Translational AI Center (TrAC) Seminar Spring 2025

Ying Li

February 25th at 1:00 PM (US Central Time)

Location and zoom link: https://trac-ai.iastate.edu/event/trac-seminar-series-ying-li/

Machine Learning-accelerated Molecular Design Of Innovative Polymers: Shifting from Thomas Edison to Iron Man

Abstract

Polymeric materials are key enablers in aerospace, mechanical, civil, and environmental engineering, such as reverse osmosis membranes for water treatment and desalination, coatings for building skins, and antifouling materials, etc. Nevertheless, the design and development of innovative polymers have been an experimental-driven and trial-and-error process guided by experience, intuition, and conceptual insights. This Edisonian approach is often costly, slow, biased towards certain chemical space domains, and limited to relatively small-scale studies, which may easily miss promising compounds. A grand challenge in designing these polymeric materials is the vast design space on the order of 10100, defined by the almost infinite combinations of chemical elements, molecular structures, and synthesis conditions. To tackle this challenge, I will present our recent works on developing a data-driven molecular simulation strategy that can efficiently discover and design novel polymers with unprecedented yet predictable combinations of properties. Specifically, we use machine-learning techniques to build a meaningful chemistry-property relation for polymeric materials. Then, we utilize generative adversarial networks, combined with Reinforcement Learning models, for the inverse molecular design of innovative polymers. Eventually, we apply the experimentally validated molecular dynamics simulations to verify these molecular designs. We expect this work can address a wide range of scientific questions in computational materials design and synthesis-structure-property relationships for polymeric materials. It will also benefit the broader scientific community and industry, which are interested in developing new types of polymers for medical, automotive, packaging, building and construction applications.

Short Bio

Dr. Li joined the University of Wisconsin-Madison in August 2022 as an Associate Professor of Mechanical Engineering. From 2015 to 2022, he was an Assistant Professor of Mechanical Engineering at the University of Connecticut and was promoted to Associate Professor. He received his Ph.D. in 2015 from Northwestern University, focusing on the multiscale modeling of soft matter and related biomedical applications. His current research interests are: multiscale modeling, computational materials design, mechanics and physics of polymers, and machine learning-accelerated polymer design. Dr. Li's achievements in research have been widely recognized by fellowships and awards, including ACS Polymeric Material Science and Engineering (PMSE) Young Investigator Award (2023), NSF CAREER Award (2021), Air Force's Young Investigator Award (2020), 3M Non-Tenured Faculty Award (2020), and multiple best paper awards from major conferences. He has authored and co-authored more than 150 peer-reviewed journal articles, including Nature Energy, Science Advances, Nature Communications, Physical Review Letters, etc. Dr. Li's lab is supported by multi-million-dollar grants and contracts from NSF, AFOSR, AFRL, ONR, DOE/National Nuclear Security Administration, DOE/National Alliance for Water Innovation, and industries.

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