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Ab initio molecular dynamics simulations for the role of hydrogen in catalytic reactions of furfural on Pd(111)[1] WENHUA XUE, HONGLI DANG, YINGDI LIU, Univ of Tulsa, FRIEDERIKE JENTOFT, DANIEL RESASCO, University of Oklahoma, SANWU WANG, Univ of Tulsa — In the study of catalytic reactions of biomass, furfural conversion over metal catalysts with the presence of hydrogen has attracted wide attention. We report *ab initio* molecular dynamics simulations for furfural and hydrogen on the Pd(111) surface at finite temperatures. The simulations demonstrate that the presence of hydrogen is important in promoting furfural conversion. In particular, hydrogen molecules dissociate rapidly on the Pd(111) surface. As a result of such dissociation, atomic hydrogen participates in the reactions with furfural. The simulations also provide detailed information about the possible reactions of hydrogen with furfural.

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