Department of Chemistry
Lafayette College
Easton, PA 18042

Prof. Heidi P. Hendrickson

226 Hugel Science Center
(610)-330-5825
hendrihe@lafayette.edu

EDUCATION

The University of Michigan, Ann Arbor, MI — May 2015
Ph.D. degree in Chemistry
M.Sc. degree in Educational Studies

Hillsdale College, Hillsdale, MI — May 2009
B.Sc. degree in Chemistry (*cum laude*)

RESEARCH and ACADEMIC EXPERIENCE

Associate Professor of Chemistry, Lafayette College — 2025 – present
Assistant Professor of Chemistry, Lafayette College — 2017 – 2025
Utilizing multi-scale computational approaches, including quantum algorithms, to investigate protein-ligand interactions and information transfer pathways in proteins, the reactivity and toxicity of aqueous environmental pollutants, and optoelectronic properties of small molecules and polymer materials.

Postdoctoral Research in Chemistry, Yale University — 2015 – 2017
Investigated allosteric networks and charge transfer in biological macromolecules via multi-scale computational approaches.
Advised by **Prof. Victor S. Batista**

Lecturer in Chemistry, University of Michigan — 2015
Designed discussion-based course materials, lectured, held office hours, wrote and graded exams, and mentored a graduate student TA for a physical chemistry course.

Ph.D. Research in Chemistry, University of Michigan — 2009 – 2015
Utilized range-separated hybrid density functional theory to study the electronic structure of novel charge transfer systems with optoelectronic applications.
Dissertation: An Electronic Structure Approach to Charge Transfer and Transport in Molecular Building Blocks for Organic Optoelectronics — March 19, 2015
Advised by **Prof. Eitan Geva**
Prof. Barry D. Dunietz

M.Sc. Research in Chemistry Education, University of Michigan — 2010 – 2015
Studied the effects of peer-review on persistent errors in student explanations of physical chemistry concepts in an introductory physical chemistry course.
Advised by **Prof. Leah A. Bricker**
Prof. Brian P. Coppola

Graduate Research in Chemistry: Summer Institute, University of Michigan — 2009
Studied transient aspects of electron transport in model molecular junctions.
Advised by **Prof. Barry D. Dunietz**

Undergraduate Research in Chemistry: LAUREATES Program, Hillsdale College — 2008
Studied photoreduction reactions on nanostructured surfaces via surface-enhanced Raman spectroscopy.
Advised by **Prof. Matthew Young**

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PUBLICATIONS

Peer-Reviewed Research Articles

Undergraduate co-authors advised by HPH are underlined

25. Kaushik, P.; Vu, N. P.; Yeung, C.; Tadisina, S.; Boyle, L.; Venkatesh, V.; Zilberstein, M.; Sorak, N.; Subedi, K.; Azevedo Cabral, D. G.; Allen, B.; Batista, V. S.; **Hendrickson, H. P.**
Quantum Chess as a Pedagogical Tool for Teaching Quantum Information Science in High Schools.
Journal of Chemical Education, **2026***, in press*.

24. Zhang, Z.; Grace, D. N.; Vu, N. P.; Nguyen, L. A.; **Hendrickson, H. P.**; Prasse C.
Mechanistic insights into (toxic) carbonyl compound formation during ozonation of substituted phenols.
Water Research, **2026***, 300*, 125916.

23. Henesey, B.; Ingwer, S.; Tracey, H.; Obarow, E.; Holappa, R.; King, A.; **Hendrickson, H. P.**; Griffith, D.; Galloway, M. M.
Cross-Reactions of Glyoxal and Glycolaldehyde in Aqueous Aerosol Mimics: Implications for Brown Carbon Product Formation
ACS ES&T Air, **2025***, 2,* 309-318.

22. Carthy, C.; O'Leary, E.; Tadisina, S.; Griffith, D.; **Hendrickson, H. P.**; Woo, J.; Galloway, M. M.
Brown carbon formation by aqueous-phase reactions of glycolaldehyde and methylamine.
ACS Earth and Space Chemistry, **2024***, 8,* 1951–1960.

21. Li, W.; Cao, Z.; Peng, J.; **Hendrickson, H. P.**; Zheng, S.
An Insight into the Mechanism of Alkyl Side-Chain Engineering of BTCN on its Photovoltaic Properties - A Theoretical Study.
Journal of Physical Chemistry C, **2024**, *128*, 12829–12839.

20. O'Connor, M. S.; Bragg, Z. T.; Dearworth, J. R., **Hendrickson, H. P.**
Quantum Mechanics/Molecular Mechanics Calculations Predict A1, Not A2, is Present in Melanopsin (Opn4m) of Red-Eared Slider Turtles (Trachemys Scripta Elegans).
Vision Research, **2023**, *209*, 108245.

19. Vu, N. P.; Ali, L.; Chua, T. L.; Barr, D. A.; **Hendrickson, H. P.**; Trivedi, D.
Computational Insights into Prostaglandin E2 Ligand Binding and Activation of G-Protein-Coupled Receptors.
ACS Applied Bio Materials, **2024**, *7*, 579–587. (Online Publication date: April 14, 2023)

18. Soto, P.; Gloeb, G. M.; Tsuchida, K. A.; Charles, A. A.; Greenwood N. M.; **Hendrickson, H.**
Insight into the conserved structural dynamics of the C-terminus of mammal PrPC identifies structural core and possible structural role of pharmacological chaperones.
Prion, **2023**, *17*, 55-66.

17. Grace, D. N.; Lugos, E. N.; Ma, S.; Griffith, D. R.; **Hendrickson, H. P.;** Woo, J. L.; Galloway, M. M.
Brown Carbon Formation Potential of the Biacetyl−Ammonium Sulfate Reaction System.
ACS Earth and Space Chemistry, **2020,** *4*, 1104-1113.

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16. Grace, D. N.; Sharp, J. R.; Holappa, R. E.; Lugos, E. N.; Sebold, M. B.; Griffith, D. R.; **Hendrickson, H. P.;** Galloway, M. M.
Heterocyclic Product Formation in Aqueous Brown Carbon Systems.
ACS Earth and Space Chemistry, **2019,** *3,* 2472-2481.

15. Negre, C. F. A.; Morzan, U. N.; **Hendrickson, H. P.;** Pal, R.; Lisi, G. P.; Loria, J. P.; Rivalta, I.; Ho, J.; Batista, V. S.
Eigenvector Centrality for Characterization of Protein Allosteric Pathways.
Proceedings of the National Academy of Science USA, **2018**, *115,* E12201-E12208.

14. Chaudhuri, S.; Hedström, S.; Méndez-Hernández, D. D.; **Hendrickson, H. P.;** Jung, K. A.; Batista, V. S.
Quantitative first-principles predictions of electron transfer rates.
Journal of Chemical Theory and Computation **2017**, *13*, 6000-6009.

13. Jafari, M.; Welden, A. R.; Williams, K.; Winograd, B.; **Hendrickson, H. P.;** Lenard, M.; Gottfried, A.; Geva, E.
Compute-to-Learn: Authentic Learning via Development of Interactive Computer Demonstrations within a Peer-Led Studio Environment.
Journal of Chemical Education, **2017**, *94*, 1896-1903.

12. Guo, Y.; **Hendrickson, H. P.;** Videla, P. E.; Chen, Y.-N.; Ho, J.; Sekharan, S.; Batista, V. S.; Tully, J. C.; Yan, E. C. Y.
Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants.
Journal of Chemical Physics, **2017**, *146*, 215104.

11. Sarkar, S.; **Hendrickson, H. P.;** Lee, D.; DeVine, F.; Jung, J.; Geva, E.; Kim, J.; Dunietz, B. D.
Phosphorescence in Bromobenzaldehyde Can Be Enhanced through Intramolecular Heavy Atom Effect.
Journal of Physical Chemistry C, **2017**, *121*, 3771-3777.

10. Lipchock, J. M.; **Hendrickson, H. P.;** Douglas, B. B.; Bird, K. E.; Ginther, P. S.; Haynie, S. T.; Rivalta, I.; Ten, N. S.; Batista, V. S.; Loria, J. P.
Characterization of PTP1B Inhibition by Chlorogenic Acid and Cichoric Acid.
Biochemistry, **2017**, *56*, 96-106.

9. Schloss, A. C.; Liu, W.; Williams, D. M.; Kaufman, G.; **Hendrickson, H. P.;** Rudshteyn, B.; Fu, L.; Wang, H.; Batista, V. S.; Osuji, C.; Yan, E. Y. C.; Reagan, L. J.
Fabrication of Modularly Functionalizable Microcapsules Using Protein-Based Technologies.
ACS Biomaterials Science & Engineering, **2016**, *2*, 1856–1861.

8. Lisi, G. P.; Manley, G. A.; **Hendrickson, H. P.;** Rivalta, I.; Batista, V. S.; Loria, J. P.
Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators.
Structure, **2016**, *24*, 1155–1166.

7. Zheng, Z.; Manna, A.; **Hendrickson, H. P.;** Hammer, M.; Song, C.; Geva, E.; Dunietz, B. D.
Molecular Structure, Spectroscopy and Photo Induced Kinetics in Tri-nuclear Cyanide Bridged Complex in Solution: A First Principle Perspective.
Journal of the American Chemical Society, **2014**, *136*, 16954–16957.

6. **Phillips, H.;** Zheng, Z.; Geva, E.; Dunietz, B. D.
Orbital Gap Predictions for Rational Design of Organic Photovoltaic Materials.
Organic Electronics, **2014**, *15*, 1509-1520.

5. **Phillips, H**.; Geva, E.; Dunietz, B. D.
Calculating Off-Site Excitations in Symmetric Donor–Acceptor Systems via Time-Dependent Density Functional Theory with Range-Separated Density Functionals.
Journal of Chemical Theory and Computation, **2012**, *8*, 2661-2668.

4. Zheng, S.; **Phillips, H.;** Geva, E.; Dunietz, B. D.
Ab Initio Study of the Emissive Charge-Transfer States of Chromophore-Functionalized Silsesquioxanes.
Journal of the American Chemical Society, **2012**, *134*, 6944-6947.

3. **Phillips, H**.; Zheng, S.; Hyla, A.; Laine, R.; Goodson III, T.; Geva, E.; Dunietz, B. D.
Ab Initio Calculation of the Electronic Absorption of Functionalized Octahedral Silsesquioxanes via Time-Dependent Density Functional Theory with Range-Separated Hybrid Functionals.
Journal of Physical Chemistry A, **2012**, *116*, 1137-1145.

2. **Phillips, H.;** Prociuk, A.; Dunietz, B. D.
Bias-Induced Electronic Spectral Effects of Molecular Junctions: A Computational Analysis.
Journal of Chemical Physics, **2011**, *134*, 054708.

1. Prociuk, A.; **Phillips, H.;** Dunietz, B. D.
Modeling Transient Aspects of Coherence-Driven Electron Transport.
Journal of Physics: Conference Series, **2010**, *220,* 012008.

Peer-Reviewed Perspectives

3. Dutta, R.; Cabral D. G. A.;, Lyu, N.; Vu, N. P.; Wang, Y.; Allen, B.; Dan, X.; Cortiñas, R. G.; Khazaei, P.; Smart, S. E.; Nie, S.; Devoret, M. H.; Mazziotti, D. A.; Narang, P.; Wang, C.; Whitfield, J. D.; Wilson, A. K.; **Hendrickson, H. P.**; Lidar, D. A.; Pérez-Bernal, F.; Santos, L. F.; Kais, S.; Geva, E.; Batista, V. S.
Simulating Chemistry on Bosonic Quantum Devices.
Journal of Chemical Theory and Computation, **2024**, *20*, 6426-6441.

2. Anderson, K.; Arradondo, S.; Ball, K. A.; Bruce, C.; Gomez, M. A.; He, K.; **Hendrickson, H.**; Madison, L.; McDonald, A. R.; Nagan, M. C.; Scott, C. E.; Soto, P.; Tomlinson, A.; Varner, M.; Parish, C.
The Impacts of the Molecular Education and Research Consortium in Undergraduate Computational Chemistry on the Careers of Women in Computational Chemistry.
Journal of Chemical Information & Modeling, **2022**, *62*, 6316–6322.

1. Ball, K. A.; He, K.; **Hendrickson, H. P.**
Engaging Undergraduate Students in Computational Chemistry Research: A Tutorial for New Assistant Professors.
International Journal of Quantum Chemistry, **2020**, *120*, e26341.

Book Chapters (Peer-Reviewed)

1. **Hendrickson, H. P.**; Lenn, K. M.; Vázquez, F. X.; Williams, K. L.; Winograd, B. A.; Mulvihill, E. A.; Geva, E.
The Compute-to-Learn Pedagogy and Its Implementation in the Chemistry Curriculum.
In Teaching Programming across the Chemistry Curriculum; McDonald, A. R., Nash, J. A., Eds.; ACS Symposium Series; American Chemical Society, Vol. 1387; American Chemical Society, **2021**; pp 69-87.

Book Reviews

1. Miller, K. F.; **Phillips, H.**
   Book Review: *Cultural Foundations Learning: East and West* by Jin Li.
   The Journal of Asian Studies, **2014**, *73*(01), 199-200.

Other Perspectives (Invited)

2. Lugos, E. N.; Gandhi, Z.; O'Connor, M. S.; Kaplan, E. L.; **Hendrickson, H. P.**
   Becoming a Scientist: Engaging the Next Generation of Chemists in Computational Research at a Primarily Undergraduate Institution.
   Council on Undergraduate Research (CUR) Chemistry News, **2019**, *4*(1), 7-10.

1. **Hendrickson, H. P.**
   November Research Bio: Dr. Heidi P. Hendrickson.
   The Octagon: Newsletter of the Lehigh Valley Section of the American Chemical Society, **2018**, *101*(8), 3-4.

Preprints

1. Chua, T. L.; Welch, L. J.; Qian, C.; Feldblyum, J. I.; **Hendrickson, H. P.**
   Computational Investigation of the Optoelectronic Properties of Ferrocene-based Polymers.
   ChemRxiv. Cambridge: Cambridge Open Engage; 2022; This content is a preprint and has not been peer-reviewed. https://doi.org/10.26434/chemrxiv-2022-5hbl9

TEACHING and MENTORING

Course Instructor

Professor, Chemistry, Lafayette College — 2017 – present
- **CHEM 107: General Chemistry I**
- **CHEM 122: General Chemistry II**
- **CHEM 341: Survey of Physical Chemistry**
- **CHEM 342: Physical Chemistry I (w/lab)**
- **CHEM 343: Physical Chemistry II**
- **CHEM 365/366: Course-based Research Experience in Chemistry**
- **CHEM 380/390/391/392/394: Independent Study/Research**
- **CHEM 445: Special Topics in Physical Chemistry** (Computational Chemistry)

- **PHYS 391: Independent Study**

Lecturer, Chemistry, University of Michigan — 2015
- **CHEMISTRY 260: Chemical Principles**
- **CHEMISTRY 261: Introduction to Quantum Chemistry**

Instructor, English Language and Literature, University of Michigan — 2014
- **ENGLISH 125: Writing and Academic Inquiry**

Graduate Student Instructor, Chemistry, University of Michigan
- **CHEMISTRY 130: General Chemistry** — 2015
- **CHEMISTRY 260: Chemical Principles** — 2010
- **CHEMISTRY 261: Introduction to Quantum Chemistry**

Honors Studio Facilitator, Chemistry, University of Michigan 2010 – 2014
CHEMISTRY 260 Honors: Chemical Principles

Thesis Advisor/Committee Member

Graduate Thesis Committee Member

Cristabella Fortna (Lehigh University) 2026-present
TBA

Isabelle Herlinger (Lehigh University) 2025-present
TBA

Undergraduate Honors Thesis Advisor (CHEM 495/496: Honors Thesis)

Jaly Chimbo Macancela (Biochemistry) 2025-2026
Information Transfer and G-Protein Selectivity in Prostaglandin E2 Receptors

Carter Brand (Biochemistry) 2024-2025
Computational Investigation of Neurofibrillary Tangle Chromophores in Relation to Alzheimer's Disease

Michael O'Connor (Biochemistry) 2021-2022
A computational investigation of chromophore binding in Red-eared turtle melanopsin

Undergraduate Honors Thesis Committee Member

Ava Katz (Chemistry) 2026-present
Reactions of Gold (I) Compounds with Aryl Boronic Acids

Qinwen Deng (Electrical and Computer Engineering) 2026
Quantum Convolutional Neural Network for Mammography Classification

Natwongsatorn Boonkongchuen (Chemical Engineering) 2025-2026
Machine Learning Models for Catalytically Relevant Transition Metal Carbide Surfaces

Isabella Allen (Biochemistry) 2025
Impact of Per- and Polyfluoroalkyl Substances and Polystyrene Nanoparticles on Solid-Supported Lipid Bilayers

Nam Vu (Electrical and Computer Engineering) 2025
Towards Gas Classification with Portable, AI-integrated Sensor Modules

Bridget Corpus (Biochemistry) 2024
Determination of chaperone requirements for yeast prion propagation and elimination using protein ortholog substitutions

Olivia Hofmann (Biology) 2023-2024
Structural and functional characterization of the Phytophthora infestans auxiliary activity 17 family gene PITG_13520

Anthony McBain (Biochemistry) 2023-2024
Cellular Locations of Melanopsin (Opn4) Transcripts in the Irises of Turtles

Samantha Ganser (Biochemistry) 2023
Prion Interactions and Overlapping Functions of J-Domain Proteins in Saccharomyces cerevisiae

Anna Kunz (Biology) 2022-2023
Gene Expression Analysis of Phytophthora infestans Glycoside Hydrolase Family 28 Genes in Infected Potato Plants

Isaiah Osei-Gyening (Biology) 2021-2022
Comparing the Association between Genetic Ancestry, DNA Methylation, and Patient Survival in African Americans and European Americans with Lung Cancer

Alex Ashley (Chemical Engineering) 2021-2022
Manipulation of the Degradation of PEO-b-PCL through Preparation Techniques and Thermal Variations

Yiru Gu (Chemistry) 2021
In-Silico Prediction for Inhibiting of Lin-28/Pre-let 7 reaction with Synthesized Small Molecules for Pancreatic Cancer

Sarah Miller (Biochemistry) 2021
Effects of Amino Acid Content on the Requirement of Swa2 on Artificial Prion Propagation

Jason Corcoran (Chemistry) 2019
Synthesis and catalytic ability of pyridyl-substituted NHC-palladium complexes

Sierra Cole (Biochemistry) 2019
Analyzing Hsp40 primary sequence dependence for chaperone-prion interactions

Scott Berger (Biochemistry) 2019
The role of J-proteins in Hsp104 overexpression-mediated curing of the prion [PSI$^+$]: A closer look at Apj1

Workshop Facilitator

Computational Chemistry in the Classroom Workshop

MARM 2026, Hershey, PA May 2026
BCCE 2024, Lexington, KY July 2024
MARM 2024, University Park, PA (*workshop organizing chair*) June 2024
BCCE 2022, West Lafayette, IN July 2022
Co-designed activities and held a workshop on incorporating computational chemistry software (WebMO) in high school or college chemistry classes.

WebMO Hands-On Workshop, Biennial Conference on Chemistry Education, Lexington, KY July 2024
Facilitated a workshop for chemistry instructors on how to use the various features of the WebMO software in their high school or college chemistry classes.

Quantum Games for Quantum Computing

Pathways Summer Scholars, Pathways to Science, Yale University July 2024
IEEE Integrated STEM Education Conference (ISEC ’24), Princeton University February 2024
Co-designed activities, mentored undergraduate research students, and held a workshop for high school students on using a Quantum Chess game to demonstrate principles in quantum information science.

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Schrödinger Educator's Week: Teaching with Maestro Demo (*Invited*), Schrödinger Inc, New York, NY — May 2024
Designed a workshop with hands-on activities to demonstrate the Teaching with Schrodinger software, titled "Real-life Teaching with Schrödinger Example: Excerpts from a Course-based Undergraduate Research Experience (CURE)."

Molecular Modeling Workshop: Bringing Computational Chemistry into the Classroom, Lehigh Valley American Chemical Society (LV-ACS) — January 2023
Co-designed activities and held a workshop on incorporating computational chemistry software (WebMO) in college chemistry classes.

MolSSI Quantum Mechanics Tools Workshop, Furman University — July 2022
Co-designed activities and held a workshop on python programming for quantum chemistry calculations for undergraduate researchers. The workshop was supported by the Molecular Science Software Institute (MolSSI).

Compute-to-Learn (C2L) Workshop, Lafayette College — October 2018
Designed and held a workshop on the Compute-to-Learn pedagogy for faculty at Lafayette and various academic institutions in the surrounding area.

Pathways Summer Scholars, Pathways to Science, Yale University — 2016 – 2017
The Role of the Reader in Scientific Writing
Investigating the Molecular Interactions Behind our Sense of Smell
Designed science writing workshop and computational chemistry workshops for local high school students participating in a summer enrichment program.

Sweetland Center for Writing, University of Michigan — 2014 – 2015
Written Communication in Science
Keeping a Laboratory Notebook
Personal Statements for Medical School
Academic Writing
Designed science writing workshops within summer research programs for STEM undergraduate students in traditionally underrepresented groups.

Research Mentor — *Mentored student co-authors on publications and preprints underlined*

Current Students

7.	Cora Davia	Undergraduate, Lafayette College	2026 – present
6.	Elizabeth Green	Undergraduate, Lafayette College (2025)	2025 – present
5.	Genevieve Chukwuonye	Undergraduate, Lafayette College	2024 – present
4.	Bodhi Colvin	Undergraduate, Lafayette College	2024 – present
3.	Tran Hoang	Undergraduate, Lafayette College	2024 – present
2.	Maya Zilberstein	Undergraduate, Lafayette College	2023 – present
1.	Vedit Venkatesh	Undergraduate, Lafayette College	2022 – present

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Former Students

69.	Lan Anh Nguyen	Undergraduate, Grand Valley State University	2025 – 2026
68.	Dylan Eschinger	Undergraduate, Lafayette College	2025 – 2026
67.	Skyler Chang	Undergraduate, Lafayette College	2025 – 2026
66.	Anthony Clerici	Undergraduate, Lafayette College	2024 – 2026
65.	Anthony Lin	Undergraduate, Lafayette College	2024 – 2026
64.	Leah Boyle	Undergraduate, Lafayette College	2024 – 2026
63.	Crystal Yeung	Undergraduate, Lafayette College	2024 – 2026
62.	Kusum Subedi	Undergraduate, Lafayette College	2023 – 2026
61.	Jaly Chimbo Macancela	Undergraduate, Lafayette College	2023 – 2026
60.	Brody Farace	Undergraduate, Lafayette College	2023 – 2026
59.	Daisy Grace	Graduate, Johns Hopkins University	2021 – 2026
58.	Guanming Hong	Undergraduate, Lafayette College	2024 – 2025
57.	Tuna Akin	Undergraduate, Lafayette College	2024 – 2025
56.	Nick Sorak	Undergraduate, Lafayette College	2023 – 2025
55.	Carter Brand	Undergraduate, Lafayette College	2023 – 2025
54.	Alexa Jindal	Undergraduate, Lafayette College	2023 – 2025
53.	Lucas Villamil	Undergraduate, Lafayette College	2023 – 2025
52.	Padmanabh Kaushik	Undergraduate, Lafayette College	2023 – 2025
51.	Swetha Tadisina	Undergraduate, Lafayette College	2023 – 2025
50.	Nam Vu	Undergraduate, Lafayette College	2022 – 2025
49.	Sam Anthony	Undergraduate, Lafayette College	2023 – 2024
48.	Zhixiang (Damon) Kang	Undergraduate, Lafayette College	2023
47.	Luke Ali	Graduate, Clarkson University	2022 – 2023
46.	Yixiang Zeng	Undergraduate, Lafayette College	2023
45.	Caroline Schaeffer	Undergraduate, Lafayette College	2022 – 2023
44.	Marc Cui	Undergraduate, Lafayette College	2022 – 2023
43.	Haleigh Marzano	Undergraduate, Lafayette College	2021 – 2023
42.	Zoey Bragg	Undergraduate, Lafayette College	2021 – 2023
41.	Eman Shahzad	Undergraduate, Lafayette College	2021 – 2023
40.	Theresa Chua	Undergraduate, Lafayette College	2020 – 2023
39.	Kelsey Wong	Undergraduate, Lafayette College	2022
38.	Nate Kopelan	Undergraduate, Lafayette College	2022
37.	Onori Luchera	Undergraduate, Lafayette College	2022
36.	Michael O'Connor	Undergraduate, Lafayette College	2019 – 2022
35.	Congyu (Alex) Qian	Undergraduate, Lafayette College	2020 – 2021
34.	Maria Giambruno-Fuge	Undergraduate, Lafayette College	2021
33.	Rachel Petzoldt	Undergraduate, Lafayette College	2020 – 2021
32.	Zahra Gandhi	Undergraduate, Lafayette College	2018 – 2021
31.	Ella Kaplan	Undergraduate, Lafayette College	2017 – 2021
30.	Philip Weiss	Undergraduate, Lafayette College	2020
29.	Emily Lugos	Undergraduate, Lafayette College	2018 – 2020
28.	Liza Welch	Undergraduate, Lafayette College	2018 – 2019

27.	Heather Harrington	Undergraduate, Yale University	2016 – 2018
26.	Meghana Jaladanki	High School, Jonathan Law High School	2017
25.	Subhajyoti Chaudhuri	Graduate, Yale University	2016 – 2017
24.	Kenneth Jung	Graduate, Yale University	2016 – 2017
23.	Rajshekhar Basak	Graduate, Yale University	2016 – 2017
22.	Michael Mascaro	Undergraduate, Yale University	2016 – 2017
21.	Nicholas Ten	Undergraduate, Yale University	2015 – 2016
20.	Srijana Bhandari	Graduate, Kent State University	2015
19.	Kyle Williams	Graduate, University of Michigan	2015
18.	Kevin Fenk	Undergraduate, Ohio State University	2015
17.	Sarah Choi	Undergraduate, University of Michigan	2014 – 2015
16.	Daphne Porat	Undergraduate, University of Michigan	2013 – 2015
15.	Francis DeVine	Undergraduate, University of Michigan	2010 – 2015
14.	Richard Sutherland	Undergraduate, University of Michigan	2014
13.	Michael Gysin	Undergraduate, University of Michigan	2012 – 2014
12.	Kari Chen	Undergraduate, University of Michigan	2011 – 2013
11.	Jessica Shost	Undergraduate, University of Michigan	2012
10.	Pavel Okun	Undergraduate, University of Michigan	2012
9.	Andrew Ichikawa	High School, Skyline High School	2012
8.	Morgan Hammer	Undergraduate, Ohio Northern University	2012
7.	Elliot MacNeille	Undergraduate, University of Michigan	2012
6.	Daniel Cummins	Undergraduate, University of Michigan	2010 – 2012
5.	Victoria Washington	Undergraduate, University of Michigan	2011
4.	Chenchen Song	Undergraduate, Tsinghua University	2011
3.	Jacob Smith	Undergraduate, University of Chicago	2011
2.	Aaron Goodman	Undergraduate, University of Michigan	2010 – 2011
1.	Alexander Hyla	Undergraduate, University of Michigan	2010 – 2011

Supplemental Instruction Mentor **indicates student was an SI for multiple semesters*

Supplemental Instructor for General Chemistry I

Brody Farace Nam Vu*	2024 (Fall)
Bridget McNish Li Yun (Angela) Tsai	2023 (Fall)
Nam Vu*	2022 (Fall)
Alex Ashley*	2021 (Fall)
Theresa Chua	2021 (Spring)
Alex Ashley* Isabella Santangelo Hannah Spitzer	2019 (Fall)
Jessica Luo*	2018 (Fall)
Emily Lugos	2017 (Fall)

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Supplemental Instructor for General Chemistry II

Maya Zilberstein	2025 (Fall)
Nam Vu*	2025 (Spring)
Jessie Grewal	2022 (Spring)
Alex Ashley*	
Katie Kavanagh	2018 (Fall)
Jessica Luo*	2018 (Spring)

Scholarship of Teaching & Learning and Professional Development

ACS Leadership Institute, American Chemical Society (*Invited*) — January 2026, Atlanta, GA
Participated in the ACS Leadership Institute, an annual invitation-only conference where ACS leaders come together to learn both management and leadership skills to enable them to be successful leaders within the American Chemical Society.
Completed the Local Section track.
Completed the Leading Without Authority workshop.

ACT-CMS Faculty Fellows Workshop, Molecular Science Software Institute (MolSSI) — June 2025, Blacksburg, VA
Participated in a week-long Curriculum Development Bootcamp focused on curriculum development and assessment training to enable creation of a reusable curriculum module that uses programming and computation in STEM.

Math in PChem Community of Practice, LABSIP Collaborative — 2023 – present, Virtual
Organized a nation-wide community of practice for physical chemists focused on identifying and developing solutions for math-related issues students experience in physical chemistry. Created CoP sub-groups to enable regular meetings.
Leader of a subgroup for the 2023-2026 AYs.

Scholarship of Teaching and Learning Community of Practice, Lafayette College — 2019 – 2024, Easton, PA
Member of a community of practice focused on designing and providing feedback on individual or collaborative pedagogical research studies

Enhancing Science Courses by Integrating Python (ESCIP) Workshop (*Invited*), New York University — April 2023, New York, NY
A small group workshop on developing course materials, learning new skills, and discussing best practices for using Python in undergraduate science courses

Introduction to Computational Antibody Engineering, Schrödinger Online Learning — March 2023, Virtual
Completed the Schrödinger Online Learning Course and earned a certificate.
Learned to use Schrödinger's BioLuminate software for antibody discovery and design in order to determine how the software could be utilized in a future course-based research project for CHEM 365/366.

Teaching Python for Computational Molecular Science, Molecular Science Software Institute (MolSSI) — August 2022, West Lafayette, IN
Workshop hosted by the MolSSI at the 2022 Biennial Conference on Chemistry Education on how instructors can teach Python coding in various chemistry courses, focusing on specific lesson examples and live coding demonstration skills.

POGIL-PCL Workshop, POGIL-PCL (Physical Chemistry Lab) — July 2020, Virtual
Virtual workshop demonstrating physical chemistry experiments students can carry out in their kitchens and analyze using Google Colab or Jupyter Notebooks.

Personalized Learning in Chemistry: Addressing Student Success, Equity, and Retention in Your Chemistry Course (*Invited*), McGraw-Hill Education — February 2020, Irvine, CA
Small group discussion on future and direction of the Chemistry course, expectations for learning and skill development, fostering conceptual understanding and application, designing effective learning resources.

POGIL Summer 3-Day Workshop, Simmons University — June 2019, Boston, MA
Workshop on process-oriented guided-inquiry learning (POGIL), an evidence-based, student-centered, group-learning instructional strategy and philosophy.

Center for the Integration of Research, Teaching, and Learning (CIRTL) Network
Various virtual workshops on professional development topics including:

Using an ePortfolio to Promote Reflection and Integration of Knowledge	November 2020
Course-based Undergraduate Research Experience	October 2020
Reducing Math Anxiety Among Your Students	October 2020
How Can We Interrupt and Mitigate Implicit Bias When We Witness It?	October 2018
How Can We Identify Implicit Biases in Ourselves and Others?	October 2018
How Pervasive Is Implicit Bias in STEM?	September 2018
Faculty Advising workshop	August 2018
Equity-Oriented, Inclusive Teaching in STEM	February 2018
Topics in STEMinism	November 2017

GRANTS, FELLOWSHIPS, and AWARDS

Computational Resource Grants and Programs

Principal Investigator of the "**Investigation of Turtle Melanopsin Activation/ Deactivation Mechanisms via QM/MM Calculations and Molecular Dynamics Simulations**," provided by the National Science Foundation's XSEDE Startup Allocation. (TG-BIO210086: 22,000 SUs) — June 2021 – June 2025

Google Cloud Research Innovator. Competitive program promoting trans-disciplinary collaborations and providing access to Google Cloud Project services. — April 2021 – April 2022

Principal Investigator of the "**Modeling Electron Transport in Bacterial Nanowires for Sustainable Bioenergy Applications**," provided by the National Science Foundation's XSEDE Startup Allocation. (TG-CHE160025: 150,000 SUs) — April 2016 – April 2017

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Interdisciplinary Program Grants

"Quantum Student Interest Group," funded by the NSF CC* PA Science DMZ. ($3000) PI: **Hendrickson, H. P.** — 2026

"The art and science of photography and conservation," funded by the Lafayette Arts' Arts and Technology via the Sherman Fairchild Foundation. ($550) PI: **Hendrickson, H. P.** — 2025

"Lehigh Valley Symposium on CRISPR Implementation and Ethics," funded by Lehigh Valley Association of Independent Colleges (LVAIC) Funding for Collaborative Programs. ($1,000) Organizing committee chair: **Hendrickson, H. P.** Co-organizers: Wightman, B., Vora, N., Davis, D. — 2022

Teaching Grants (Lafayette College)

"Using the Mechanisms App for Acid/Base Reactions," funded by Lafayette College's Teaching with Technology Grant
Provided support for purchasing the Mechanisms App used in Chem 122 — August 2018 – December 2018

"Using the Mechanisms App for Acid/Base Reactions in General Chemistry II (CHEM 122)," funded by Lafayette College's Meta-Mindset Grant
Objective: For students to understand acid-base reactions at a deeper level by using the Mechanisms app, which enables them to visualize and manipulate the reaction mechanism in acid- base reactions. — August 2018 – December 2018

"Utilizing Compute-to-Learn pedagogy within CHEM 324," funded by Lafayette College's Meta-Mindset Grant
Objective: Enable students to collaboratively construct demonstrations of physical chemistry topics using the Mathematica software to achieve a deeper understanding of and to explore the limits of these concepts and theories. — January 2018 – May 2018

Research Grants (University of Michigan)

Co-Principal Investigator of the "***Compute-To-Learn*: Designing interactive, computer-based demonstrations of physical chemistry concepts,**" funded by the University of Michigan's Transforming Learning for the Third Century – Quick Wins Program. ($25,000) PI: Geva, E. Co-PI's: **Hendrickson, H. P.**, Jafari, M., Welden, A. R., Williams, K., & Winograd, B. — September 2015 – December 2016

Co-Principal Investigator of the "**Developing a student-generated study-resource for CHEM 260,**" funded by the University of Michigan Instructional Technology Committee's Level I Faculty Grant. ($3,940) PI: Zgid, D. Co-PI's: **Phillips, H.**, Gysin, M., Porat, D. — June 2014 – June 2015

Co-Principal Investigator of the "**Using the STEM Studio to Design Science-Related Learning Experiences and Artifacts: A Transdisciplinary Collaboration**," funded by the University of Michigan's Transforming Learning for the Third Century – Quick Wins Program. ($24,968.70) PI: Bricker, L. A. Co-PI's: Barnard, R. A., Crocker, K. C., Kademian, S. M., **Phillips, H.**, Prater, K. E., Reicher, M. A., & Zaidi, S. Z. — October 2013 – April 2015

Co-Principal Investigator of the "**Developing a student-generated wiki-textbook for CHEM 260,**" funded by the University of Michigan Instructional Technology Committee Level II Faculty Grant. ($13,668) PI: Sension, R. Co-PI: Geva, E., **Phillips, H.** — September 2012 – May 2014

Fellowships

Accelerating Curricular Transformation in the Computational Molecular Sciences Faculty Fellowship, Molecular Science Software Institute (MolSSI) — 2025 – 2027
The goal of ACT-CMS is to transform science curricula by accelerating the integration of programming and computation into existing molecular science courses through faculty training and the development of open and reusable curricular modules.

SoTL Scholar, Center for Integration of Teaching and Learning, Lafayette College — 2022 – 2023
Scholarship of Teaching and Learning fellowship providing support to conduct a study in a learning environment during the academic year.

Junior Fellowship, Sweetland Center for Writing, University of Michigan — 2014 – 2015
Seminar for graduate students and faculty from multiple disciplines who share a commitment to integrating writing in their courses. Culminates in course design and teaching a discipline-specific writing composition course.

NSF Graduate Research Fellowship, National Science Foundation — 2011 – 2014

Rackham Merit Fellowship, Rackham Graduate School, University of Michigan — 2009 – 2011
Promotes diversity and inclusion by funding students with superior academic achievement who represent a broad array of life experiences and perspectives.

Awards and Recognition

Excellence in Teaching at Small Colleges Award — 2026
Lehigh Valley Section of the American Chemical Society

MERCURY Conference Poster Session Faculty Mentor Award — 2024
Amazon Web Services and the MERCURY Consortium

Recognized for the "Thank a Professor or Staff Member" Initiative — Fall 2023, Fall 2024
Lafayette College Center for Integration of Teaching, Learning, and Scholarship

Nominated for the Aaron O. Hoff Award for Superior Teaching – Sciences and Engineering — 2022, 2023, 2024
Lafayette College Leadership Education Committee

Faculty All-Star Award — 2019
Lafayette College Department of Athletics and Student-Athlete Advisory Council

Recognized at "Faculty Appreciation Night" Volleyball Game — 2018, 2019
Lafayette College Women's Volleyball Team

Reviewer of the Month — 2019
International Journal of Quantum Chemistry

Baruch '60 Center for Biochemical Solar Energy Research Award of Excellence — 2017
Eastern Regional Photosynthesis Conference

Best Poster Award — 2015
Midwest Theoretical Chemistry Conference

Robert & Carolyn Buzzard Graduate Chemistry Student Leadership Award — 2013
Chemistry Department, University of Michigan
Awarded $500 for leadership and service to the chemistry department.

Poster Session Travel Award 2010 & 2011
Vaughan Symposium, University of Michigan Chemistry Department
David M. and Charlotte W. Trout Memorial Award 2009
Hillsdale College
Awarded $3000 as an outstanding science major pursuing graduate education.

Travel Grants
DoE Travel Award for the 32nd Inter-American Photochemical Society Winter Conference, US Department of Energy 2025
Postdoctoral Scholars Travel Fund, Office of Postdoctoral Affairs, Yale University 2016
Rackham Conference Travel Grant, Rackham Graduate School, University of Michigan 2010 – 2014

Competitive Scholarships (Hillsdale College)
LAUREATES Summer Research Scholarship 2008
Elizabeth Schermerhorn Women Commissions Scholarship 2008 – 2009
Hillsdale Merit Award – Presidential Scholarship 2005 – 2007

Honor Societies
Iota Sigma Pi, Women in Chemistry Honorary
Faculty advisor for students organizing and initiating the Protactinium Chapter of ISP in the Lehigh Valley Metropolitan region. 2023 – present
Treasurer, Protactinium Chapter 2024 – 2025
Vice-President, Hillsdale College Members at Large 2008 – 2009
Phi Sigma Tau, Philosophy Honorary
Treasurer, Kappa Chapter 2008 – 2009
Sigma Pi Sigma, Physics Honorary
Chapter #467 2008 – 2009
Sigma Zeta, Math/Science Honorary
Alpha Psi Chapter 2007 – 2009

SERVICE

Professional Affiliations and Societies
Iota Sigma Pi, Women in Chemistry Honorary 2008, 2023 – present
MERCURY Consortium (Molecular Education and Research Consortium in Undergraduate computational chemistRY) 2018 – present
MoleCVUE (Molecular Computation and Visualization in Undergraduate Education) 2018 – present
American Chemical Society 2008 – present
Local Section membership: Lehigh Valley ACS
Division membership: CHED, COMP, PHYS
Inter-American Photochemical Society 2024 – 2025

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Professional Service

Journal Referee (Reviewed 28 articles for the following publications) 2018 – present

ACS Books
ACS Neuroscience
ACS Omega
Biochemistry
Chemistry Select
International Journal of Quantum Chemistry (*Reviewer of the Month – June 2019*)
Journal of Chemical Education
Journal of Chemical Physics
Journal of Molecular Graphics and Modelling
Journal of Physical Chemistry
New Journal of Chemistry
Physical Chemistry Chemical Physics
Organic Electronics
Solar RRL
Spectrochimica Acta: Part A
The FEBS Journal (Federation of European Biochemical Societies)

External Reviewer for Promotion and Tenure

State University of New York at Oneonta
Furman University
University of Hartford

American Chemical Society

National Meetings

Oral Session Presider

Served as a presider for an in-person PHYS – QIS for Chemistry and Chemistry for QIS oral presentation session during the ACS Spring 2025 National Meeting. 2025

Served as a presider for a virtual COMP – Materials Science oral presentation session during the ACS Spring 2022 National Meeting. 2022

Poster Session Judge

Served as a judge for the COMP undergraduate student poster awards 2023 – 2026

Served as a judge for the PHYS student poster awards 2025

Regional Meetings: MARM (Mid-Atlantic Regional Meeting of the ACS)

Symposium and workshop organizer 2024

Organized a "Computational Chemistry in the Classroom" symposium, featuring 18 talks, a panel discussion titled "Computation and Visualization in Chemistry Education: Challenges and Strategies for the Future", and a complementary "Computational Chemistry in the Classroom" workshop University Park, PA

Local Section: Lehigh Valley Section of the American Chemical Society (LVACS)

LVACS Chair-elect 2026

Organized the programming for AY 2026-2027 and performed other executive activities as required by the LVACS chair

Meeting Organizer — October 2025
Organized a LVACS local section meeting at Lafayette College

NSF PA Science DMZ – Quantum Student Interest Group — 2026 – present
Faculty Mentor
Led team of three student leaders to run a weekly, online interest group on quantum computing and information science for students from PA Science DMZ institutions (Penn State, Indiana University of PA, Lafayette, Swarthmore)

Math in PChem Community of Practice (CoP), LABSIP Collaborative
CoP Sub-Group Leader — 2023 – present
CoP Organizer — 2023
Organized a nation-wide community of practice for physical chemists focused on identifying and developing solutions for math-related issues students experience in physical chemistry. Created CoP sub-groups to enable regular meetings. Leader of a subgroup for the 2023-2025 AYs.

CyberAccelerate Poster Session, KINBERCON 2025 — October 2025
Poster Session Faculty Lead — Lancaster, PA
Faculty lead organizer for the NSF Pennsylvania Science DMZ CyberAccelerate student poster session during the Kinber Conference, which aims to enable a more inclusive and innovative digital future.

Community of Communities Gathering 2025 (*Invited*), Community of Communities — June 2025
Workshop Participant — Holland, MI
A small group workshop with the goal to build strong and lasting bridges between chemistry communities of practice to improve chemistry teaching and learning across the entire chemistry community.

NSF CCI Center for Quantum Dynamics on Modular Quantum Devices — 2023 – 2024
Director of Education, Outreach, and Training
Led the development of QIS workshops for high school students. Coordinated education, outreach, and training efforts across the CCI.

MoleCVUE 2024 — 2023 – 2024
Meeting Organizer — University Park, PA
Organizing chair for the annual MoleCVUE consortium meeting, which was held prior to the MARM 20204 meeting at Penn State in 2024.

NSF/UKRI Bilateral Workshop on Quantum Information Science in Chemistry (*Invited*), National Science Foundation — February 2024
Workshop Participant — Alexandria, VA
A small group workshop with the goal to define and articulate unique "chemistry-centric" opportunities for research directions and open questions at the interface between chemistry and quantum information science.

Lowering Activation Barriers to Success in Physical Chemistry (LABSIP) In-Person Workshop (*Invited*), LABSIP Collaborative — July 2023, Tucson, AZ
Workshop Participant
A small group workshop with the goal to 1) develop a consensus set of content-independent learning goals for Physical Chemistry courses, and 2) identify the most impactful support structures to achieve these learning goals.

Women in Science and Engineering (WISE) Forum — 2018
Mentor
Served as a mentor to high school women interested in science during a networking and mentoring event sponsored by the Da Vinci Science Center.

Faculty Service – Lafayette College

Events

YQuantum Hackathon Trip, PA Science DMZ — 2026
Faculty Organizer
Organized a trip to Yale University for seven (7) Lafayette students and one (1) Indiana University of PA student to attend the YQuantum Hackathon.

Trip to NYC – Brooklyn Center for Theatre Research, Lafayette College — 2025
Organizer
Organized a trip to NYC for an interdisciplinary group of students to see the play *Doomers* by Matthew Gasda at the Brooklyn Center for Theatre Research. *Doomers* explores the ethical implications of artificial intelligence via a fictionalized take on Sam Altman's ousting from OpenAI in November 2023.

Quantum Unlocked – IBM Qiskit Fall Fest, Lafayette College — 2024
Organizing committee faculty chair
Advised students organizing the Quantum Unlocked event, an IBM sponsored event for the 2024 Qiskit Fall Fest, including a QIS panel discussion with five invited panelists; a staged reading of the play *Copenhagen* by Michael Frayn; and a Qiskit workshop co-led by Yale graduate students and Lafayette students. https://sites.google.com/lafayette.edu/qiskitfallfest2024/home

World Piano Day Celebration, Lafayette College — 2024
Co-organizer
Organized the World Piano Day Celebration incorporating three events to highlight the interconnections between science and music: a student panel on their experiences connecting musical and scientific academic interests, an invited guest lecture on quantum information science and music, and a piano concert.

Trip to NYC – Schrodinger, Inc and the Metropolitan Museum of Art, Lafayette College — 2023
Organizer
Organized a trip to NYC for an interdisciplinary group of students for a career panel and tour of a computational chemistry company (Schrodinger, Inc.), and a tour of the Met Museum photograph and time-based media conservation labs.

Summer Tie-Dye Event, Lafayette College 2023
Organizer
Organized a campus-wide, summer tie-dye event with the aim to strengthen the campus community by engaging students, faculty, and staff across all divisions in a shared activity.

Lehigh Valley Symposium on CRISPR Implementation and Ethics, Lafayette College 2021 – 2022
Organizing committee faculty chair
Provided support for students to organize the LV-SCIE, an interdisciplinary, day-long event on the Nobel Prize winning CRISPR-Cas9 gene-editing technology. Raised $20,000 in funding for the symposium. Participated in planning, organizing, and running the symposium.
https://sites.google.com/lafayette.edu/lv-scie

Committees

Summer Research Programming, Lafayette College 2026 – present
Committee member
Planning on-campus programming for summer research scholars and their faculty mentors.

Interdisciplinary Action Team, Lafayette College 2025 – present
Committee member
Working to expand opportunities for social innovation, creative scholarship and activity, entrepreneurial mindsets, and inclusive collaboration and integration across centers, the libraries, and academic departments and programs.

NSF PA Science DMZ – Science Driver Committee, Lafayette College 2024 – present
Committee member
Providing leadership on the science drivers for the NSF CC*-funded project: "CC* Regional Networking: The Pennsylvania Science DMZ supporting under resourced colleges and universities (PA Science DMZ)".

High-Performance Computing Advisory Committee, Lafayette College 2019 – present
Committee member
Providing guidance for the use, procurement, and prioritization of HPC-related resources shared across Lafayette campus.

College Writing Program Advisory Committee, Lafayette College 2019 – present
Committee member
Integrating the practice of writing into courses across the curriculum and supporting writing through faculty development and writing associates program.

Visiting Faculty Search Committee, Biology Department, Lafayette College 2023
Committee member
Departmental search committee to fill visiting assistant professor position.

Research and High-performance Computing Manager Search Committee, Division of Information Technology Services, Lafayette College — 2023
Committee member
Divisional search committee charged with hiring a manager for the HPC cluster responsible for maintaining existing capabilities and developing new functionality.

Teaching and Learning Committee, Lafayette College — 2018 – 2020, 2021 – 2022
Elected committee member
Supported faculty development of teaching practice, scholarship on teaching and learning, and evaluation of teaching methods in the classroom.
Specific contributions: Co-led focus groups on faculty perceptions of student evaluation of teaching (SET) forms; analyzed quantitative data from survey of faculty perceptions of SET; assisted in the transition to online SET; drafted memos to PTR, department heads and program chairs, etc.

Subcommittee member: Joint T&L/Promotion, Tenure, and Review
Conducted review of criteria for distinctive teaching
Specific contributions: Co-led open meetings on potential revisions to criteria.

Other service

Minerva, Lafayette College — 2017 – present
Member
Participating in various activities and events to promote inclusion of women and underrepresented faculty members in STEM disciplines.

Summer Scholars Book Club, Lafayette College — 2021, 2022, 2025
Book Club Leader
Initiated an inclusive book club for summer research students.
The Housekeeper and the Professor by Yoko Ogawa — 2026
The Anxious Generation: How the Great Rewiring of Childhood Is Causing an Epidemic of Mental Illness by Dr. Jonathan Haidt — 2025
Social by Nature: The Promise and Peril of Sociogenomics by Dr. Catherine (Rina) Bliss — 2022
A Crack in Creation: Gene Editing and the Unthinkable Power to Control Evolution by 2020 Nobel Laureate Dr. Jennifer Doudna and Dr. Sam Sternberg — 2021
https://today.lafayette.edu/2021/06/29/a-crack-in-creation/

Coffee with Chemists, XLC Admissions Event, Lafayette College — 2018, 2020, 2023, 2025, 2026
Participant
Participated in the chemistry department's "Coffee with Chemists" XLC spring recruitment event for admitted students.

Biophysics Research Group, Lafayette College — 2018 – 2022
Member
Participating in meetings and presentations to promote interdisciplinary research across the biophysical sciences.

2019-2020 Community Reading, Lafayette College — 2019
Faculty discussion facilitator
Created discussion materials and facilitated discussion for an FYS section on Ross Gay's *Book of Delights.*

Faculty Service – Chemistry Department

Lafayette Chemistry Alumni Symposium, Chemistry Department, Lafayette College — 2025 – present
Team leader
Led (along with department head and other faculty members), the organization of a chemistry alumni symposium for Lafayette College's Bicentennial Celebration.

Iota Sigma Pi, Protactinium Chapter — 2023 – present
Faculty Advisor
Advising students on initiating a new chapter of Iota Sigma Pi, the Women in Chemistry honorary, in the Lehigh Valley metropolitan area.

Assessment Team, Chemistry Department, Lafayette College — 2020 – present
Team Leader
Leading a team of four other faculty in overseeing and improving chemistry department assessment plan.

Institute for Future PUI Faculty (IFPF), Chemistry Department, Lafayette College
Faculty Mentor — 2022, 2023, 2025
Mentored IFPF participant in teaching general/physical chemistry courses
Session leader — 2025, 2026
Student-Centered Teaching/Active Learning Strategies session leader: co-led a discussion on teaching a Course-based Undergraduate Research Experience.

Women & Inclusion in The Sciences, Chemistry Department, Lafayette College — 2017 – 2024
WITS Organizing Committee member
Planning and participating in various activities and events to promote inclusion of women in STEM disciplines.

Faculty Search Committee, Chemistry Department, Lafayette College — 2024, 2025
Committee member
Departmental search committee charged with filling a tenure-track assistant professor position (physical chemistry, 2025; biochemistry, 2024)

Visiting Faculty Search Committee, Chemistry Department, Lafayette College — 2018, 2020, 2022
Committee member
Departmental search committee charged with filling visiting assistant professor positions (two in 2018, one in 2020, one in 2022).

Departmental Clerk, Chemistry Department, Lafayette College — 2017 – 2018
Clerk of the Chemistry Department
Recorded the meeting minutes for all department meetings during AY 17-18.

Invited Speakers and Departmental Seminars, Lafayette College

21. Mr. Michael O'Connor '22, The University of Wisconsin - Madison (Career event for CHEM 342 class)	November 2025
20. Prof. Christina Vizcarra, Barnard College (Lehigh Valley ACS event)	October 2025
19. Prof. Anne Vazquez, St. John's University (Iota Sigma Pi event)	April 2025
18. Prof. Aron Huckaba, University of Kentucky	January 2025
17. Mr. Christopher Bishop, Podcaster (Quantum Unlocked panelist)	November 2024
16. Dr. Layla Hormozi, Brookhaven National Lab (Quantum Unlocked panelist)	November 2024
15. Dr. Marlou Slot, NIST & University of Colorado – Boulder (Quantum Unlocked panelist)	November 2024
14. Dr. Francesco Valenti, IBM Quantum (Quantum Unlocked panelist)	November 2024
13. Prof. Chen Wang, UMass Amherst (Quantum Unlocked panelist)	November 2024
12. Prof. Victor Batista, Yale University (World Piano Day speaker)	March 2024
11. Dr. Anda Trifan, Glaxo-Smith-Klein (GSK) (WITS event)	February 2024
10. Prof. Elizabeth Thrall, Fordham University (WITS event)	January 2024
9. Dr. Kaitlin McCardle, Nature Computational Science, Nature Portfolio (WITS event)	November 2023
8. Prof. Tania Lupoli, New York University (WITS event)	March 2023
7. Prof. Jeremy Feldblyum, University at Albany, SUNY	January 2023
6. Prof. Glen Hocky, New York University	October 2022
7. Prof. K. Joy Karnas, Cedar Crest College (Lehigh Valley Symposium on CRISPR Implementation and Ethics speaker)	September 2022
6. Prof. Bruce Wightman, Muhlenberg College (Lehigh Valley Symposium on CRISPR Implementation and Ethics speaker)	September 2022
5. Prof. Rina Bliss, Rutgers University (Lehigh Valley Symposium on CRISPR Implementation and Ethics Keynote)	September 2022
4. Prof. Sam Sternberg, Columbia University (Lehigh Valley Symposium on CRISPR Implementation and Ethics Keynote)	September 2022
5. Prof. Lisa Fredin, Lehigh University (WITS event)	October 2021
4. Ms. Laramie Jensen, Oceanography PhD student at Texas A&M (WITS event)	November 2019
3. Dr. Kira Armacost, Merck & Co., Inc. (WITS event, part of Women in STEM week)	April 2019
2. Dr. Spencer Stober, Exxon Mobil Research and Engineering Corporate Strategic Research	November 2018
1. Ms. Ellen Mulvihill, Chemistry PhD student at the University of Michigan	October 2018

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Post-doctoral Service

Chemistry Education Group, Chemistry Department, Yale University 2016 – 2017
Co-founder
Established an organization for graduate students, post-docs, and faculty interested in education research and practice within the chemical sciences.

Girls Science Investigations, Physics Department, Yale University 2015 – 2017
Session Leader
Facilitated hands-on activity sessions to guide middle school girls in discovering and understanding various topics in physics.

Younger Chemists Committee, American Chemical Society, New Haven, CT 2015 – 2017
Committee member
Visited local universities to serve on career panels addressing education and research questions from undergraduate students. Organized and served as a presentation judge at the New Haven ACS Undergraduate Research Symposium.

Graduate Service

Chemical Sciences at the Interface of Education (CSIE|UM), University of Michigan 2014 – 2015
Organization Committee member
Organized speakers, panels, and other events addressing various topics in chemistry education.
Presented original research, literature discussions, and served as panel speaker.

STEM Studio, University of Michigan 2013 – 2015
Studio facilitator and participant
Developed studio-based learning experiences and artifacts within STEM disciplines as part of trans-disciplinary collaboration.

Instructional Technology Committee, University of Michigan 2010 – 2015
Graduate student member
Reviewed grant proposals to support innovative use of instructional technology in University of Michigan courses.

The Vaughan Symposium Organizing Committee, University of Michigan 2012 – 2013
Committee Chair (2013), Chair-elect (2012)
Led a committee of graduate students in organizing a department-wide chemical research symposium.
Initiated the inclusion of chemistry education research in the symposium.

Chemistry Graduate Student Council, University of Michigan 2010 – 2013
Vice-President, Treasurer
Organized events to enhance chemistry graduate student experiences, and served as a liaison between the graduate student body and department faculty & staff.

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INVITED PRESENTATIONS

Conference Presentations

16/17. ACS Spring 2026 (National Meeting of the American Chemical Society) — March 2026
(1) Engaging the next-generation of computational chemists: Vignettes from an undergraduate research group at a liberal arts college — Atlanta, GA
(2) Incorporating computation and programming across the chemistry curriculum: Engaging with communities of practice can help!

15. ACS Fall 2025 (National Meeting of the American Chemical Society) — August 2025
Using WebMO to explore symmetry elements and point groups — Washington, DC

13/14. ACS Spring 2025 (National Meeting of the American Chemical Society) — March 2025
(1) Developing quantum machine learning algorithms to predict electrophilicity — San Diego, CA
(2) Course-based research experience in chemistry at Lafayette College

12. 32nd Inter-American Photochemical Society (I-APS) Winter Conference — January 2025
Characterizing the Environmental Effect on Chromophore Absorption in Turtle Melanopsin using Computational Chemistry — Miramar Beach, FL
Received "DOE Travel Award"

11. MARM 2024 (Mid-Atlantic Regional Meeting of the American Chemical Society) — June 2024
Predicting the chromophore identity in turtle melanopsin using quantum mechanics/molecular mechanics calculations and molecular dynamics simulations — University Park, PA

10. Teaching & Learning Colloquium — October 2023
Utilizing student-generated Mathematica demonstrations in general chemistry courses — Center Valley, PA
Co-presented with undergraduate Vedit Venkatesh

9. Schrödinger Educator's Week — June 2023
Developing Computational Activities for a Course-Based Research Experience (CURE) — Virtual

8. ACS Spring 2023 (National Meeting of the American Chemical Society) — March 2023
Utilizing student-generated Mathematica demonstrations in general chemistry courses — Indianapolis, IN

7. BCCE 2022 (Biennial Conference on Chemistry Education) — July 2022
Using the Compute-to-Learn pedagogy in physical and general chemistry courses — West Lafayette, IN

6. MARM 2022 (Mid-Atlantic Regional Meeting of the American Chemical Society) — June 2022
Undergraduate researchers use density functional theory to investigate ferrocene-based polymers — Ewing, NJ

5. Amber Developer's Meeting — February 2020
Modeling the Optoelectronic Properties of Fc-based Polymers: Considerations for Force-Field Development — Safety Harbor, FL

4. Cambridge Crystallographic Date Centre (CCDC) User Group Meeting — August 2018
Computational Investigation of the Antagonist Binding Site in PTGER3 Using the CSD-Discovery Suite — Boston, MA

3. CECAM Workshop: Computational Insight into Photo-induced Processes at Interfaces — October 2016
Linker Rectifiers for Covalent Attachment of Catalysts to Semiconductor Surfaces — Bremen, Germany

2. Gordon Research Conference on Molecular Interactions and Dynamics — July 2016
Mechanisms for Allosteric Inhibition of Protein Tyrosine Phosphatase 1B — Stonehill, MA

1. Midwest Undergraduate Computational Chemistry Consortium Conference — July 2013
Predictive Computational Methods for Charge Transfer in Organic Photovoltaic Systems — Ann Arbor, MI

Seminars

14. Binghamton Local Section of the American Chemical Society — April 2026
Making Chemistry Accessible with Molecular Visualization Software — Binghamton, NY

13. The Amazing Chemistry Insights and Discussions (ACID) Series — June 2025
An Introduction to Computational Chemistry using WebMO — Virtual

12. New Jersey City University STEM Faculty Development Seminar — December 2024
Developing a Course-Based Research Experience (CURE): Designing Computational Activities using Teaching with Schrodinger — Jersey City, NJ

11. Lafayette College IEEE Club Seminar — October 2024
My Career Pathway Toward Engaging the Next-Generation of Computational Chemists in Quantum Computing — Easton, PA

10. Stevens Institute of Technology Chemistry and Chemical Biology Department Seminar — August 2024
Real-life Teaching with Schrödinger Example: Excerpts from a Course-based Undergraduate Research Experience (CURE) — Hoboken, NJ

9. New York University Chemistry Department Seminar — March 2024
Engaging the Next-Generation of Computational Chemists in Undergraduate Research at a Liberal Arts College — New York, NY

8. Barnard College Chemistry Department Seminar — October 2023
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers Calculated using Density Functional Theory — New York, NY

7. Fordham University Chemistry Department Seminar — September 2023
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers Calculated using Density Functional Theory — New York, NY

6. Lafayette College SoTL Scholar Presentation — April 2023
Utilizing Student-Generated Mathematica Demonstrations in General Chemistry Courses — Easton, PA

5. Lehigh University Chemistry Department Seminar — March 2022
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers Calculated using Density Functional Theory — Bethlehem, PA

4. Lafayette College ARC Works-in-Progress Talk — April 2019
Designing molecules and materials with insights from computational chemistry. — Easton, PA

3. Lafayette College Biophysics Research Group Seminar — October 2018
Eigenvector Centrality for Characterization of Protein Allosteric Pathways. — Easton, PA

2. Yale Physical Chemistry Club Seminar — October 2015
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices — New Haven, CT

1. Hillsdale College Chemistry Department Seminar — October 2012
Using Computational Chemistry to Understand Systems with Optoelectronic Applications — Hillsdale, MI

Panel Discussions

16. How to Set Your Students Up for Success with Molecular Modeling Skills (Schrodinger Educator's Week) — April 2026
Discussion on integrating computational molecular modeling in teaching and research — Virtual

15. Narrating Knowledge: New Dimensions in Molecular Science Communication and Teaching (Women Chemists Committee – ACS Spring 2026) — March 2026
Discussion with panelists, including ACS President, President-Elect, and Immediate Past President, on communicating science outside traditional academic formats — Atlanta, GA

14. Being a Tenure-line Faculty Member (New Faculty Orientation – Lafayette College) — August 2025
Discussion on experiences as a tenure-line faculty member at Lafayette — Easton, PA

13. Women in STEM Tea (Tri Beta – Lafayette College) — March 2025
Discussion on experiences of women in STEM — Easton, PA

12. Minerva Panel Discussion on Working with Research Students (Lafayette College) — November 2024
Discussion on working with research students for underrepresented women faculty — Easton, PA

11. Institute for Future PUI Faculty Panel Discussion (Lafayette College) — July 2024
Discussion for IFPF applicants on PUI Faculty Careers — Virtual (Easton, PA)

10. Graduate Division at UC Merced (University of California, Merced) — July 2024
Discussion for graduate students on PUI Faculty Careers — Merced, CA

9. Mental Health Initiative (Lafayette College) — May 2021
Discussion for college community on student mental health awareness — Virtual (Easton, PA)

8. Academic Mentor "Morning Coffee Hour" (ACS Computers in Chemistry Division) — April 2021
Discussion on academic careers in computational chemistry for interested students — Virtual

7. Women in STEM Tea (Tri Beta – Lafayette College) — March 2021
Discussion on experiences of women in STEM — Virtual (Easton, PA)

6. Yale Resonance Conference (Yale Scientific Magazine) — December 2016
Discussion for High School Students: "Your Pathway through Science" — New Haven, CT

5. YCC Careers in Chemistry (Fairfield University) — April 2016
Discussion for Undergraduate Students by the ACS Younger Chemists Committee — Fairfield, CT

4. YCC Careers in Chemistry (New Haven University) — October 2015
Discussion for Undergraduate Students by the ACS Younger Chemists Committee — West Haven, CT

3. Chemical Sciences at the Interface of Education (CSIE|UM) — May 2015
Discussion on Honors Chemistry Courses: "What is Honors?" — Ann Arbor, MI

2. Enriching Scholarship Conference (University of Michigan) — May 2012
Discussion for Undergraduate Students: "How I Became Involved in Computational Chemical Research" — Ann Arbor, MI

1. CyberInfrastructure Days Conference (University of Michigan) — December 2011
Discussion for Undergraduate Students: "How I Became Involved in Computational Chemical Research" — Ann Arbor, MI

CONTRIBUTED PRESENTATIONS

Oral Presentations

29/30. BCCE 2024 (Biennial Conference on Chemistry Education) — July 2024 — Lexington, KY
(1) Quantum Chess Workshops as a Method to Introduce Quantum Information Science Through Quantum Superposition for High School Students
(2) Investigating the impact of student-generated Mathematica demonstrations developed using the Compute-to-Learn approach

27/28. ACS Spring 2024 (National Meeting of the American Chemical Society) — March 2024 — New Orleans, LA
(1) Investigating the impact of student-generated Mathematica demonstrations developed using the compute-to-learn approach
Co-presented with undergraduate Vedit Venkatesh
(2) Computational investigation of charge transfer in ferrocene-based metallopolymers of intrinsic microporosity

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26. IEEE Integrated STEM Education Conference (ISEC '24) — March 2024
Impact of Quantum Mechanics-Based Workshops on Developing High School Students' Interest and Intuition in Quantum Information Science — Princeton, NJ
Co-presented with undergraduate Padmanabh Kaushik

25. LABSIP Math in PChem CoP workshop — January 2024
Reflections on How to Get the Most Out of Organizing a LABSIP Community of Practice — Virtual

24. Teaching & Learning Colloquium — October 2023
Quantum Chess as a Method to Introduce Quantum Superposition in General Chemistry — Center Valley, PA

22/23. CERM 2023 (Central Regional Meeting of the American Chemical Society) — June 2023
(1) Utilizing student-generated Mathematica demonstrations in general chemistry courses — Dearborn, MI
(2) Computational investigation of charge transfer in ferrocene-based polymer materials

21. LABSIP Fall 2022 — November 2022
Using the Compute-to-Learn Pedagogy in Physical Chemistry — Virtual

20. MoleCVUE 2022 — June 2022
A CANDO (Computer Aided Nanomaterial Design and Optimization) Attitude Towards Undergraduate Chemistry Education — Oneonta, NY

19. ACS Spring 2022 (National Meeting of the American Chemical Society) — March 2022
Computational investigation of charge transfer in ferrocene-based polymer materials — Virtual

18. ACS Spring 2021 (National Meeting of the American Chemical Society) — April 2021
Computational investigation of structure-property relationships in ferrocene-based polymer materials — Virtual

17. *Cancelled due to COVID*- 2020 Biennial Conference on Chemistry Education — *July 2020*
Adapting the compute-to-learn pedagogy: From a research university to a liberal arts college — *Corvallis, OR*
Abstract accepted March 31, 2020. Because of the global COVID-19 pandemic, the 2020 Biennial Conference on Chemical Education was terminated on April 2, 2020, by the Executive Committee of the Division of Chemical Education, American Chemical Society; and, therefore, this presentation could not be given as intended.

16. MoleCVUE 2020 — June 2020
Updates on: Adapting the compute-to-learn pedagogy to a liberal arts college — Virtual

14/15. *Cancelled due to COVID* –
ACS Spring 2020 (National Meeting of the American Chemical Society) — *March 2020*
(1) Computational investigation of structure-property relationships in ferrocene-based polymer materials — *Philadelphia, PA*

(2) Adapting the compute-to-learn pedagogy from a research university to a liberal arts college

Abstracts were accepted but conference was cancelled due to Covid-19

13. MoleCVUE 2019 — June 2019
Adapting the compute-to-learn pedagogy to a liberal arts college — Middletown, CT

12. ACS Spring 2018 (National Meeting of the American Chemical Society) — March 2018
Towards the rational design of alternative, eco-friendly herbicides targeting PSII — New Orleans, LA

11. 2017 Eastern Regional Photosynthesis Conference — April 2017
Towards the Rational Design of Alternative, Eco-Friendly Herbicides Targeting Photosystem II — Woods Hole, MA

Awarded "Baruch '60 Center for Biochemical Solar Energy Research Award of Excellence"

10. ACS Spring 2017 (National Meeting of the American Chemical Society) — April 2017
Mechanisms for Allosteric Inhibition of Protein Tyrosine Phosphatase 1B — San Francisco, CA

7/8/9. ACS Spring 2016 (National Meeting of the American Chemical Society) — March 2016
(1) DFT-NEGF Study of Conducting Protein Filaments for Solar Energy Harvesting — San Diego, CA
(2) QM/MM Studies of Rhodopsin Thermal Decay
(3) Multiple Dimensions of "Wrong": Using Student Generated Explanations of Quantum Chemistry Topics to Explore Student Conceptual Understanding

6. Midwest Theoretical Chemistry Conference — June 2015
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices — Ann Arbor, MI

5. National Association of Research in Science Teaching — April 2015
Multiple Dimensions of "Wrong": Using Student Generated Explanations of Quantum Chemistry Topics to Explore Student Conceptual Understanding — Chicago, IL

4. Biennial Conference on Chemistry Education — August 2014
Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model — Grand Rapids, MI

3. Gordon Research Seminar on Computational Chemistry — July 2014
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices — West Dover, VT

2. ACS Fall 2013 (National Meeting of the American Chemical Society) — September 2013
Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach — Indianapolis, IN

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1. CERM 2013 (Central Regional Meeting of the American Chemical Society) — May 2013
Predictive Computational Methods for Charge Transfer in Functionalized Silsesquioxanes: Building Blocks for Photovoltaic Applications — Mt. Pleasant, MI

Poster Presentations

36. ACS Spring 2023 (National Meeting of the American Chemical Society) — March 2023
Using molecular dynamics simulations and transfer entropy pathway calculations to investigate binding of P2E to prostaglandin EP receptors — Indianapolis, IN

35. *Cancelled due to COVID –*
ACS Spring 2020 (National Meeting of the American Chemical Society) — *March 2020*
Adapting the compute-to-learn pedagogy from a research university to a liberal arts college — *Philadelphia, PA*
Selected for Sci-Mix Interdisciplinary Poster Session
Abstract was accepted but conference was cancelled due to Covid-19

34. Gordon Research Conference on Computational Chemistry — July 2018
Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations — West Dover, VT

33. ACS Spring 2018 (National Meeting of the American Chemical Society) — March 2018
Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations — New Orleans, LA
Selected for Sci-Mix Interdisciplinary Poster Session

32. Gordon Research Conference on Molecular Interactions and Dynamics — July 2016
Investigating Conductivity in Bacterial Nanowires for Solar Energy Harvesting — Stonehill, MA

31. ACS Spring 2016 (National Meeting of the American Chemical Society) — March 2016
Multiple Dimensions of "Wrong": Using Student Generated Explanations of Quantum Chemistry Topics to Explore Student Conceptual Understanding — San Diego, CA
Selected for Sci-Mix Interdisciplinary Poster Session

30. Midwest Theoretical Chemistry Conference — June 2015
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices — Ann Arbor, MI
Awarded "Best Poster Award"

28/29. CSIE|UM Symposium — June 2015
(1) *Compute-to-Learn:* Designing Interactive, Computer-Based Demonstrations of Physical Chemistry Concepts — Ann Arbor, MI
(2) Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model

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26/27. 2014 Vaughan Symposium — July 2014
(1) Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Photovoltaic Materials — Ann Arbor, MI
(2) Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model

25. Gordon Research Conference on Computational Chemistry — July 2014
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices — West Dover, VT

24. Organic Photovoltaic Symposium — April 2014
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Photovoltaic Materials — Kent, OH

23. CyberInfrastructure Days — November 2013
A Computational Approach to Rational Design for Organic Optoelectronic Devices — Ann Arbor, MI

21/22. ACS Fall 2013 (National Meeting of the American Chemical Society) — September 2013
(1) Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach — Indianapolis, IN
Selected for Sci-Mix Interdisciplinary Poster Session

(2) Predictive Computational Methods for Organic Optoelectronic Materials
Selected for Sci-Mix Interdisciplinary Poster Session

20. Gordon Research Conference on TDDFT — August 2013
Predictive Computational Methods for Organic Optoelectronic Materials — Biddeford, ME

19. 2013 Vaughan Symposium — August 2013
Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach — Ann Arbor, MI

18. Midwest Theoretical Chemistry Conference — May 2013
Predictive Computational Methods for Charge-Transfer in Organic Optoelectronic Materials — Urbana-Champaign, IL

17. Organic Photovoltaic Symposium — April 2013
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials — Kent, OH

16. CyberInfrastructure Days — November 2012
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials — Ann Arbor, MI

15. Center for Solar and Thermal Energy Conversion External Workshop — October 2012
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials — Ann Arbor, MI

14. Midwest Theoretical Chemistry Conference — June 2012
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications — Madison, WI

13. Michigan State University- Graduate Academic Conference — March 2012
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications — East Lansing, MI

12. Rackham Centennial Symposium- Graduate Students in the World — February 2012
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications — Ann Arbor, MI

11. CyberInfrastructure Days — December 2011
Using High Performance Computing to Study the Role of Symmetry in Electron Transfer for Photovoltaic Materials via Density Functional Theory — Ann Arbor, MI

10. 2011 Vaughan Symposium — August 2011
A Time-Dependent Density Functional Theory Analysis of the Charge Transfer Properties in Dye-Functionalized Silsesquioxane — Ann Arbor, MI
Awarded "Poster Session Travel Award"

9. American Theoretical Chemistry Conference (ACTC) — July 2011
A Time-Dependent Density Functional Theory Analysis of the Charge Transfer Properties in Dye-Functionalized Silsesquioxane — Telluride, CO

8. Center for Solar and Thermal Energy Conversion Annual Workshop — May 2011
On the Nature of Excited Charge Transfer States in Functionalized Silsesquioxanes — Ann Arbor, MI

7. CyberInfrastructure Days — November 2010
Using High-Performance Computing to Study Electron Transfer in Photovoltaic Materials Using Density Functional Theory — Ann Arbor, MI

6. 8th International Conference on Electroluminescence & Organic Optoelectronics — October 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time-dependent Density Functionals — Ann Arbor, MI

5. 2010 Vaughan Symposium — August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time-dependent Density Functionals — Ann Arbor, MI
Awarded "Poster Session Travel Award"

4. Michigan Quantum Summer School — August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time-dependent Density Functionals — Ann Arbor, MI

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3. Center for Solar and Thermal Energy Conversion Annual Workshop — August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time-dependent Density Functionals — Ann Arbor, MI

2. Theoretical, Computational, and Experimental Challenges to Exploring Coherent Quantum Dynamics in Complex Many-Body Systems — May 2010
Quantum Transport and Dynamics in Materials and Biosystems: From Molecular Mechanisms to Mesoscopic Functionality — Dublin, Ireland
(1) Probing Conjugation Effects on Charge Transfer Using TDDFT
(2) Symmetry Effects on the Electronic Spectra of Simple Molecular Junctions

1. PittCon 2009 — March 2009
Following the Surface-Induced Photoreduction of 4-Nitrobenzenethiol on Ag Nanoparticles Using Surface-Enhanced Raman Spectroscopy — Chicago, IL

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STUDENT PRESENTATIONS of MENTORED RESEARCH PROJECTS

Oral Presentations

MARM 2026 (Mid-Atlantic Regional Meeting of the American Chemical Society) — May 2026
Evaluating Machine Learning Models Trained on Computational Data to Predict Experimental Electrophilicity and Nucleophilicity — Hershey, PA
Presented by undergraduate researcher Bodhi Colvin

ACS Spring 2024 (National Meeting of the American Chemical Society) — March 2024
(1) Investigating the impact of student-generated Mathematica demonstrations developed using the compute-to-learn approach — New Orleans, LA
Co-presented by undergraduate researcher Vedit Venkatesh

(2) Computational model for rational design of L. plantarum AIP agonists
Presented by undergraduate researcher Carter Brand

IEEE Integrated STEM Education Conference (ISEC '24) — March 2024
(1) Impact of Quantum Mechanics-Based Workshops on Developing High School Students' Interest and Intuition in Quantum Information Science — Princeton, NJ
Co-presented by undergraduate researcher Padmanabh Kaushik

(2) Quantum Games for Quantum Computing (workshop)
Co-facilitated by undergraduate researchers Leah Boyle, Nick Sorak, Swetha Tadisina, Vedit Venkatesh, Crystal Yeung

Teaching & Learning Colloquium — October 2023
Utilizing student-generated Mathematica demonstrations in general chemistry courses — Center Valley, PA
Co-Presented by undergraduate researcher Vedit Venkatesh

ACS Spring 2021 (National Meeting of the American Chemical Society) — April 2021
Probing protein-protein interactions via SFG and MD simulations — Virtual
Presented by undergraduate researcher Zahra Gandhi

Cancelled due to COVID –
ACS Spring 2020 (National Meeting of the American Chemical Society) — *March 2020*
Density functional theory investigation of brown carbon species in aqueous aerosol mimics — *Philadelphia, PA*
To Be Presented by undergraduate researcher Emily Lugos
Abstracts were accepted but conference was cancelled due to Covid-19

Amber Developers' Meeting — February 2020
Computational investigation of melanopsin photoreception in freshwater and marine turtles — Tampa, FL
Presented by undergraduate researcher Michael O'Connor

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Lafayette College ARC Student Research Presentations — July 2019, Easton, PA
Density functional theory investigation of brown carbon species in aqueous aerosol mimics
Presented by undergraduate researcher Emily Lugos

Poster Presentations

Lafayette Bicentennial Chemistry Alumni Symposium — April 2026, Easton, PA
(1) Quantum Algorithmic Approaches to Conformational Optimization in Conjugated Polyenes
Presented by undergraduate researcher Skyler Chang

(2) Investigating Information Transfer Pathways in Prostaglandin E2 Receptors using Molecular Dynamics Simulations.
Presented by undergraduate researcher Genevieve Chukwuonye

(3) Impacts of Solvents on the Absorption Energies of Brown Carbon Molecules
Presented by undergraduate researcher Dylan Eschinger

Lehigh Valley Section of the ACS Annual Undergraduate Research Poster Session — April 2026, Center Valley, PA
Evaluating Machine Learning Models Trained on Computational Data to Predict Experimental Electrophilicity and Nucleophilicity
Presented by undergraduate researcher Bodhi Colvin

ACS Spring 2026 (National Meeting of the American Chemical Society) — March 2026, Atlanta, GA
(1) Quantum chess workshops as a method to introduce quantum information science through quantum superposition for high school students
Presented by undergraduate researcher Maya Zilberstein

(2) Investigating information transfer pathways in prostaglandin E2 receptors using molecular dynamics simulations
Presented by undergraduate researcher Genevieve Chukwuonye

(3) Computational analysis of information transfer and selectivity in prostaglandin E2 Receptors
Presented by undergraduate researcher Jaly Chimbo Macancela

(4) Impacts of solvents on the absorption energies of brown carbon molecules
Presented by undergraduate researcher Dylan Eschinger

(5) Grover adaptive search applied to polyene conformational problem
Presented by undergraduate researcher Skyler Chang

(6) Mechanistic insights into toxic carbonyl compound formation during ozonation of substituted phenols
Presented by undergraduate researcher Lan Anh Nguyen

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CyberAccelerate @ KINBERCON 2025 October 2025
Comparing classical machine learning models against quantum machine learning models for predicting the electrophilicity and nucleophilicity of molecules Lancaster, PA
Presented by undergraduate researcher Bodhi Colvin
Awarded the Honorable Mention poster award

2025 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference July 2025
(1) Developing Quantum Machine Learning Algorithms to Predict Electrophilicity Pittsburgh, PA
Presented by undergraduate researcher Anthony Lin

(2) Comparing classical machine learning models against quantum machine learning models for predicting the electrophilicity and nucleophilicity of molecules
Presented by undergraduate researcher Bodhi Colvin

(3) Developing a User-Friendly Post-processing Package to Convert Molecular Dynamics Trajectories to Electronic Structure Input
Presented by undergraduate researcher Brody Farace

(4) Impacts of Solvents on the Absorption Energies of Brown Carbon Molecules
Presented by undergraduate researcher Dylan Eschinger

(5) Computational Investigation of Information Transfer Pathways in Prostaglandin E2 Receptors
Presented by undergraduate researcher Genevieve Chukwuonye

(6) Using Density Functional Theory to Investigate Acidic Properties of Atmospheric Aerosols
Presented by undergraduate researcher Elizabeth Green

(7) Drug-Target Affinity Prediction through Quantum Machine Learning and Comparison to Classical Machine Learning
Presented by undergraduate researcher Skyler Chang

(8) Generating Descriptors for Electrophilicity and Nucleophilicity Prediction
Presented by undergraduate researcher Tran Hoang

ACS Spring 2025 (National Meeting of the American Chemical Society) March 2025
(1) Electrophilicity prediction with quantum machine learning models San Diego, CA
Presented by undergraduate researcher Swetha Tadisina

(2) Investigating the impact of descriptor quality on electrophilicity predictions from machine-learning models
Presented by undergraduate researcher Vedit Venkatesh

(3) Investigating information transfer in proteins using molecular dynamics simulations
Presented by undergraduate researcher Lucas Villamil

(4) Mechanistic Insights into (toxic) carbonyl compound formation during ozonation of substituted phenols
Presented by undergraduate researcher Nam Vu
Selected for Sci-Mix Interdisciplinary Poster Session

32nd Inter-American Photochemical Society (I-APS) Winter Conference — January 2025
Using Computational Methods to Determine the Chromophore of Visual Receptor Proteins — Miramar Beach, FL
Presented by undergraduate researcher Brody Farace

2024 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference — July 2024
(1) Developing Quantum Machine Learning Algorithms to Predict Electrophilicity and Teaching High Schoolers About Quantum Information Science — Merced, CA
Presented by undergraduate researcher Leah Boyle

(2) Computational Analysis of Information Transfer in Prostaglandin E2 Receptors Using MD Simulations
Presented by undergraduate researcher Jaly Chimbo Macancela

(3) Tackling Subgraph Isomorphism Puzzles with the Power of Gaussian Boson Sampling
Presented by undergraduate researcher Nam Vu

(4) Variational Preparation of Quantum State in a Superconducting Quantum Processor
Presented by undergraduate researcher Crystal Yeung

ACS Spring 2024 (National Meeting of the American Chemical Society) — March 2024
(1) Using student-generated Mathematica demonstrations in general chemistry courses — New Orleans, LA
Presented by undergraduate researcher Vedit Venkatesh

(2) Computational investigation of porosity in ferrocene-based polymer materials
Presented by undergraduate researcher Samuel Anthony

(3) Computational model for protein-ligand optimization in L. plantarum quorum sensing
Presented by undergraduate researcher Carter Brand

(4) Using molecular dynamics simulations to determine the identity of the chromophore, A1 or A2, in melanopsin (Opn4m) of red-eared slider turtles (Trachemys scripta elegans)
Presented by undergraduate researcher Alexa Jindal

(5) Investigating the impact of descriptor quality on electrophilicity predictions from machine-learning models
Presented by undergraduate researcher Vedit Venkatesh

(6) Computational investigation of information transfer pathways in prostaglandin E2 (EP) receptors
Presented by undergraduate researcher Nam Vu

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2023 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference — July 2023, Greenville, SC

(1) Using molecular dynamics simulations and quantum mechanics/molecular mechanics calculations to determine the chromophore in red-eared slider turtle melanopsin
Presented by undergraduate researcher Brody Farace

(2) Using Time-Dependent Density Functional Theory to Calculate UV Absorption in Aqueous Aerosols
Presented by undergraduate researcher Swetha Tadisina

(3) Investigating information transfer in proteins using molecular dynamics simulations
Presented by undergraduate researcher Lucas Villamil

Lafayette College's 2022 Spring Student Research Poster Session — April 2023, Easton, PA

(1) Molecular Dynamics Investigation of Opn4m and Opn4x in red-eared slider (Trachemys scripta elegans)
Presented by undergraduate researcher Zoey Bragg

(2) Molecular dynamics simulations and time-dependent density functional theory to determine chromophore identity in freshwater and marine turtle melanopsin
Presented by undergraduate researcher Haleigh Marzano

Lehigh Valley Section of the ACS Annual Undergraduate Research Poster Session — April 2023, Center Valley, PA

(1) Molecular Dynamics Investigation of Opn4m and Opn4x in red-eared slider (Trachemys scripta elegans)
Presented by undergraduate researcher Zoey Bragg

(2) Computational investigation of conjugation and porosity in metallocene polymers of intrinsic microporosity
Presented by undergraduate researcher Caroline Schaeffer

(3) Molecular dynamics simulations and time-dependent density functional theory to determine chromophore identity in freshwater and marine turtle melanopsin
Presented by undergraduate researcher Haleigh Marzano

(4) Computational modeling of intramolecular Diels-Alder reactions as a way of predicting product outcome
Presented by undergraduate researcher Elizabeth Foker

(5) Benchmarking Density Functional Theory Methods for Toxicity Prediction in Aqueous Electrophiles
Presented by undergraduate researcher Zheyu (Marc) Cui

(6) Using molecular dynamics simulations and transfer entropy pathway calculations to investigate binding of P2E to prostaglandin EP receptors
Presented by undergraduate researcher Nam Vu

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ACS Spring 2023 (National Meeting of the American Chemical Society) March 2023
(1) Utilizing student-generated Mathematica demonstrations in general chemistry courses Indianapolis, IN
Presented by undergraduate researcher Theresa Chua

(2) Computational investigation of conjugation and porosity in metallocene polymers of intrinsic microporosity
Presented by undergraduate researcher Caroline Schaeffer

Lafayette College's 2022 Fall Student Research Poster Session November 2022
Computational benchmarking study of chromophore absorption in freshwater and marine turtle melanopsin Easton, PA
Presented by undergraduate researcher Zoey Bragg

The Lehigh Valley Symposium on CRISPR Implementation and Ethics (LV-SCIE) September 2022
(1) Molecular dynamics simulations and time-dependent density functional theory to determine chromophore identity in freshwater and marine turtle melanopsin Easton, PA
Presented by undergraduate researcher Haleigh Marzano

(2) Investigating Activation and Inhibition Mechanisms in Prostaglandin E2 Receptors
Presented by undergraduate researcher Nam Vu

(3) Benchmarking Density Functional Theory Methods for Toxicity Prediction in Aqueous Electrophiles
Presented by undergraduate researcher Zheyu (Marc) Cui

(4) Tunable Porosity and Conjugation in Ferrocene-based Main-Chain Polymers
Presented by undergraduate researcher Theresa Chua

2022 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference July 2022
(1) Molecular dynamics simulations and time-dependent density functional theory to determine chromophore identity in freshwater and marine turtle melanopsin Greenville, SC
Presented by undergraduate researcher Haleigh Marzano

(2) Investigating Activation and Inhibition Mechanisms in Prostaglandin E2 Receptors
Presented by undergraduate researcher Nam Vu

(3) Benchmarking Density Functional Theory Methods for Toxicity Prediction in Aqueous Electrophiles
Presented by undergraduate researcher Zheyu (Marc) Cui

Lafayette College's 2022 Spring Student Research Poster Session April 2022
(1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles Easton, PA
Presented by undergraduate researcher Michael O'Connor

(2) Tunable Porosity and Conjugation in Ferrocene-based Main-Chain Polymers
Presented by undergraduate researcher Theresa Chua

Lehigh Valley Section of the ACS Annual Undergraduate Research Poster Session — April 2022
(1) Computational benchmarking study of chromophore absorption in freshwater and marine turtle melanopsin — Center Valley, PA
Presented by undergraduate researcher Zoey Bragg

(2) Computational investigation of porosity and conjugation in metallocene polymers of intrinsic micro porosity
Presented by undergraduate researcher Eman Shahzad

ACS Spring 2022 (National Meeting of the American Chemical Society) — March 2022
Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles — Virtual
Presented by undergraduate researcher Michael O'Connor

Lafayette College's 2021 Fall Student Research Poster Session — October 2021
(1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles — Virtual
Presented by undergraduate researcher Michael O'Connor

(2) Tunable Porosity and Conjugation in Ferrocene-based Main-Chain Polymers
Presented by undergraduate researcher Theresa Chua

ACS Spring 2021 (National Meeting of the American Chemical Society) — April 2021
Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles — Virtual
Presented by undergraduate researcher Michael O'Connor

2021 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference — August 2021
(1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles — Virtual
Presented by undergraduate researcher Michael O'Connor

(2) Investigation of UV-Vis Absorption in Ferrocene-based Polymer Materials using Time-Dependent Density Functional Theory
Presented by undergraduate researcher Alex Qian

Lafayette College's 2020 Fall Student Research Poster Session — September 2020
(1) Determining A1 or A2 chromophore in Red-Eared Slider Melanopsin — Virtual
Presented by undergraduate researcher Michael O'Connor

(2) Investigating the effects of solvating environments on UV-Vis absorption in aqueous aerosols using density functional theory
Presented by undergraduate researcher Rachel Petzoldt

Cancelled due to COVID –
ACS Spring 2020 (National Meeting of the American Chemical Society) *March 2020*
(1) Probing protein-protein interactions via SFG and MD simulations *Philadelphia, PA*
To Be Presented by undergraduate researcher Zahra Gandhi
Travel supported by GSSPC ACS Undergraduate Travel Grant

(2) Computational investigation of melanopsin photoreception in freshwater and marine turtles
To Be Presented by undergraduate researcher Michael O'Connor
Abstracts were accepted but conference was cancelled due to Covid-19

Lafayette College's 2019 Fall Student Research Poster Session October 2019
(1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations Easton, PA
Presented by undergraduate researcher Zahra Gandhi

(2) Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3 Receptor
Presented by undergraduate researcher Ella Kaplan

(3) Density functional theory investigation of brown carbon species in aqueous aerosol mimics
Presented by undergraduate researcher Emily Lugos

(4) 3-D Homology Model of Melanopsin in Painted Turtles (*Chrysemys picta bellii*)
Presented by undergraduate researcher Michael O'Connor

2019 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference July 2019
(1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations Greenville, SC
Presented by undergraduate researcher Zahra Gandhi

(2) Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3 Receptor
Presented by undergraduate researcher Ella Kaplan

(3) Density functional theory investigation of brown carbon species in aqueous aerosol mimics
Presented by undergraduate researcher Emily Lugos

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MACC-NYAGIM Symposium — May 2019
Computational investigation of structure-property relationships in ferrocene-based polymer materials — New York, NY
Presented by undergraduate researcher Liza Welch

Lafayette College's 2019 Spring Student Research Poster Session — April 2019
(1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations — Easton, PA
Presented by undergraduate researcher Zahra Gandhi

(2) Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3 Receptor
Presented by undergraduate researcher Ella Kaplan

(3) Density functional theory investigation of brown carbon species in aqueous aerosol mimics
Presented by undergraduate researcher Emily Lugos

ACS Spring 2019 (National Meeting of the American Chemical Society) — April 2019
(1) Density functional theory investigation of brown carbon species in aqueous aerosol mimics — Orlando, FL
Presented by undergraduate researcher Emily Lugos
Travel supported by ACS Bridge Travel Award

(2) Computational investigation of structure-property relationships in ferrocene-based polymer materials
Presented by undergraduate researcher Liza Welch

Lafayette College's 2018 Fall Student Research Poster Session — October 2018
(1) Computational investigation of semiconducting properties in ferrocene-based polymer materials — Easton, PA
Presented by undergraduate researcher Liza Welch

(2) Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3 Receptor
Presented by undergraduate researchers Zahra Gandhi, Ella Kaplan, and Emily Lugos

2018 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference — July 2018
Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3 Receptor — Greenville, SC
Presented by undergraduate researchers Zahra Gandhi and Ella Kaplan

2017 Eastern Regional Photosynthesis Conference — April 2017
Designing synthetic acceptor ligands to enhance electron transfer efficiency in PSII — Woods Hole, MA
Presented by undergraduate researcher Heather Harrington

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CERM 2013 (Central Regional Meeting of the American Chemical Society) May 2013
(1) Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach Mt. Pleasant, MI

Presented by undergraduate researchers Kari Chen and Michael Gysin

(2) Predictive Computational Methods for Organic Optoelectronic Materials

Presented by undergraduate researcher Francis DeVine