

### The Effect of Hydrogen Bonding on Glucose Solubility in Water-mediated Ionic Liquids

김호신, 하성호<sup>1</sup>, Rakee Pani<sup>2</sup>, Abhishek Singh<sup>2</sup>, 이원길, Yaroslava G. Yingling<sup>2</sup>, 구윤모\*  
인하대학교; <sup>1</sup>한남대학교; <sup>2</sup>Dept. of Material Science and Engineering, North Carolina State  
University  
(ymkoo@inha.ac.kr\*)

The low solubility of glucose in ionic liquids (ILs) has hindered enzymatic synthesis of sugar ester. The restriction of low solubility of glucose in ILs can be overcome by mixing an aqueous glucose solution into ILs followed by water removal from the solution. The change in molecular interactions in water-mediated [Emim][TfO] system and pure [Emim][TfO] system was explored using all-atoms molecular dynamics simulations. We found that diffusivity of all components in the system ([Emim]<sup>+</sup>, [TfO]<sup>-</sup>, and glucose) in water-mediated [Emim][TfO] tends to be higher than that in pure [Emim][TfO]. Through the hydrogen bonding occupancy statistics and radial distribution function analysis, glucose molecules are found to interact more with water and anion, but less with other glucose molecules in water-mediated [Emim][TfO] as compared to those in pure [Emim][TfO]. Our simulation study shows that water acts as a co-solvent that disrupts glucose-anion and glucose-glucose interactions which consequently increases glucose solubility.