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First-principles quantum-mechanical investigations: The role of water in catalytic conversion of furfural on Pd(111)[1] WENHUA XUE, University of Tulsa, MIGUEL GONZALEZ BORJA, DANIEL E. RESASCO, University of Oklahoma, SANWU WANG, University of Tulsa — In the study of catalytic reactions of biomass, furfural conversion over metal catalysts with the presence of water has attracted wide attention. Recent experiments showed that the proportion of alcohol product from catalytic reactions of furfural conversion with palladium in the presence of water is significantly increased, when compared with other solvent including dioxane, decalin, and ethanol. We investigated the microscopic mechanism of the reactions based on first-principles quantum-mechanical calculations. We particularly identified the important role of water and the liquid/solid interface in furfural conversion. Our results provide atomic-scale details for the catalytic reactions.

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