

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Bioinspired Nanocellulose Based Hybrid Materials With Novel Interfacial Properties SINAN KETEN, Northwestern University — This talk will overview a simulation-based approach to enhancing the mechanical properties of nanocomposites by utilizing cellulose – the most abundant and renewable structural biopolymer found on our planet. Cellulose nanocrystals (CNCs) exhibit outstanding mechanical properties exceeding that of Kevlar, serving as reinforcing domains in nature’s toughest hierarchical nanocomposites such as wood. Yet, weak interfaces at the surfaces of CNCs have so far made it impossible to scale these inherent properties to macroscopic systems. In this work, I will discuss how surface functionalization of CNCs influences their properties in their self-assembled films and nanocomposites with engineered polymer matrices (Xin et al. Nano Letters, 2015, Fox et al. Applied Materials and Interfaces, 2016). Specifically, the role of ion exchange based surface modifications and polymer conjugation will be discussed, where atomistic and coarse-grained simulations will reveal new insights into how superior mechanical properties can potentially be attained by hybrid constructs.

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Date submitted: 20 Oct 2016

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