Y. N.; Nam, W. A Mononuclear Non-Heme Manganese(IV)–Oxo Complex Binding Redox-Inactive Metal Ions. *J. Am. Chem. Soc.* **2013**.  
- Highlighted in “Metal model mimics metalloenzymes.” (Phys.org – August 12, 2013)
  34. **Davis, K. M.**; Mattern, B. A.; Pacold, J. I.; Zakharova, T.; Brewe, D.; Kosheleva, I.; Henning, R. W.; Graber, T. J.; Heald, S. M.; Seidler, G. T.; Pushkar, Y. Fast Detection Allowing Analysis of Metalloprotein Electronic Structure by X-ray Emission Spectroscopy at Room Temperature. *J. Phys. Chem. Lett.* **2012**, *3*, 1858.
  35. Wu, X.; Seo, M. S.; **Davis, K. M.**; Lee, Y.-M.; Chen, J.; Cho, K.-B.; Pushkar, Y.; Nam, W. A Highly Reactive Mononuclear Non-Heme Manganese(IV)-Oxo Complex That Can Activate the Strong C-H Bonds of Alkanes. *J. Am. Chem. Soc.* **2011**, *133*, 20088.

## PATENT APPLICATIONS

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3. Seyedsayamdost, M. R., Chiotti V. T., **Davis, K. M.**, McWhorter, K. L. Glycopeptide Antibiotic Combination Therapy Against Clostridia. *U.S. Provisional Patent No. 63/225,607*, 2021.
2. Seyedsayamdost, M. R., Zhang, Y., Chandler, J. R., Klaus, J. R., **Davis, K. M.**, McWhorter, K. L. Antibacterial Combination Therapy to Treat Burkholderia Infections. Provisional Patent Filed 11/10/2020.
1. Seyedsayamdost, M. R.; Xu, F.; Wu, Y.; Bushin, L.; **Davis, K. M.** Cryptic Metabolites and Method for Activating Silent Biosynthetic Gene Clusters in Diverse Microorganisms. *U.S. Patent No. 11,549,950-B2*, 2023.

## PRESENTATIONS

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### Invited Talks

30. Seminar – Dept. of Chemistry, University of Siena, (June 17, 2024). “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
29. Seminar – Dept. of Chemistry, Utah State University, (March 20, 2024). “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
28. Seminar – Dept. of Physics, Western Kentucky University, (March 11, 2024). “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
27. Seminar – Dept. of Chemistry, University of Texas at San Antonio, (March 8, 2024). “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
26. Seminar – Dept. of Chemistry, Mississippi State University, (February 29, 2024), “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
25. Symposium – 28<sup>th</sup> Enzyme Mechanisms Conference, (January 6, 2024). “Examining the structural and dynamic basis for atypical heme enzyme reactivity”.
24. Seminar – Dept. of Chemistry, Auburn University (March 30, 2023), “Structural insights into the biosynthesis and bioactivity of natural products”.
23. Seminar – BioTechnology Institute, University of Minnesota (Nov. 10, 2022), “Structural insights into the biosynthesis and bioactivity of natural products”.
22. Symposium – Regional Beckman Symposium, Georgia Institute of Technology (Aug. 3, 2022), “X-rays shine light on the synergy between metalloenzyme structure and electronics”.

21. Seminar – University of Georgia, Dept. of Chemistry (Feb. 21, 2022), “Structure and dynamics of enzyme-ligand interactions”.
20. Symposium – Pacificchem, RiPP Natural Products: Biosynthesis, Function, and Engineering (Dec. 16, 2021), “Structural insights into peptide recognition and modification by RiPP biosynthetic enzymes”.
19. Seminar – Emory University, Dept. of Physics (April 28, 2020), “Using X-rays to Probe Protein Dynamics”.

*Before Emory*

18. Honors Colloquium Speaker – University of Louisville, Dept. of Physics and Astronomy (April 5, 2019), “Using X-rays to Probe Protein Dynamics”.
17. Seminar – University of Wisconsin, Madison, Dept. of Chemistry (March 7, 2019), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
16. Seminar – University of North Carolina, Dept. of Applied Physical Sciences (Feb. 28, 2019), “Using X-rays to Probe Protein Dynamics”.
15. Seminar – Carnegie Mellon, Dept. of Physics (Feb. 21, 2019), “Using X-rays to Probe Protein Dynamics”.
14. Outreach Seminar – Presentation Academy, Louisville, KY (Feb. 19, 2019), “Girls in Science Go Everywhere”.
13. Seminar – University of Kentucky, Dept. of Chemistry (Feb. 14, 2019), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
12. Seminar – University of Florida, Dept. of Physics (Feb. 12, 2019), “Using X-rays to Probe Protein Dynamics”.
11. Seminar – University of California, Santa Barbara, Dept. of Chemistry (Jan. 31, 2019), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
10. Seminar – Purdue University, Dept. of Chemistry (Jan. 24, 2019), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
9. Seminar – Emory University, Dept. of Chemistry (Dec. 10, 2018), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
8. Seminar – Columbia University, Dept. of Chemistry (Dec. 7, 2018), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
7. Seminar – New York University, Dept. of Chemistry (Dec. 3, 2018), “X-rays Illuminate Metalloenzymes: Photosystem II and Radical SAM enzymes”.
6. Symposium – American Society for Biochemistry and Molecular Biology (ASBMB) Annual Meeting, San Diego, CA, (Apr. 24, 2018), “Structural Insights into Peptide Recognition and Modification by the Radical SAM Enzyme SuiB”.
5. Seminar – Advanced Photon Source, Argonne National Lab (Mar. 17, 2017), “Structural Characterization of a Novel RiPP-modifying Radical SAM Enzyme”.
3. Seminar – Simmons College Department of Physics and Chemistry (Nov. 9, 2015) “Physics, Chemistry and Spinach: Investigating How Plants Split Water”.
3. Seminar – University of Louisville Physics Department (Sept. 12, 2014) “X-ray Emission Analysis of the S-state Intermediates of the Photosystem II Protein Complex”.
2. Seminar – DESY CFEL, Hamburg, Germany (July 17, 2014) “X-ray Emission Analysis of the S-state Intermediates of the Photosystem II Protein Complex”.
1. Symposium – APS User Meeting, Argonne National Lab. (May 12-15, 2014) “X-ray Emission Analysis of the S-state Intermediates of the Photosystem II Protein Complex”.

**TEACHING EXPERIENCE**

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*Emory*

- 2025      Spring  
**Chem 205 – Light and Matter**
- 2024      Summer  
**Chem 370W – Special Topics: Chemistry of Italian Art**
- Spring  
**Chem 575R – Physical Biochemistry**
- 2023      Fall  
**Chem 205 – Light and Matter**
- 2022      Fall  
**Chem 205 – Light and Matter**
- 2021      Fall  
**Chem 575R – Physical Biochemistry**
- 2020      Fall  
**Chem 575R – Physical Biochemistry**

*Pre-Emory*

- 2018      **The Pennsylvania State University**  
Teaching Assistant, Penn State Bioinorganic Workshop  
Co-taught a hands-on crystallography workshop
- 2015      **Princeton University**  
Guest Lecturer – Biophysical Chemistry I, Department of Chemistry
- 2013      **Purdue University**  
Guest Lecturer – Biophysics II, Department of Physics and Astronomy
- 2008 – 2009      **University of Louisville**  
Teaching Assistant – Mechanics, Heat, and Sound Lab, Dept. of Physics and Astronomy
- 2007 – 2009      **University of Louisville**, Resources for Academic Achievement Center  
Physics and Mathematics Tutor  
Introductory courses through differential equations/modern physics
- 2007 – 2009      **University of Louisville**, Resources for Academic Achievement Center  
Supplemental Lecturer for Introductory Physics Courses  
Introduction to Mechanics & Introduction to Electricity and Magnetism
- 2007 – 2008      **University of Louisville**  
Grader for Linear Algebra, Department of Mathematics

**PROFESSIONAL DEVELOPMENT**

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- 2023      **NSF Career Academy**, ECAS Office of Research and CFDE
- 2023      **STEM/Community-Engaged Learning Workshop**, CFDE
- 2022      **Managing Bias**, Office of Diversity, Equity, and Inclusion
- 2022      **Diversity: Inclusion in the Modern Workplace**, Office of Diversity, Equity, and Inclusion
- 2021      **It's About Flipping Time**, Center for Faculty Development and Excellence (CFDE)
- 2020      **Emory College Online Teaching Strategies (ECOTS)**

2020  
2019**Faculty Showcase on Blended and Hybrid Courses, CFDE**  
**The PI Crash Course: Skills for Future or New Lab Leaders, Columbia University****STUDENT SUPERVISION**

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**Current Group Members**Chemistry Graduate Students

2020 –	Stacey Jones	2021 NSF Graduate Research Fellowship
2020 –	Kendra Ireland	2021 NSF Graduate Research Fellowship
2020 –	Kirklín McWhorter	
2020 –	Samantha Horwitz	2022 NSF Graduate Research Fellowship
2021 –	Benjamin Dratch	
2021 –	Lidia Waidmann	2023 NSF Graduate Research Fellowship
2022 –	Gabe DeLong	
2023 –	Tiffany Alvarez	
2023 –	Jesus Vazquez Hernandez	

Physics Graduate Students

2020 –	Sahand Emamian
2024 –	Drisha Sehgal

Undergraduate Students

2022 –	Riddhi Jhunjunwala ('25)
2023 –	Varun Karry ('26)
2023 –	Lorenzo Layug ('26)
2023 –	Madeline Garcia ('26)
2023 –	Abbas Khambatti ('25)
2024 –	Ryan Jones ('26)
	Brandon Colella (LGS-SOAR summer student)

**Group Alumni**Graduate Students

2020 – 2023	Tamra Blue	Honorable Mention – 2021 Ford Fndn. & 2020 NSF GRF <b>Currently</b> – Assistant Prof. Carleton College & Postdoc in the Booker Lab at PSU
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Undergraduate Students

2022 – 2024	Ken Dorazio ('24)	Highest honors, current: <i>student at Georgia Tech</i>
2021 – 2023	Joe Ambarian ('23)	NSF GRF '23, highest honors, current: <i>student Caltech</i>
2022	Evan Nie ('24)	
2021 – 2022	Andrea Mancina ('24)	IRES Lyon, current: researcher in the Liotta Lab
2020 – 2022	Nithin Bagal ('22)	Highest honors, current: <i>student at Princeton</i>
2020 – 2022	Sina Djafari-Rouhani ('22)	Highest honors, current: <i>Post-bac at the Broad Institute</i>
2020 – 2022	Cindy Amaya Lopez ('22)	Current: <i>Epic Systems Corporation</i>
2020 – 2021	Eray Schulz ('21)	Current: <i>student at IUPUI</i>

Visiting Faculty

2020 – 2021	Prof. C. L. Davis (U. of Louisville)
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**Other Graduate Thesis Committees**Department of Chemistry:

- |                                |                               |
|--------------------------------|-------------------------------|
| 1. Aimee Sanford (PhD 2022)    | 5. Jessalyn Rogers (PhD 2023) |
| 2. Thomas Persinger (PhD 2022) | 6. Erika Diosdado (MS 2023)   |
| 3. Joel Schmitz (PhD 2022)     | 7. Evy Kimbrough (PhD 2023)   |
| 4. Amber Scharnow (PhD 2022)   | 8. Tiffany Trieu              |

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|--------------------------------------|-----------------------------|
| 9. Noah Jaffe                        | 17. Sydney Elebra           |
| 10. Yusha Imtiaz                     | 18. Andres Socorro Gonzalez |
| 11. Martina Golden                   | 19. Elise Bezold            |
| 12. Mohamed Husaini Bin Abdul Rahman | 20. Tram Nguyen             |
| 13. Taylor Blackburn                 | 21. Giao Vu                 |
| 14. Chris Nielson                    | 22. Chipo Kambarami         |
| 15. Angele Bruce                     | 23. Sophia Lee              |
| 16. Maia Vierengel                   |                             |

Department of Physics:

1. Wei Li (PhD 2023)

**Other Undergraduate Thesis Committees**Department of Chemistry:

1. Kristina Trifonova ('23)
2. Brian Wang ('23)
3. Rea Yoza ('24)
4. Ritika Pandey ('24)
5. Christina Hastings ('24)
6. Kenneth Wingate ('24)
7. Sophie Barthel ('25)

*Pre-Emory***The Pennsylvania State University (2016 – 2018)**Undergraduate Thesis Mentor – Madison Altmyer, Boal Lab

Project: Structural analysis of iron(II) and 2-(oxo)-glutarate-dependent oxygenases with alternate reactivities

**Princeton University (2015 – 2016)**Undergraduate Thesis Mentor – Emily Adler, Ando Lab

Project: Structural characterization of proteins in an antibiotic biosynthesis pathway using small angle x-ray scattering and x-ray crystallography

**Purdue University (2010-2014)**Research Mentor, Pushkar Lab

Trained first year graduate students, undergraduates and REU participants in practical and theoretical aspects of laboratory research.

**TEACHING/MENTORING RECOGNITION**

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| 2023 | Identified by student who was elected to Phi Beta Kappa as a faculty member "who has encouraged and helped students to excel, and who exemplifies intellectual rigor and enthusiasm for scholarly pursuits." |
| 2020 | Identified by first-year student as a faculty member who has been "particularly helpful to their transition to Emory."   |

**SERVICE***Internal to Emory***Committees***Department of Chemistry*

2022 – 2023	Senior Faculty Search Committee
2022 –	Biomolecular Seminar Program Coordinator
2022 –	Operations Committee
2021	Emerson Postdoctoral Fellows Program Committee
2020 – 2022	Graduate Committee - Proposal writing course sub-committee (2021)

*ECAS*

2022 – 2023	See above for search committee membership
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*University*

2022	Achievement Rewards for College Scientists (ARCS) Scholars Selection Committee
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**Chemistry Major Advising**

2024 –	Ryan Jones, Dean Kamenev, Halle Wulff
2023 –	Julia Kamara, Erika Ono, Steven Tibbetts, Jr., Stella Fox
2022 –	Jack Timmons, Rea Yoza
2022	Ankitha Kumar
2021 – 2022	Peter Liu
2021 – 2022	Marissa Hollingsworth

**Pre-major Advising**

2022 – 2023	Nate Hu, Katharine Haspel, Jiya Shah, Luke Hibbeln
2021 – 2022	Kearya Tendall, Kaicheng Chen, Dana Catalano, Roja Ayyadurai
2020 – 2021	Dan Kim, Ashley Kim, Shawn Kim, Aditya Kolisetti

**Other Service**

2023	Interviewed by Emory's Biotech Consulting Club
2023	Poster judge at 13th Annual Southeast Enzyme Conference
2023	AWIS Women in STEM Panelist
2023 –	FirstSTEM Faculty Fellow (formerly STEM Pathways)
2022 –	LGS SOAR Faculty Partner (reviewed applications, offered to host summer students)
2022	Undergraduate Research Panelist for the Biology and Chemistry Cohort
2021 –	STEM Pathways Faculty Partner (organized lab tours, attended luncheons with students)
2020 – 2022	SIRE Program Mentor

*External to Emory***Peer Review Activity**

2024 –	<i>Biochimie, Communications Biology, Protein Science</i>
2023 –	<i>ACS Bio &amp; Med Chem Au, Communications Biology</i>
2022 –	<i>Communications Biology, Biochemistry, Current Opinions in Chemical Biology, Nature Communications</i>
2021 –	<i>Nature Communications, Nature Chemical Biology, ChemBioChem</i>

**Proposal Review Activity**

2023	Early Career Research Program, Office of Basic Energy Sciences, DOE
2022	NIH Special Emphasis Panel
2021 –	Pump-Probe Review Panel, Advanced Photon Source, Argonne National Lab
2019 – 2021	Fellowship Review Panel, Arnold and Mabel Beckman Foundation

### Professional Memberships

2023 – Biological Discovery through Chemical Innovation (BDCI) at Emory  
2018 – American Society for Biochemistry and Molecular Biology  
2017 – American Chemical Society  
2009 – 2014 Women in Physics (WIP), Purdue University  
2009 – 2014 Women in Science Programs (WISP), Purdue University  
2007 – American Physical Society

### Leadership Roles in Service Pre-Emory

2013 – 2014 **Secretary**, Forum on Graduate Student Affairs, American Physical Society  
2013 – 2014 **Executive Committee**, Physics Graduate Student Association, Purdue University  
2008 – 2009 **President**, Society of Physics Students, University of Louisville  
2007 – 2008 **President**, Mathematics Club, University of Louisville