Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Dynamic Structural Disorder in Supported Nanoparticles[1] F.D. VILA, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195, S.D. KELLY, S.R. BARE, UOP LLC, Des Plaines, IL 60016 — Supported Pt based nanoclusters are of wide interest in nano-scale physics and have many industrial applications, yet an understanding of their structure is far from complete. Experimental probes such as x-ray absorption spectroscopy (XAS) only yield globally averaged properties, e.g., mean bond distances and mean-square radial disorder (MSRD), which can give a misleading characterization of such complex systems. To obtain a more detailed picture we have carried out finite temperature DFT/MD simulations[2] of Pt and PtSn nanoclusters up to 600 K (*operando* conditions). These show that the nano-scale structure and charge distribution are inhomogeneous and dynamically fluctuating over several time-scales, ranging from fast (200-400 fs) bond vibrations to slow fluxional bond breaking (>10 ps). In particular the anomalous behavior of the MSRD is not static, but rather due to "dynamic structural disorder" (DSD) driven by stochastic motion of the center of mass over 1-4 ps time-scales. In addition the nanoclusters exhibit a semi-melted, Sn-rich surface. These findings show that, and how an improved XAS interpretation of supported nano-scale structure must take into account DSD and other structural inhomogeneities.

[1]Supported by NSF Grant PHY-0835543 with computer support from DOE - NERSC.
[2]F. Vila *et al.*, *UW preprint* (2012).

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Date submitted: 08 Nov 2012 Electronic form version 1.4