Pierre Kawak, Ph.D.

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- Computational chemist and software engineer with 7+ years of experience in molecular simulations, materials modeling, and high-performance computing (HPC).

- Developed and deployed scalable molecular dynamics (MD) & Monte Carlo (MC) workflows using LAMMPS, GROMACS, and Gaussian across HPC environments, accelerating polymer crystallization, vitrification, and additive manufacturing insights.

- Proficient in Python, C++, and CUDA for algorithm development, Bayesian optimization, and GPU-accelerated simulations.

- Applied statistical modeling and data fitting techniques to extract physical insights from large simulation datasets.

- Collaborated on interdisciplinary projects spanning materials design and AI integration, presenting findings at 27+ international conferences.

- Committed to rigorous documentation, reproducibility, and mentoring in scientific software practices.

Research Experience

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

- Developed and deployed large-scale MD simulations using LAMMPS, GROMACS, Gaussian, and OPLS to model polymer composites, enabling nanoscale insights into stress relaxation and deformation mechanisms.

- Engineered analysis pipelines to extract nonlinear rheological properties from simulation data, identifying nanoscale toughening mechanisms aligned with high-performance rubber design.

- Simulated coarse-grained and atomistic copolymer sequences to optimize thermal stability, predicting glass transition temperatures (T_g) without modifying feedstock or processing conditions.

- Applied Bayesian optimization to fit polymer relaxation data (e.g., self-intermediate scattering functions) with multiple dynamic modes, enabling accurate T_g extraction from complex simulation outputs.

- Optimized supercomputing workflows using SLURM, bash scripting, and job arrays to balance core-hour usage and maximize simulation throughput across distributed clusters with large datasets (>50TB), reducing compute time by 90% and earning an NSF Discover ACCESS Compute Grant (2023).

- Mentored 11 researchers in HPC best practices, version control (Git), and molecular simulations, earning the APS Career Mentor Fellowship (2023) for impactful training and collaboration.

- Presented results at 17+ national and international conferences, winning poster awards at the Gordon Research Conference (2024) and USF Postdoc Symposium (2023).

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

- Developed, optimized, & deployed GPU-accelerated Monte Carlo simulations in C/CUDA, achieving $100\times$ speedup in property computes, enabling experimental comparison.

- Automated high-throughput simulations using Python, C++, bash, MATLAB, & R, reducing paramter-sweep runtimes & enabling large-scale polymer crystal studies.

- Constructed the first-ever 3D free energy landscapes for polymer crystallization, differentiating order-formation pathways inaccessible to classical simulations.

- Developed advanced phase diagrams & applied order parameters for crystalline & orientational order, quantifying phase transitions in complex molecular landscapes.

- Visualized & analyzed large datasets of 3D molecular configurations using VMD & OVITO, extracting key structural & kinetic insights.

- Mentored 4 undergraduate researchers, co-authoring 2 journal articles & 6 conference abstracts, thereby supporting their transition to graduate-level careers.

- Secured research awards, e.g., APS Forum on Intl. Physics Distinguished Student Award (2022) & BYU Grad. Student Society Professional Presentation Award (2021).

- Contributed critical preliminary findings that supported the successful NSF CAREER Award ($500,000) proposal for continued crystallization research.

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

- Designed ultrasound-sensitive drug delivery systems to improve chemotherapy efficiency, winning the AUS Biomedical Engineering Symposium Best Talk Award (2016).

- Engineered estrone-functionalized phospholipid liposomal drug carriers, enhancing breast cancer drug delivery precision.

- Formulated & optimized self-assembling chemotherapy nanoparticles using the dry film method, enhancing drug stability & controlled release kinetics.

- Validated encapsulation efficiency & nanoparticle integrity through NMR & DLS assays, ensuring high drug-loading capacity & structural robustness.

- Quantified ultrasound-triggered drug release across frequency & intensity gradients, identifying optimal acoustic parameters for clinical performance & stability.

- Standardized lab protocols to improve reproducibility, collaboration, & data integrity, increasing research efficiency across teams.

- Published findings in a peer-reviewed journal & presented at 3 conferences, disseminating contributions to biomedical engineering & drug delivery research.

Leadership & Community Engagement

President   Early Career Researchers in Polymer Physics   2022 – Present

- Led a 550-member global Slack community, organizing networking, technical, self-development, & conference prep events, improving belonging of polymer researchers.

- Organized the 2023 Virtual Polymer Physics Symposium, a 2-day intl. event with 150+ attendees, 4 technical sessions, a DEI discussion, & a diverse career panel.

President and Founder   USF Postdoctoral Scholar Association   2023 – Present

- Served 200+ postdocs through career programming, networking events, & advocacy, e.g., ELEVATE Talk Series, funded by NPA IMPACT Fellowship (2023, 6% acc. rate).

President and Founder   BYU Chem. Eng. Graduate Student Council   2019 – 2022

- Organized dept. recruitment, social & outreach events, social content, & financial well-being initiatives, e.g., Recruitment Poster Event (2019–2021) & BBQ Socials (2018–2021).

- Administered a financial health survey to assess graduate student well-being, influencing department policy discussions (2021).

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 and updated list of publications and presentations available online at `linktr.ee/pkawak`