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Effects of hydroxylated γ-Al_2O_3 support and H adsorbate on the Geometry and Electronic Structure of Pt Nanoparticles[1] GHAZAL SHAFAI, University of Central Florida, Orlando, FL, 32816, SAMPYO HONG, University of Central Florida, Orlando, FL, 32816, University of North Florida, Jacksonville, FL, 32224, TALAT S. RAHMAN, University of Central Florida, Orlando, FL, 32816 — We have studied the effects of hydroxylated γ-Al_2O_3(110) support and H adsorbate on the geometry and electronic structures of Pt_x (n=22,44) nanoparticles (NP) using DFT. We find that Pt_{22} interacts more strongly with a less hydrated support, while Pt_{44} more with a hydroxylated one. We also find a structural transition of the Pt_{22} (and not Pt_{44}) from a biplanar to a 3D-like shape as a function of hydroxilation. H induces a much larger shift in the unoccupied d-band center than does the support. Also, these shifts are well correlated with metal-support interaction. The increased hydroxylation on γ-Al_2O_3(110) causes weaker metal-support interaction. As a result, the d-band width of a Pt NP decreases causing the center of the unoccupied d band to shift to lower energy (red shift). In the light of these results, we will discuss the features of XANES spectra obtained for γ-Al_2O_3(110) supported Pt nanoparticles [1].

[1] Behafarid et al, Phys. Chem. Chem. Phys. 14, 11766 (2012).

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