Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Galactose adsorption on Ru(0001) MATTI ALATALO, MIKKO PUISTO, Lappeenranta University of Technology — In order to understand the valorisation of biomass, it is essential to study the behavior of sugar molecules on catalytic surfaces. We have studied the adsorption of galactose molecules on the Ru(0001) surface using first principles calculations. We present results for the fully relaxed configurations of the molecule at different adsorption sites. We also compare the effect of the inclusion of the van der Waals interactions on both the energetics of the free galactose molecule and the adsorption energy of galactose on Ru(0001). We compare our results, obtained using periodically repeated supercells, to those obtained with cluster calculations.

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Date submitted: 15 Nov 2013 Electronic form version 1.4