

Translational AI Center (TrAC) Seminar

Fall 2025

Wenjie Xia

October 28th at 1:00 PM (US Central Time)

Location and zoom link: <https://trac-ai.iastate.edu/event/trac-seminar-hybrid-wenjie-xia/>

Multiscale Modeling and Machine Learning-Enabled Materials by Design for Functional Polymers

Abstract

Multifunctional polymeric materials, such as semiconductive polymers, crosslinked network, and thin film membranes, are driving innovation across optoelectronics, energy storage, structural and functional coatings. This presentation highlights recent advances from our group that leverage insights from modeling and computation to reveal the optoelectronic, structural, interfacial, and thermomechanical characteristics of these advanced materials. To accelerate the discovery and design of next-generation polymers, we introduce a data-driven, high-throughput modeling framework that integrates multiscale simulations with AI/ML to enhance the design of those polymeric materials, focusing on critical features such as glass-transition temperature, microstructures, and interfacial characteristics. Through the integration of modeling, AI/ML, and experiments, we uncover the molecular mechanisms underlying the multifunctional performance of these polymers, offering a roadmap for the modeling-driven design of high-performance multifunctional materials.

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Short Bio

Dr. Wenjie Xia is currently an Associate Professor in the Department of Aerospace Engineering at Iowa State University. He received his Ph.D. from Northwestern University in 2016, followed by his postdoc training at National Institute of Standards and Technology. His research focuses on the computational design and modeling of multifunctional materials, and he has authored over 120 peer-reviewed papers in leading journals such as Advanced Materials, Matter, Science Advances, Nano Letters, and ACS Nano. His research has been supported by NSF, ONR, ARO, DOE, NIST, and NASA. He is the recipient of several prestigious awards, including the NSF CAREER Award, ASME Rising Star of Mechanical Engineering, ACS PMSE Young Investigator Award, and Materials Genome Initiative (MGI) Fellowship. His contribution has been recognized by NIST through the NIST-MML Accolade for Technical Excellence "for leading the development of a new multiscale modeling approach for glass-forming polymer materials".

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