Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Decarboxylation of furfural on Pd(111): Ab initio molecular dynamics simulations[1] WENHUA XUE, HONGLI DANG, DARWIN SHIELDS, YINGDI LIU, The University of Tulsa, FRIEDERIKE JENTOFT, DANIEL RESASCO, The University of Oklahoma, SANWU WANG, The University of Tulsa — Furfural conversion over metal catalysts plays an important role in the studies of biomass-derived feedstocks. We report *ab initio* molecular dynamics simulations for the decarboxylation process of furfural on the palladium surface at finite temperatures. We observed and analyzed the atomic-scale dynamics of furfural on the Pd(111) surface and the fluctuations of the bondlengths between the atoms in furfural. We found that the dominant bonding structure is the parallel structure in which the furfural plane, while slightly distorted, is parallel to the Pd surface. Analysis of the bondlength fluctuations indicates that the C-H bond is the aldehyde group of a furfural molecule is likely to be broken first, while the C=O bond has a tendency to be isolated as CO. Our results show that the reaction of decarbonylation dominates, consistent with the experimental measurements.

[1] Supported by DOE (DE-SC0004600). Simulations and calculations were performed on XSEDE's and NERSC's supercomputers.

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Date submitted: 08 Nov 2012

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