

# Pierre Kawak, Ph.D.

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Senior Scientist with 7+ years of experience applying molecular modeling, polymer physics, & material characterization to advance next-generation material solutions. Expertise includes free energy analysis, mechanical property prediction, polymer crystallization, & multiscale simulations using molecular dynamics (MD), Monte Carlo (MC), & CUDA-based models. Proven ability to connect structure & property through simulation & experimental validation (e.g.,  $T_g$  tuning, drug release kinetics, NMR/DLS). Passionate about solving high-impact R&D problems & driving innovation in polymer technology.

## 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 multiscale MD models using LAMMPS & GROMACS to investigate stress relaxation & nanoscale reinforcement in polymer composites, enabling predictive links between molecular structure & mechanical performance.
- Created novel Python-based analysis methods for nonlinear rheology & deformation behavior, supporting simulation-driven property optimization of filled rubber.
- Simulated copolymer thermal behavior using atomistic & coarse-grained MD (OPLS), identifying high- $T_g$  formulations with statistical validation without changing processing or feedstock chemistry, validating performance outcomes through structure-property modeling & cross-functional collaboration with experimentalists.
- Optimized 50TB+ HPC workflows in bash/Python, improving simulation throughput by 90% & enabling rapid iteration across product development cycles; awarded NSF ACCESS Compute Resource Grant (2023).
- Mentored 11 junior researchers in HPC simulation & data workflows, boosting collaboration, productivity, & earning APS Career Mentor Fellowship (2023).
- Presented findings at 17 industrial, & academic conferences, highlighting advancements in polymer characterization & modeling & earning poster awards at the Gordon Research Conference (2024) & the USF Postdoc Research Symposium (2023).

<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, achieving 100× speedup in property computes, enabling experimental comparison.
- Automated high-throughput simulations using Python, C++, MATLAB, & R, reducing statistically significant parameter-sweep runtimes for data-driven characterization.
- Constructed first-ever 3D free energy landscapes to map ordering pathways & phase behavior, offering first-principles insights into molecular crystallization processes.
- Created advanced phase diagrams using custom order parameters to quantify phase transitions & molecular ordering via design of experiments, delivering new crystallization metrology tools.
- Visualized & analyzed large datasets of 3D molecular configurations using VMD & 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**

- Designed ultrasound-sensitive drug delivery systems to improve chemotherapy efficiency, winning the AUS Biomedical Engineering Symposium Best Talk Award (2016).
- Engineered estrone-functionalized liposomal drug carriers, enhancing breast cancer drug delivery precision.
- 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 assays, ensuring high drug-loading capacity & structural robustness.
- Quantified ultrasound-triggered drug release across frequency & intensity gradients, identifying optimal acoustic parameters for clinical performance & stability.
- Standardized lab protocols to improve reproducibility, collaboration, & data integrity, increasing research efficiency across teams.
- Published findings in a peer-reviewed journal & presented at 3 conferences, disseminating contributions to biomedical engineering & drug delivery research.

## **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](https://linktr.ee/pkawak)