Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Multiscale Modeling of Catalysis and its Application to Hydrogen Production through the Water Gas Shift Reaction on Nanoparticles[1]

ALTAF KARIM, JAMES T. MUCKERMAN, Brookhaven National Lab — We describe a density functional kinetic Monte Carlo approach enabling us to study and simulate the steady-state condition of the water gas shift (WGS) reaction on Cu and Au nano-particles supported on ZnO(0001) surfaces. We have adopted a multiscale modeling paradigm in which density functional theory can be used to determine the behavior of systems at much larger length and time scales by coupling it with kinetic Monte Carlo methods. In the first step, density functional theory is used to obtain the energetics of the relevant atomistic processes of the WGS reaction on Cu and Au nanoparticles. Subsequently, the kinetic Monte Carlo method is employed, which accounts for the spatial distribution, fluctuations, and evolution of chemical species under steady-state conditions. Our simulations show that, in agreement with experiments, the hydrogen production rate strongly depends on size and structure of the nanoparticles.

[1]DOE, Division of Chemical Science, Contract No. DE-AC02-98CH10886 and NERSC computational resources

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Date submitted: 21 Nov 2008 Electronic form version 1.4