Zeke A. Piskulich

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Education

Ph.D., Chemistry, University of Kansas - Lawrence, KS, Advisors: Ward H. Thompson and Brian B. Laird.	2017–2021
"Beyond Arrhenius: Fluctuation Theory for Dynamics"	
B.S., Physics, University of Missouri - Columbia, MO, Advisors: Donald L. Thompson and Thomas D. Sewell.	2011-2017
(Molecular Simulations of Energy Transfer in Shock Tubes)	

Professional Appointments

Consultant, ATTMOS Inc	Mar. 2025–Present
Software and Scientific Consulting for Problems Related to Small-Molecule Drug Discovery	
Postdoctoral Associate , <i>Rutgers University - Piscataway, NJ</i> , Advisor: Darrin York. (Small Molecule Drug Discovery in RNA)	Aug. 2024–Present
Postdoctoral Associate , <i>Boston University</i> - <i>Boston, MA</i> , Advisor: Qiang Cui. (Nanoparticle Interactions at the Interface of Lipid Membranes)	2021–Jun. 2024

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### **Key Achievements**

| Marnie and Bill Argersinger Award for Outstanding Doctoral Dissertation in STEM, University of Kansas, Link.         | 2022   |
|----------------------------------------------------------------------------------------------------------------------|--------|
| <ul> <li>Awarded for "the best dissertation in science, technology, engineering, and mathematics"</li> </ul>         |        |
| <ul> <li>Nominated for the ProQuest Council of Graduate Schools Distinguished Dissertation Award</li> </ul>          |        |
| Justin Jankunas Doctoral Dissertation Award in Chemical Physics, American Physical Society, Link.                    | 2022   |
| <ul> <li>Award for "doctoral thesis research of outstanding quality and achievement in chemical physics"</li> </ul>  |        |
| • Citation: "For the development of fluctuation theory to enable direct calculation of Arrhenius activation energies |        |
| and volumes at a single temperature."                                                                                |        |
| Young Scientist, Lindau Nobel Laureate Meetings.202                                                                  | 0-2022 |
| National Science Foundation Graduate Research Opportunities World Wide Award.                                        | 2019   |
| <ul> <li>Awarded to work with Prof. Damien Laage for 3 months in France.</li> </ul>                                  |        |
| National Science Foundation Graduate Research Fellow. 201                                                            | 8–2021 |

#### **Grants for Computational Resources**

**Principal Investigator**, *National Science Foundation Advanced Cyberinfrastructure Coordination Ecosystem*, **2023-2024** #CHE-230043, 200,000 ACCESS Credits. Characterization of the Impact of Crowding Agents on the Composition and 2D-Infrared Spectroscopy of Fused-in-Sarcoma Condensates

### Other Fellowships, Awards, and Scholarships

| <b>Director's Award for Excellence</b> , <i>Department of Chemistry</i> , Boston University.<br>• Award given in recognition of "tremendous efforts" as a postdoctoral scholar.                                                       | 2024 |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|
| <b>Invited Attendee</b> , <i>NC State Building Future Faculty Workshop</i> , Office of Diversity, Equity, and Inclusion.                                                                                                              | 2023 |
| Air Force Office of Scientific Research Scholar, American Conference on Theoretical Chemistry.                                                                                                                                        | 2022 |
| <ul> <li>Higuchi Doctoral Progress Award, Department of Chemistry, University of Kansas.</li> <li>Award given "to a superior, post-comprehensive graduate student in his or her final year."</li> </ul>                               | 2021 |
| <b>Paul and Hellen Gilles Award in Physical Chemistry</b> , <i>Department of Chemistry</i> , University of Kansas.<br>• Award given "for superior academic performance and research accomplishments by an advanced graduate student." | 2020 |
| Graduate Scholarly Presentation Fund, Graduate Studies, University of Kansas.                                                                                                                                                         | 2019 |

| Helen and Paul Gilles Travel Fund Award, Department of Chemistry, University of Kansas.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 2018, 2019                         |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------|
| <b>Cornelius McCollum Research Scholarship</b> , <i>Department of Chemistry</i> , University of Kansas.<br>• Research scholarship "awarded to outstanding advanced graduate students."                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 2019                               |
| Graduate Travel Fund Award, Research Excellence Initiative, University of Kansas.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2019                               |
| Graduate Writing Incentive Award, Research Excellence Initiative, University of Kansas.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 2018                               |
| <ul> <li>H.P. Cady Award, Department of Chemistry, University of Kansas.</li> <li>Award given "to a first-year graduate student for excellent performance."</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 2018                               |
| Phi Beta Kappa Honor Society, University of Missouri.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 2018                               |
| Bailey Scholarship, University of Kansas.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 2017                               |
| Leadership                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                    |
| <ul> <li>Terriers F1RSTS Advocate, Newbury Center, Boston University.</li> <li>The Terrier F1RSTS Advocate program trains faculty and staff to better support first generation college and gradu</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                            | <b>2023-2024</b><br>uate students. |
| <ul> <li>Advocacy Committee Chair, Co-Chair (member since 2021), Boston Postdoctoral Association, Boston</li> <li>Represented advocacy efforts for all 19 Boston-area universities</li> <li>Reorganized the committee to have greater connection to local postdoc association efforts</li> <li>Organized a "Life as a Postdoc" seminar series that included data-driven talks on postdoc advocacy</li> <li>Organized immigration webinars with a variety of law firms for international postdocs</li> </ul>                                                                                                                                                            | , MA. <b>2022-2024</b>             |
| Gordon Research Seminar Co-Chair, 2019 Chemistry and Physics of Liquids, Holderness, NH.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 2017-2019                          |
| <ul> <li>Constructed an interdisciplinary conference program that highlights the current understanding of the liquid phase.</li> <li>Fundraised from Academic, Industrial, and Federal sources.</li> <li>Designed a mentorship panel focused on student career exploration.</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                 |                                    |
| President, Vice President, Chemistry Graduate Student Organization, Lawrence, KS.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 2018-2020                          |
| <ul> <li>Spearheaded effort to develop GSO into an official student organization.</li> <li>Assisted in the creation of a weekly professional development series in collaboration with other departments.</li> <li>Increased graduate student membership in departmental committees.</li> <li>Organized an alumni panel discussion that included alumni from PUI's, R1 Institutions, and Industry.</li> <li>Organized a "Fund Yourself" workshop to connect graduate students with external funding opportunities in 2019 a</li> <li>Organized a "Research Open House" that connected undergraduates and 1<sup>st</sup>-year graduate students with research</li> </ul> | nd 2020.<br>opportunities.         |
| Academic Service                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                    |
| <ul> <li>Developer, Amber Molecular Dynamics, AMBER.</li> <li>Contributed software to calculate Relative Binding Free Energies of Nucleic Acid targets to the Amber Drug Discovery Boost Package</li> <li>Tested and implemented bug fixes in the AmberTools 2025 release.</li> <li>Instructor for the 2024 Amber Free Energy Workshop</li> </ul>                                                                                                                                                                                                                                                                                                                      | 2024-Present                       |
| <b>Early Career Member at Large</b> , <i>Division of Chemical Physics Executive Committee</i> , American Physical Sc<br>• Nominated to run for election by unanimous vote of DCP Executive Committee                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ciety. 2024-2025                   |
| Member, Presentation Peer Review Team, Center for Sustainable Nanotechnology.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 2022-2024                          |
| Member, Seed Committee, Center for Sustainable Nanotechnology.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 2021-2024                          |
| <ul> <li>NSF Fellowship Information Session, Speaker, University of Kansas, Lawrence, KS.</li> <li>Discussed my experiences and advice for graduate and undergraduate students applying to the NSF GRFP.</li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 2019, Sep. 2019                    |
| <b>Chemistry and Chemical Engineering REU Programs</b> , <i>Speaker</i> , University of Kansas, Lawrence, KS.<br>• Developed materials for and led a discussion titled "How to apply to the NSF Graduate Research Fellowship Progr                                                                                                                                                                                                                                                                                                                                                                                                                                     | <b>Jul. 2019</b><br>am".           |
| Undergraduate Research Symposium, Session Chair, University of Kansas, Lawrence, KS.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Apr. 2018, 2019                    |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |

## **Peer Reviews**

| 1 Reviews, Discover Applied Sciences.                  | 2025 |
|--------------------------------------------------------|------|
| 2 Reviews, Journal of Chemical Theory and Computation. | 2024 |
| 1 Review, PLOS Computational Biology.                  | 2024 |

| <b>1 Review</b> , Comptes Rendus Chimie Comptes Rendus Chimie. | 2023 |
|----------------------------------------------------------------|------|
| 2 Reviews, Physical Chemistry Chemical Physics.                | 2023 |
| <b>1 Review</b> , Nature Communications Materials.             | 2023 |
| <b>1 Review</b> , Journal of Chemical Theory and Computation.  | 2023 |
| <b>1 Review</b> , Journal of the American Chemical Society Au. | 2022 |
| <b>1 Review</b> , Journal of Physical Chemistry.               | 2022 |
| <b>1 Review</b> , Physical Chemistry Chemical Physics.         | 2021 |
|                                                                |      |

#### Outreach

| Volunteer, Deer Creek Intermediate School, Center for Sustainable Nanotechnology.                                                                                                                          | 2023       |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| Judge, Batelle Climate Challenge, Future Engineers.                                                                                                                                                        | 2023       |
| Volunteer, STEM Pathways: Science Club for Girls, "Insulation Experiment Packing".                                                                                                                         | 2023       |
| Judge, NASA TechRise Challenge, Future Engineers.                                                                                                                                                          | 2021, 2022 |
| Judge, NASA Artemis Moon Pod Essay Contest, Future Engineers.                                                                                                                                              | 2021       |
| Participant, Lindau Sciathon, "Digital Notebooks for Enhanced Accessibility to Research".                                                                                                                  | 2021       |
| Participant, Lindau Sciathon, "Graduate Admissions During and After COVID-19".                                                                                                                             | 2020       |
| Judge, NASA Name the Rover Challenge, Future Engineers.                                                                                                                                                    | 2019–2020  |
| <b>Carnival of Chemistry</b> , <i>Volunteer</i> , University of Kansas, Lawrence, KS.<br>• Designed an activity that taught nearly 300 children about different types of stars, as well as emission lines. | Nov. 2018  |
| Hillcrest Science Night, Volunteer, Hillcrest Elementary School, Lawrence, KS.                                                                                                                             | Jan. 2018  |

• Worked directly with a classroom of elementary school children to help with studying different methods of propulsion.

• Helped students design experiments for evaluating the performance of model rockets propelled by different techniques.

#### **Teaching Experience**

| Course Assistant (Informal), Rutgers University, Piscataway, NJ.                     | 2024 |
|--------------------------------------------------------------------------------------|------|
| <ul> <li>Assisted with a graduate-level Quantum Chemistry course.</li> </ul>         |      |
| <ul> <li>Assisted PI with course grading and office hours.</li> </ul>                |      |
| <ul> <li>Co-led a guest lecture on matrix algebra and python programming.</li> </ul> |      |

Instructor, Amber Free Energy Workshop, San Diego, CA.

2024

2023

Fall 2017, 2018

| Guest Lecturer, Boston University, Boston, MA.                                                 |  |
|------------------------------------------------------------------------------------------------|--|
| <ul> <li>Guest lecture on "Second Quantization" for Molecular Quantum Mechanics III</li> </ul> |  |

#### Teaching Assistant, University of Kansas, Lawrence, KS.

• Lecture Teaching Assistant Physical Chemistry for Engineers for Dr. Ward H. Thompson

- Actively participated in the development of homework assignments, quizzes, and exams.
- Collaboratively taught a discussion section with a fellow graduate student.
- Lecture Teaching Assistant General Chemistry I for Dr. Krzysztof Kuczera
  - Planned content for and led class discussion sections to promote student learning.
  - Implemented active learning activities to take place during the lecture.

#### **Mentoring Experience**

| Harsh Amin, Graduate Student, Rutgers University, Piscataway, NJ.                     | 2024-Present |
|---------------------------------------------------------------------------------------|--------------|
| Zhengyi (Kevin) Tang, Graduate Student, Boston University, Boston, MA.                | 2023-2024    |
| Alexandra Wright, Undergraduate, Senior Honors Thesis, Boston University, Boston, MA. | 2021-2022    |
| Carolyn Smith, Undergraduate, University of Kansas, Lawrence, KS.                     | 2019         |
| Sahan M. Godahewa, Graduate Student, University of Kansas, Lawrence, KS.              | 2019-2020    |
| Allyson L. Leicht, Graduate Student, University of Kansas, Lawrence, KS.              | 2019-2020    |
| Ashley Borkowski, Graduate Student, University of Kansas, Lawrence, KS.               | 2018-2020    |

| Micah Welsch, Graduate Student, University of Kansas, Lawrence, KS.          | 2018-2019 |
|------------------------------------------------------------------------------|-----------|
| Carl Heroneme, Undergraduate, University of Kansas, Lawrence, KS.            | 2018-2019 |
| Trevor Neal, Undergraduate, REU Program, University of Kansas, Lawrence, KS. | 2017      |
| Alondra Garcia-Arevalo, Undergraduate, University of Kansas, Lawrence, KS.   | 2017      |

#### **Publications**

**24.** Andrew K. Gillespie, Adam D. Smith, Sean Sweeny, Makr Sweeny, **Zeke A. Piskulich**, Ernest Knight, Matthew Prosniewski, Samantha M. Gillespie, David Stalla, "Biowaste-Derived Activated Carbon from Spent Coffee Grounds for Volumetric Hydrogen Storage," Cleaner Chem. Eng., **11**, 100155, (2025). (From Undergrad), Link.

**23.** <u>Zeke A. Piskulich</u>, and Qiang Cui, "Hydrogen Bonding Blues: Vibrational Spectroscopy of the TIP3P Water Model", *J. Chem. Phys.*, **162**, 014104, (2025). (*Co-Corresponding Author, Editor's Choice, Cover Article*), Link.

**22.** Qing Xia, Harini A. Perera, Rylie Bolarinho, <u>Zeke A. Piskulich</u>, Zhongyue Guo, Jiaze Yin, Hongjian He, Mingsheng Li, Xiaowei Ge, Qiang Cui, Olof Ramstrom, Mingdi Yan, and Ji-Xin Cheng, "Click-free imaging of carbohydrate trafficking in live cells using an azido photothermal probe", *Science Advances*, **10**, eadq0294 (2024), Link.

**21.** <u>Zeke A. Piskulich</u>, Damien Laage, and Ward H. Thompson, "A Structure-Dynamics Relationship Enables Prediction of the Water Hydrogen Bond Exchange Activation Energy from Experimental Data", *Chem. Sci.* **15**, 2197-2204 (2024), Link.

**20.** <u>Zeke A. Piskulich</u>, Ashley K. Borkowski and Ward H. Thompson, "A Maxwell Relation for Dynamical Timescales. Application to the Pressure and Temperature Dependence of Water Self-Diffusion", *Phys. Chem. Chem. Phys.*, **25**, 12820 (2023), Link.

**19.** Laura Kesner\*, <u>Zeke A. Piskulich\*</u>, Qiang Cui, and Zeev Rosenzweig, "Untangling the Interactions between Anionic Polystyrene Nanoparticles and Lipid Membranes using Laurdan Fluorescence Spectroscopy and Molecular Simulations", *J. Am. Chem. Soc.*, **145**, 7962-7973 (2023), \**Equal Contributions*, Link.

18. <u>Zeke A. Piskulich</u> and Qiang Cui, "Machine Learning Assisted Phase Transition Temperatures from Generalized Replica Exchange Simulations of Dry Martini Lipid Bilayers", *J. Phys. Chem. Lett.*, 13, 6481-6486 (2022), Link.

17. Axel Gomez, <u>Zeke A. Piskulich</u>, Ward H. Thompson, and Damien Laage, "Water Diffusion Proceeds via a Hydrogen-Bond Jump Exchange Mechanism", *J. Phys. Chem. Lett.*, **13**, 4660-4666 (2022), Link.

16. <u>Zeke A. Piskulich</u>, Damien Laage, and Ward H. Thompson, "Using Activation Energies to Elucidate Mechanisms of Water Dynamics", *J. Phys. Chem. A*, 125, 9941-9952, (2021), Link.

**15.** Sean Roget, <u>Zeke A. Piskulich</u>, Ward H. Thompson and Michael D. Fayer, "Identical Water Dynamics in Acrylamide Hydrogel, Polymer and Monomer Solutions: Ultrafast IR Spectroscopy and Molecular Dynamics Simulations", *J. Am. Chem. Soc.*, **143**, 14855-14868, (2021), Link.

**14.** <u>Zeke A. Piskulich</u>, and Brian B. Laird, "Molecular Simulations of Phase Equilibria and Transport Properties in a Model CO<sub>2</sub>-Expanded Lithium Perchlorate Electrolyte", *J. Phys. Chem. B.*, **125**, 9341-9349 (2021), Link.

**13.** <u>Zeke A. Piskulich</u>, and Ward H. Thompson, "Examining the Role of Different Molecular Interactions on Activation Energies and Activation Volumes in Liquid Water", *J. Chem. Theor. Comput.*, **17**, 2659-2671 (2021), Link.

**12.** <u>Zeke A. Piskulich</u>, Damien Laage, and Ward H. Thompson, "On the Role of Hydrogen Bond Exchanges in the Spectral Diffusion of Water", *J. Chem. Phys.*, **154**, 064501, (2021), Link.

**11.** Ashley K. Borkowski, <u>Zeke A. Piskulich</u>, and Ward H. Thompson, "Examining the Hofmeister Series through Activation Energies. Water Diffusion in Aqueous Alkali-Halide Solutions", *J. Phys. Chem. B.*, **125**, p. 350-359, (2020), Link.

**10.** <u>Zeke A. Piskulich</u>, and Ward H. Thompson, "Temperature Dependence of the Water Infrared Spectrum: Driving Forces, Isosbestic Points, and Predictions", *J. Phys. Chem. Lett.*, **11**, 7762-7768 (2020), Link.

**9.** <u>Zeke A. Piskulich</u>, Damien Laage, and Ward H. Thompson, "Activation Energies and the Extended Jump Model: How Temperature Affects Reorientation and Hydrogen-Bond Exchange Dynamics in Water", *J. Chem. Phys.*, **153**, 074110 (2020), Link.

8. <u>Zeke A. Piskulich</u> and Ward H. Thompson, "The Dynamics of Supercooled Water Can Be Predicted From Room Temperature Dynamics", J. Chem. Phys., **152**, 074505 (2020), Link.

7. <u>Zeke A. Piskulich</u> and Ward H. Thompson, "On the Temperature Dependence of Liquid Structure", *J. Chem. Phys.*, **152**, 011102 (2020), Link.

6. Camina H. Mendis, <u>Zeke A. Piskulich</u>, and Ward H. Thompson, "Tests of the Stokes-Einstein Relation through the Shear Viscosity Activation Energy of Water", *J. Phys. Chem. B*, **123**, 5857-5865 (2019), Link.

5. Zeke A. Piskulich, Oluwaseun O. Mesele, and Ward H. Thompson, "Activation Energies and Beyond", J. Phys. Chem. A, 123, 7185-7194 (2019), (Invited Feature Article, ACS Editor's Choice, ACS Weekend Read, Cover Article), Link.

4. Zeke A. Piskulich, and Ward H. Thompson, "The Activation Energy for Water Reorientation Differs Between IR Pump-Probe and NMR Measurements", J. Chem. Phys. 149, 164504 (2018), (Editor's Pick), Link.

3. Zeke A. Piskulich, Oluwaseun O. Mesele, and Ward H. Thompson, "Expanding the Calculation of Activation Volumes: Self-Diffusion in Liquid Water", J. Chem. Phys. 148, 134105 (2018), Link.

2. Zeke A. Piskulich, Oluwaseun O Mesele, and Ward H. Thompson, "Removing the Barrier to the Calculation of Activation Energies. Diffusion and Reorientation of Water", J. Chem. Phys. 147, 134103 (2017), (Editor's Pick, Editor's Choice Collection). Link.

1. G. Sreenivasulu, P. Qu, E. Piskulich, V.M. Petrov, Y.K. Fetisov, A.P. Nosov, Hongwei Qu and G. Srinivasan, "Shear Strain Mediated Magneto-Electric Effects in Composites of Piezoelectric Lanthanum Gallium Silicate or Tantalate and Ferromagnetic Alloys", Appl. Phys. Lett. 105, 032409 (2014), Link.

#### **Publications In Preparation**

1. Zeke A. Piskulich, Zeev Rosenzweig, and Qiang Cui, "Polystyrene Perturbs Hydration around Laurdan within Lipid Membranes" (Working Title), In Preparation (2024).

2. Cheng-Hsin Huang, Riley Lewis, Sara Thomas, Zhengyi Tang, Jasmine Jones, Sara Nason, Nubia Zuverza-Mena, Zeke A. Piskulich, Tana L. O'Keefe, Beza Tuga, Antavia Paredes-Beaulieu, Vasilis Vasiliou, Qiang Cui, Joseph J. Dalluge, Jason C. White, Christy L. Haynes, "Designing Ultraporous Mesostructured Silica Nanoparticles for the Remediation of Per- and Polyfluoroalkyl Substances, In Preparation (2024).

#### **Book Chapters**

1. Sanjoy Paul, Sayantan Mondal, Zeke A. Piskulich, and Qiang Cui, "Lipid membrane remodeling by (bio)polymers and nanoparticles: mechanistic insights from multi-scale simulations", Membrane Shape and Biological Function, Editors: Jose Carlos Bozelli Jr. and Richard Epand In Press (2024).

#### Presentations

| Relative Binding Free Energies in a Model Gaunine Riboswitch (Title Changed) .<br>Talk, Poster, APS March Meeting Anaheim, CA                                                                         | Mar. 2025 |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| Molecular interactions in Action:Insights into Activation Energies and the Nanoplastic-Membrane Interface.<br>Invited Talk, Notre Dame Department of Chemistry South Bend, IN                         | Jan. 2025 |
| Untangling perturbations to lipid membrane hydration induced by polystyrene nanoplastics .<br>Talk, APS March Meeting Minneapolis, MN                                                                 | Mar. 2024 |
| Molecular interactions in Action:Insights into Activation Energies and the Nanoplastic-Membrane Interface.<br>Invited Talk, St. Louis University Department of Chemistry St. Louis, MO                | Dec. 2023 |
| Untangling the interactions between nanoplastics and fluid lipid membranes through multiscale simulation. Talk, Poster, Chemistry and Physics of Liquids GRS and GRC, respectively. Holderness, NH    | July 2023 |
| Untangling the interactions between nanoplastics and fluid lipid membranes through multiscale simulation. Lightning Talk, Poster, International High Performance Computing Summer School, Atlanta, GA | July 2023 |
| Understanding the interaction between polystyrene nanoplastics and model cell membranes through multiscale simulation.                                                                                | June 2023 |
| Talk, ACS Northeast Regional Meeting, Boston, MA                                                                                                                                                      |           |
| Mapping Lipid Phase Transition Temperatures using Machine Learning and Generalized Replica Exchange Simulations.                                                                                      | June 2023 |
| Poster, MolSSI Workshop Machine Learning and Chemistry: Are We There Yet?, College Park, MD                                                                                                           |           |
| Molecular Interactions in Action: Insights into Activation Energies and the Nanoplastic-Membrane Interface.                                                                                           | Mar. 2023 |
| Invited Talk, NC State Department of Chemistry, Raleigh, NC                                                                                                                                           |           |
| Untangling Interactions at the Interface Between Nanoplastics and Model Cell Membranes.                                                                                                               | Nov. 2022 |

Talk, Boston University Postdoctoral Seminar Series, Boston, MA

| Machine-learning assisted determination of lipid phase transition temperatures.<br>Poster, American Conference on Theoretical Chemistry, Tahoe, CA                                      | Jul. | 2022 |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|------|
| Polystyrene Penetrates Lipid Vesicles.<br>Poster, Center for Sustainable Nanotechnology, All-Hands Meeting, Dunwoody, GA                                                                | Apr. | 2022 |
| Beyond Arrhenius: Fluctuation Theory for Dynamics.<br>Poster, American Physical Society March Meeting, Chicago, IL                                                                      | Mar. | 2022 |
| Beyond Arrhenius: Fluctuation Theory for Dynamics.<br>Invited Talk, American Physical Society March Meeting, Chicago, IL                                                                | Mar. | 2022 |
| On the Relationship Between Structure and Dynamics in Liquid Water.<br>Invited Talk, Statistical Thermodynamics and Molecular Simulation Seminar, Virtual                               | Feb. | 2021 |
| Carbon-Dioxide Expanded Acetonitrile as an Ion-Transport Medium.<br>Lightning Talk, Virtual Conference on Theoretical Chemistry, Virtual                                                | July | 2020 |
| Bringing Supercooled Water in from the Cold: Signatures at Room Temperature.<br>Talk, Pacific Conference on Spectroscopy and Dynamics, San Diego, CA                                    | Jan. | 2020 |
| <b>The Dynamics and Structure of Supercooled Water can be Predicted from Room Temperature Simulations</b> .<br>Poster, Chemistry and Physics of Liquids GRC, Holderness, NH             | Aug. | 2019 |
| Getting Something for (Almost) Nothing: New Methods for the Calculation of Activation Energies.<br>Poster, Pacific Conference on Spectroscopy and Dynamics, San Diego, CA               | Jan. | 2019 |
| Getting Something for (Almost) Nothing: New Methods for the Calculation of Activation Energies.<br>Invited Talk, Oakland University Chemistry Departmental Seminar, Rochester Hills, MI | Dec. | 2018 |
| <b>The Activation Energy for Water Reorientation Differs Between IR Pump-Probe and NMR Measurements</b> .<br>Poster, Water and Aqueous Solutions GRS and GRC, Holderness, NH            | Aug. | 2018 |
| Phase Equilibria, Transport Properties, and Structure of CO <sub>2</sub> -Expanded Ethylene Oxide and Methanol.<br>Talk, ACS Midwest Regional Meeting, Lawrence, KS                     | Oct. | 2017 |
| Removing the Barrier to the Calculation of Activation Energies and Volumes: Diffusion and Reorientation in Water.                                                                       | Oct. | 2017 |
| Talk, ACS Midwest Regional Meeting, Lawrence, KS                                                                                                                                        |      |      |
| Phase Equilibria and Structure of CO <sub>2</sub> -Expanded Ethylene Oxide and Methanol and Direct Calculation of Activation Energies of Diffusion and Reorientation.                   | Aug. | 2017 |
| Poster, Chemistry and Physics of Liquids GRS and GRC, Holderness, NH                                                                                                                    |      |      |
| <b>Phase Equilibria and Structure of CO</b> <sub>2</sub> - <b>Expanded Ethylene Oxide and Methanol</b> .<br>Poster, American Conference on Theoretical Chemistry, Boston, MA            | Jul. | 2017 |
| Breaking Barriers: Direct Calculation of Activation Energies of Diffusion and Reorientation.<br>Talk, CEBC Industrial Advisory Board Meeting, Lawrence, KS                              | Oct. | 2017 |
| <b>Tunability of Phase Equilibria in Gas-Expanded Liquids: The Carboxylation of Ethylene Oxide</b> .<br>Poster, Kansas Physical Chemistry Symposium, Lawrence, KS                       | Jan. | 2017 |
| Tunability of Phase Equilibria in Gas-Expanded Liquids: The Carboxylation of Ethylene Oxide.<br>Talk, ACS Midwest Regional Meeting, Manhattan, KS                                       | Oct. | 2016 |
| Vibrational Relaxation of HF in Argon Fluid.<br>Poster, APS Shock Compression of Condensed Matter, Tampa, FL                                                                            | Jun. | 2015 |
| Boron-Doped Graphene-Like Carbons for Hydrogen Gas Storage.<br>Talk, Physics Leaders Meeting, Columbia, MO                                                                              | Oct. | 2013 |
| Boron-Doped Graphene-Like Carbons for Hydrogen Gas Storage.<br>Talk, Summer Research Forum, Columbia, MO                                                                                | Jul. | 2013 |