

Theoretical investigate of solvent-dependent performance of glucose isomerization on hydrotalcite

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Glucose is the most abundant species of monosaccharides and is also readily available as main sources of cellulosic biomass such as furandicarboxylic acid. However, the direct use of glucose as a raw material is very difficult because glucose can be easily changed to many kinds of byproducts. In this regard, some researchers reported that the use of glucose can be maximized by isomerization of glucose to fructose using hydrotalcite catalyst. Herein, we propose how to improve performance of highly selective production of fructose using solvents. To investigate the solvent effects on the fructose selectivity, several solvents (e.g. water, GVL, DMF, and butanol) were considered. The initiation and following conversion mechanisms for the isomerization reaction from glucose to fructose were calculated on the basic hydrotalcite surface via density functional theory calculation. Under the butanol solvent condition, the high selectivity in the isomerization of glucose to fructose was achieved. The results showed large yield and high purity of fructose.