

EDUCATION

The University of Michigan , Ann Arbor, MI Ph.D. degree in Chemistry M.Sc. degree in Educational Studies	May 2015
Hillsdale College , Hillsdale, MI B.Sc. degree in Chemistry (<i>cum laude</i>)	May 2009

Maroon text indicates activities carried out at Lafayette College

RESEARCH and ACADEMIC EXPERIENCE

Assistant Professor of Chemistry , Lafayette College Utilizing multi-scale computational approaches to investigate optoelectronic properties of small molecules and polymer materials; protein-ligand interactions and information transfer pathways in proteins; and the reactivity and toxicity of aqueous environmental pollutants.	2017 – present
Postdoctoral Research in Chemistry , Yale University Investigated allosteric networks and charge transfer in biological macromolecules via multi-scale computational approaches. Advised by Prof. Victor S. Batista	2015 – 2017
Lecturer in Chemistry , University of Michigan Designed discussion-based course materials, lectured, held office hours, wrote and graded exams, and mentored a graduate student TA for a physical chemistry course.	2015
Ph.D. Research in Chemistry , University of Michigan 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 Advised by Prof. Eitan Geva Prof. Barry D. Dunietz	2009 – 2015 March 19, 2015
M.Sc. Research in Chemistry Education , University of Michigan 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	2010 – 2015
Graduate Research in Chemistry: Summer Institute , University of Michigan Studied transient aspects of electron transport in model molecular junctions. Advised by Prof. Barry D. Dunietz	2009
Undergraduate Research in Chemistry: LAUREATES Program , Hillsdale College Studied photoreduction reactions on nanostructured surfaces via surface-enhanced Raman spectroscopy. Advised by Prof. Matthew Young	2008

PUBLICATIONS

Peer-Reviewed Research Articles

Undergraduate co-authors advised by HPH are underlined

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.; 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. (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.
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

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, 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 (Previously CHEMISTRY 121: General Chemistry I)	
CHEM 122: General Chemistry II	
CHEM 341: Survey of Physical Chemistry (Previously CHEM 311: Elementary Physical Chemistry)	
CHEM 342: Physical Chemistry I (w/lab) (Previously CHEM 323/325: Physical Chemistry I (w/lab))	
CHEM 343: Physical Chemistry II (Previously CHEMISTRY 324/326: Physical Chemistry II (w/lab))	
CHEM 365: Course-based Research Experience in Chemistry	
CHEM 380/390/391/392/394: Independent Study/Research	
Computational investigation of light absorbing pigments in freshwater and marine turtle species.	2022-2023
Predicting the environmental toxicity of aqueous electrophiles using density functional theory and machine learning.	2022-2023
Computational investigation of the optoelectronic properties of ferrocene-based polymers.	2018-2022
Density functional theory investigation of brown carbon species in aqueous aerosol mimics	2019-2020
Molecular mechanics/quantum mechanics Investigation of antagonist binding mechanisms in the prostaglandin EP3 receptor protein	2019,2022-2023
CHEM 445: Special Topics in Physical Chemistry	
Honors Thesis Advisor (CHEM 495/496: Honors Thesis)	
Michael O'Connor <i>A computational investigation of chromophore binding in Red-eared turtle melanopsin</i>	2021-2022
Honors Thesis Committee Member	
Bridget Corpus (Biochemistry) TBA	2024 – present
Olivia Hofmann (Biology) TBA	2023 – present
Anthony McBain (Biochemistry) TBA	2023 – present
Samantha Ganer (Biochemistry) <i>Prion Interactions and Overlapping Functions of J-Domain Proteins in Saccharomyces cerevisiae</i>	2023
Anna Kunz (Biology) <i>Gene Expression Analysis of Phytophthora infestans Glycoside Hydrolase Family 28 Genes in Infected Potato Plants</i>	2022-2023
Isaiah Osei-Gyening (Biology) <i>Comparing the Association between Genetic Ancestry, DNA Methylation, and Patient Survival in African Americans and European Americans with Lung Cancer</i>	2021-2022

Alex Ashley (Chemical Engineering) <i>Manipulation of the Degradation of PEO-b-PCL through Preparation Techniques and Thermal Variations</i>	2021-2022
Yiru Gu (Chemistry) <i>In-Silico Prediction for Inhibiting of Lin-28/Pre-let 7 reaction with Synthesized Small Molecules for Pancreatic Cancer</i>	2021
Sarah Miller (Biochemistry) <i>Effects of Amino Acid Content on the Requirement of Swa2 on Artificial Prion Propagation</i>	2021
Jason Corcoran (Chemistry) <i>Synthesis and catalytic ability of pyridyl-substituted NHC-palladium complexes</i>	2019
Sierra Cole (Biochemistry) <i>Analyzing Hsp40 primary sequence dependence for chaperone-prion interactions</i>	2019
Scott Berger (Biochemistry) <i>The role of J-proteins in Hsp104 overexpression-mediated curing of the prion [PSI⁺]: A closer look at Apj1</i>	2019
Lecturer, Chemistry, University of Michigan CHEMISTRY 260: Chemical Principles CHEMISTRY 261: Introduction to Quantum Chemistry	2015
Instructor, English Language and Literature, University of Michigan ENGLISH 125: Writing and Academic Inquiry	2014
Graduate Student Instructor, Chemistry, University of Michigan CHEMISTRY 130: General Chemistry CHEMISTRY 260: Chemical Principles CHEMISTRY 261: Introduction to Quantum Chemistry	2015 2010
Honors Studio Facilitator, Chemistry, University of Michigan CHEMISTRY 260 Honors: Chemical Principles	2010 – 2014
<u>Workshop Facilitator</u> Quantum Games for Quantum Computing Easton Area High School IEEE Integrated STEM Education Conference (ISEC '24) 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.	2024
Molecular Modeling Workshop: Bringing Computational Chemistry into the Classroom , Lehigh Valley American Chemical Society (LV-ACS) Co-designed activities and held a workshop on incorporating computational chemistry software (WebMO) in college chemistry classes.	2023

- Computational Chemistry in the Classroom Workshop**, Biennial Conference on Chemistry Education 2022
Co-designed activities and held a workshop on incorporating computational chemistry software (WebMO) in high school or college chemistry classes.
- MolSSI Quantum Mechanics Tools Workshop**, Furman University 2022
Co-designed activities and held a workshop on python programming for quantum chemistry calculations for undergraduate researchers.
- Compute-to-Learn (C2L) Workshop**, Lafayette College 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

Undergraduate co-authors underlined

Current Students

- | | | | |
|-----|-----------------------|----------------------------------|----------------|
| 17. | Leah Boyle | Undergraduate, Lafayette College | 2024 – present |
| 16. | Crystal Yeung | Undergraduate, Lafayette College | 2024 – present |
| 15. | Tuna Akin | Undergraduate, Lafayette College | 2024 – present |
| 14. | Nick Sorak | Undergraduate, Lafayette College | 2023 – present |
| 13. | Maya Zilberstein | Undergraduate, Lafayette College | 2023 – present |
| 12. | Kusum Subedi | Undergraduate, Lafayette College | 2023 – present |
| 11. | Jaly Chimbo Macancela | Undergraduate, Lafayette College | 2023 – present |
| 10. | Carter Brand | Undergraduate, Lafayette College | 2023 – present |
| 9. | Sam Anthony | Undergraduate, Lafayette College | 2023 – present |
| 8. | Alexa Jindal | Undergraduate, Lafayette College | 2023 – present |
| 7. | Lucas Villamil | Undergraduate, Lafayette College | 2023 – present |
| 6. | Padmanabh Kaushik | Undergraduate, Lafayette College | 2023 – present |
| 5. | Brody Farace | Undergraduate, Lafayette College | 2023 – present |
| 4. | Swetha Tadisina | Undergraduate, Lafayette College | 2023 – present |
| 3. | Vedit Venkatesh | Undergraduate, Lafayette College | 2022 – present |

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|----|-----------------------------|------------------------------------|----------------|
| 2. | Nam Vu | Undergraduate, Lafayette College | 2022 – present |
| 1. | Daisy Grace | Graduate, Johns Hopkins University | 2021 – present |

Former Students

- | | | | |
|-----|----------------------------------|---------------------------------------|-------------|
| 48. | 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. | 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.	<u>Morgan Hammer</u>	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.	<u>Chenchen Song</u>	Undergraduate, Tsinghua University	2011
3.	Jacob Smith	Undergraduate, University of Chicago	2011
2.	Aaron Goodman	Undergraduate, University of Michigan	2010 – 2011
1.	<u>Alexander Hyla</u>	Undergraduate, University of Michigan	2010 – 2011

Supplemental Instruction Mentor

**indicates student was an SI for multiple semesters*

Supplemental Instructor for General Chemistry I

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

Supplemental Instructor for General Chemistry II

Jessie Grewal	2022 (Spring)
Alex Ashley*	
Katie Kavanagh	2018 (Fall)
Jessica Luo*	2018 (Spring)

Scholarship of Teaching and Professional Development

Math in PChem Community of Practice, LABSIP Collaborative	2023 – present
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 and leading a subgroup for the 2023-2024 AY.	
Scholarship of Teaching and Learning Community of Practice, Lafayette College	2019 – present
Member of a community of practice focused on designing and providing feedback on individual or collaborative pedagogical research studies	

NSF/UKRI Bilateral Workshop on Quantum Information Science in Chemistry (Invited), National Science Foundation

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.

February 2024
Alexandria, VA

Lowering Activation Barriers to Success in Physical Chemistry (LABSIP) In-Person Workshop (Invited), LABSIP Collaborative

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.

July 2023
Tucson, AZ

Enhancing Science Courses by Integrating Python (ESCIP) Workshop (Invited), New York University

A small group workshop on developing course materials, learning new skills, and discussing best practices for using Python in undergraduate science courses

April 2023
New York, NY

Introduction to Computational Antibody Engineering, Schrödinger Online Learning

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.

March 2023
Virtual

Personalized Learning in Chemistry: Addressing Student Success, Equity, and Retention in Your Chemistry Course (Invited), McGraw-Hill Education

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.

February 2020
Irvine, CA

POGIL Summer 3-Day Workshop, Simmons University

Workshop on process-oriented guided-inquiry learning (POGIL), an evidence-based, student-centered, group-learning instructional strategy and philosophy.

June 2019
Boston, MA

GRANTS, FELLOWSHIPS, and AWARDS

Currently Under Review

Co-Principal Investigator of the “**NSF CCI: Center for Quantum Dynamics on Modular Quantum Devices (CQD-MQD)**” NSF Centers for Chemical Innovation: Phase II, submitted 10/2023.

October 2023
Under review

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 – present

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

Interdisciplinary Program Grants

“**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

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

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

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

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

Department of Chemistry
Lafayette College
Easton, PA 18042

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Honor Societies

Iota Sigma Pi , Women in Chemistry Honorary Members at Large, Vice-President (Hillsdale College)	2021 – present 2008 – 2009
Phi Sigma Tau , Philosophy Honorary Kappa Chapter, Treasurer	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

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

Professional Service

Journal Referee

ACS Books
ACS Neuroscience
ACS Omega
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)

MoleCVUE 2024 2023 – present

Meeting Organizer

Serving as organizing chair for the annual MoleCVUE meeting in 2024.

MARM 2024 (Mid-Atlantic Regional Meeting of the ACS) 2024

Symposium and workshop organizer

Organizing a “Computational Chemistry in the Classroom” symposium, including an invited panel discussion titled “Computation and Visualization in Chemistry Education: Challenges and Strategies for the Future”, and a complementary “Computational Chemistry in the Classroom” workshop

ACS Spring 2022 2022

Oral Session Presider

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

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

- 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 to tour the computational chemistry company Schrodinger, Inc.'s office and to tour 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.

Committees

- Science Driver Committee, Penn State University/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 charged with filling 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 – 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.

Biophysics Research Group, Lafayette College 2018 – present
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

Iota Sigma Pi, Lehigh Valley 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.

Assessment Team , Chemistry Department, Lafayette College <i>Team Leader</i> Leading a team of four other faculty in overseeing and improving chemistry department assessment plan.	2020 – present
Women & Inclusion in The Sciences , Chemistry Department, Lafayette College <i>WITS Organizing Committee member</i> Planning and participating in various activities and events to promote inclusion of women in STEM disciplines.	2017 – present
Chemistry Book Club , Chemistry Department, Lafayette College <i>Book Club Leader</i> Initiated an inclusive chemistry book club for summer research students to read books by scientists written for the general public (e.g., 2020 Nobel Laureate Jennifer Doudna’s book “A Crack in Creation”).	2021, 2022
Visiting Faculty Search Committee , Chemistry Department, Lafayette College <i>Committee member</i> Departmental search committee charged with filling visiting assistant professor positions (two in 2018, one in 2020, one in 2022).	2018, 2020, 2022
Invited Speakers and Departmental Seminars , Lafayette College	
12. Dr. Victor Batista, Yale University	March 2024
11. Dr. Anda Trifan, Glaxo-Smith-Klein (GSK) (WITS event)	February 2024
10. Dr. Elizabeth Thrall, Fordham University (WITS event)	January 2024
9. Dr. Kaitlin McCardle, Nature Computational Science, Nature Portfolio (WITS event)	November 2023
8. Dr. Tania Lupoli, New York University (WITS event)	March 2023
7. Dr. Jeremy Feldblyum, University at Albany, SUNY	January 2023
6. Dr. Glen Hocky, New York University	October 2022
5. Dr. Lisa Fredin, Lehigh University (WITS event)	October 2021
4. Laramie Jensen, Oceanography PhD student at Texas A&M (WITS event)	November 2019
3. Dr. Kira Armacost, Merck & Co., Inc. (WITS event)	April 2019
2. Dr. Spencer Stober, Exxon Mobil Research and Engineering Corporate Strategic Research	November 2018
1. Ellen Mulvihill, Chemistry PhD student at the University of Michigan	October 2018

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.

INVITED PRESENTATIONS

Conference Presentations

- | | |
|--|------------------------------------|
| 10. Teaching & Learning Colloquium
Utilizing student-generated Mathematica demonstrations in general chemistry courses
<i>Co-presented with undergraduate Vedit Venkatesh</i> | October 2023
Center Valley, PA |
| 9. Schrödinger Educator's Week
Developing Computational Activities for a Course-Based Research Experience (CURE) | June 2023
Virtual |
| 8. ACS Spring 2023 (National Meeting of the American Chemical Society)
Utilizing student-generated Mathematica demonstrations in general chemistry courses | March 2023
Indianapolis, IN |
| 7. BCCE 2022 (Biennial Conference on Chemistry Education)
Using the Compute-to-Learn pedagogy in physical and general chemistry courses | July 2022
West Lafayette, IN |
| 6. MARM 2022 (Mid-Atlantic Regional Meeting of the American Chemical Society)
Undergraduate researchers use density functional theory to investigate ferrocene-based polymers | June 2022
Ewing, NJ |
| 5. Amber Developer's Meeting
Modeling the Optoelectronic Properties of Fc-based Polymers: Considerations for Force-Field Development | February 2020
Safety Harbor, FL |
| 4. Cambridge Crystallographic Data Centre (CCDC) User Group Meeting
Computational Investigation of the Antagonist Binding Site in PTGER3 Using the CSD-Discovery Suite | August 2018
Boston, MA |
| 3. CECAM Workshop: Computational Insight into Photo-induced Processes at Interfaces
Linker Rectifiers for Covalent Attachment of Catalysts to Semiconductor Surfaces | October 2016
Bremen, Germany |
| 2. Gordon Research Conference on Molecular Interactions and Dynamics
Mechanisms for Allosteric Inhibition of Protein Tyrosine Phosphatase 1B | July 2016
Stonehill, MA |
| 1. Midwest Undergraduate Computational Chemistry Consortium Conference
Predictive Computational Methods for Charge Transfer in Organic Photovoltaic Systems | July 2013
Ann Arbor, MI |

Seminars

- | | |
|--|------------------------------|
| 9. New York University Chemistry Department Seminar
Engaging the Next-Generation of Computational Chemists in Undergraduate Research at a Liberal Arts College | March 2024
New York, NY |
| 8. Barnard College Chemistry Department Seminar
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers Calculated using Density Functional Theory | October 2023
New York, NY |

- 7. Fordham University Chemistry Department Seminar**
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers
Calculated using Density Functional Theory
September 2023
New York, NY
 - 6. Lafayette College SoTL Scholar Presentation**
Utilizing Student-Generated Mathematica Demonstrations in General Chemistry Courses
April 2023
Easton, PA
 - 5. Lehigh University Chemistry Department Seminar**
Investigating the Porosity and Conjugation in Main-Chain Ferrocene-Based Polymers
Calculated using Density Functional Theory
March 2022
Bethlehem, PA
 - 4. Lafayette College ARC Works-in-Progress Talk**
Designing molecules and materials with insights from computational chemistry.
April 2019
Easton, PA
 - 3. Lafayette College Biophysics Research Group Seminar**
Eigenvector Centrality for Characterization of Protein Allosteric Pathways.
October 2018
Easton, PA
 - 2. Yale Physical Chemistry Club Seminar**
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices
October 2015
New Haven, CT
 - 1. Hillsdale College Chemistry Department Seminar**
Using Computational Chemistry to Understand Systems with Optoelectronic Applications
October 2012
Hillsdale, MI
- Panel Discussions*
- 8. Mental Health Initiative (Lafayette College)**
Discussion for college community on student mental health awareness
May 2021
Virtual (Easton, PA)
 - 7. Women in STEM Tea (Tri Beta – Lafayette College)**
Discussion on experiences of women in STEM
March 2021
Virtual (Easton, PA)
 - 6. Yale Resonance Conference (Yale Scientific Magazine)**
Discussion for High School Students: “Your Pathway through Science”
December 2016
New Haven, CT
 - 5. YCC Careers in Chemistry (Fairfield University)**
Discussion for Undergraduate Students by the ACS Younger Chemists Committee
April 2016
Fairfield, CT
 - 4. YCC Careers in Chemistry (New Haven University)**
Discussion for Undergraduate Students by the ACS Younger Chemists Committee
October 2015
West Haven, CT
 - 3. Chemical Sciences at the Interface of Education (CSIE|UM)**
Discussion on Honors Chemistry Courses: “What is Honors?”
May 2015
Ann Arbor, MI

2. Enriching Scholarship Conference (University of Michigan)

Discussion for Undergraduate Students: "How I Became Involved in Computational Chemical Research"

May 2012
Ann Arbor, MI

1. CyberInfrastructure Days Conference (University of Michigan)

Discussion for Undergraduate Students: "How I Became Involved in Computational Chemical Research"

December 2011
Ann Arbor, MI

CONTRIBUTED PRESENTATIONS

Oral Presentations

23. ACS Spring 2024 (National Meeting of the American Chemical Society)

(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

March 2024
New Orleans, LA

22. IEEE Integrated STEM Education Conference (ISEC '24)

Impact of Quantum Mechanics-Based Workshops on Developing High School Students' Interest and Intuition in Quantum Information Science

Co-presented with undergraduate Padmanabh Kaushik

March 2024
Princeton, NJ

21. LABSIP Winter 2024

Reflections on How to Get the Most Out of Organizing a LABSIP Community of Practice

January 2024
Virtual

20. Teaching & Learning Colloquium

Quantum Chess as a Method to Introduce Quantum Superposition in General Chemistry

October 2023
Center Valley, PA

19. CERM 2023 (Central Regional Meeting of the American Chemical Society)

(1) Utilizing student-generated Mathematica demonstrations in general chemistry courses

(2) Computational investigation of charge transfer in ferrocene-based polymer materials

June 2023
Dearborn, MI

18. LABSIP Fall 2022

Using the Compute-to-Learn Pedagogy in Physical Chemistry

November 2022
Virtual

17. MoleCVUE 2022

A CANDO (Computer Aided Nanomaterial Design and Optimization) Attitude Towards Undergraduate Chemistry Education

June 2022
Oneonta, NY

16. ACS Spring 2022 (National Meeting of the American Chemical Society)

Computational investigation of charge transfer in ferrocene-based polymer materials

March 2022
Virtual

15. ACS Spring 2021 (National Meeting of the American Chemical Society)

Computational investigation of structure-property relationships in ferrocene-based polymer materials

April 2021
Virtual

- 14. 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.
- 13. MoleCVUE 2020** June 2020
Updates on: Adapting the compute-to-learn pedagogy to a liberal arts college Virtual
- 12. 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 Philadelphia, PA
polymer materials
(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
- 11. MoleCVUE 2019** June 2019
Adapting the compute-to-learn pedagogy to a liberal arts college Middletown, CT
- 10. 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
- 9. 2017 Eastern Regional Photosynthesis Conference** April 2017
Towards the Rational Design of Alternative, Eco-Friendly Herbicides Targeting Woods Hole, MA
Photosystem II
Awarded "Baruch '60 Center for Biochemical Solar Energy Research Award of Excellence"
- 8. 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. 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 Ann Arbor, MI
Optoelectronic Devices

- 5. National Association of Research in Science Teaching**
Multiple Dimensions of “Wrong”: Using Student Generated Explanations of Quantum Chemistry Topics to Explore Student Conceptual Understanding
April 2015
Chicago, IL
- 4. Biennial Conference on Chemistry Education**
Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model
August 2014
Grand Rapids, MI
- 3. Gordon Research Seminar on Computational Chemistry**
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices
July 2014
West Dover, VT
- 2. ACS Fall 2013 (National Meeting of the American Chemical Society)**
Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach
September 2013
Indianapolis, IN
- 1. CERM 2013 (Central Regional Meeting of the American Chemical Society)**
Predictive Computational Methods for Charge Transfer in Functionalized Silsesquioxanes: Building Blocks for Photovoltaic Applications
May 2013
Mt. Pleasant, MI
- Poster Presentations
- 33. ACS Spring 2023 (National Meeting of the American Chemical Society)**
Using molecular dynamics simulations and transfer entropy pathway calculations to investigate binding of P2E to prostaglandin EP receptors
March 2023
Indianapolis, IN
- 32. Cancelled due to COVID – ACS Spring 2020 (National Meeting of the American Chemical Society)**
Adapting the compute-to-learn pedagogy from a research university to a liberal arts college
March 2020
Philadelphia, PA
Selected for Sci-Mix Interdisciplinary Poster Session
Abstract was accepted but conference was cancelled due to Covid-19
- 31. Gordon Research Conference on Computational Chemistry**
Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations
July 2018
West Dover, VT
- 30. ACS Spring 2018 (National Meeting of the American Chemical Society)**
Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations
March 2018
New Orleans, LA
Selected for Sci-Mix Interdisciplinary Poster Session
- 29. Gordon Research Conference on Molecular Interactions and Dynamics**
Investigating Conductivity in Bacterial Nanowires for Solar Energy Harvesting
July 2016
Stonehill, MA

- 28. ACS Spring 2016 (National Meeting of the American Chemical Society)**
Multiple Dimensions of "Wrong": Using Student Generated Explanations of Quantum Chemistry Topics to Explore Student Conceptual Understanding
Selected for Sci-Mix Interdisciplinary Poster Session
March 2016
San Diego, CA
- 27. Midwest Theoretical Chemistry Conference**
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices
Awarded "Best Poster Award"
June 2015
Ann Arbor, MI
- 26. CSIE|UM Symposium**
(1) *Compute-to-Learn*: Designing Interactive, Computer-Based Demonstrations of Physical Chemistry Concepts
(2) Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model
June 2015
Ann Arbor, MI
- 25. 2014 Vaughan Symposium**
(1) Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Photovoltaic Materials
(2) Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model
July 2014
Ann Arbor, MI
- 24. Gordon Research Conference on Computational Chemistry**
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Optoelectronic Devices
July 2014
West Dover, VT
- 23. Organic Photovoltaic Symposium**
Using Range-Separated Hybrid Density Functional Theory for Rational Design of Organic Photovoltaic Materials
April 2014
Kent, OH
- 22. CyberInfrastructure Days**
A Computational Approach to Rational Design for Organic Optoelectronic Devices
November 2013
Ann Arbor, MI
- 21. ACS Fall 2013 (National Meeting of the American Chemical Society)**
(1) Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach
Selected for Sci-Mix Interdisciplinary Poster Session
(2) Predictive Computational Methods for Organic Optoelectronic Materials
Selected for Sci-Mix Interdisciplinary Poster Session
September 2013
Indianapolis, IN
- 20. Gordon Research Conference on TDDFT**
Predictive Computational Methods for Organic Optoelectronic Materials
August 2013
Biddeford, ME
- 19. 2013 Vaughan Symposium**
Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A Design-Based Research Approach
August 2013
Ann Arbor, MI

- 18. Midwest Theoretical Chemistry Conference**
Predictive Computational Methods for Charge-Transfer in Organic Optoelectronic Materials
May 2013
Urbana-Champaign, IL
- 17. Organic Photovoltaic Symposium**
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials
April 2013
Kent, OH
- 16. CyberInfrastructure Days**
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials
November 2012
Ann Arbor, MI
- 15. Center for Solar and Thermal Energy Conversion External Workshop**
Predictive Computational Methods for Charge-Transfer in Organic Photovoltaic Materials
October 2012
Ann Arbor, MI
- 14. Midwest Theoretical Chemistry Conference**
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications
June 2012
Madison, WI
- 13. Michigan State University- Graduate Academic Conference**
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications
March 2012
East Lansing, MI
- 12. Rackham Centennial Symposium- Graduate Students in the World**
Using Time-Dependent Density Functional Theory to Understand Charge Transfer in Systems with Photovoltaic Applications
February 2012
Ann Arbor, MI
- 11. CyberInfrastructure Days**
Using High Performance Computing to Study the Role of Symmetry in Electron Transfer for Photovoltaic Materials via Density Functional Theory
December 2011
Ann Arbor, MI
- 10. 2011 Vaughan Symposium**
A Time-Dependent Density Functional Theory Analysis of the Charge Transfer Properties in Dye-Functionalized Silsesquioxane
Awarded "Poster Session Travel Award"
August 2011
Ann Arbor, MI
- 9. American Theoretical Chemistry Conference (ACTC)**
A Time-Dependent Density Functional Theory Analysis of the Charge Transfer Properties in Dye-Functionalized Silsesquioxane
July 2011
Telluride, CO
- 8. Center for Solar and Thermal Energy Conversion Annual Workshop**
On the Nature of Excited Charge Transfer States in Functionalized Silsesquioxanes
May 2011
Ann Arbor, MI
- 7. CyberInfrastructure Days**
Using High-Performance Computing to Study Electron Transfer in Photovoltaic Materials
Using Density Functional Theory
November 2010
Ann Arbor, MI

- 6. 8th International Conference on Electroluminescence & Organic Optoelectronics** October 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time- Ann Arbor, MI
dependent Density Functionals
- 5. 2010 Vaughan Symposium** August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time- Ann Arbor, MI
dependent Density Functionals
Awarded "Poster Session Travel Award"
- 4. Michigan Quantum Summer School** August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time- Ann Arbor, MI
dependent Density Functionals
- 3. Center for Solar and Thermal Energy Conversion Annual Workshop** August 2010
Electron Transfer Studies in Functionalized Silsesquioxane Complexes using Novel Time- Ann Arbor, MI
dependent Density Functionals
- 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 Dublin, Ireland
Mechanisms to Mesoscopic Functionality
(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 Chicago, IL
Nanoparticles Using Surface-Enhanced Raman Spectroscopy

STUDENT PRESENTATIONS of MENTORED RESEARCH PROJECTS

Oral Presentations

ACS Spring 2024 (National Meeting of the American Chemical Society)

(1) Investigating the impact of student-generated Mathematica demonstrations developed using the compute-to-learn approach
Co-presented by undergraduate Vedit Venkatesh

March 2024
New Orleans, LA

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

IEEE Integrated STEM Education Conference (ISEC '24)

Impact of Quantum Mechanics-Based Workshops on Developing High School Students' Interest and Intuition in Quantum Information Science
Co-presented by undergraduate Padmanabh Kaushik

March 2024
Princeton, NJ

Teaching & Learning Colloquium

Utilizing student-generated Mathematica demonstrations in general chemistry courses
Co-Presented by undergraduate researcher Vedit Venkatesh

October 2023
Center Valley, PA

ACS Spring 2021 (National Meeting of the American Chemical Society)

Probing protein-protein interactions via SFG and MD simulations
Presented by undergraduate researcher Zahra Gandhi

April 2021
Virtual

Cancelled due to COVID –

ACS Spring 2020 (National Meeting of the American Chemical Society)

Density functional theory investigation of brown carbon species in aqueous aerosol mimics
To Be Presented by undergraduate researcher Emily Lugos
Abstracts were accepted but conference was cancelled due to Covid-19

March 2020
Philadelphia, PA

Amber Developers' Meeting

Computational investigation of melanopsin photoreception in freshwater and marine turtles
Presented by undergraduate researcher Michael O'Connor

February 2020
Tampa, FL

Lafayette College ARC Student Research Presentations

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

July 2019
Easton, PA

Poster Presentations

ACS Spring 2024 (National Meeting of the American Chemical Society)

(1) Using student-generated Mathematica demonstrations in general chemistry courses
Presented by undergraduate researcher Vedit Venkatesh

March 2024
New Orleans, LA

- (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

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](#)

ACS Spring 2023 (National Meeting of the American Chemical Society)

March 2023
Indianapolis, IN

(1) Utilizing student-generated Mathematica demonstrations in general chemistry courses

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
Easton, PA

Computational benchmarking study of chromophore absorption in freshwater and marine turtle melanopsin

Presented by undergraduate researcher [Zoey Bragg](#)

The Lehigh Valley Symposium on CRISPR Implementation and Ethics (LV-SCIE)

September 2022
Easton, PA

(1) 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](#)

(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
Greenville, SC

- (1) 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](#)

- (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
Easton, PA

- (1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles
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
Center Valley, PA

- (1) Computational benchmarking study of chromophore absorption in freshwater and marine turtle melanopsin
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
Virtual

- Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles
Presented by undergraduate researcher [Michael O'Connor](#)

Lafayette College's 2021 Fall Student Research Poster Session

October 2021
Virtual

- (1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles
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)

Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles

Presented by undergraduate researcher [Michael O'Connor](#)

April 2021

Virtual

2021 MERCURY (Molecular Education and Research Consortium in Undergraduate computational chemistRY) Conference

(1) Computational investigation of the melanopsin photoreceptor in freshwater and marine turtles

Presented by undergraduate researcher [Michael O'Connor](#)

August 2021

Virtual

(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

(1) Determining A1 or A2 chromophore in Red-Eared Slider Melanopsin

Presented by undergraduate researcher [Michael O'Connor](#)

September 2020

Virtual

(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)

(1) Probing protein-protein interactions via SFG and MD simulations

To Be Presented by undergraduate researcher [Zahra Gandhi](#)

Travel supported by GSSPC ACS Undergraduate Travel Grant

March 2020

Philadelphia, PA

(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

(1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations

Presented by undergraduate researcher [Zahra Gandhi](#)

October 2019

Easton, PA

(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
Greenville, SC

- (1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations
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](#)

MACC-NYAGIM Symposium

May 2019
New York, NY

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

Lafayette College's 2019 Spring Student Research Poster Session

April 2019
Easton, PA

- (1) Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations
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
Orlando, FL

- (1) Density functional theory investigation of brown carbon species in aqueous aerosol mimics
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

(1) Computational investigation of semiconducting properties
in ferrocene-based polymer materials

Presented by undergraduate researcher Liza Welch

October 2018
Easton, PA

(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**

Computational Investigation of the Antagonist Binding Site in Prostaglandin EP3
Receptor

Presented by undergraduate researchers Zahra Gandhi and Ella Kaplan

July 2018
Greenville, SC

2017 Eastern Regional Photosynthesis Conference

Designing synthetic acceptor ligands to enhance electron transfer efficiency in PSII

Presented by undergraduate researcher Heather Harrington

April 2017
Woods Hole, MA

CERM 2013 (Central Regional Meeting of the American Chemical Society)

(1) Using Writing to Teach Pedagogy in an Introductory Physical Chemistry Course: A
Design-Based Research Approach

Presented by undergraduate researchers Kari Chen and Michael Gysin

May 2013
Mt. Pleasant, MI

(2) Predictive Computational Methods for Organic Optoelectronic Materials

Presented by undergraduate researcher Francis DeVine