

# Pierre Kawak, Ph.D.

+1 (801) 762-7999 • [pskawak@gmail.com](mailto:pskawak@gmail.com) • [linktr.ee/pkawak](https://linktr.ee/pkawak)

- Computational materials scientist with 11+ years of experience in molecular dynamics, polymer simulations, and high-performance computing workflows.
- Skilled in Python, C++, CUDA, & LAMMPS for building scalable, reproducible tools.
- Hands-on experience with GPU-accelerated molecular simulations, workflow automation, and data-driven property prediction.
- Proven track record in optimizing computational pipelines, mentoring interdisciplinary teams, and contributing to open science through 5 publications and 27+ presentations.
- Eager to advance next-generation battery technologies by bridging molecular modeling with AI and HPC at SES AI.

## Technical Skills

---

- **Programming & Automation:** Python, C++, C, CUDA, MATLAB, Bash, R, Git
- **Simulation & Modeling:** LAMMPS, GROMACS, Gaussian, AMBER, OPLS, Monte Carlo, Molecular Dynamics, Multi-Scale Modeling, Free Energy Calculations
- **Machine Learning & Optimization:** Bayesian Optimization, Model Fitting, Data-driven Property Prediction
- **HPC & Workflow Engineering:** Slurm, OpenMPI, Cluster Resource Management, Parallelization, Workflow Automation, Large-Scale Data Processing (50TB+)
- **Data Analysis & Visualization:** VMD, OVITO, NumPy, Pandas, Matplotlib
- **Experimental Techniques:** Drug Encapsulation, DLS, NMR, Liposomal Formulations, Nanoparticle Synthesis
- **Communication & Leadership:** Technical Mentorship, DEI Advocacy, Public Speaking (27+ conferences), Scientific Writing (5 publications), Event Coordination

## Research Experience

---

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

- Develop, optimize, & deploy scalable LAMMPS molecular simulations of rubber deformation to extract nanoscale insights for stress response & composite optimization.
- Collaborate with chemists to identify copolymer sequences with enhanced thermal stability via targeted simulations without feedstock or process changes.
- Develop custom, rigorous, well-documented mechanics & dynamics analysis tools in Python/C++ & integrate them into in-house simulation workflows.
- Streamline molecular simulations & maximize resource utilization via Slurm across HPC clusters of 50+ TB simulation datasets, earning NSF ACCESS grant.

- Mentor 11 researchers on Git, HPC scripting, & simulation methods, earning APS Career Mentor Fellowship.
- Present award-winning research at 17 conferences, including GRC 2024 & USF 2023, on rubber dynamics & copolymer design.

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

- Designed 2 C++/CUDA Monte Carlo simulation packages (internal GitHub repos).
- Resolved computational bottlenecks through iterative profiling, debugging, & code redesign to enable GPU-accelerated, high-accuracy simulations.
- Implemented statistical mechanics pipelines to extract free energies from noisy data with rigorous replication strategies.
- Analyzed large 3D simulation datasets with custom crystalline & orientational order parameters to extract key structural & kinetic insights.
- Mentored 4 undergraduates, co-authoring 2 papers & 6 abstracts, supporting careers.
- Contributed data & writing to a successful \$500K NSF CAREER proposal.
- Earned APS Distinguished Student Award (2022) & BYU Presentation Award (2021) for research excellence & scientific communication.

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

- Validated nanoparticle encapsulation & release kinetics using DLS & NMR, optimizing formulation parameters & ultrasonic parameters for breast cancer treatment.
- Standardized lab workflows to improve reproducibility, collaboration, & data quality.
- Presented award-winning research at AUS Biomedical Engineering 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](https://linktr.ee/pkawak)