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Title: The Solvation Structures of Cellulose Microfibrils in Ionic Liquids

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The use of ionic liquids for non-derivatized cellulose dissolution promises an alternative method for the thermochemical pretreatment of biomass that may be more efficient and environmentally acceptable than more conventional techniques in aqueous solution. Here, we performed equilibrium MD simulations of a cellulose microfibril in the ionic liquid 1-butyl-3-methylimidazolium chloride (BmimCl) and compared the solute structure and the solute-solvent interactions at the interface with those from corresponding simulations in water. The results indicate a higher occurrence of solvent-exposed orientations of cellulose surface hydroxymethyl groups in BmimCl than in water. Moreover, spatial and radial distribution functions indicate that hydrophilic surfaces are a preferred site of interaction between cellulose and the ionic liquid. In particular, hydroxymethyl groups on the hydrophilic fiber surface adopt a different conformation from their counterparts oriented towards the fiber's core. Furthermore, the glucose units with these solvent-oriented hydroxymethyls are surrounded by the heterocyclic organic cation in a preferred parallel orientation, suggesting a direct and distinct interaction scheme between cellulose and BmimCl.