

Pierre Kawak

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Professional Summary

Computational scientist with expertise in **molecular modeling, scientific computing, crystallization, and mechanical deformation**. Skilled in **Python, C++, HPC, ML, and molecular simulations** for materials science and engineering. Strong background in **material modeling and characterization, free energy simulations, and computational chemistry**. Passionate about applying computational methods to solve real-world challenges in pharma and biotech.

Technical Skills

- **Programming & Computing:** Python, C++, R, bash, CUDA, Open MPI, High-Performance Computing, Machine Learning
- **Computational Chemistry & Modeling:** Molecular dynamics, Atomistic simulations, Statistical mechanics, Phase behavior, Free energy calculations and analysis
- **Software & Tools:** Linux/UNIX, LAMMPS, MATLAB, Gaussian, GROMACS, AMBER
- **Polymer Physics:** Viscoelasticity, Copolymers, Vitrification, Rouse Modes Analysis, Nucleation Theory
- **Drug Delivery:** Liposomes, Chemotherapy, Surface functionalization, Breast cancer, Ultrasound

Research Experience

- | Postdoctoral Researcher | University of South Florida | 2022 – Present |
|--|--------------------------------|----------------|
| Established new understanding of nanocomposite toughening mechanisms & how to rationally control them | | |
| <ul style="list-style-type: none">• Developed predictive molecular dynamics simulators to study rheology of filled rubber.• Analyzed nonlinear rheology via novel local metrics to identify nanoscale toughness origins.• Identified nanoscale toughness origins via novel locally resolved measurements of stress response.• Communicated results via two peer-reviewed publications and 11 conference talks and posters. | | |
| Developed guidance for copolymer thermal stability enhancement via chemical sequence control | | |
| <ul style="list-style-type: none">• Identified, created, and simulated atomistic copolymer with specified sequences to tune T_g.• Analyzed segmental and chain dynamics of automated quench simulations to calculate T_g.• Developed simulation/analysis software suites, boosting team-wide collaboration and productivity.• Mentored 11 students in high-performance coding, version control, and molecular simulations.• Communicated findings via a conference talk and poster. | | |
| Doctoral Researcher | Brigham Young University | 2017 – 2022 |
| Accelerated polymer crystal phase predictions via targeted free energy simulations and GPU computation | | |
| <ul style="list-style-type: none">• Implemented rapid & targeted Monte Carlo simulations in C++/CUDA to study crystallization.• Designed predictive models to enhance material characterization and experimental comparison.• Developed customized Python/C++ scripts for molecular simulations and automated data analysis.• Characterized material phases using crystalline (structure factor, Steinhardt) and orientational (Maier-Saupe, Legendre Polynomial) order parameters.• Communicated results via two peer-reviewed publications and six conference talks and posters. | | |
| Masters Researcher | American University of Sharjah | 2015 – 2017 |
| Improved breast cancer targeting via ultrasound-sensitive smart drug delivery liposomal systems | | |
| <ul style="list-style-type: none">• Synthesized phospholipids reacted with estrone ligands for active breast cancer targeting.• Created self-assembled liposomal chemotherapy formulations via dry film method.• Validated functionalization, structural integrity, and encapsulation via NMR assays, DLS, and lysis.• Characterized release efficacy of novel nanoparticle carrier via sonification in a spectrofluorometer.• Developed/modernized team-wide lab protocols, encouraging collaboration & effective record taking.• Communicated results via a peer-reviewed publication and three conference talks. | | |

Selected Peer-Reviewed Publications

- [4] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "On the origin of heating-induced stiffening and enthalpic reinforcement in elastomeric nanocomposites" (2025). arXiv: [2501.06971](https://arxiv.org/abs/2501.06971) [[cond-mat.soft](#)].
- [3] **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](https://doi.org/10.1021/acs.macromol.4c00489).
- [2] **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](https://doi.org/10.1103/PhysRevMaterials.8.075606).
- [1] **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](https://doi.org/10.1063/5.0067788).

Selected Synergistic Activities

Honors & Awards

National Postdoctoral Association (NPA) IMPACT Fellowship	2023 – 2024
National Science Foundation (NSF) Discover ACCESS Compute Resource Grant	Nov. 2023
AUS College of Engineering Hall of Fame Inductee	2023
American Physical Society (APS) Career Mentor Fellowship	2023
USF Annual Postdoctoral Research Symposium Best Poster Award	Mar. 2023
APS Forum on International Physics Distinguished Student Award	Fall 2022
BYU University Accessibility Center Banquet Scholarship Award	Fall 2021
Delta Alpha Pi (DAPi) International Honor Society Inductee	2021
oSTEM Professional Development Summit Participant	Mar. 2021

Volunteer Work

Elected to American Physical Society Committee on International Freedom of Scientists	2025 – 2026
Founded USF Postdoctoral Scholar Association & chaired executive committee	2023 –
Organized 2023 Virtual Polymer Physics Symposium (150 attendees)	Aug. 2023
Peer-reviewed 15 manuscript and proposal submissions	2021 –
Facilitated 550-member Early Career Researchers in Polymer Physics online community	2021 –
Served oSTEM as scholarship coordinator, conference volunteer, representative, and mentor	2021 – 2023
Frequent service to K-12 schools (science fair judge, visiting scholar, teacher mentorship)	2019 –

Education

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