Pierre Kawak, Ph.D.

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Education & Training

University of South Florida (USF)	Postdoctoral Scholarship	2022 – 2025
Advisor: David S. Simmons		
Brigham Young University (BYU)	Ph.D. Chemical Engineering	2017 – 2022
Advisor: Douglas R. Tree	*Funded Assistantship; 3.81 GPA*	
Dissertation: Simulation of Crystal Nucleation in a Polymer Melt		
American University of Sharjah (AUS)	M.S. Chemical Engineering	2015 – 2017
Advisor: Ghaleb A. Husseini	*Full Scholarship; 4.0 GPA*	
Dissertation: Ultrasound Triggered Release of Estrone-Targeted Liposomes		
American University of Sharjah (AUS)	B.S. Chemical Engineering	2010 – 2015
Minor Economics	*Partial Scholarship*	

Publications

Peer-Reviewed Journal Articles

[5] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Origin of Heating-Induced Softening and Enthalpic Reinforcement in Elastomeric Nanocomposites". *ACS Macro Letters* 14 (2025). DOI: 10.1021/acsmacrolett.5c00442.

[4] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Central Role of Filler-Polymer Interplay in Nonlinear Reinforcement of Elastomeric Nanocomposites". *Macromolecules* 57 (2024). DOI: 10.1021/acs.macromol.4c00489.

[3] **Pierre Kawak**, Christopher Akiki, and Douglas R. Tree. "Effect of local chain stiffness on oligomer crystallization from a melt". *Physical Review Materials* 8 (2024), p. 075606. DOI: 10.1103/PhysRevMaterials.8.075606.

[2] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Semiflexible oligomers crystallize via a cooperative phase transition". *Journal of Chemical Physics* 155 (2021), p. 214902. DOI: 10.1063/5.0067788.

[1] Najla M. Salkho, Vinod Paul, **Pierre Kawak**, Rute F. Vitor, Ana M. Martins, Mohammad Al Sayah, and Ghaleb A. Husseini. "Ultrasonically controlled estrone-modified liposomes for estrogen-positive breast cancer therapy". *Artificial Cells, Nanomedicine, and Biotechnology* 46 (2018), pp. 462–472. DOI: 10.1080/21691401.2018.1459634.

Preprints

[4] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Fracture of Elastomeric Nanocomposites Due to Filler Pillar Formation" (in preparation).

[3] **Pierre Kawak**, William F. Drayer, Mark E. Mackura, and David S. Simmons. "Amorphous Molecular Dynamics Analysis Toolkit (AMDAT): A Software Package for Analysis of Simulations of Structure and Dynamics in Supercooled Liquids and Complex Fluids" (in preparation).

[2] Douglas R. Tree and **Pierre Kawak**. "The Search for a Molecular-Level Understanding of Nucleation in Polymer Crystallization" (in preparation).

[1] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Glassy interphases reinforce elastomeric nanocomposites by enhancing percolation-driven volume expansion under strain" (2025). DOI: 10.48550/arXiv.2509.04755.

Software

[1] David Simmons, **Pierre Kawak**, William Drayer, and Mark Mackura. *Amorphous Molecular Dynamics Analysis Toolkit (AMDAT)*. Version 1.0.1. 2025. DOI: 10.5281/zenodo.17417166.

Awards & Fellowships

Research Grants & Fellowships

National Postdoctoral Association (NPA) IMPACT Fellowship 2023 – 2024
One of six selected out of 100 applicants nationwide for funding & mentorship of proposed project.

National Science Foundation (NSF) CoPI Discover ACCESS Compute Resource Grant Nov. 2023
Awarded NSF funding for access to high performance computing resources.

American Physical Society (APS) Career Mentor Fellowship 2023
Received mentorship training, administered career talk at USF, & judged young trainee talks.

Relevant Program Acceptance & Participation

Torrey Pines Foundations of Leadership Development Program Participant 2024 – 2025
NSF & SACNAS Grant Writing & Peer Review Workshop Attendance Aug. 2023
Future Faculty Workshop Diverse Leaders for the Future Workshop Attendance June 2023
Out in Science, Tech., Engineering, & Maths Professional Development Summit Participant Mar. 2021
UCSD SDSC High Performance Computing Summer Institute Attendee Jul. 2018

Conference Awards

Outstanding Poster Award at Gordon Research Conference on Polymer Physics July 2024
USF Annual Postdoctoral Research Symposium Best Poster Award $200 Mar. 2023
APS Forum on International Physics Distinguished Student Award Fall 2022

Excellence, Leadership & Service Awards

AUS College of Engineering Hall of Fame Inductee 2023
BYU Chemical Engineering Department Graduate Student of the Month Sept. 2022
BYU University Accessibility Center Banquet Scholarship Award $1,500 Fall 2021
BYU Graduate Student Society Professional Presentation Award $500 Fall 2021
BYU Chemical Engineering Department Travel Award Fall 2021
Delta Alpha Pi (DAPi) International Honor Society Inductee 2021
AUS Biomedical Engineering Symposium Best Overall Talk Award $700 Fall 2016
AUS 3× Dean's List for Academic Excellence 2013 – 2014

Research Mentorship Experience

Amanda Sharrer *Ph.D. Candidate, USF* *2024-2025*

- Onboarded and provided ongoing technical guidance for a project on molecular sequence selection for additive compatibilizers in mixed waste plastics.
- Assisted in building molecular configurations and simulation protocols (equilibration/production, validation).
- Supported analysis and visualization workflows using Python and OVITO to probe interfacial phenomena.

Luis Zepeda *Ph.D. Candidate, USF* *2024-2025*

- Provided technical guidance for simulations of thin polymer films near supported and free surfaces.
- Helped establish reliable simulation protocols to study structure and dynamics near interfaces.
- Supported Python post-processing and visualization to extract interfacial trends and communicate results clearly.

Harshad Bhapkar *Ph.D. Candidate, USF* *2022-2025*

- Directly supervised day-to-day research activities focused on mechanical response of polymer nanocomposites.
- Provided hands-on mentorship spanning simulation planning, troubleshooting, analysis strategy, and interpretation of mechanical/structural metrics.
- Served as a primary technical point-of-contact to maintain momentum, prioritize tasks, and ensure method rigor.

Makayla Branham *Ph.D. Candidate, USF* *2023-2025*

- Directly mentored and collaborated on research studying copolymer sequence effects on glass transition behavior.
- Guided analysis, planning and interpretation to connect sequence-level descriptors with relaxation metrics.

Bao Ma *Ph.D. Candidate, USF* *2023-2025*

- Onboarded and provided technical guidance for thin-film polymer simulations near interfaces.
- Supported development of simulation protocols and Python analysis for interfacial structure and dynamics.

Alyna Williams *Undergraduate Researcher, USF* *2024-2025*

- Mentored end-to-end research execution: scientific computing, HPC usage, simulation workflows, and polymer physics literature grounding.
- Co-developed generalized relaxation characterization pipeline across diverse molecular systems.
- Provided career mentorship and wrote letters of reference in support of professional opportunities.

Tianna Virgo *Undergraduate Researcher, USF* *2024*

- Onboarded into simulation-based polymer physics research with structured guidance in scientific computing workflows, high-performance computing procedures, and best practices.

Dr. Peijing Yue *Ph.D. Candidate, USF* *2022-2024*

- Provided sustained professional development/guidance during the Ph.D. to industry transition.
- Helped translate research strengths into industry-ready narratives and practical application materials.

Annelise Curtin *M.S. Student, USF* *2024*

- Provided career guidance for graduate-school prep; placed as Ph.D. at the University of Minnesota.

Austin Hartley *Undergraduate Researcher, USF* *2023*

- Provided career guidance for graduate-school prep; placed as Ph.D. at the Penn State University.

Dr. William F. Drayer *Ph.D. Candidate, USF* *2022-2023*

- Provided professional development and career guidance during transition from Ph.D. to postdoc.

Christopher Akiki *Undergraduate Researcher, BYU* *2020-2022*

- Co-authored a peer-reviewed manuscript on sensitivity of polymer crystallization to force-field choices.
- Collaborated on development of the Order-Parameter Wang–Landau (OPWL) simulation engine in C++, a generalized rare-event sampler for free energies and densities of states.
- Provided technical guidance on literature review and methodological approaches to polyethylene crystallization.
- Provided career guidance for graduate-school prep; placed as Ph.D. at University of Minnesota.

Dr. Dakota S. Banks *Undergraduate Researcher, BYU* *2018-2019*

- Co-authored a peer-reviewed manuscript on minimum free energy path for polymer crystal nucleation.
- Collaborated on the design and implementation of a GPU-accelerated Monte Carlo Polymer Crystallization (MCPC) simulation engine in C++/CUDA.
- Provided career guidance for graduate-school prep; placed as Ph.D. at Brigham Young University.

Beverly S. Delgado *Undergraduate Researcher, BYU* *2019*

- Supported onboarding into molecular simulations and polymer physics with literature and resources.

Andrew S. Gibson *Undergraduate Researcher, BYU* *2018*

- Collaborated on development of the Monte Carlo Polymer Crystallization (MCPC) simulation engine in C++/CUDA and provided onboarding training in simulation workflows.

Paul Kawak *M.S. Student, AUS* *2015-2017*

- Provided onboarding/mentorship on a project developing albumin-targeted smart nanocarriers for cancer treatment (synthesis, validation, and release studies probing ultrasonic-triggered response).

Teaching Experience

Graduate Teaching Assistant *Brigham Young University*	**Thermodynamics**	Winter 2021
	Separations Engineering	Fall 2021
	Heat & Mass Transfer	2018 – 2021 (3x)
	Process Dynamics & Control	Fall 2018
Volunteer Course Instructor; *University of the People*	**College Algebra**	Spring 2018
Graduate Instructor; *American University of Sharjah*	**Principles of ChemE**	2016 – 2017 (3x)
Graduate Teaching Assistant *American University of Sharjah*	**Corrosion Lab**	2016 – 2017 (2x)
	ChemE Lab I	2015 – 2016 (2x)
	Graduate Desalination	Spring 2015
	Wastewater Treatment	Spring 2015
Undergraduate Teaching Assistant *American University of Sharjah*	**Mass Transfer**	2014 – 2015 (3x)
	Kinetics	Fall 2014
	Thermodynamics	Spring 2014
Private Tutor	**Maths, Engineering, Business, etc.**	2008 – now

Community & Service

Peer Review

American Chemical Society Macromolecules	9× Reviews
American Chemical Society Journal of Chemical Information and Modeling	2× Reviews
American Chemical Society Petroleum Research Fund (PRF)	2× Review
Freiburg Institute for Advanced Studies Early Career Fellowship Programme	1× Review
Wiley Journal of Polymer Science	1× Review

Professional Society & Conference Leadership

Co-Chair of 2026 Gordon Research Seminar on Polymer Physics

American Physical Society (APS)

Member of Committee on International Freedom of Scientists 2025-2026
Member of Division of Polymer Physics (DPOLY) Membership Committee 2024-2025
Session Chair "Polymer Structure & Dynamics across Lengths & Timescales" Mar 2024, 2025
Session Organizer "Polymer Structure & Dynamics across Lengths & Timescales" Mar 2024, 2025
Organizer & Winner of Inaugural DPOLY T-Shirt Design Competition Mar 2024
Ranked Undergraduate Talks & Posters as Career Mentoring Fellow 2022 – 2023
Session Chair "Polymers & Composites for Energy Storage & Conversion I" Mar 2023

Early Career Researchers in Polymer Physics

Administrator of 550 member Slack channel for collaboration & networking 2022 – present
Organizer of 2023 Virtual Polymer Physics Symposium with 150 Global Attendees Aug 2023
Cofounder & Organizer of Self-Development Seminar series 2022 – present

Out in Science Technology Engineering & Mathematics (oSTEM), Inc.

Table Representative at MAA MathFest 2023 Aug 2023
Annual Conference Volunteer & Organizer Nov. 2022
Annual Conference Merchandise Team Organizer Nov. 2022

Departmental & Institutional Service

University of South Florida (USF) Postdoctoral Scholar Association (PSA)

Founded & Chaired PSA Executive Committee at USF serving 200 postdocs 2023 – present
Organized Inaugural ELEVATE Talk Series 2024 – 2025
Led Postdoc Highlight Interviews, Socials, & Orientations 2023 – present

BYU Chemical Engineering Graduate Student Council (GSC)

President & Cofounder 2018 – 2021
Organizer of Department Recruitment Poster Event 2019, 2020, 2021
Department BBQ Social Organizer 2018 – 2021
Department-Wide Survey Administrator on Graduate Student Financial Health Fall 2021
Social Media Accounts Manager Fall 2021

Outreach, Inclusion & Public Engagement

White House Presidential AI Challenge volunteer judge and mentor 2025 – present
State Science & Engineering Fair of Florida (SSEF Florida) volunteer judge 2023, 2024

American Chemical Society (ACS)

Science Coach (Education Outreach Initiative) 2023 – 2024
Lecture series facilitator for high school students at Bradenton Christian School 2023 – 2024

University of South Florida (USF)

Great American Teach In Martinez Middle School Visit June 2023
Highschoolers Programming & Scientific Computing Summer Workshop Facilitator June 2023

American Society for Engineering Education (ASEE)

Facilitator of Trans Allyship Safe Zone Ally Training Workshop Mar. 2023
Member of ASEE LGBTQ+ Advocacy in STEM Virtual Community of Practice 2022 – present

American Physical Society (APS)

Member of National Mentoring Community 2022 – present
Physicists To-Go Public Engagement Program Participant 2022 – 2024

Josephine C. Locke Elementary School visiting scholar talk 2022

Out in Science Technology Engineering & Mathematics (oSTEM), Inc.

Scholarship Coordinator (Lead review of $>$ 200 applicants for 20 scholarships) 2022 – present

Mentorship Program Volunteer 2021 – present

Technical Presentations

[29] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Low-Strain Reinforcement as a Volume-Expansion Effect in Filled Elastomers with Glassy Interphases". Global Physics Summit. American Physical Society. Denver, CO, 2026.

[28] **Pierre Kawak**. "Molecular Simulations and Machine Learning for Sustainable Polymer Innovation". Southeast Polymer Forum. University of Georgia, Athens. Athens, GA, 2025.

[27] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Exploring the Role of Polymer-Filler Interactions in Modulating Elastomeric Reinforcement". Global Physics Summit. American Physical Society. Anaheim, CA, 2025.

[26] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Tuning Polymer-Filler Interactions to Modulate Elastomeric Reinforcement". Rubber Division Spring Technical Meeting. American Chemical Society. Lake Buena Vista, FL, 2025.

[25] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Tuning Reinforcement, Void Formation, and Fracture in Elastomeric Nanocomposites: Toward High-Performance, Sustainable Tire Materials". Chemical, Biological, & Materials Engineering Department Seminar. University of South Florida. Tampa, FL, 2025.

[24] **Pierre Kawak**. "Molecular Simulations for Greener Polymers: From Theory to Reality". Annual Meeting. American Institute of Chemical Engineers. San Diego, CA, 2024.

[23] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Contrasting Reinforcement Mechanisms in Elastomeric Nanocomposites". Annual Meeting. American Institute of Chemical Engineers. San Diego, CA, 2024.

[22] **Pierre Kawak**. "Filler-Filler Contacts Reinforce Filled Elastomers at High Strains". GRC Polymer Physics. Gordon Research Conferences. South Hadley, MA, 2024.

[21] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Filler-Filler Contacts Reinforce Filled Elastomers at High Strains". Annual Postdoctoral Research Symposium. University of South Florida. Tampa, FL, 2024.

[20] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Polymer-Filler Competition-Driven Reinforcement Beyond the Payne Effect in Elastomeric Nanocomposites". March Meeting. American Physical Society. Minneapolis, MN, 2024.

[19] Harshad Bhapkar, **Pierre Kawak**, and David S. Simmons. "Exploring the Effects of Nanoparticle Loading, Dispersion and Structure on the Stress Response of Elastomeric Nanocomposites". March Meeting. American Physical Society. Minneapolis, MN, 2024.

[18] **Pierre Kawak**, David S. Simmons, and Douglas R. Tree. "Rational Sustainable Polymer Materials Design Using Multiscale Simulation and Theory". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.

[17] **Pierre Kawak**, Makayla Branham, William F. Drayer, and David S. Simmons. "Tuning Polymer Dynamics Via Sequence Control". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.

[16] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Elucidating the Molecular Origins of Reinforcement in Filled Elastomers Via Spatial- and Species-Resolved Stresses from Molecular Dynamics Simulations". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.

[15] Harshad Bhapkar, **Pierre Kawak**, and David S. Simmons. "Insights into the Dependence of Elastomeric Nanocomposite Mechanics on Nanoparticulate Properties". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.

[14] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Dissecting the Payne Effect: How Filler-Polymer Competition Reinforces Elastomeric Nanocomposites". IOP Polymer Physics Group Graduate Symposium. Institute of Physics. Virtual, 2023.

[13] **Pierre Kawak**. "Career Paths in Physics". Physics Colloquia Series. University of South Florida Department of Physics. Tampa, FL, 2023.

[12] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Exploring Mechanisms of Enhanced Dissipation in Nanoparticle-filled Rubber Using Molecular Dynamics". Annual Postdoctoral Research Symposium. University of South Florida. Tampa, FL, 2023.

[11] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Exploring mechanisms of enhanced dissipation in nanoparticle-filled rubber using molecular dynamics". March Meeting. American Physical Society. Las Vegas, NV, 2023.

[10] Douglas R. Tree and **Pierre Kawak**. "Free Energy Analysis of Crystal Nucleation of Semiflexible Polymers". March Meeting. American Physical Society. Las Vegas, NV, 2023.

[9] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Spatially resolving energy dissipation in molecular dynamics of polymer nanocomposites". March Meeting. American Physical Society. Las Vegas, NV, 2023.

[8] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Acute Sensitivity of Polymer Crystallization Phase Behavior to Intermolecular Interactions". Annual Meeting. American Institute of Chemical Engineers. Phoenix, AZ, 2022.

[7] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Free Energy Analysis of Polymer Crystal Nucleation Indicates Cooperative Crystallization and Nematic Alignment". March Meeting. American Physical Society. Chicago, IL, 2022.

[6] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Free Energy Surfaces for Homogeneous Nucleation in a Polymer Melt". Annual Meeting. American Institute of Chemical Engineers. Boston, MA, 2021.

[5] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "GPU-accelerated Wang-Landau Simulation of Polymer Crystallization". March Meeting. American Physical Society. Virtual, 2021.

[4] **Pierre Kawak**, Andrew S. Gibson, Logan S. Brown, Beverly Delgado, Douglas R. Tree, and Dakota S. Banks. "Investigating Primary Nucleation in Polymer Melts using GPU-Accelerated Wang-Landau Simulations". Annual Meeting. American Institute of Chemical Engineers. Virtual, 2020.

[3] **Pierre Kawak**, Andrew S. Gibson, Logan S. Brown, Beverly Delgado, and Douglas R. Tree. "Wang-Landau Simulation of the Free Energy Surface of Crystallization in a Polymer Melt". March Meeting. American Physical Society. Virtual, 2020.

[2] **Pierre Kawak**, Vinod Paul, Paul Kawak, Rita Kassermally, Fatme Lahib, Rute F. Vitor, Mohammad Al-Sayah, and Ghaleb A. Husseini. "Doxorubicin-Encapsulated, Estrone-Appended Liposomes Triggered by Ultrasound for the Treatment of Breast Cancer". Graduate Students Research Conference. UAE Ministry of Education. Khalifa University, Abu Dhabi, UAE, 2017.

[1] **Pierre Kawak**, Christian C. Momah, Mohamed A. Elkhodiry, Shaima R. Suwaidi, Dina Gadalla, Fatehia M. Banamah, Rute F. Vitor and Hesham G. Moussa, Ana M. Martins and Mohammad Al-Sayah, and Ghaleb A. Husseini. "A Peptide-Targeted Nanodelivery System Triggered by Ultrasound for Anticancer Therapy". Life Sciences Grand Challenges Conference. Institute of Engineering and Electronics Engineering. Khalifa University, Abu Dhabi, UAE, 2016.

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