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Tailoring Molecular Topology to Control the Mechanical Properties of Polymeric and Nanoparticle Networks



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ABSTRACT:

In this talk, I will summarize recent advances in computational design of new macromolecular materials that make use of nanoscale topologies, such as brushes, networks, and folded loops, that result in exceptional mechanical properties. I will first present physics-based and data-driven reduced order modeling approaches that were developed to describe molecular and mesoscale mechanics of polymers and polymer-grafted nanoparticle systems. Following this, I will present strategies for achieving higher strength, toughness, and impact tolerance in soft materials. The first strategy involves the use of star polymers, crosslinked network topologies or polymer grafted nanoparticles to improve diametric mechanical properties such as modulus and toughness, while also controlling the time-dependent characteristics of the response. The second strategy involves creating nanoparticle interfaces with looped tethers that take inspiration from catch bonds in biological adhesion proteins, which results in molecular seat-belt type interfaces that self-strengthen at high strain rates like shear-thickening fluids. I will conclude with some thoughts on how to translate these findings to new material concepts that could be explored further with synergistic experiments and simulations.

BIOGRAPHY:

Sinan Keten is the June and Donald Brewer Professor of Civil & Environmental Engineering and Mechanical Engineering at Northwestern University. He joined Northwestern University faculty in 2010 after obtaining his Ph.D. from MIT. His research expertise is on computational materials design and mechanics with an emphasis on soft matter, and he has co-authored over a hundred journal articles in this area. Prof. Keten has received a number of honors including the Presidential Early Career Award for Scientists and Engineers (PECASE), Office of Naval Research (ONR) Young Investigator Program (YIP) Award, Society of Engineering Science Young Investigator Medal, ASME Sia Nemat Nasser Award, ASME Thomas J. R. Hughes Young Investigator Award, and ASCE Huber Prize. He is a Fellow of the American Physical Society and serves as an Associate Editor for the Journal of Applied Mechanics and npj Computational Materials.