

Abstract Submitted  
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**Structural and charge inhomogeneity in supported Pt clusters<sup>1</sup>**

F.D. VILA, J.J. REHR, U. of Washington, A.I. FRENKEL, Yeshiva U. — Nanoparticle materials are ubiquitous in heterogeneous catalytic processes and there is broad interest in their physical and chemical properties. However, global probes such as XAS and XPS reveal their ensemble properties, missing details of their internal architecture. We have previously shown<sup>2</sup> that a combination of theoretical and experimental techniques is needed to understand the intra-particle heterogeneity of these systems.<sup>3</sup> Recent studies of CO- and H-covered Pt clusters on C and SiO<sub>2</sub> exhibit a variety of spectral and structural trends as a function of temperature. Here we present DFT simulations showing opposite shifts in XES and XAS, as well as bond contraction with increasing temperature both arise from local electronic and structural changes upon desorption. For example, upon single CO adsorption, the Pt-Pt bonds formed by coordinated Pt atoms are locally expanded by 5%, with little change in the rest of the particle. Coordination also has a large effect on the net charge of the Pt atoms, with a net loss of charge upon adsorption. Finally, we show how high coverage inverts the charge distribution in the clusters.

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<sup>2</sup>F.D. Vila *et al.*, Phys. Rev. B **78**, 121404(R) (2008).

<sup>3</sup>J.J. Rehr and F.D. Vila, J. Chem. Phys. **140**, 134701 (2014).

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