

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Atomic-Scale Mechanism for Hydrogenation of *o*-Cresol on Pt Catalysis¹ YAPING LI, University of Tulsa, ZHIMIN LIU, University of Oklahoma, WENHUA XUE, University of Tulsa, STEVEN CROSSLEY, University of Oklahoma, FRIEDERIKE JENTOFT, University of Massachusetts Amherst, SANWU WANG, University of Tulsa — Biofuels derived from lignocellulosic biomass have received significant attention lately due to increasing environmental concerns. With first-principles density-functional theory and *ab initio* molecular dynamic simulations, we investigated the atomic-scale mechanism of *o*-cresol hydrogenation on the Pt(111) surface. The formation of 2-methyl-cyclohexanone (the intermediate product) was found to involve two steps. The first step is the dehydrogenation, that is, the H atom in the hydroxyl group moves to the Pt surface. The second step is the hydrogenation, that is, the H atoms on Pt react with the carbon atoms in the aromatic ring. The first step involves a smaller barrier, suggesting that dehydrogenation occurs first, followed by hydrogenation of the ring. In particular, tautomerization is found to occur via a two-step process over the catalyst. On the other hand, 2-methyl-cyclohexanol (the final product) is produced through two paths. One is direct hydrogenation of the aromatic ring. Another pathway includes partial hydrogenation of the ring, dehydrogenation of -OH group, finally hydrogenation of remaining C atoms and the O atom. Our theoretical results agree well with the experimental observations.

¹Supported by DOE (DE-SC0004600). This research used the supercomputer resources of NERSC, XSEDE, TACC

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Date submitted: 03 Dec 2015

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