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The effect of support on the characteristics of Pt Nanoparticles[1]

GHAZAL SHAFAI ERFANI, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, FL 32816 — We have carried out density functional theory calculations within the projector augmented wave scheme (PAW) and the pseudopotential approach to evaluate the effect of the support (γ-alumina and titania) on geometric and electronic structural properties of Pt22, Pt33, Pt44, Pt55 nanoparticles (NPs) with the shape previously characterized by extended X-ray absorption fine structure spectroscopy (EXAFS) [1]. We are in particular interested in the electronic structural changes of the perimeter atoms, as we expect them to play a major role in catalysis. We find stabilization of the NP on the substrate to depend critically on the existence of oxygen vacancies on the surface and the effect to be more prominent for titania than for alumina. On both substrates the average bond-length (first nearest-neighbor distance) expands (1 to 3%) as compared to that of unsupported NPs. We present results for the charge transfer and local density of states of the atoms at the interface and make comparisons with available experimental data on the propensity of these atoms to be chemically active.

[1] Roldan Cuenya et. al. Phys. Rev. B 84, 245438 (2011).

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