

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

- Postdoctoral Associate**, *Boston University - Boston, MA*, Advisor: Qiang Cui. **2021–Present**
"Nanoparticle Interactions at the Interface of Lipid Membranes"

Key Achievements

- Marnie and Bill Argersinger Award for Outstanding Doctoral Dissertation in STEM**, *University of Kansas*. **2022**
◦ Awarded for "the best dissertation in science, technology, engineering, and mathematics".
◦ Nominated for the ProQuest Council of Graduate Schools Distinguished Dissertation Award
- Justin Jankunas Doctoral Dissertation Award in Chemical Physics**, *American Physical Society*. **2022**
◦ Award for "doctoral thesis research of outstanding quality and achievement in chemical physics."
◦ 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*. **2020-2022**
- National Science Foundation Graduate Research Opportunities World Wide Award**. **2019**
◦ Awarded to work with Prof. Damien Laage for 3 months in France.
- National Science Foundation Graduate Research Fellow**. **2018–2023**

Publications

- 19.** Laura Kesner, [Zeke A. Piskulich](#), 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.*, Accepted (2023).
- 18.** [Zeke A. Piskulich](#) 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, [Zeke A. Piskulich](#), 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.** [Zeke A. Piskulich](#), 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, [Zeke A. Piskulich](#), 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.** [Zeke A. Piskulich](#), and Brian B. Laird, "Molecular Simulations of Phase Equilibria and Transport Properties in a Model CO₂-Expanded Lithium Perchlorate Electrolyte", *J. Phys. Chem. B.*, **125**, 9341-9349 (2021), [Link](#).
- 13.** [Zeke A. Piskulich](#), 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.** [Zeke A. Piskulich](#), 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, [Zeke A. Piskulich](#), 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. [Zeke A. Piskulich](#), 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. [Zeke A. Piskulich](#), 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. [Zeke A. Piskulich](#) and Ward H. Thompson, "The Dynamics of Supercooled Water Can Be Predicted From Room Temperature Dynamics", *J. Chem. Phys.*, **152**, 074505 (2020), [Link](#).
7. [Zeke A. Piskulich](#) and Ward H. Thompson, "On the Temperature Dependence of Liquid Structure", *J. Chem. Phys.*, **152**, 011102 (2020), [Link](#).
6. Camina H. Mendis, [Zeke A. Piskulich](#), 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](#), Ashley K. Borkowski and Ward H. Thompson, "A Maxwell Relation for Dynamical Timescales. Application to the Pressure and Temperature Dependence of Water Self-Diffusion", *In Preparation* (2022).
2. [Zeke A. Piskulich](#), and Ward H. Thompson, "The Water Hydrogen Bond Jump Activation Energy can be Inferred from Experimental Data", *In Preparation* (2022).

Other Fellowships, Awards, and Scholarships

Air Force Office of Scientific Research Scholar , <i>American Conference on Theoretical Chemistry.</i>	2022
Higuchi Doctoral Progress Award , <i>Department of Chemistry</i> , University of Kansas.	2021
○ Award given "to a superior, post-comprehensive graduate student in his or her final year."	
Paul and Hellen Gilles Award in Physical Chemistry , <i>Department of Chemistry</i> , University of Kansas.	2020
○ Award given "for superior academic performance and research accomplishments by an advanced graduate student."	
Graduate Scholarly Presentation Fund , <i>Graduate Studies</i> , University of Kansas.	2019
Helen and Paul Gilles Travel Fund Award , <i>Department of Chemistry</i> , University of Kansas.	2018, 2019
Cornelius McCollum Research Scholarship , <i>Department of Chemistry</i> , University of Kansas.	2019
○ Research scholarship "awarded to outstanding advanced graduate students."	
Graduate Travel Fund Award , <i>Research Excellence Initiative</i> , University of Kansas.	2019
Graduate Writing Incentive Award , <i>Research Excellence Initiative</i> , University of Kansas.	2018
H.P. Cady Award , <i>Department of Chemistry</i> , University of Kansas.	2018
○ Award given "to a first-year graduate student for excellent performance."	
Phi Beta Kappa Honor Society , University of Missouri.	2018
Bailey Scholarship , University of Kansas.	2017

Leadership

Terriers F1RSTS Advocate, *Newbury Center*, Boston University. **2023-Present**

The Terrier F1RSTS Advocate program trains faculty and staff to better connect with and support first generation college and graduate students.

Advocacy Committee Chair, Co-Chair (member since 2021), *Boston Postdoctoral Association*, Boston, MA. **2022-Present**

- Represented advocacy efforts for all 19 Boston-area universities
- Reorganized the committee to have greater connection to local postdoc association efforts
- Organized a "Life as a Postdoc" seminar series that included data-driven talks on postdoc advocacy
- Organized immigration webinars with a variety of law firms for international postdocs

Gordon Research Seminar Co-Chair, *2019 Chemistry and Physics of Liquids*, Holderness, NH. **2017–2019**

- Constructed an interdisciplinary conference program that highlights the current understanding of the liquid phase.
- Fundraised from Academic, Industrial, and Federal sources.
- Designed a mentorship panel focused on student career exploration.

President, Vice President, *Chemistry Graduate Student Organization*, Lawrence, KS. **2018–2020**

- Spearheaded effort to develop GSO into an official student organization.
- Assisted in the creation of a weekly professional development series in collaboration with other departments.
- Increased graduate student membership in departmental committees.
- Organized an alumni panel discussion that included alumni from PUI's, R1 Institutions, and Industry.
- Organized a "Fund Yourself" workshop to connect graduate students with external funding opportunities in 2019 and 2020.
- Organized a "Research Open House" that connected undergraduates and 1st-year graduate students with research opportunities.

Academic Service

Member, *Seed Committee*, Center for Sustainable Nanotechnology. **2021-Present**

NSF Fellowship Information Session, *Speaker*, University of Kansas, Lawrence, KS. **Jul. 2019, Sep. 2019**

- Discussed my experiences and advice for graduate and undergraduate students applying to the NSF GRFP.

Chemistry and Chemical Engineering REU Programs, *Speaker*, University of Kansas, Lawrence, KS. **Jul. 2019**

- Developed materials for and led a discussion titled "How to apply to the NSF Graduate Research Fellowship Program".

Undergraduate Research Symposium, *Session Chair*, University of Kansas, Lawrence, KS. **Apr. 2018, 2019**

- Presided over two sessions of talks given by undergraduate researchers in STEM and Humanities fields.

Outreach

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**

Carnival of Chemistry, *Volunteer*, University of Kansas, Lawrence, KS. **Nov. 2018**

- Designed an activity that taught nearly 300 children about different types of stars, as well as emission lines.

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 and Mentoring Experience

Teaching Assistant, *University of Kansas*, Lawrence, KS. **Fall 2017, 2018**

- 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.

Undergraduate Students: Alexandra Wright (Honors Thesis), Carolyn Smith, Carl Heroneme, Trevor Neal, Alondra Garcia-Arevalo.

Graduate Students: Micah Welsch, Ashley K. Borkowski, Allyson L. Leicht, Sahan M. Godahewa.

Selected Presentations

- 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.** Jul. 2022
Poster, American Conference on Theoretical Chemistry, Tahoe, CA
- Polystyrene Penetrates Lipid Vesicles.** Apr. 2022
Poster, Center for Sustainable Nanotechnology All-Hands Meeting, Dunwoody, GA
- Beyond Arrhenius: Fluctuation Theory for Dynamics.** Mar. 2022
Poster, American Physical Society March Meeting, Chicago, IL
- Beyond Arrhenius: Fluctuation Theory for Dynamics.** Mar. 2022
Invited Talk, American Physical Society March Meeting, Chicago, IL
- On the Relationship Between Structure and Dynamics in Liquid Water.** Feb. 2021
Invited Talk, Statistical Thermodynamics and Molecular Simulation Seminar, Virtual
- Carbon-Dioxide Expanded Acetonitrile as an Ion-Transport Medium.** July 2020
Lightning Talk, Virtual Conference on Theoretical Chemistry, Virtual
- Bringing Supercooled Water in from the Cold: Signatures at Room Temperature.** Jan. 2020
Talk, Pacific Conference on Spectroscopy and Dynamics, San Diego, CA
- The Dynamics and Structure of Supercooled Water can be Predicted from Room Temperature Simulations.** Aug. 2019
Poster, Chemistry and Physics of Liquids GRC, Holderness, NH
- Getting Something for (Almost) Nothing: New Methods for the Calculation of Activation Energies.** Jan. 2019
Poster, Pacific Conference on Spectroscopy and Dynamics, San Diego, CA
- Getting Something for (Almost) Nothing: New Methods for the Calculation of Activation Energies.** Dec. 2018
Invited Talk, Oakland University Chemistry Departmental Seminar, Rochester Hills, MI
- The Activation Energy for Water Reorientation Differs Between IR Pump-Probe and NMR Measurements.** Aug. 2018
Poster, Water and Aqueous Solutions GRS and GRC, Holderness, NH
- Phase Equilibria, Transport Properties, and Structure of CO₂-Expanded Ethylene Oxide and Methanol.** Oct. 2017
Talk, ACS Midwest Regional Meeting, Lawrence, KS
- 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 CO₂-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
- Phase Equilibria and Structure of CO₂-Expanded Ethylene Oxide and Methanol.** Jul. 2017
Poster, American Conference on Theoretical Chemistry, Boston, MA
- Breaking Barriers: Direct Calculation of Activation Energies of Diffusion and Reorientation.** Oct. 2017
Talk, CEBC Industrial Advisory Board Meeting, Lawrence, KS
- Tunability of Phase Equilibria in Gas-Expanded Liquids: The Carboxylation of Ethylene Oxide.** Jan. 2017
Poster, Kansas Physical Chemistry Symposium, Lawrence, KS
- Tunability of Phase Equilibria in Gas-Expanded Liquids: The Carboxylation of Ethylene Oxide.** Oct. 2016
Talk, ACS Midwest Regional Meeting, Manhattan, KS
- Vibrational Relaxation of HF in Argon Fluid.** Jun. 2015
Poster, APS Shock Compression of Condensed Matter, Tampa, FL
- Boron-Doped Graphene-Like Carbons for Hydrogen Gas Storage.** Oct. 2013
Talk, Physics Leaders Meeting, Columbia, MO

Boron-Doped Graphene-Like Carbons for Hydrogen Gas Storage.

Talk, Summer Research Forum, Columbia, MO

Jul. 2013