

Pierre Kawak, Ph.D.

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Senior Computational Scientist with 7 years of experience in molecular modeling & simulation, & 4 years in experimental drug delivery & liposomal formulation. Expertise spans molecular dynamics (LAMMPS, GROMACS, AMBER), free energy calculations, GPU-accelerated simulations, & Python-based workflow automation, including:

- Executed high-throughput simulations for nanoscale materials using HPC infrastructure, earning an NSF ACCESS Compute Resource Grant (2023).
- Developed ultrasound-sensitive liposomal drug delivery systems & nanoparticle formulations, improving chemotherapy efficiency & stability.
- Mentored 16+ junior researchers, authored 5 peer-reviewed articles, & presented at 27+ conferences, with national recognition (APS Career Mentor Fellowship, GRC Best Poster Award, NPA IMPACT Fellowship). Eager to apply computational chemistry & simulation-driven design to accelerate molecular glue discovery at Neomorph.

Research Experience

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

- Simulated nanoscale mechanical response of polymer composites using high-throughput molecular dynamics (LAMMPS, OPLS), revealing deformation pathways that inform molecular design of toughened materials.
- Engineered a rheology analysis framework of stress-strain from simulations, enabling discovery of nanoscale relaxation mechanisms linked to material failure resistance.
- Modeled thermal performance of copolymers across atomistic & coarse-grained scales, identifying novel sequences with enhanced glass transition temperature T_g without altering composition or processing routes.
- Automated processing of 50TB+ simulation datasets via Python & bash, reducing analysis time by 90% & securing NSF ACCESS Compute Resource Grant (2023).
- Elevated group research capacity by mentoring 11 researchers in molecular simulation, HPC, & version control, earning the APS Career Mentor Fellowship (2023).
- Disseminated findings at 17 int'l venues, receiving poster awards for innovations in computational polymer mechanics (USF Postdoc Symposium 2023, GRC 2024).

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

- Accelerated Monte Carlo simulations 100× via GPU-optimized CUDA/C++ pipelines, enabling tractable modeling of polymer crystallization & experimental comparison.
- Deployed automated simulation workflows using Python, Bash, & R to run parametric sweeps across molecular architectures, facilitating large-scale crystallization studies.
- Constructed first-ever 3D free energy landscapes & derived kinetic pathways for polymer order formation, offering new mechanistic insight inaccessible to classical models.
- Designed phase diagrams using custom order parameters to map crystalline & orientational transitions, supporting predictive modeling of material phase behavior.

- Visualized complex molecular configurations with VMD & OVITO, extracting structural signatures from thousands of simulation frames for downstream analysis.
- Mentored 4 undergraduates, co-authoring 2 journal papers & 6 conference abstracts, supporting their successful entry into competitive graduate programs.
- 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 Hussein 2015 – 2017

- Engineered ultrasound-responsive liposomal drug carriers with estrone surface ligands, enhancing breast cancer targeting & release precision.
- Formulated self-assembling chemotherapy nanoparticles using the dry film method, improving drug encapsulation stability & sustained release profiles.
- Quantified ultrasound-triggered drug release across acoustic parameters, identifying optimal frequencies for controlled release & clinical viability.
- Validated nanoparticle integrity & drug-loading efficiency through NMR & dynamic light scattering, ensuring structural robustness & reproducibility.
- Standardized lab protocols to improve reproducibility, collaboration, & data integrity, increasing research efficiency across teams.
- Presented findings at 3 conferences & peer-reviewed publication, earning Best Talk Award at the AUS Biomed. Eng. Symposium (2016) for innovation in drug delivery.

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