Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Bridging the materials gap in catalytic kinetics via first principles coarse-grained kinetic Monte Carlo simulations ALTAF KARIM, DION VLACHOS, University of Delaware — We describe a first principles coarse-grained kinetic Monte Carlo technique enabling us to simulate catalysis under different technologically relevant conditions. By implementing coarse-grained KMC, various simulations are performed efficiently at much larger time and length scales. Using this approach, we studied catalytic oxidation of CO on different metal surfaces. Especially, we tried to understand the role of defects in catalytic kinetics such as steps, kinks, and multiple facets. These studies led us to some interesting results bridging the material gap in catalysis.

Altaf Karim
University of Delaware

Date submitted: 25 Nov 2006 Electronic form version 1.4