Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

**Nanosecond Dynamics in Pt Nanoparticles**[1] F.D. VILA, J.M. MOORE, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195 — Understanding the physical and chemical behavior of supported catalysts is of fundamental and technological importance. However, due to the complex nature of their structure and dynamics at operando temperatures, their nanoscale behavior remains poorly understood. We have shown that DFT/MD calculations provide fundamental insight into the few ps dynamic structure of the nanoparticles, but such methods can be very computationally intensive.[2,3] In order to examine relaxation dynamics in the ns regime here we present finite temperature MD simulations based on a modified Sutton-Chen (SC) model potential, supplemented with Lennard-Jones potentials for the interaction with the support. We find that bulk SC parameters tend to produce nanoparticles with less fluxional dynamics than those in ab initio simulations. To address this issue, we have determined modified SC parameters that capture the DFT dynamics. Nanosecond simulations reveal regimes controlled by internal particle melting and activation of surface mobility. The approach is illustrated for nano-catalysts of Pt/$\gamma$-alumina and compared with ab initio DFT/MD results.

[1]Supported in part by DOE grant DE-FG02-03ER15476 (F.D.V and J.J.R) and by NSF grant PHY-1262811, REU Site: University of Washington Physics (J.M.M.), with computer support from DOE - NERSC.
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Date submitted: 15 Nov 2013 Electronic form version 1.4