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, Ovito, VMD, 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**

Researched nanoscale material behavior to enhance durability and performance of polymer composites.

- **Designed and implemented molecular dynamics simulations** to model nanoscale deformation, relaxation, and stress distribution, improving understanding of material toughening mechanisms.
- **Developed novel analysis methods** to analyze nonlinear rheology, identifying key nanoscale factors that enhance material resilience.
- **Applied advanced simulation techniques** to quantify stress response and reinforcement behavior in nanocomposites, informing strategies for improved material design.
- **Published findings in peer-reviewed journals** and presented at 11 conferences, contributing to advancements in filled rubber mechanics and computational materials science.

Developed guidance to enhance thermal stability of copolymers via chemical sequence control.

- **Designed and simulated atomistic copolymers** with controlled sequences to fine-tune glass transition temperature (T_g) at constant composition, improving stability with minimal process or feedstock change.
- **Analyzed molecular dynamics & phase behavior**, determining sequences with superior thermal stability.
- **Developed Python/C++ automation tools** for molecular modeling and free energy calculations, streamlining team-wide computational workflows and improving research efficiency.
- **Trained and mentored 11 researchers** in high-performance computing, version control, and molecular simulations, boosting collaboration, productivity, and technical skill development.
- **Presented findings at institutional and academic conferences,** highlighting advancements in copolymer theory and polymer dynamics modeling.

Doctoral Researcher — **Brigham Young University** — **2017 – 2022**

Developed computational models to predict polymer crystallization behavior, improving material characterization, accelerating simulation workflows, and resolving long-standing scientific debate.

- **Implemented high-performance Monte Carlo simulations in C++/CUDA** to model polymer crystallization, achieving 100× speedup in property computation and enabling experimental comparison.
- **Automated molecular simulation workflows** by developing Python/C++ tools, significantly increasing efficiency in large-scale molecular studies sweeping large multi-dimensional parameter spaces.
- **Applied advanced molecular characterization techniques** to distinguish complex phase transitions, enabling insights into controlling parameters.

- **Mapped multi-dimensional phase transitions** using **first-of-their-kind** 3D free energy landscapes, enabling differentiation of order-formation pathways that are inaccessible to classical simulation.
- **Resolved long-standing debates in polymer crystallization theory** by distinguishing competing mechanisms of phase transitions, advancing scientific understanding.
- **Published findings in peer-reviewed journals** and presented at six conferences, supporting a funded NSF CAREER proposal for continued research.

Masters Researcher **American University of Sharjah** **2015 – 2017**

Engineered ultrasound (US) sensitive drug delivery systems to enhance breast cancer treatment efficacy.

- **Designed and synthesized targeted liposomal drug carriers** by functionalizing phospholipids with estrone ligands, improving tumor-specific drug delivery.
- **Formulated and optimized self-assembling liposomal chemotherapy systems** with enhanced stability and controlled drug release using the dry film method.
- **Validated drug encapsulation and nanoparticle integrity** through NMR and DLS assays.
- **Characterized drug release kinetics**, optimizing US frequency & intensity for future clinical application.
- **Standardized lab protocols** to improve reproducibility, collaboration, and data integrity across teams.
- **Published findings in a peer-reviewed journal** and presented at three conferences.

Education

Brigham Young University (BYU) *Advisor: Douglas R. Tree*	Ph.D. Chemical Engineering *Funded Assistantship; 3.81 GPA*	2017 – 2022
American University of Sharjah (AUS) *Advisor: Ghaleb A. Husseini*	M.S. Chemical Engineering *Full Scholarship; 4.0 GPA*	2015 – 2017
American University of Sharjah (AUS) Minor Economics	B.S. Chemical Engineering *Partial Scholarship*	2010 – 2015

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 [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.

[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.

[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.

Honors, Awards, & Service

Elected to American Physical Society (APS) Committee on International Freedom of Scientists	2025 – 2026
Founded USF Postdoctoral Scholar Association & chaired executive committee	2023 –
Awarded National Postdoctoral Association (NPA) IMPACT Fellowship	2023 – 2024
Inducted to AUS College of Engineering Hall of Fame	2023
Awarded American Physical Society (APS) Career Mentor Fellowship	2023
Granted National Science Foundation (NSF) Discover ACCESS Compute Resource Grant	Nov. 2023
Organized & Fundraised for 2023 Virtual Polymer Physics Symposium (150 attendees)	Aug. 2023
Awarded APS Forum on International Physics Distinguished Student Award	Fall 2022
Facilitated 550-member Early Career Researchers in Polymer Physics online community	2021 –
Served oSTEM as scholarship coordinator, conference volunteer, representative, and mentor	2021 – 2023