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Water adsorption on surface-modified cellulose nanocrystals ZONGHUI WEI, ROBERT SINKO, SINAN KETEN, ERIK LUIJTEN, Northwestern Univ — Cellulose nanocrystals (CNCs) have attracted much attention as a filler phase for polymer nanocomposites due to their impressive mechanical properties, low cost, and environmental sustainability. Despite their promise for this application, there are still numerous obstacles that prevent optimal performance of CNC–polymer nanocomposites, such as poor filler dispersion and high levels of water absorption. One way to mitigate these negative effects is to modify CNC surfaces. Computational approaches can be utilized to obtain direct insight into the properties of modified CNC surfaces and probe the interactions of CNCs with other materials to facilitate the experimental design of nanocomposites. We use atomistic grand-canonical Monte Carlo simulations to study how surface modification of ion-exchanged sulfated cellulose nanocrystals (Na-CNCs) impacts water adsorption. We find that methyl(triphenyl)phosphonium-exchanged CNCs adsorb less water than Na-CNCs at the same relative humidity, supporting recent experimental dynamic vapor sorption measurements. By characterizing the distribution and configuration of water molecules near the modified CNC surfaces we determine how surface modifications disrupt CNC–water interactions.

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