

Abstract Submitted
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Thermodynamic description of cellulose chain collapse using coarse grain modeling RITANKAR DAS, JHHH-WEI CHU, UC Berkeley — Biomass contains abundant amounts of cellulose as crystalline microfibrils. A limiting step to using cellulose as an alternative energy source, however, is the hydrolysis of the biomass and subsequent transformation into fuels. Cellulose is insoluble in most solvents including organic solvents and water, but it is soluble in some ionic liquids like BMIM-Cl. This project aims to find alternative solvents that are less expensive and are more environmentally benign than the ionic liquids. All-atom molecular dynamics simulations were performed on dissociated glucan chains separated by multiple (4-5) solvation shells, in the presence of several novel solvents and solvent mixtures. The solubility of the chains in each solvent was indicated by contacts calculations after the equilibration of the molecular dynamics. It was discovered that pyridine and imidazole acted as the best solvents because their aromatic electronic structure was able to effectively disrupt the inter-sheet interactions among the glucan chains in the axial direction, and because perturbation of the solvent interactions in the presence of glucan chains was minimal.

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