Pierre Kawak, Ph.D.

+1 (801) 762-7999 pskawak@gmail.com linktr.ee/pkawak

Professional Summary

Computational polymer physicist with expertise in molecular simulation, statistical mechanics, and polymer theory. Extensive experience leading collaborative projects at the intersection of materials science, chemical engineering, and polymer physics.

- Expert in developing, optimizing, and deploying molecular dynamics and Monte Carlo simulations to uncover structure–property relationships in polymers and soft materials.
- Experienced in leading cross-functional teams, managing up to 11 researchers, and mentoring graduate and undergraduate students on computational methods and scientific communication.
- Proven ability to architect and accelerate analysis pipelines for polymer simulations, including profiling and optimizing in-house codes in Python, C++, and CUDA.
- Demonstrated success translating molecular insights into design principles for tough, recyclable, and sustainable materials, including elastomeric nanocomposites and copolymer systems.
- Strong record of scientific communication with multiple invited talks, publications in top journals, and community leadership in the polymer physics community.
- Passionate about building inclusive scientific communities, with leadership experience organizing professional development events, symposia, and mentoring programs.

Technical Skills

- **Simulation and Modeling:** Molecular dynamics (MD), Monte Carlo (MC), coarse-grained modeling, polymer chain modeling, non-equilibrium simulations, phase behavior analysis, free energy calculations.
- **Software Development:** Architecting, profiling, and deploying scientific software in Python, C++, CUDA, Bash, and FORTRAN; experience with collaborative software development using Git.
- **Simulation Packages:** LAMMPS, HOOMD-blue, GROMACS, OpenMM, Lattice-based MC codes, in-house simulation and analysis tools.
- **Analysis and Data Processing:** Custom analysis pipelines for molecular simulation data using Python (NumPy, SciPy, Matplotlib, Pandas), bash scripting, and parallel computation.
- **High-Performance Computing:** Experience with HPC job scheduling (SLURM), running simulations on national supercomputing facilities (XSEDE, ACCESS), and GPU-accelerated computing (CUDA, Nsight, nvprof).

- **Data Visualization and Reporting:** Scientific visualization with Matplotlib, Plotly, and VMD; automated report generation in LaTeX.
- **Process Simulation and Thermodynamics:** Experience with process simulation tools (Aspen HYSYS) and instruction in thermodynamic modeling.
- **Leadership and Project Management:** Leading cross-functional teams, mentoring junior researchers, organizing professional development workshops and symposia.

Research Experience

Postdoctoral Researcher, University of South Florida *2022 – Present*
Advisor: Prof. David Simmons

Material Simulation and Analysis

- Developed molecular dynamics models (LAMMPS, GROMACS, OPLS) to investigate stress relaxation, deformation, and nanoscale reinforcement in polymer nanocomposites.
- Simulated thermo-elastoplastic deformation and rheology of rubber and copolymers, identifying nanoscale toughening mechanisms.
- Modeled copolymer sequences with enhanced glass transition temperatures without altering processing or feedstock chemistry.
- Applied Bayesian optimization to fit relaxation dynamics and extract glass transition behavior.
- Led multi-dimensional parameter sweeps (nanoparticle size, chemistry, volume fraction) to optimize nanocomposite and copolymer designs.
- Collaborated with experimentalists to validate molecular predictions against thermal and mechanical performance targets.
- Designed statistical models and applied machine learning to extract insights from large molecular datasets.

Software Development and Automation

- Architected Python/C++/CUDA simulation and analysis tools to enable high-throughput, physics-informed property prediction.
- Developed modular, reusable rheology and stress analysis toolkits integrated into team-wide simulation workflows.
- Automated data analysis pipelines handling 50+ TB datasets, reducing turnaround time by 90%.
- Built bash, Slurm, and MPI automation for large-scale HPC job orchestration, checkpointing, and storage.

- Documented group codebases and created tutorials for reproducible scientific computing.
- Integrated local stress analysis tools to study mechanical response under deformation.

High-Performance Computing Optimization and Workflow Acceleration

- Led optimization of 50+ TB data pipelines across HPC clusters, improving data throughput by 90%.
- Streamlined multi-node CPU and GPU workflows for molecular simulations.
- Reduced simulation runtime by 90% through parallelization and high-performance computing resource optimization.
- Awarded NSF ACCESS Compute Resource Grant for advancing scalable HPC-enabled molecular simulations.

Debugging, Profiling, and Performance Tuning

- Debugged and profiled C++/Python group codebases using GDB, valgrind, and profiling tools (nsight, nvprof), resolving memory leaks and runtime bottlenecks.
- Improved software modularity, runtime, and scalability for multi-month, high-dimensional simulations.
- Led efforts to standardize code maintainability and scientific reproducibility through internal documentation and technical presentations.

Leadership, Mentorship, and Community Engagement

- Led and mentored 11+ researchers in HPC, molecular simulation, version control, and scientific computing practices.
- Designed structured onboarding programs, documentation, and tutorials to train new users.
- Organized professional development workshops, DEI programs, and research symposia for 200+ researchers across multiple organizations.
- Presented research at 17+ institutional, industrial, and academic conferences, earning multiple awards (GRC 2024, USF 2023).
- Recognized with the APS Career Mentor Fellowship for leadership in mentoring and community building.

Ph.D. Researcher, Brigham Young University *2017 – 2022*
Advisor: Prof. Douglas Tree

Software Development and GPU Acceleration

- Built two GPU-accelerated Monte Carlo engines in C++/CUDA to simulate polymer crystallization and free energy landscapes.

- Developed advanced sampling algorithms (Configurational Bias Monte Carlo, Wang-Landau) to efficiently explore high-dimensional molecular states.
- Designed GPU-optimized data structures (cell lists) and pairwise interaction search algorithms, achieving significant performance improvements.
- Utilized NVIDIA profiling tools (nsight, nvprof) to debug, optimize, and scale GPU-accelerated codes.

Structure–Property Analysis and Data Processing

- Developed numerical algorithms to quantify nanoscale crystalline and orientational order from 3D simulation trajectories.
- Processed large-scale simulation data to generate thermodynamic observables, including free energy derivatives and heat capacity profiles.
- Extracted phase diagrams and structure–property relationships through systematic parameter sweeps and automated analysis pipelines.

High-Performance Computing and Workflow Optimization

- Leveraged HPC resources to perform long-timescale, high-throughput Monte Carlo simulations using GPU acceleration.
- Automated simulation and data analysis workflows to enable reproducible exploration of high-dimensional parameter spaces.

Scientific Communication and Collaboration

- Collaborated with interdisciplinary teams to apply simulation methods to polymer crystallization and glass transition problems.
- Presented research findings at academic conferences, advancing understanding of nanoscale phenomena in polymer materials.

Graduate Researcher, American University of Sharjah *2015 – 2017*
Advisor: Prof. Ghaleb Husseini

- Synthesized estrone-functionalized drug nanocarriers; enhanced release control for chemotherapy applications.
- Validated drug stability & kinetics with DLS/NMR; optimized ultrasonic parameters.
- Standardized lab protocols; boosted reproducibility and cross-lab collaboration.
- Presented at 3 conferences; awarded Best Talk at AUS Biomedical Symposium.

Leadership & Community Engagement

- **President**, Early Career Researchers in Polymer Physics (2022–Present): Led 550+ member global network, organized 150+ attendee virtual symposium.

- **Founder & President**, USF Postdoctoral Scholar Association (2023–Present): Launched NPA-funded ELEVATE Talk Series and DEI programs for 200+ postdocs.
- **Founder & President**, BYU Chem. Eng. Graduate Council (2019–2022): Shaped department policies and spearheaded outreach and recruitment.

Selected Peer-Reviewed Publications

[4] **P. Kawak**, H. Bhapkar, and D. Simmons. "On the origin of heating-induced stiffening and enthalpic reinforcement in elastomeric nanocomposites". In: (2025). arXiv: 2501.06971.

[3] **P. Kawak**, H. Bhapkar, and D. Simmons. "Central role of filler-polymer interplay in nonlinear reinforcement of elastomeric nanocomposites". In: *Macromolecules* 57 (2024). DOI: 10.1021/acs.macromol.4c00489.

[2] **P. Kawak**, C. Akiki, and D. Tree. "Effect of local chain stiffness on oligomer crystallization from a melt". In: *Phys. Rev. Mater.* 8 (2024). DOI: 10.1103/PhysRevMaterials.8.075606.

[1] **P. Kawak**, D. Banks, and D. Tree. "Semiflexible oligomers crystallize via a cooperative phase transition". In: *J. Chem. Phys.* 155 (2021). DOI: 10.1063/5.0067788.

Education

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

Full list of publications and presentations available at linktr.ee/pkawak