



HOWARD
UNIVERSITY

HowU Connect ChEminar Series

HOSTED BY THE DEPARTMENT OF
CHEMICAL ENGINEERING

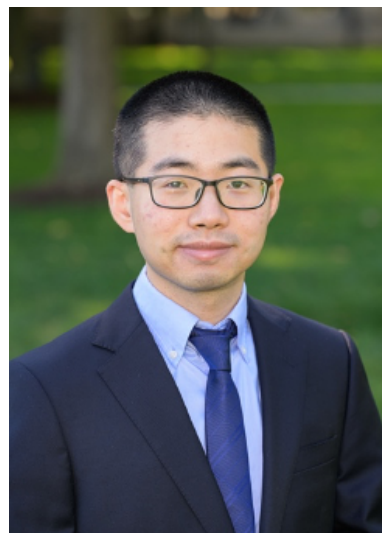
AI for Macromolecular Engineering: Interpretable Similarity Learning and Sequence-Aware Prediction

WITH **Dr. Jiale Shi**

Assistant Professor, The University of Toledo

Bio:

Dr. Jiale Shi is an Assistant Professor in the Department of Chemical Engineering at University of Toledo. His research focuses on AI and graph theory for macromolecular engineering. His group develops interpretable AI methods, graph-based representations, and generative models to understand and design polymers, soft materials, and biomacromolecular systems, with applications in healthcare, sustainability, and energy. Before joining UToledo, he conducted postdoctoral research at Boston University (2025–2026) with Prof. Qiang Cui and at the Massachusetts Institute of Technology (2022–2025) under the mentorship of Prof. Bradley Olsen and Dr. Debra Audus of the National Institute of Standards and Technology (NIST). He received his Ph.D. in Chemical Engineering, with a minor in Computer Science and Engineering, from the University of Notre Dame in 2022 under the supervision of Prof. Jonathan Whitmer. He earned his B.S. in Chemistry from Peking University in 2017.



Abstract:

Macromolecular engineering is central to many problems in chemical engineering, including advanced materials, separations, energy, healthcare, and sustainability. However, polymer design remains challenging because macromolecular systems span enormous chemical spaces, and many complex structure-property relationships remain unknown. These challenges create significant opportunities for AI, but they also demand AI models that are interpretable, scientifically grounded, and capable of going beyond black-box prediction. In this talk, I will present two complementary directions in my research toward interpretable and predictive AI for macromolecular engineering. First, I will discuss interpretable similarity learning for macromolecules. Rather than relying solely on black-box input-output prediction, this work begins with similarity as a physically and chemically meaningful way to compare polymer structures. I will show how similarity can serve as a scientifically meaningful foundation for AI, starting from the definition and computation of macromolecular similarity and extending to graph-neural-network-based acceleration and similarity-based embedding methods. As a related application of graph theory, I will briefly discuss protein allostery, showing how quantitative comparisons of communication networks reveal mutation-induced changes in allosteric pathways. Second, I will discuss sequence-aware prediction for sequence-defined polymers. In these systems, monomer order can directly influence material properties, which requires AI models that explicitly represent sequence information. I will present language-model-based approaches that learn sequence-aware representations and improve both property prediction and conditional generative design for sequence-defined macromolecules. Together, these efforts aim to develop AI methods for chemical engineering that are both scientifically grounded and effective for complex macromolecular systems.

WHERE

Microsoft Teams

<https://teams.microsoft.com/join/222986309901355?p=q2GEx90rLXBD8EkrE2>

Meeting ID: 222 986 309 901 355
Passcode: Fb25Ri7j

WHEN

Monday, Oct. 19th, 2026

1 – 2 pm

FOR MORE INFORMATION:

Dr. Cristiano Reis

cristiano.reis@howard.edu

Dr. Patrick Ymele-Leki

patrick.ymeleleki@howard.edu

<https://che.howard.edu/>



The mission of the Department of Chemical Engineering at Howard University is to produce outstanding chemical engineering graduates prepared to become technological, managerial and public service leaders with a keen sense of ethical and social responsibility, grounded in a holistic appreciation of technology. The faculty and staff are committed to providing a learning environment that instills creative and critical thinking, a solid technical foundation, competence and facility in information technology use, and a sensitivity to environmental and safety issues.

