



CASE SCHOOL  
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UNIVERSITY

Department of Civil and Environmental Engineering  
Case Western Reserve University  
Bingham Bldg, Room 208  
10900 Euclid Ave  
Cleveland, OH 44106

## Civil and Environmental Engineering Department Seminar

### Multiscale Modeling of Nanoconfinement and Interfaces in Polymeric Structural Materials

**Wenjie Xia**, BS11 (CWRU)

Assistant Professor of Civil and Environmental Engineering, North Dakota State University

*Date:* Wednesday October 7, 2020, 10:30-11:30 PM

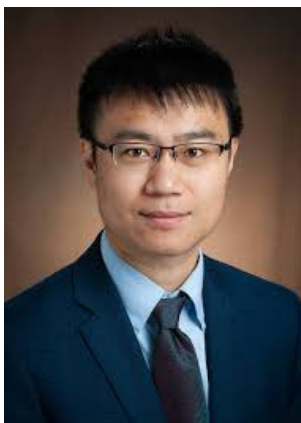
*Zoom Meeting ID:* 913 9974 3238 *Passcode:* 576579

<https://cwru.zoom.us/j/91399743238?pwd=QlVTVWJFVUFGZDVON2ZMVmZleFlxdz09>

#### Abstract

Natural and engineered load-bearing polymers and composites often achieve remarkable mechanical performance by confining their microphases in smaller dimensions. However, understanding and predicting their thermomechanical behaviors are inherently challenging due to their complex hierarchical microstructures and interfaces within the systems. In this presentation, I will present a multi-scale modeling paradigm for understanding these complex phenomena occurring in nanocomposite materials. I will first present scale-bridging computational techniques for simulating complex materials such as polymers and 2D materials at extended time and length scales. Following this, I will discuss cases where the coupling between nanoconfinement and interface leads to intriguing phenomena in polymers materials. Using multiscale modeling, in conjunction with machine learning, I will illustrate how understanding interfaces can help us design better load-bearing composites using renewable materials, such as nanocellulose.

#### About the speaker:



Dr. Wenjie Xia is currently an Assistant Professor in the Department of Civil and Environmental Engineering at NDSU. He obtained his Ph.D. in Civil & Environmental Engineering from Northwestern University (2016) and his B.S. in Civil Engineering from CASE (2011). Prior to joining NDSU in 2018, he was an MGI (Materials Genome Initiative) Postdoctoral Fellow at the National Institute of Standards and Technology (NIST). His research focuses on computational design of complex materials via multiscale modeling. He has published 38 peer-review journal publications in computational and nanoscale science, including Science Advances, ACS Nano, Nano Letters, and Macromolecules. He has received several honors and awards, including the NIST-MML Accolade for Technical Excellence (2019), the finalist for the APS Padden Award (2016), and the Chinese Government Award for outstanding students abroad (2015).