Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles quantum-mechanical investigations of biomass conversion at the liquid-solid interfaces[1] HONGLI DANG, WENHUA XUE, YINGDI LIU, The University of Tulsa, FRIEDERIKE JENTOFT, DANIEL RESASCO, University of Oklahoma, SANWU WANG, The University of Tulsa — We report first-principles density-functional calculations and *ab initio* molecular dynamics (MD) simulations for the reactions involving furfural, which is an important intermediate in biomass conversion, at the catalytic liquid-solid interfaces. The different dynamic processes of furfural at the water-Cu(111) and water-Pd(111) interfaces suggest different catalytic reaction mechanisms for the conversion of furfural. Simulations for the dynamic processes with and without hydrogen demonstrate the importance of the liquid-solid interface as well as the presence of hydrogen in possible catalytic reactions including hydrogenation and decarbonylation of furfural.

[1]Supported by DOE (DE-SC0004600). This research used the supercomputer resources of the XSEDE, the NERSC Center, and the Tandy Supercomputing Center.

Hongli Dang
Univ of Tulsa

Date submitted: 15 Nov 2013 Electronic form version 1.4