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Effects of γ-Al_2O_3 Support on the Morphology and Electronic Structure of Pt Nanoparticles GHAZAL SHAFAI, SAMPYO HONG, TALAT S. RAHMAN, University of Central Florida — We have studied the effects of pristine and hydroxylated γ-Al_2O_3(110) support on the morphology and electronic structure of clean and H-covered Pt nanoparticles (NP) containing 22 and 44 atoms (Pt_{22} and Pt_{44}) using density functional theory (DFT) based calculations. We find a morphology change from 3 dimensional (3D) to a bi-planar shape for Pt_{22} upon adsorption on pristine and partially hydroxylated γ-Al_2O_3(110) surface. This shape change is not found for higher hydroxylation coverage (0.325 monolayer (ML) and higher) or for Pt_{44}, indicating that the aforementioned effect is size and OH coverage dependent. Furthermore, the relative position of the d-band center of the unoccupied orbitals of the nanoparticles is sensitive to the presence of the support and the extent to which it is hydroxylated. A competing and even dominating effect on the electronic structure of the nanoparticles comes from adsorbed hydrogen. At higher temperatures when the effect of adsorbates is minimal, the shift in the d-band center of the unoccupied orbitals is found to correlate with the extent of metal-support interaction In the light of these results, we conclude that an accurate description of the local environment of nanoparticles (support, hydroxylation of the support, adsorbed hydrogen) is necessary in order to understand the preferred shape and electronic structure of these nanoparticles.

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