Polymer Physics Meets Machine Learning: A Synergistic Approach to Complex Polymer Design

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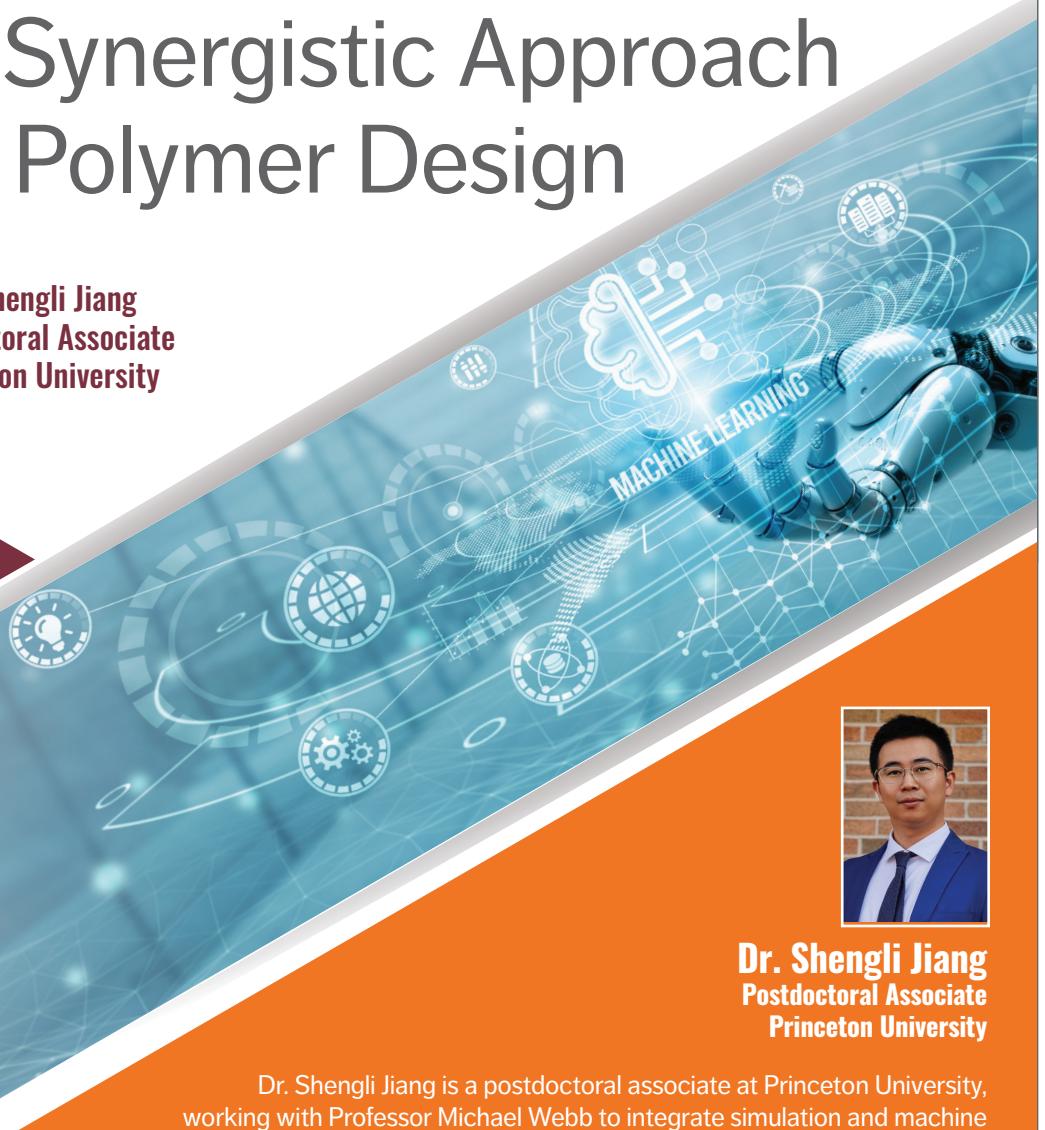
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Dr. Shengli Jiang is a postdoctoral associate at Princeton University, working with Professor Michael Webb to integrate simulation and machine learning for polymer design. He received his Ph.D. in Chemical Engineering from the University of Wisconsin-Madison under the supervision of Professor Victor Zavala, focusing on machine learning applications in sensor design, solvent systems, electrochemistry, and sustainability. He earned his B.S. in Chemical Engineering from the University of California, San Diego, where he worked with Professor Zheng Chen on lithium-ion battery cathode design. He was also a Givens Associate at Argonne National Laboratory, working on neural architecture search and uncertainty quantification, and an intern at Dow on electricity price forecasting and language models.

Polymers exhibit rich and tunable properties governed by their topological, compositional, and chemical complexity. However, navigating this vast design space to identify optimal materials remains a grand challenge. While artificial intelligence and machine learning have significantly advanced materials design, their application to polymers has been largely restricted to simpler systems, particularly linear polymers. Furthermore, the limited availability and heterogeneous nature of the requisite data continue to pose ongoing challenges for these computational methods.

In this talk, I will outline our recent efforts that combine simulation, machine learning, and polymer physics to navigate complex design spaces and reveal structure-function relationships. First, I will demonstrate how generative machine learning models can address combinatorial challenges in designing chain architectures with targeted conformational properties. Building on this, I will describe a physics-guided closed-loop learning approach that directs simulations for designing viscosity-modifying polymers under shear flow. Finally, I will present our work on embedding polymer physics directly into machine learning architectures to improve model transferability and reduce data dependence in copolymer property prediction.