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The stability of cellulose TONGYE SHEN, S. GNANAKARAN, T-Division, LANL — Stabilities and dynamics of known forms of crystalline cellulose (an ordered assembly of beta-glucose polysaccharide chains) are dominated by hydrogen bonding (HB) interactions. A detailed understanding on how HB interactions contribute to overall thermostability of crystalline cellulose is essential for efficient enzymatic degradation of cellulosic structures and the eventual conversion to ethanol. We construct a statistical mechanical model of cellulose at the resolution of explicit HB networks. This model takes into account the essential physical interaction in terms of both intramolecular bonding between neighboring glucose units within a chain and intermolecular bonding between different cellulose chains. These calculations reveal stabilities of HB networks under various conditions, and the microscopic details (at the resolution of individual bonds) of breaking of HB network that leads to instability. By combining these observations with all-atom replica exchange dynamics simulations of short cellulose chains, we are able to capture the local disorder and amorphous nature of crystalline cellulose where the directionality of HB interactions play a critical role.

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