

# Pierre Kawak, Ph.D.

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- 7 years of computational expertise in molecular modeling, material characterization, free energy analysis, computational chemistry, crystallization, & material mechanics.
- 4 years of experimental expertise in breast cancer treatment, liposomal formulations, surface functionalization, active targeting, drug delivery kinetics, & ultrasonification.
- Authored 5 peer-reviewed articles, contributing to advancements in copolymer theory, polymer dynamics modeling, filled rubber mechanics, & cancer drug delivery.
- Presented at 27 institutional, national, & intl. conferences (e.g., APS, ACS, AIChE, USE, AUS, GRC, IoP, etc.) to diverse audiences from industry, govt., & academia.
- Passionate about using computation to solve challenges in materials & pharma.

## Technical Skills

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- **Programming & Automation:** Python, C++, C, CUDA, MATLAB, Bash, R
- **Simulation & Modeling:** LAMMPS, GROMACS, Gaussian, AMBER, OPLS, Monte Carlo methods, Molecular Dynamics, Atomistic, Coarse-Graining
- **Data Analysis & Visualization:** VMD, OVITO, NumPy, Pandas, Matplotlib, Free Energy Calculations
- **HPC & Workflow Optimization:** Slurm, Open MPI, Cluster Management, Parallelization, Large-Scale Data Processing (50TB+)
- **Experimental Techniques:** Drug Encapsulation, DLS, NMR, Liposomal Formulations, Nanoparticle Synthesis
- **Communication & Leadership:** Public Speaking (27+ conferences), Scientific Writing (5 publications), Mentoring, DEI Advocacy, Event Coordination

## Research Experience

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<b>Postdoc</b>	<b>University of South Florida</b>	<b>Prof. David Simmons</b>	<b>2022 – Present</b>
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- Simulate polymer deformation & stress, generating high-throughput nanoscale insights for composite design.
- Improve copolymer  $T_g$  by simulating specific sequences, optimizing stability without altering feedstock or process.
- Develop custom polymer rheology & dynamics analysis tools & extend in-house codebase, streamlining group workflows & accelerating junior researchers' productivity.
- Streamline HPC workflows to process 50+ TB datasets, accelerating studies by 90% & earning an NSF ACCESS grant.
- Mentor 11 researchers in HPC, Git, & simulation methods, fostering collaboration & earning APS Career Mentor Fellowship.

- Present at 17 conferences, winning awards at GRC (2024) & USF Symposium (2023) for research on rubber & copolymer design.

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

- Wrote two Monte Carlo simulation codes in C++/CUDA from scratch, accelerating crystallization studies 100× & enabling published 3D free energy landscapes.
- Constructed advanced phase diagrams using custom crystalline & orientational order parameters, quantifying key molecular transitions.
- Analyzed large 3D datasets via VMD & OVITO, extracting structural & kinetic insights across crystallization pathways.
- Mentored 4 undergraduates, co-authoring 2 papers & 6 conference abstracts, & supporting their admission to graduate programs.
- Earned APS Distinguished Student Award (2022) & BYU Presentation Award (2021) for scientific communication & research excellence.
- Played key role in a successful \$500K NSF CAREER proposal.

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

- Designed & synthesized estrone-functionalized ultrasound-sensitive drug carriers, improving drug stability & controlled release in breast cancer chemotherapy.
- Validated & characterized encapsulation & release kinetics using DLS & NMR, optimizing ultrasonic parameters for clinical stability and efficacy.
- Standardized lab protocols to improve reproducibility, collaboration, & data integrity, increasing research efficiency across teams.
- 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](https://linktr.ee/pkawak)