

## **Theoretical Insights into Alcohol Solvent Effects on Glucose Transformation Chemistry in Modified UiO-66**

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Solvents can significantly affect the rates and selectivities of acid-catalyzed transformations. Metal-organic frameworks (MOFs) can offer larger pore sizes that can aid in configuring solvent environments to stabilize transition states and promote catalytic transformations. In this work, we examined different pathways over modified UiO-66 for glucose-to-fructose isomerization and the side reaction involving the etherification of glucose with alcohol as well as the influence of different alcohol solvents (methanol and propanol) using density functional theory (DFT) and a cluster-based UiO-66 model. Our studies show that propanol promotes the rate-determining hydride shift step in glucose-to-fructose isomerization more than methanol whereas a lower barrier is seen for the etherification reaction of glucose with methanol than propanol. This is attributed to their different hydrogen-bonding and solvation abilities as well as alkoxide basicities which result in a higher fructose selectivity in propanol solvent. Ongoing investigations involve exploration of other solvents that can selectively drive these transformations as well as understanding their adsorption behavior.