Conversion of Biomass to Fuels and Chemicals

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ABSTRACT

Lignocellulosic biomass is an alternate and renewable source of carbon and it can be used to produce fuels and chemicals without putting any stress on the nutritional needs of world population. However, conversion of biomass is technologically challenging since it is a solid material and needs a solvent for liquid phase catalytic processing, and carbon – oxygen bonds need to be cleaved selectively without breaking carbon – carbon bonds. Acid catalyzed dehydration of sugars to intermediates like 5 – hyroxymethyl furfural (HMF) is one of the key reactions in biomass conversion. Since the economic analysis of the process has shown that the cost of HMF is most sensitive to the cost of fructose, high conversion and selectivity to HMF are desired. Experimental investigations have shown that pH of reaction mixture has a significant effect on the conversion and selectivity. It is believed that pH affects the conversion and selectivity in the reaction of fructose to HMF by altering the local arrangement of water molecules around fructose. The local arrangement of water molecules around the sugar can possibly influence the protonation of fructose, which is the first step in the dehydration reaction. Since the protonation of selected oxygens in fructose only leads to the formation of HMF, the site specificity of protonation can alter the reaction selectivity. In the present work, systems of different hydronium ion concentrations i.e. varying number of HCl molecules in glucose – water mixtures, were simulated using ab initio molecular dynamics to study the changes of fructose solvation in water medium as a function of pH. Simulations were performed using the Car – Parrinello scheme, and the planewave pseudopotential implementation of the Kohn – Sham density functional theory. Molecular dynamic trajectories were analyzed using radial pair distribution functions and spatial distribution functions. Our simulation results showed that the local arrangement of water molecules around selected oxygens of the sugar gets significantly altered as the hydronium ion concentration in the system changes. The change in the intermolecular hydrogen bonding in water due to the presence of hydronium ion also alters the sugar – water interaction. The findings of the present work have helped us better understand the effect of pH on the solvation of fructose in water, which has an effect on its conversion to HMF.