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Structure and dynamics of PtSn/γAl$_2$O$_3$[1] F.D. VILA, J.J. REHR, U. of Washington, S.D. KELLY, EXAFS Analysis, S.R. BARE, UOP LLC — Supported metal clusters have many industrial applications, especially in heterogeneous catalysis. Their activity and durability is determined by their internal atomic and electronic structure, as well as by their interaction with the support. We have previously shown[2] that unusual phenomena such as large structural disorder and negative thermal expansion in supported Pt clusters can be understood by using a combination of MD and x-ray absorption spectroscopy simulations. Here we present results for prototypical $Pt_{10}Sn_{10}$ alloy clusters on γAl_2O_3. Our simulations show that the internal structure and surface location of the clusters varies dynamically on a time scale of a few ps. While the Sn atoms are especially mobile, the clusters have well defined Pt-Pt and Pt-Sn coordination shells at $\sim$2.75Å. Moreover, at any instant there are between 2 and 5 bonds between the Pt/Sn and the O atoms in the surface. Finally, we present simulations of the XANES spectra and their relation to charge transfers between atoms in the cluster and between the cluster and the surface.

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[2]F. Vila *et al.*, Phys. Rev. B **78**, 121404(R) (2008).

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