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# Optimizing the mechanical properties of cellulose nanopaper through surface energy and critical length scale considerations.

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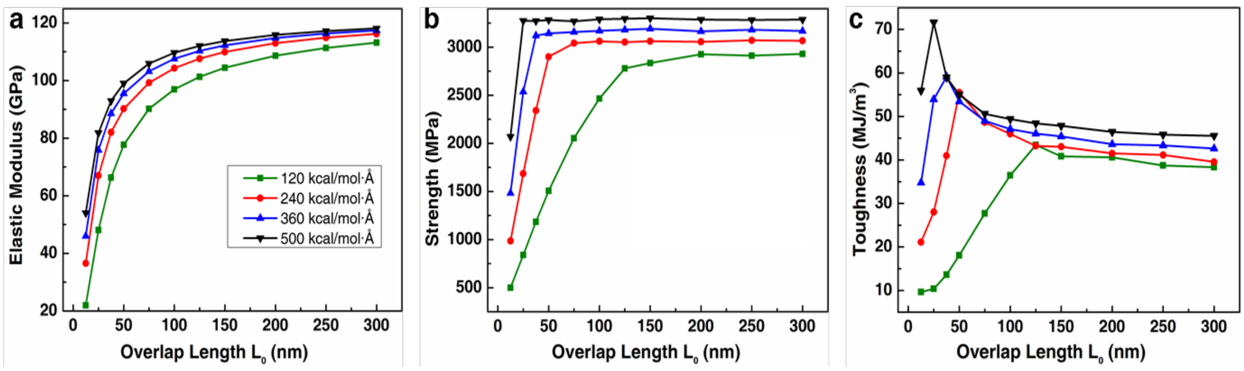


***Caption:*** Dependence of CNC nanopaper mechanical properties on the overlap length and interfacial properties for: an elastic modulus, b strength, and c toughness, where 240 kcal/mol·Å case corresponds to native CNC nanopaper.

## Scientific Achievement

We address the challenge to link macroscale properties of cellulose nanopaper and thin films to the nanoscale properties of constituent CNCs and their structural arrangements by establishing an atomistically informed coarse-grained model for CNCs. We carried out mesoscale simulations to extract mechanical properties including elastic modulus, strength, and toughness. We showed that the modulus and strength of the nacre-inspired nanopaper with brick-and-mortar structures increase with increasing overlap length and saturate at critical length scales which is dominated by the failure mechanisms transitioning from CNC sliding to fibril fracture, and maximum toughness is reached when the interface and CNC failure occur concurrently. These mechanical properties can be further tuned with surface modifications of individual CNCs readily for desired nanopaper performance.

## Significance

With our established CG model for CNCs, the mechanical properties of cellulose nanomaterials with bioinspired structures can be efficiently and accurately studied. Our model generates broadly applicable insights into factors governing the performance of self-assembling thin film materials made from 1D nanostructures

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