Pierre Kawak, Ph.D.

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- Computational scientist with 11 years of experience designing atomistic simulations, automating high-throughput modeling workflows, and analyzing large structural datasets in materials and therapeutic systems.
- Skilled in Python, C, cloud computing, & simulation such as LAMMPS & GROMACS.
- Developed custom codebases and data pipelines (>50TB) to accelerate insights into copolymer design and molecular crystallization.
- Experience includes sequence-specific copolymer modeling for property optimization and initial cheminformatics tool development (e.g., RDKit).
- Passionate about applying AI/ML and molecular modeling to drug discovery.

Technical Skills

- **Programming & Software Development**: Python, R, C++, CUDA, Bash, GitHub, Jupyter, Linux (CLI), Object-Oriented Design, Unit Testing, Benchmarking
- **Molecular Modeling & Simulation**: Gaussian, Molecular Dynamics (LAMMPS, GROMACS), Free Energy Calculations, Coarse-Graining, Atomistic Force Fields (AMBER, OPLS), Monte Carlo Methods, RDKit, Sequence-Structure-Property Relationships
- **Data Science & Visualization**: Scikit-learn, Bayesian Optimization, NumPy, Pandas, Matplotlib, VMD, OVITO, High-Dimensional Large-Scale Data Analysis (>50TB)
- **HPC & Cloud Infrastructure**: Slurm, Open MPI, Cluster Management, Parallelization
- **Communication & Leadership**: Scientific Writing (5 publications), Public Speaking (27+ talks), Mentorship (15+ trainees), DEI Advocacy, Event Coordination

Research Experience

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

- Automated sequence-specific copolymer screening to identify formulations with elevated glass transition temperatures (T_g).
- Simulated deformation via molecular dynamics to create design rules for composites.
- Curated & analyzed >50TB of simulation data using parallel Python/C++ pipelines, improving study turnaround time by 90% and securing NSF HPC grant.
- Mentored 15+ researchers in simulation, Git workflows, & cloud computing practices; selected for APS Career Mentorship Fellowship.
- Delivered 17+ conference talks & won sci. comm. awards at GRC (2024) & USF (2023).

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

- Built two Monte Carlo simulation codes (C++/CUDA) from scratch, enabling 100× faster crystallization studies & published 3D free energy landscapes.

- Iteratively tested, benchmarked, and profiled algorithms to ensure accurate structure–property predictions and scalable performance.
- Designed custom order parameters to analyze large 3D structural datasets, quantify molecular transitions and crystallization dynamics.
- Mentored 4 undergrads and co-authored 2 papers & 6 conference abstracts.
- Played key role in a successful $500K NSF CAREER grant.
- Earned APS Distinguished Student & BYU Presentation Award for science comm.

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

- Designed estrone-functionalized ultrasound-sensitive liposomes for breast cancer therapy, enhancing drug stability & controlled release.
- Validated encapsulation & release kinetics using DLS & NMR, optimizing ultrasonic parameters for therapeutic viability.
- Standardized lab protocols across teams, boosting reproducibility & collaboration.
- Presented at 3 conferences; earned Best Talk Award at AUS Biomedi. 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

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" (2025). arXiv: 2501.06971.

[3] **P. Kawak**, H. Bhapkar, and D. Simmons. "Central role of filler-polymer interplay in nonlinear reinforcement of elastomeric nanocomposites". *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". *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". *J. Chem. Phys.* 155 (2021). DOI: 10.1063/5.0067788.

Comprehensive & updated **list of publications & presentations** available online at linktr.ee/pkawak