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Solvent effect in biomass conversions: Catalytic reactions of cresol at the liquid-solid interface[1] YAPING LI, University of Tulsa, ZHIMIN LIU, STEVEN CROSSLEY, University of Oklahoma, FRIEDERIKE JENTOFT, University of Massachusetts Amherst, SANWU WANG, University of Tulsa — Liquid water plays a very important role in biomass conversions. The specific mechanisms for the solvent effect in various catalytic reactions remain elusive, however. We employed first-principles density functional theory and *ab initio* molecular dynamic simulations to explore the mechanism for the catalytic hydrogenation of *o*-cresol at the water/Pt(111) interface. We found that the hydrogen atom of the hydroxyl group of *o*-cresol dissociates into water with a barrier of essentially 0 kJ/mol. We also found that the reaction barriers for the stepwise hydrogenation of *o*-cresol at the water/Pt(111) interface are lower by 10-30 kJ/mol than those on the Pt(111) surface in the absence of water, suggesting that water promotes hydrogenation of *o*-cresol. In addition, we determined the detailed configurations for the transition states. Furthermore, we found that, while 2-methyl-cyclohexanone is an intermediate product when water is absent, the barrier for further hydrogenation of 2-methyl-cyclohexanone is significantly reduced when water is present, indicating that water facilitates the formation of the final product, 2-methyl-cyclohexanonal.

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