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Theoretical Investigation of Hydrogen Bonding Networks in Cellulose Iα and Iβ XIANGHONG QIAN, Department of Mechanical Engineering, Colorado State University — The cellodextrins in native crystalline cellulose Iα and Iβ are unusually stable compared to other polysaccharides, not easily prone to hydrolysis even with chemical or biological catalysts. The stability of crystalline celluloses is most likely due to theirs highly enhanced hydrogen-bonding (HB) networks. We carried out *ab initio* calculations to determine the atomic and conformational structures of native crystalline celluloses Iα and Iβ. The differences in their HB networks will be discussed and compared with available experimental data. A theoretical model based on competition between hydrogen bonding energy and electronic energy was constructed to explain the size of native crystalline celluloses.

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