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Title: Block co-polymer self-assembly: A Coarse-grain model for natural cellulose fibrils

Name: Srinivas, Goundla

Affiliation: Oak Ridge National Lab

Understanding biomass structure and dynamics on a range of time and length scales is important for the development of cellulosic biofuels. In an effort to extend length and timescale of biomass simulations, we develop a coarse grain (CG) model for molecular dynamics (MD) simulations of cellulose fibrils in implicit and explicit water environments based on fully target observables from fully atomistic simulations. The present constraint-free CG model is used to generate a series of non-crystalline fibril structures with the help of a coupling parameter between fully crystalline and fully amorphous potentials. Simulations show that in water the transition between crystalline and amorphous states occur at larger values of ? (transition parameter) compared to solvent-free case, revealing that the presence of solvent-presence favors crystalline state. The present method provides an accurate and constraint-free approach to derive CG models for cellulose in water with a wide range of crystallinity, suitable for incorporation into large-scale models of lignocellulosic biomass.