Abstract Submitted
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The Effect of Water Molecules on Mechanical Properties of Bamboo Microfibrils[1] NIMA RAHBAR, Worcester Polytechnic Institute — Bamboo fibers have higher strength-to-weight ratios than steel and concrete. The unique properties of bamboo fibers come from their natural composite structures that comprise mainly cellulose nanofibrils in a matrix of intertwined hemicellulose and lignin called lignin-carbohydrate complex (LCC). Here, we have utilized atomistic simulations to investigate the mechanical properties and mechanisms of interactions between these materials, in the presence of water molecules. Our results suggest that hemicellulose exhibits better mechanical properties and lignin shows greater tendency to adhere to cellulose nanofibrils. Consequently, the role of hemicellulose found to be enhancing the mechanical properties and lignin found to be providing the strength of bamboo fibers. The abundance of Hbonds in hemicellulose chains is responsible for improving the mechanical behavior of LCC. The strong van der Waals forces between lignin molecules and cellulose nanofibrils is responsible for higher adhesion energy between LCC/cellulose nanofibrils. We also found out that the amorphous regions of cellulose nanofibrils is the weakest interface in bamboo Microfibrils. In presence of water, the elastic modulus of lignin increases at low water content (less than 10

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