Simulations of coarse-grained cellulose 1-beta

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We have built a coarse-grained model of cellulose 1-beta where each beta-D-glucose molecule was represented by eight beads, allowing approximately three-fold reduction in the number of particles. The bonded interactions were derived from atomistic trajectories of single glucose chains using Boltzmann statistics. The non-bonded interactions were derived using the least squares force-matching scheme. Water molecules were modeled as single beads. We have applied the model to study the mechanical properties of crystalline cellulose 1-beta in water. We are particularly interested in studying the twisting and possible bending of long crystalline cellulose fibrils.