Pierre Kawak, Ph.D.

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- Scientific software developer with 11+ years of experience using Python and C++ to build high-throughput molecular simulation tools and force field-based models.
- Specialized in atomistic and coarse-grained polymer simulations using OPLS and custom physics-based molecular dynamics and Monte Carlo frameworks to study material properties with experimental accuracy.
- Passionate about writing clean, test-driven code and advancing molecular modeling to accelerate discovery in chemistry, materials, and therapeutics.

Technical Skills

- **Simulation & Molecular Modeling**: Atomistic & Coarse-Grained Simulation, Force Field Parameterization, Monte Carlo Sampling, Molecular Dynamics, Free Energy Calculations, Model Validation, LAMMPS, GROMACS, Gaussian, OPLS, AMBER
- **Programming & Software Development**: Python, C++, C, CUDA, MATLAB, Bash, R, Object-Oriented Programs, Unit Testing, Modular Code Design, Git, Version Control, Scientific Software Engineering
- **Data Analysis & Visualization**: VMD, OVITO, NumPy, Pandas, Matplotlib, 3D Scientific Visualization, Simulation Output Parsing
- **HPC & Workflow Optimization**: Slurm, Open MPI, HPC Cluster Management, Workflow Automation, Parallelization, Large-Scale Data Processing (50TB+)
- **Scientific Domains**: Polymer Physics, Glass Transition, Crystallization, Nanoparticles, Drug Delivery, Rheology
- **Collaboration & Communication**: Public Speaking (27+ conferences), Scientific Writing (5 publications), Technical Documentation, Mentoring, DEI Advocacy

Research Experience

Postdoc **University of South Florida** **Prof. David Simmons** **2022 – Present**

- Simulate atomistic copolymers with OPLS force field with high accuracy to identify sequences with enhanced thermal stability without altering feedstock or processing.
- Develop modular Python/bash/C tools for rheology analysis with automated workflows spanning 500+ sequential/parallel jobs & 6-month-long simulations.
- Perform high-throughput parameter sweeps across nanoparticle size, volume fraction, monomer chemistry, etc. to optimize nanocomposite & copolymer performance.
- Document & validate internal codebases, & created structured tutorials to onboard 11 mentees in simulation, HPC workflows, & technical practices.
- Streamline large-scale HPC pipelines (50+ TB), reducing analysis time by 90%+ & earning an NSF ACCESS award.

- Present at 17 conferences, receiving recognition at GRC (2024) & USF Symposium (2023) for simulation-driven rubber & copolymer design.

Ph.D. **Brigham Young University** **Prof. Douglas Tree** **2017 – 2022**

- Built 2 modular Monte Carlo codes (35K+ lines each in C++/CUDA) to accelerate crystallization modeling (100×) & explore complex free energy landscapes.
- Designed reusable interaction modules to support diverse chemistries and sampling strategies in custom molecular simulations.
- Constructed 3D phase diagrams using custom crystalline & orientational order parameters to reveal molecular transition mechanisms.
- Analyzed 3D structural data to extract kinetic & thermodynamic insights.
- Mentored 4 undergraduates, co-authoring 2 papers & 6 abstracts, supporting careers.
- Played key role in a successful $500K NSF CAREER proposal & received national awards for scientific communication.

M.S. **American University of Sharjah** **Prof. Ghaleb Husseini** **2015 – 2017**

- Engineered liposomal drug carriers with estrone targeting & ultrasound-triggered release, enhancing delivery control for breast cancer chemotherapy.
- Characterized encapsulation & release kinetics using DLS & NMR, gaining insight into nanoscale interactions and delivery efficiency.
- Standardized lab protocols to boost reproducibility, collaboration, & data integrity.
- Presented at 3 conferences, earning Best Talk Award at AUS Biomed. Eng. Symposium.

Leadership & Community Engagement

- **President, Early Career Researchers in Polymer Physics (2022–):** Led a global 550-member community & organized the 2023 Virtual Symposium with 150+ attendees.
- **President & Founder, USF Postdoctoral Scholar Association (2023–):** Served 200+ postdocs via career events, DEI initiatives, & the NPA-funded ELEVATE Talk Series.
- **President & Founder, BYU Chem. Eng. Grad. Student Council (2019–2022):** Directed recruitment, outreach, & well-being programs impacting department policy.

Education

Ph.D.	Chemical Engineering	Brigham Young University	2022
M.S.	Chemical Engineering	American University of Sharjah	2017
B.S.	Chemical Engineering (Econ. Minor)	American University of Sharjah	2015

Comprehensive & updated list of publications & presentations available online at linktr.ee/pkawak