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Molecular computation for bioengineering

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Abstract

The rapid development of high-performance computing has enabled unprecedented advances in the mechanistic understanding of molecular biomaterials. We direct the power of our “computational microscope” to investigate complex biological molecular systems, to understand when and how these systems function in health and break down in disease. We also develop computational methods for the multiscale and data-driven characterization and design of novel functional biomaterials from the nanoscale, for medical and engineering applications, drawing inspiration from natural design principles. I will present recent work that combines multiscale modeling and big data frameworks to probe and predict behavior of complex biomolecular systems.

Biography

Dr. Anna Tarakanova is Assistant Professor in the Department of Mechanical Engineering and Biomedical Engineering at the University of Connecticut. Her research focuses on advancing molecular, multiscale and data-driven modeling methods to study the structure, function and mechanics of complex nanoscale biological materials. These tools provide the foundation to ask essential questions about the behavior of tissues such as arterial elastic tissue and bone, and to repurpose molecules for new functions like improved immunogenicity, thermal stability or resilience in aging. In particular, her work aims to characterize extracellular matrix proteins including elastin, collagen and fibrillin, and their role in the context of aging and human disease. She received her BS from Cornell University, and her MS and PhD from the Massachusetts Institute of Technology. Dr. Tarakanova is a recipient of the NSF Career Award.