

Simulation of Water-Mediated Supersaturation of Glucose in Ionic Liquid Using Molecular Dynamics

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The low solubility of glucose in ionic liquids (ILs) has restricted enzymatic synthesis of sugar ester. In order to overcome the solubility limit of glucose in ILs, our group developed water-mediated supersaturation method which involves mixing of an aqueous glucose solution into ILs followed by water removal from the solution. By using water-mediated supersaturation method, significantly increased dissolved glucose concentration in ILs compared to its solubility limit in ILs at 25°C as well as much faster reaction rate were obtained. To identify the mechanisms responsible for these results, molecular dynamics (MD) simulations were carried out. When solvated glucose molecules in two different solvents ([Emim][TfO] and water-mediated supersaturated [Emim][TfO]) were examined with a series of explicit solvent MD simulations, it was found that glucose molecules in [Emim][TfO] strongly interact with each other compared to those in water-mediated supersaturated [Emim][TfO]. It was also observed that water molecules in the shell around glucose in water-mediated supersaturated [Emim][TfO] were most replaced by [TfO]⁻ through strong hydrogen bonding between [TfO]⁻ and glucose.