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*)

Maroon text indicates activities carried out at Lafayette College

RESEARCH and ACADEMIC EXPERIENCE

Assistant Professor of Chemistry, Lafayette College — 2017 – present
Utilizing multi-scale computational approaches to investigate optoelectronic properties of small molecules and polymer materials, as well as protein-ligand interactions in G-protein coupled receptor proteins

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 Articles

Undergraduate co-authors advised by HPH are underlined

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.

Invited Perspectives

3. 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.

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.

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Book Chapters

1. **Hendrickson, H. P.***; Lenn, K. M.; Vázquez, F. X.; Williams, K. L.; Winogrrad, 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, 2021. *(In Press)*

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.

TEACHING and MENTORING

Course Instructor

Professor, Chemistry, Lafayette College — 2017 – present

CHEMISTRY 121: General Chemistry I
CHEMISTRY 122: General Chemistry II
CHEMISTRY 324/326: Physical Chemistry II
CHEMSITRY 311: Elementary Physical Chemistry
CHEMISTRY 380/390/392: Independent Study/Research

- Computational investigation of the optoelectronic properties of ferrocene-based polymers. — 2018-2021
- 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

Honors Thesis Committee Member (CHEMISTRY 495: Honors Thesis)

- Yiru Gu — 2021
  Prediction for Inhibiting of Lin-28/Pre-let 7 reaction with Synthesized Small Molecules for Pancreatic Cancer
- Sarah Miller — 2021
  Effects of Amino Acid Content on the Requirement of Swa2 on Artificial Prion Propagation
- Jason Corcoran — 2019
  Synthesis and catalytic ability of pyridyl-substituted NHC-palladium complexes
- Sierra Cole — 2019
  Analyzing Hsp40 primary sequence dependence for chaperone-prion interactions
- Scott Berger — 2019
  The role of J-proteins in Hsp104 overexpression-mediated curing of the prion [PSI^{+}]: A closer look at Apj1

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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

Workshop Facilitator

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

6.	Daisy Grace	Graduate, Johns Hopkins University	2021 – present
5.	Zoey Bragg	Undergraduate, Lafayette College	2021 – present
4.	Eman Shahzad	Undergraduate, Lafayette College	2021 – present
3.	Alex Qian	Undergraduate, Lafayette College	2020 – present
2.	Theresa Chua	Undergraduate, Lafayette College	2020 – present
1.	Michael O'Connor	Undergraduate, Lafayette College	2019 – present

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Former Students

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

Scholarship of Teaching and Professional Development

Scholarship of Teaching and Learning Community of Practice, Lafayette College — 2019 – present
Community of practice focused on designing and providing feedback on individual or collaborative pedagogical research studies

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

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 – present

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

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

Teaching Grants (Lafayette College)

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

"Using the Mechanisms App for Acid/Base Reactions in General Chemistry II (CHEM 122)," funded by Lafayette College's Meta-Mindset Grant — August 2018 – December 2018
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.

"Utilizing Compute-to-Learn pedagogy within CHEM 324," funded by Lafayette College's Meta-Mindset Grant — January 2018 – May 2018
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.

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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

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

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

Honor Societies
Iota Sigma Pi, Members at Large (Hillsdale College) 2008 – 2009
Women in Chemistry Honorary, Vice-President
Phi Sigma Tau, Kappa Chapter 2008 – 2009
Philosophy Honorary, Treasurer
Sigma Pi Sigma, Chapter #467 2008 – 2009
Physics Honorary
Sigma Zeta, Alpha Psi Chapter 2007 – 2009
Math/Science Honorary

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
National Science Foundation External Grant Reviewer 2019, 2021

Journal Referee
Chemistry Select
International Journal of Quantum Chemistry (*Reviewer of the Month – June 2019*)
Journal of Chemical Physics
Journal of Molecular Graphics and Modelling
Journal of Physical Chemistry
New Journal of Chemistry
Organic Electronics
Solar RRL
The FEBS Journal (Federation of European Biochemical Societies)

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Faculty Service – Lafayette College

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.

Teaching and Learning Committee, Lafayette College — 2018 – present
Committee member
Supporting 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.

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.

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

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

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

Chemistry Book Club, Chemistry Department, Lafayette College — 2021 – present
Book Club Leader
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 Jennnifer Doudna's book "A Crack in Creation").

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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

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

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

Invited Speakers and Departmental Seminars, Lafayette College

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

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

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Seminars

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

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

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

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

15. 259th National Meeting of the American Chemical Society — April 2021
Computational investigation of structure-property relationships in ferrocene-based polymer materials — Virtual

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14. *Cancelled* - 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* - 257th 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

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

10. 255th 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 Photosystem II — Woods Hole, MA

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

8. 253th National Meeting of the American Chemical Society — April 2017
Mechanisms for Allosteric Inhibition of Protein Tyrosine Phosphatase 1B — San Francisco, CA

7. 251th 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. 246th 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

1. 44th 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

32. *Cancelled* - 257th 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

31. 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

30. 255th 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

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

28. 251th 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

27. 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"

26. 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

25. 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

24. 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

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

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

21. 46th 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

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

STUDENT PRESENTATIONS of MENTORED RESEARCH PROJECTS

Oral Presentations

259th 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* - 257th 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 Developer's Meeting — February 2020
Computational investigation of melanopsin photoreception in freshwater and marine turtles — Tampa, FL
Presented by undergraduate researcher Michael O'Connor

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

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Poster Presentations

Lafayette College's 2020 Fall Student Research Poster Session — September 2020, Virtual

(1) Determining A1 or A2 chromophore in Red-Eared Slider Melanopsin
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* - 257th National Meeting of the American Chemical Society** — *March 2020, Philadelphia, PA*

(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

(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, 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
Travel supported by ACS Bridge Travel Award

(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
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

257th 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

(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

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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

44th 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