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, 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**

Copolymer Sequence Specific Effects on Glass Transition (Tg) with Dr. David S. Simmons

- Identify, create, and simulate atomistic copolymer with specified sequences to tune Tg.
- Analyze segmental and chain dynamics of automated quench simulations to calculate Tg.
- Develop/maintain team-wide simulation/analysis software suites.
- Communicated findings via a conference talk and poster.

Molecular Origins of Polymer Nanocomposite Toughness (PNC) with Dr. David S. Simmons

- Develop equilibrium (eq.) & non-eq. LAMMPS MD simulators to study rheology of filled rubber.
- Analyze nonlinear rheological response via local & global metrics to identify nanoscale toughness origins.
- Communicated results via two peer-reviewed publications and 11 conference talks and posters.

Ph.D. Researcher **Brigham Young University** **2017 – 2022**

GPU Accelerated Polymer Crystal Simulation with Dr. Douglas R. Tree

- Implemented GPU-accelerated Wang-Landau simulations to study polymer crystallization.
- Designed property prediction models to enhance material characterization and experimental comparison.
- Developed custom 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.

M.S. Researcher **American University of Sharjah** **2015 – 2017**

Ultrasound-sensitive smart drug delivery systems with Dr. Ghaleb Husseini

- Synthesize, validate and test novel nanoparticle carrier for treatment of breast cancer cells.
- Develop/modernize team-wide lab protocols.
- Communicated results via a peer-reviewed publication and two conference talks and posters.

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

Education & Training

University of South Florida — 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*