Pierre Kawak, Ph.D.

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- Scientific programmer with 11+ years of experience building modular, well-documented tools in Python & C++ for high-throughput simulation & analysis in materials science.
- Developed 2 object-oriented C++ Monte Carlo codes from scratch & created collaborative Python frameworks for job submission & data processing across diverse teams.
- Passionate about writing clean, testable code & translating scientific insight into maintainable software infrastructure.
- Seeking to contribute strong software engineering practices & a deep scientific background to impactful drug discovery.

Technical Skills

- **Programming & Software Development**: Python, C++, C, CUDA, MATLAB, Bash, R, Object-Oriented Programs, Unit Testing, Modular Code Design, Git, Version Control, Scientific Software Design, Codebase Maintenance
- **Scientific Computing & Simulation**: Monte Carlo, Molecular Dynamics, Free Energy Calculations, LAMMPS, GROMACS, Gaussian, OPLS, Atomistic, Coarse-Graining
- **Analysis & Visualization**: VMD, OVITO, NumPy, Pandas, Matplotlib, Advanced Scientific Visualization (3D schematics, configuration rendering, scientific illustration)
- **HPC & Workflow Optimization**: Slurm, Open MPI, Cluster Management, Workflow Automation, Parallelization, Large-Scale Data Processing (50TB+)
- **Scientific Domains**: Material Simulation, Polymer Physics, 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**

- Lead targeted simulations of nanocomposites & copolymers, sweeping high-dimensional design spaces (e.g., nanoparticle size, chemistry) to identify optimal performance.
- Develop modular Python/bash/C tools for analysis & job automation, supporting workflows with 500+ sequential/parallel jobs & 6-month-long simulations.
- Document tools extensively & create structured tutorials to onboard 11 mentees in technical, scientific, & communication skills.
- Streamline large-scale HPC pipelines (50+ TB), reducing analysis time by 90%+ & earning an NSF ACCESS award.
- Mentor 11 researchers in HPC, Git, & simulations, earning APS Mentor Fellowship.

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

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

- Designed & implemented 2 modular Monte Carlo codes (35K+ lines each in C++/CUDA) to explore crystallization behavior, accelerating discovery 100×.
- Applied object-oriented design principles to build reusable simulation modules supporting diverse chemistries & sampling strategies.
- Integrated unit tests to ensure long-term reliability & minimize regression.
- 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, optimizing ultrasonic parameters for clinical stability & efficacy.
- 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