A DFT study of the water effects on the catalytic behavior of acid catalysts for aldol condensation.

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The aldol condensation of furfurals and ketones is important to upgrade the quality of biofuels by extending carbon-carbon length. Acid catalysts have been studied due to the high concentration of carboxylic acids in the reactants, but low activity towards the target product is still a major challenge. The hydroxyl groups on transition metal surface have been shown to enhance activity for aldol condensation, making the enol intermediate in equilibrium with ketones stable through intermolecular hydrogen bonding. Density functional theory (DFT) calculations were used to understand the formation of hydroxyl group on the pristine surface and the effects on the stability of the intermediate using three different acid catalysts (ZnO, ZrO_2, TiO_2). Then, the dopant is incorporated into the surface to adjust the activity of the aldol reaction. Our research will give us insight into the promising catalysts for biofuels.