

# Pierre Kawak, Ph.D.

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Computational Modeling Researcher with 7+ years of experience in developing & deploying first-principles & molecular simulations to investigate polymer thermal & mechanical properties, drug delivery systems, & crystallization. Career highlights include leading large-scale modeling campaigns using LAMMPS, GROMACS, AMBER, & Python; optimizing data workflows to process 50TB+ datasets; & mentoring 11 junior researchers in HPC methods. Seeking to leverage deep computational expertise & team leadership to drive modeling innovation & reactor/process development at ExxonMobil.

## Research Experience

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<b>Postdoctoral Researcher</b>	<b>University of South Florida (USF)</b>	<b>2022 – Present</b>
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- Developed & applied first-principles molecular dynamics (MD) simulations using LAMMPS & GROMACS to probe stress relaxation & deformation mechanics in polymer composites, yielding physical predictions to guide macroscopic performance.
- Designed custom Python-based analysis frameworks to extract nonlinear rheological behavior from simulation data, linking simulation outputs to phenomenological insights relevant for advanced rubber design & performance/process optimization.
- Simulated coarse-grained & atomistic copolymer sequences using OPLS & multi-scale MD approaches to identify  $T_g$ -enhancing formulations, enabling improved thermal properties without feedstock or process changes.
- Architected HPC workflows using bash & Python to process >50TB of simulation data, reducing data pipeline runtime by 90% & enabling real-time iteration across modeling efforts; awarded NSF Discover ACCESS Compute Grant (2023).
- Mentored & trained 11 researchers in HPC-enabled simulation, version control (Git), & data management practices, strengthening team modeling capacity & earning the APS Career Mentor Fellowship (2023).
- Presented modeling innovations & materials simulation & theory advancements at 17+ academic & industry venues, earning Outstanding Poster honors at Gordon Research Conference (2024) & USF Postdoctoral Symposium (2023) for contributions to predictive polymer performance modeling.

<b>Doctoral Researcher</b>	<b>Brigham Young University</b>	<b>2017 – 2022</b>
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- Developed, optimized, & deployed GPU-accelerated Monte Carlo simulations in C/CUDA to investigate polymer crystallization thermodynamics, achieving 100× speedup in property computes, enabling experimental comparison.
- Automated high-throughput, multi-variate simulations using Python, C++, bash, MATLAB, & R to explore polymer morphology & crystallization kinetics, reducing parameter-sweep runtimes & enabling large-scale polymer crystal studies.
- Constructed first-ever 3D free energy landscapes for polymer crystallization, differentiating metastable states & ordering pathways inaccessible to classical methods.
- Derived advanced phase diagrams & applied custom order parameters to quantify crystalline & orientational order, classifying phase transitions in complex landscapes.
- Visualized molecular datasets in OVITO, extracting key structural & kinetic insights.
- Mentored 4 undergraduate researchers, co-authoring 2 journal articles & 6 conference abstracts, thereby supporting their transition to graduate-level careers.

- 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.

#### **Masters Researcher                      American University of Sharjah                      2015 – 2017**

- Developed ultrasound-responsive drug delivery systems for targeted chemotherapy, integrating mechanistic understanding of acoustic propagation with kinetic drug release modeling; awarded Best Talk at AUS Biomedical Engineering Symposium (2016).
- Designed & synthesized estrone-functionalized phospholipid liposomes to improve tumor-targeting precision, enhancing selective drug uptake in breast cancer treatment.
- Formulated & optimized self-assembling chemotherapy nanoparticles using the dry film method, enhancing drug stability & controlled release kinetics.
- Validated encapsulation efficiency & nanoparticle integrity through NMR & DLS, ensuring high drug-loading capacity & structural robustness.
- Quantified & optimized ultrasound-triggered drug release kinetics, identifying ideal acoustic frequency & intensity parameters to maximize on-demand release profiles—bridging lab-scale kinetics to potential clinical translation.
- Standardized cross-lab protocols & workflows to improve reproducibility, collaboration, & data integrity across research units.
- Disseminated findings in a peer-reviewed publication & 3 conference presentations, contributing novel methods to the field of responsive drug delivery.
- Served as Instructor of Record for a Principles of Chemical Engineering recitation, teaching unit operation modeling in ASPEN HYSYS (e.g., reactors, pumps, separators); redesigned syllabus to emphasize industry-relevant software features.

## **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.
- Directed 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).
- Designed & 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](https://linktr.ee/pkawak)