

# Pierre Kawak, Ph.D.

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## Key Skills & Achievements

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- 7 years of computational expertise in **molecular modeling, material characterization, free energy analysis, computational chemistry, crystallization, and mechanical deformation.**
- 4 years of experimental expertise in **breast cancer treatment, liposomal formulations, surface functionalization, passive & active targeting, drug delivery kinetics, and sonification.**
- Authored & edited 5 peer-reviewed articles, contributing to advancements in copolymer theory, polymer dynamics modeling, filled rubber mechanics, and cancer drug delivery.
- Presented 27 times at institutional, national, and international conferences (e.g., APS, ACS, AIChE, USF, AUS, GRC, IoP, etc.)
- BS, MS, PhD, & postdoc in Chemical Engineering from the Middle East to the USA.
- Passionate about using computational methods to solve challenges in pharma & biotech.

## Professional Experience

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- | Postdoctoral Researcher  | University of South Florida | 2022 – Present |
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| <ul style="list-style-type: none"><li>• Developed and implemented large-scale molecular dynamics simulations using LAMMPS, GROMACS, Gaussian, AMBER, and OPLS, achieving high-throughput insights into nanoscale deformation, relaxation, and stress distribution in polymer composites.</li><li>• Created novel analysis techniques for nonlinear rheology, identifying nanoscale toughening factors overlooked by previous literature that guide rubber advancements.</li><li>• Optimized copolymer thermal stability by simulating coarse-grained and atomistic sequences at constant composition, identifying novel sequences with enhanced glass transition temperatures <math>T_g</math> without changing feedstock or processing conditions.</li><li>• Leveraged high-performance and parallel computing to conduct multi-TB molecular simulations on supercomputing clusters, securing an NSF Discover ACCESS Compute Resource Grant (2023).</li><li>• Developed Python, C++, bash, Slurm, Open MPI, and R automation tools for molecular modeling of polymer dynamics and mechanics, accelerating team-wide computational workflows, streamlining multi-TB data analysis, and improving research efficiency.</li><li>• Mentored and trained 11 researchers in HPC, version control, and molecular simulations, boosting collaboration, productivity, and technical skill development and earning the APS Career Mentor Fellowship (2023).</li><li>• Presented findings at 17 institutional, industrial, and academic conferences, highlighting advancements in rubber and copolymer technology, as well as polymer theory, and earning the USF Annual Postdoctoral Research Symposium Best Poster Award (2023) and the Outstanding Poster Award at the Gordon Research Conference (2024).</li><li>• Founded and led the USF Postdoctoral Scholar Association (PSA), serving 200+ postdocs through career programming, networking events, and advocacy, including the ELEVATE Talk Series, funded by the prestigious NPA IMPACT Fellowship (2023–2024, 1 of 6 out of 100 selected globally).</li></ul> |                             |                |

**Doctoral Researcher****Brigham Young University****2017 – 2022**

- Developed, optimized, and deployed GPU-accelerated Monte Carlo simulations in C++/CUDA, achieving a  $100\times$  speedup in crystallization property computations, enabling direct comparison with experiments.
- Automated high-throughput molecular simulations using Python, C++, bash, MATLAB, and R, optimizing multi-dimensional parameter sweeps and accelerating polymer crystallization studies.
- Constructed the first-ever 3D free energy landscapes for polymer crystallization, differentiating order-formation pathways previously inaccessible to classical simulations and resolving a long-standing theoretical controversy on polymer crystallization pathways.
- Developed advanced phase diagrams and applied order parameters for crystalline and orientational order, quantifying phase transitions in complex molecular landscapes.
- Visualized and analyzed multi-TB datasets of 3D molecular configurations using VMD and OVITO, extracting key structural and kinetic insights.
- Published 2 peer-reviewed articles with 2 mentored undergraduates, supporting their entry into research careers.
- Secured multiple research and travel awards, including the APS Forum on International Physics Distinguished Student Award (2022), and the BYU Graduate Student Society Professional Presentation Award (2021).
- Presented at six conferences and directly contributed to securing an NSF CAREER Award (\$500,000) for continued polymer crystallization research by producing critical preliminary findings.
- Founded and led the BYU Chemical Engineering Graduate Student Council (GSC), organizing recruitment, social events, and financial well-being initiatives for graduate students.
- Organized & led department-wide recruitment and outreach events, including the Department Recruitment Poster Event (2019–2021) and Department BBQ Socials (2018–2021).
- Administered a financial health survey to assess graduate student well-being, influencing department policy discussions.
- Managed department social media accounts, boosting student engagement and networking.

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

- Developed ultrasound-sensitive drug delivery systems to improve targeted chemotherapy efficiency, winning the AUS Biomedical Engineering Symposium Best Overall Talk Award (2016).
- Designed and synthesized tumor-targeting liposomal drug carriers by functionalizing phospholipids with estrone ligands, improving breast cancer drug delivery precision.
- Formulated and optimized self-assembling chemotherapy nanoparticles using the dry film method, enhancing drug stability and controlled release kinetics.
- Validated encapsulation efficiency and nanoparticle integrity through NMR and DLS assays, ensuring high drug-loading capacity and structural robustness.

- Characterized and optimized ultrasound-triggered drug release kinetics, determining the ideal US frequency & intensity for future clinical applications.
- Standardized lab protocols to improve reproducibility, collaboration, and data integrity, increasing research efficiency across teams.
- Published findings in a peer-reviewed journal and presented at three conferences, disseminating contributions to biomedical engineering and drug delivery research.

## Education

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Doctorate Philosophy	Chemical Engineering	Brigham Young University	2022
Master of Science	Chemical Engineering	American University of Sharjah	2017
Bachelor of Science	Chemical Eng. (Econ. Minor)	American University of Sharjah	2015

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