

# Pierre Kawak, Ph.D.

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## Education & Training

University of South Florida (USF) <i>Advisor: David S. Simmons</i>	Postdoctoral Scholarship	2022 – 2025
Brigham Young University (BYU) <i>Advisor: Douglas R. Tree</i> Dissertation: Simulation of Crystal Nucleation in a Polymer Melt	Ph.D. Chemical Engineering <i>Funded Assistantship; 3.81 GPA</i>	2017 – 2022
American University of Sharjah (AUS) <i>Advisor: Ghaleb A. Hussein</i> Dissertation: Ultrasound Triggered Release of Estrone-Targeted Liposomes	M.S. Chemical Engineering <i>Full Scholarship; 4.0 GPA</i>	2015 – 2017
American University of Sharjah (AUS) Minor Economics	B.S. Chemical Engineering <i>Partial Scholarship</i>	2010 – 2015

## Publications

### *Peer-Reviewed Journal Articles*

- [5] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Origin of Heating-Induced Softening and Enthalpic Reinforcement in Elastomeric Nanocomposites". *ACS Macro Letters* (2025). doi: [10.1021/acsmacrolett.5c00442](https://doi.org/10.1021/acsmacrolett.5c00442).
- [4] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Central Role of Filler-Polymer Interplay in Nonlinear Reinforcement of Elastomeric Nanocomposites". *Macromolecules* 57 (2024). doi: [10.1021/acs.macromol.4c00489](https://doi.org/10.1021/acs.macromol.4c00489).
- [3] **Pierre Kawak**, Christopher Akiki, and Douglas R. Tree. "Effect of local chain stiffness on oligomer crystallization from a melt". *Physical Review Materials* 8 (2024), p. 075606. doi: [10.1103/PhysRevMaterials.8.075606](https://doi.org/10.1103/PhysRevMaterials.8.075606).
- [2] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Semiflexible oligomers crystallize via a cooperative phase transition". *Journal of Chemical Physics* 155 (2021), p. 214902. doi: [10.1063/5.0067788](https://doi.org/10.1063/5.0067788).
- [1] Najla M. Salkho, Vinod Paul, **Pierre Kawak**, Rute F. Vitor, Ana M. Martins, Mohammad Al Sayah, and Ghaleb A. Hussein. "Ultrasonically controlled estrone-modified liposomes for estrogen-positive breast cancer therapy". *Artificial Cells, Nanomedicine, and Biotechnology* 46 (2018), pp. 462–472. doi: [10.1080/21691401.2018.1459634](https://doi.org/10.1080/21691401.2018.1459634).

### *Preprints*

- [4] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Fracture of Elastomeric Nanocomposites Due to Filler Pillar Formation" (in preparation).
- [3] **Pierre Kawak**, William F. Drayer, Mark E. Mackura, and David S. Simmons. "Amorphous Molecular Dynamics Analysis Toolkit (AMDAT): A Software Package for Analysis of Simulations of Structure and Dynamics in Supercooled Liquids and Complex Fluids" (in preparation).

- [2] Douglas R. Tree and **Pierre Kawak**. “The Search for a Molecular-Level Understanding of Nucleation in Polymer Crystallization” (in preparation).
- [1] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Glassy interphases reinforce elastomeric nanocomposites by enhancing percolation-driven volume expansion under strain” (2025). doi: [10.48550/arXiv.2509.04755](https://doi.org/10.48550/arXiv.2509.04755).

### Software

- [1] David Simmons, **Pierre Kawak**, William Drayer, and Mark Mackura. *Amorphous Molecular Dynamics Analysis Toolkit (AMDAT)*. Version 1.0.1. 2025. doi: [10.5281/zenodo.17417166](https://doi.org/10.5281/zenodo.17417166).

## Awards & Fellowships

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### Research Grants & Fellowships

National Postdoctoral Association (NPA) <a href="#">IMPACT Fellowship</a>	2023 – 2024
One of six selected out of 100 applicants nationwide for funding & mentorship of proposed project.	
National Science Foundation (NSF) CoPI Discover <a href="#">ACCESS</a> Compute Resource Grant	Nov. 2023
Awarded NSF funding for access to high performance computing resources.	
American Physical Society (APS) <a href="#">Career Mentor Fellowship</a>	2023
Received mentorship training, administered career talk at USF, & judged young trainee talks.	

### Relevant Program Acceptance & Participation

<a href="#">Torrey Pines Foundations of Leadership Development Program</a> Participant	2024 – 2025
<a href="#">NSF &amp; SACNAS Grant Writing &amp; Peer Review Workshop</a> Attendance	Aug. 2023
<a href="#">Future Faculty Workshop Diverse Leaders for the Future Workshop</a> Attendance	June 2023
<a href="#">Out in Science, Tech., Engineering, &amp; Maths Professional Development Summit</a> Participant	Mar. 2021
<a href="#">UCSD SDSC High Performance Computing Summer Institute</a> Attendee	Jul. 2018

### Conference Awards

Outstanding Poster Award at Gordon Research Conference on Polymer Physics	July 2024
USF Annual Postdoctoral Research Symposium <a href="#">Best Poster Award</a> \$200	Mar. 2023
APS Forum on International Physics <a href="#">Distinguished Student Award</a>	Fall 2022

### Excellence, Leadership & Service Awards

AUS <a href="#">College of Engineering Hall of Fame Inductee</a>	2023
BYU Chemical Engineering Department Graduate Student of the Month	Sept. 2022
BYU University Accessibility Center Banquet Scholarship Award \$1,500	Fall 2021
BYU Graduate Student Society Professional Presentation Award \$500	Fall 2021
BYU Chemical Engineering Department Travel Award	Fall 2021
Delta Alpha Pi (DAPI) International Honor Society Inductee	2021
AUS Biomedical Engineering Symposium Best Overall Talk Award \$700	Fall 2016
AUS 3× Dean’s List for Academic Excellence	2013 – 2014

## Research Mentorship Experience

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<b>Amanda Sharrer</b>	<i>Ph.D. Candidate, USF</i>	2024-2025
<ul style="list-style-type: none"> <li>– Onboarded and provided ongoing technical guidance for a project on molecular sequence selection for additive compatibilizers in mixed waste plastics.</li> <li>– Assisted in building molecular configurations and simulation protocols (equilibration/production, validation).</li> <li>– Supported analysis and visualization workflows using Python and OVITO to probe interfacial phenomena.</li> </ul>		
<b>Luis Zepeda</b>	<i>Ph.D. Candidate, USF</i>	2024-2025
<ul style="list-style-type: none"> <li>– Provided technical guidance for simulations of thin polymer films near supported and free surfaces.</li> <li>– Helped establish reliable simulation protocols to study structure and dynamics near interfaces.</li> <li>– Supported Python post-processing and visualization to extract interfacial trends and communicate results clearly.</li> </ul>		
<b>Harshad Bhapkar</b>	<i>Ph.D. Candidate, USF</i>	2022-2025
<ul style="list-style-type: none"> <li>– Directly supervised day-to-day research activities focused on mechanical response of polymer nanocomposites.</li> <li>– Provided hands-on mentorship spanning simulation planning, troubleshooting, analysis strategy, and interpretation of mechanical/structural metrics.</li> <li>– Served as a primary technical point-of-contact to maintain momentum, prioritize tasks, and ensure method rigor.</li> </ul>		
<b>Makayla Branham</b>	<i>Ph.D. Candidate, USF</i>	2023-2025
<ul style="list-style-type: none"> <li>– Directly mentored and collaborated on research studying copolymer sequence effects on glass transition behavior.</li> <li>– Guided analysis, planning and interpretation to connect sequence-level descriptors with relaxation metrics.</li> </ul>		
<b>Bao Ma</b>	<i>Ph.D. Candidate, USF</i>	2023-2025
<ul style="list-style-type: none"> <li>– Onboarded and provided technical guidance for thin-film polymer simulations near interfaces.</li> <li>– Supported development of simulation protocols and Python analysis for interfacial structure and dynamics.</li> </ul>		
<b>Alyna Williams</b>	<i>Undergraduate Researcher, USF</i>	2024-2025
<ul style="list-style-type: none"> <li>– Mentored end-to-end research execution: scientific computing, HPC usage, simulation workflows, and polymer physics literature grounding.</li> <li>– Co-developed generalized relaxation characterization pipeline across diverse molecular systems.</li> <li>– Provided career mentorship and wrote letters of reference in support of professional opportunities.</li> </ul>		
<b>Tianna Virgo</b>	<i>Undergraduate Researcher, USF</i>	2024
<ul style="list-style-type: none"> <li>– Onboarded into simulation-based polymer physics research with structured guidance in scientific computing workflows, high-performance computing procedures, and best practices.</li> </ul>		
<b>Dr. Peijing Yue</b>	<i>Ph.D. Candidate, USF</i>	2022-2024
<ul style="list-style-type: none"> <li>– Provided sustained professional development/guidance during the Ph.D. to industry transition.</li> <li>– Helped translate research strengths into industry-ready narratives and practical application materials.</li> </ul>		
<b>Annelise Curtin</b>	<i>M.S. Student, USF</i>	2024
<ul style="list-style-type: none"> <li>– Provided career guidance for graduate-school prep; placed as Ph.D. at the University of Minnesota.</li> </ul>		
<b>Austin Hartley</b>	<i>Undergraduate Researcher, USF</i>	2023
<ul style="list-style-type: none"> <li>– Provided career guidance for graduate-school prep; placed as Ph.D. at the Penn State University.</li> </ul>		
<b>Dr. William F. Drayer</b>	<i>Ph.D. Candidate, USF</i>	2022-2023
<ul style="list-style-type: none"> <li>– Provided professional development and career guidance during transition from Ph.D. to postdoc.</li> </ul>		
<b>Christopher Akiki</b>	<i>Undergraduate Researcher, BYU</i>	2020-2022
<ul style="list-style-type: none"> <li>– Co-authored a peer-reviewed manuscript on sensitivity of polymer crystallization to force-field choices.</li> <li>– Collaborated on development of the Order-Parameter Wang-Landau (OPWL) simulation engine in C++, a generalized rare-event sampler for free energies and densities of states.</li> <li>– Provided technical guidance on literature review and methodological approaches to polyethylene crystallization.</li> <li>– Provided career guidance for graduate-school prep; placed as Ph.D. at University of Minnesota.</li> </ul>		

**Dr. Dakota S. Banks** *Undergraduate Researcher, BYU* 2018-2019

- Co-authored a peer-reviewed manuscript on minimum free energy path for polymer crystal nucleation.
- Collaborated on the design and implementation of a GPU-accelerated Monte Carlo Polymer Crystallization (MCPC) simulation engine in C++/CUDA.
- Provided career guidance for graduate-school prep; placed as Ph.D. at Brigham Young University.

**Beverly S. Delgado** *Undergraduate Researcher, BYU* 2019

- Supported onboarding into molecular simulations and polymer physics with literature and resources.

**Andrew S. Gibson** *Undergraduate Researcher, BYU* 2018

- Collaborated on development of the Monte Carlo Polymer Crystallization (MCPC) simulation engine in C++/CUDA and provided onboarding training in simulation workflows.

**Paul Kawak** *M.S. Student, AUS* 2015-2017

- Provided onboarding/mentorship on a project developing albumin-targeted smart nanocarriers for cancer treatment (synthesis, validation, and release studies probing ultrasonic-triggered response).

## Teaching Experience

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Graduate Teaching Assistant <i>Brigham Young University</i>	<b>Thermodynamics</b> <b>Separations Engineering</b> <b>Heat &amp; Mass Transfer</b> <b>Process Dynamics &amp; Control</b>	Winter 2021 Fall 2021 2018 – 2021 (3x) Fall 2018
Volunteer Course Instructor; <i>University of the People</i>	<b>College Algebra</b>	Spring 2018
Graduate Instructor; <i>American University of Sharjah</i>	<b>Principles of ChemE</b>	2016 – 2017 (3x)
Graduate Teaching Assistant <i>American University of Sharjah</i>	<b>Corrosion Lab</b> <b>ChemE Lab I</b> <b>Graduate Desalination</b> <b>Wastewater Treatment</b>	2016 – 2017 (2x) 2015 – 2016 (2x) Spring 2015 Spring 2015
Undergraduate Teaching Assistant <i>American University of Sharjah</i>	<b>Mass Transfer</b> <b>Kinetics</b> <b>Thermodynamics</b>	2014 – 2015 (3x) Fall 2014 Spring 2014
Private Tutor	<b>Maths, Engineering, Business, etc.</b>	2008 – now

## Community & Service

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### Peer Review

American Chemical Society <a href="#">Macromolecules</a>	9× Reviews
American Chemical Society <a href="#">Journal of Chemical Information and Modeling</a>	2× Reviews
American Chemical Society <a href="#">Petroleum Research Fund (PRF)</a>	2× Review
Freiburg Institute for Advanced Studies <a href="#">Early Career Fellowship Programme</a>	1× Review
Wiley <a href="#">Journal of Polymer Science</a>	1× Review

### Professional Society & Conference Leadership

Co-Chair of [2026 Gordon Research Seminar on Polymer Physics](#)  
*American Physical Society (APS)*

Member of <a href="#">Committee on International Freedom of Scientists</a>	2025-2026
Member of Division of Polymer Physics (DPOLY) Membership Committee	2024-2025
Session Chair "Polymer Structure & Dynamics across Lengths & Timescales"	Mar <a href="#">2024</a> , 2025
Session Organizer "Polymer Structure & Dynamics across Lengths & Timescales"	Mar <a href="#">2024</a> , 2025
Organizer & Winner of Inaugural DPOLY T-Shirt Design Competition	Mar 2024
Ranked Undergraduate Talks & Posters as <a href="#">Career Mentoring Fellow</a>	2022 – 2023
Session Chair " <a href="#">Polymers &amp; Composites for Energy Storage &amp; Conversion I</a> "	Mar 2023

#### *Early Career Researchers in Polymer Physics*

Administrator of 550 member Slack channel for collaboration & networking	2022 – present
Organizer of 2023 <a href="#">Virtual Polymer Physics Symposium</a> with 150 Global Attendees	Aug 2023
Cofounder & Organizer of <a href="#">Self-Development Seminar</a> series	2022 – present

#### *Out in Science Technology Engineering & Mathematics (oSTEM), Inc.*

Table Representative at MAA MathFest 2023	Aug 2023
Annual Conference Volunteer & Organizer	Nov. 2022
Annual Conference Merchandise Team Organizer	Nov. 2022

### **Departmental & Institutional Service**

#### *University of South Florida (USF) Postdoctoral Scholar Association (PSA)*

Founded & Chaired PSA Executive Committee at USF serving 200 postdocs	2023 – present
Organized Inaugural ELEVATE Talk Series	2024 – 2025
Led Postdoc Highlight Interviews, Socials, & Orientations	2023 – present

#### *BYU Chemical Engineering Graduate Student Council (GSC)*

President & Cofounder	2018 – 2021
Organizer of Department Recruitment Poster Event	2019, 2020, 2021
Department BBQ Social Organizer	2018 – 2021
Department-Wide Survey Administrator on Graduate Student Financial Health	Fall 2021
Social Media Accounts Manager	Fall 2021

### **Outreach, Inclusion & Public Engagement**

<i>White House</i> Presidential AI Challenge volunteer judge and mentor	2025 – present
<i>State Science &amp; Engineering Fair of Florida (SSEF Florida)</i> volunteer judge	2023, 2024

#### *American Chemical Society (ACS)*

<a href="#">Science Coach</a> (Education Outreach Initiative)	2023 – 2024
Lecture series facilitator for high school students at Bradenton Christian School	2023 – 2024

#### *University of South Florida (USF)*

Great American Teach In Martinez Middle School Visit	June 2023
Highschoolers Programming & Scientific Computing Summer Workshop Facilitator	June 2023

#### *American Society for Engineering Education (ASEE)*

Facilitator of <a href="#">Trans Allyship Safe Zone Ally Training Workshop</a>	Mar. 2023
Member of ASEE LGBTQ+ Advocacy in STEM <a href="#">Virtual Community of Practice</a>	2022 – present

#### *American Physical Society (APS)*

Member of <a href="#">National Mentoring Community</a>	2022 – present
<a href="#">Physicists To-Go</a> Public Engagement Program Participant	2022 – 2024

Josephine C. Locke Elementary School visiting scholar talk	2022
<i>Out in Science Technology Engineering &amp; Mathematics (oSTEM), Inc.</i>	
Scholarship Coordinator (Lead review of > 200 applicants for 20 scholarships)	2022 – present
Mentorship Program Volunteer	2021 – present

## Technical Presentations

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- [29] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Low-Strain Reinforcement as a Volume-Expansion Effect in Filled Elastomers with Glassy Interphases”. Global Physics Summit. American Physical Society. Denver, CO, 2026.
  - [28] **Pierre Kawak**. “Molecular Simulations and Machine Learning for Sustainable Polymer Innovation”. Southeast Polymer Forum. University of Georgia, Athens. Athens, GA, 2025.
  - [27] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Exploring the Role of Polymer-Filler Interactions in Modulating Elastomeric Reinforcement”. Global Physics Summit. American Physical Society. Anaheim, CA, 2025.
  - [26] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Tuning Polymer-Filler Interactions to Modulate Elastomeric Reinforcement”. Rubber Division Spring Technical Meeting. American Chemical Society. Lake Buena Vista, FL, 2025.
  - [25] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Tuning Reinforcement, Void Formation, and Fracture in Elastomeric Nanocomposites: Toward High-Performance, Sustainable Tire Materials”. Chemical, Biological, & Materials Engineering Department Seminar. University of South Florida. Tampa, FL, 2025.
  - [24] **Pierre Kawak**. “Molecular Simulations for Greener Polymers: From Theory to Reality”. Annual Meeting. American Institute of Chemical Engineers. San Diego, CA, 2024.
  - [23] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Contrasting Reinforcement Mechanisms in Elastomeric Nanocomposites”. Annual Meeting. American Institute of Chemical Engineers. San Diego, CA, 2024.
  - [22] **Pierre Kawak**. “Filler-Filler Contacts Reinforce Filled Elastomers at High Strains”. GRC Polymer Physics. Gordon Research Conferences. South Hadley, MA, 2024.
  - [21] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Filler-Filler Contacts Reinforce Filled Elastomers at High Strains”. Annual Postdoctoral Research Symposium. University of South Florida. Tampa, FL, 2024.
  - [20] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. “Polymer-Filler Competition-Driven Reinforcement Beyond the Payne Effect in Elastomeric Nanocomposites”. March Meeting. American Physical Society. Minneapolis, MN, 2024.
  - [19] Harshad Bhapkar, **Pierre Kawak**, and David S. Simmons. “Exploring the Effects of Nanoparticle Loading, Dispersion and Structure on the Stress Response of Elastomeric Nanocomposites”. March Meeting. American Physical Society. Minneapolis, MN, 2024.
  - [18] **Pierre Kawak**, David S. Simmons, and Douglas R. Tree. “Rational Sustainable Polymer Materials Design Using Multiscale Simulation and Theory”. Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.
  - [17] **Pierre Kawak**, Makayla Branham, William F. Drayer, and David S. Simmons. “Tuning Polymer Dynamics Via Sequence Control”. Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.

- [16] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Elucidating the Molecular Origins of Reinforcement in Filled Elastomers Via Spatial- and Species-Resolved Stresses from Molecular Dynamics Simulations". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.
- [15] Harshad Bhapkar, **Pierre Kawak**, and David S. Simmons. "Insights into the Dependence of Elastomeric Nanocomposite Mechanics on Nanoparticulate Properties". Annual Meeting. American Institute of Chemical Engineers. Orlando, FL, 2023.
- [14] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Dissecting the Payne Effect: How Filler-Polymer Competition Reinforces Elastomeric Nanocomposites". IOP Polymer Physics Group Graduate Symposium. Institute of Physics. Virtual, 2023.
- [13] **Pierre Kawak**. "Career Paths in Physics". Physics Colloquia Series. University of South Florida Department of Physics. Tampa, FL, 2023.
- [12] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Exploring Mechanisms of Enhanced Dissipation in Nanoparticle-filled Rubber Using Molecular Dynamics". Annual Postdoctoral Research Symposium. University of South Florida. Tampa, FL, 2023.
- [11] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Exploring mechanisms of enhanced dissipation in nanoparticle-filled rubber using molecular dynamics". March Meeting. American Physical Society. Las Vegas, NV, 2023.
- [10] Douglas R. Tree and **Pierre Kawak**. "Free Energy Analysis of Crystal Nucleation of Semiflexible Polymers". March Meeting. American Physical Society. Las Vegas, NV, 2023.
- [9] **Pierre Kawak**, Harshad Bhapkar, and David S. Simmons. "Spatially resolving energy dissipation in molecular dynamics of polymer nanocomposites". March Meeting. American Physical Society. Las Vegas, NV, 2023.
- [8] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Acute Sensitivity of Polymer Crystallization Phase Behavior to Intermolecular Interactions". Annual Meeting. American Institute of Chemical Engineers. Phoenix, AZ, 2022.
- [7] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Free Energy Analysis of Polymer Crystal Nucleation Indicates Cooperative Crystallization and Nematic Alignment". March Meeting. American Physical Society. Chicago, IL, 2022.
- [6] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "Free Energy Surfaces for Homogeneous Nucleation in a Polymer Melt". Annual Meeting. American Institute of Chemical Engineers. Boston, MA, 2021.
- [5] **Pierre Kawak**, Dakota S. Banks, and Douglas R. Tree. "GPU-accelerated Wang-Landau Simulation of Polymer Crystallization". March Meeting. American Physical Society. Virtual, 2021.
- [4] **Pierre Kawak**, Andrew S. Gibson, Logan S. Brown, Beverly Delgado, Douglas R. Tree, and Dakota S. Banks. "Investigating Primary Nucleation in Polymer Melts using GPU-Accelerated Wang-Landau Simulations". Annual Meeting. American Institute of Chemical Engineers. Virtual, 2020.
- [3] **Pierre Kawak**, Andrew S. Gibson, Logan S. Brown, Beverly Delgado, and Douglas R. Tree. "Wang-Landau Simulation of the Free Energy Surface of Crystallization in a Polymer Melt". March Meeting. American Physical Society. Virtual, 2020.
- [2] **Pierre Kawak**, Vinod Paul, Paul Kawak, Rita Kassermally, Fatme Lahib, Rute F. Vitor, Mohammad Al-Sayah, and Ghaleb A. Hussein. "Doxorubicin-Encapsulated, Estrone-Appended Liposomes Triggered by Ultrasound for the Treatment of Breast Cancer". Graduate Students Research Conference. UAE Ministry of Education. Khalifa University, Abu Dhabi, UAE, 2017.

- [1] **Pierre Kawak**, Christian C. Momah, Mohamed A. Elkhodiry, Shaima R. Suwaidi, Dina Gadalla, Fatehia M. Banamah, Rute F. Vitor and Hesham G. Moussa, Ana M. Martins and Mohammad Al-Sayah, and Ghaleb A. Hussein. "A Peptide-Targeted Nanodelivery System Triggered by Ultrasound for Anti-cancer Therapy". Life Sciences Grand Challenges Conference. Institute of Engineering and Electronics Engineering. Khalifa University, Abu Dhabi, UAE, 2016.

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