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**Dynamic structure in Pt nanoclusters on $\gamma$-alumina**[1] F. VILA, J.J. REHR, J. KAS, Dept. of Physics, U. of Washington, R.G. NUZZO, Dept. of Chemistry, U. of Illinois at Urbana-Champaign, A.I. FRENKEL, Yeshiva U. — Pt nanoclusters on $\gamma$-alumina exhibit a number of unusual phenomena including large structural disorder and bond-length contraction with increasing temperature. We investigate this behavior for a prototypical 10-atom Pt cluster using real-time, temperature-dependent simulations combining density functional theory/molecular dynamics and x-ray spectroscopy theory. We find that the cluster structure is dynamically varying in shape and topology on a time scale long compared with internal vibrations. Moreover, the clusters are not rigidly attached to the surface and occasionally pick up or discard a Pt-O bond. This real-time approach suggests that these nanoclusters are comprised of two distinct populations of Pt atoms depending on the charge transfer from the surface, and reproduces many of their unusual properties.

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