Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Catalytic hydrogenation of cresol: first-principles density-functional calculations and *ab initio* molecular dynamics simulations[1]
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[1]Supported by DOE (DE-SC0004600). This research used the supercomputer resources at NERSC, of XSEDE, at TACC and at the Tandy Supercomputing Center.

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Date submitted: 13 Nov 2014 Electronic form version 1.4