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A DFT study of the effects of preparation conditions on the reactivity of Pt/α-alumina catalysts VALENTINO R. COOPER, ANDREW M. RAPPE, University of Pennsylvania — In this paper, we present a density functional theory study on how the presence of water products on the surface of an α-alumina substrate affects the adsorption of Pt adatoms and dimers on the stoichiometric (Al_T) and oxygen terminated(O_T) surfaces. Studies have shown that the catalytic activity of oxide-supported clusters are sensitive to preparation conditions, with catalysts prepared through the impregnation of alumina with a metal ion solution exhibiting increased rates of reactivity. Here, we demonstrate that changes in the charge distribution at the metal-oxide interface and the partial pressures of water and Pt atoms affect the stability and adsorption sites of Pt adatoms and dimers to the alumina surface. Finally, we show that these differences have a significant effect on the electronic properties of the Pt adsorbates, thereby affecting the interaction of CO and NO at the metal surface.

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