Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

A novel Pd_3O_9@α-Al_2O_3 catalyst under hydroxylated effect: high activity in CO oxidation reaction

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For further investigation of the hy-3Pd@α-Al_2O_3 model, the total electron density and the charge density difference are dominated in Fig 1S. The results show hydroxylation has litter influence on Pd_3O_9 clusters. What's more, Pd, Al and H atoms lose electrons and O atoms get electrons. O-H bond is greatly covalent, while Pd-O and Al-O band is basically electrovalent.

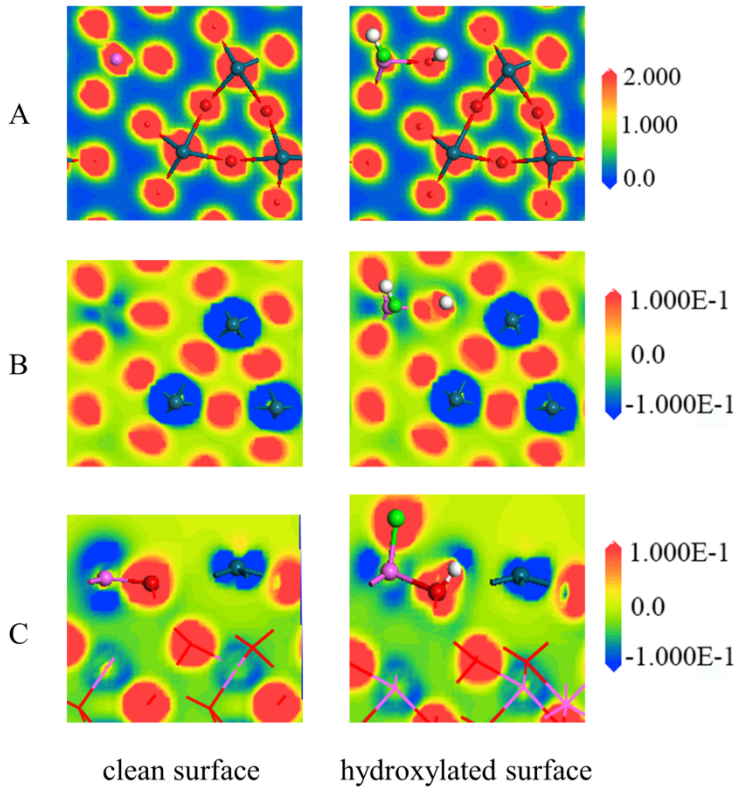

Fig. 1S. The total electron density (A, top view) and the charge density difference (B, top view and C, side view) of hy-Pd_3O_9@α-Al_2O_3 model.

The total density of states (DOS) of a clean α-Al_2O_3(0001) surface, Pd-doped clean and hydroxylated Pd-doped α-Al_2O_3(0001) surface are shown in Fig. 2S, which depicts a clear splitting at the Fermi energy and some states shifting down in energy above the Fermi energy.

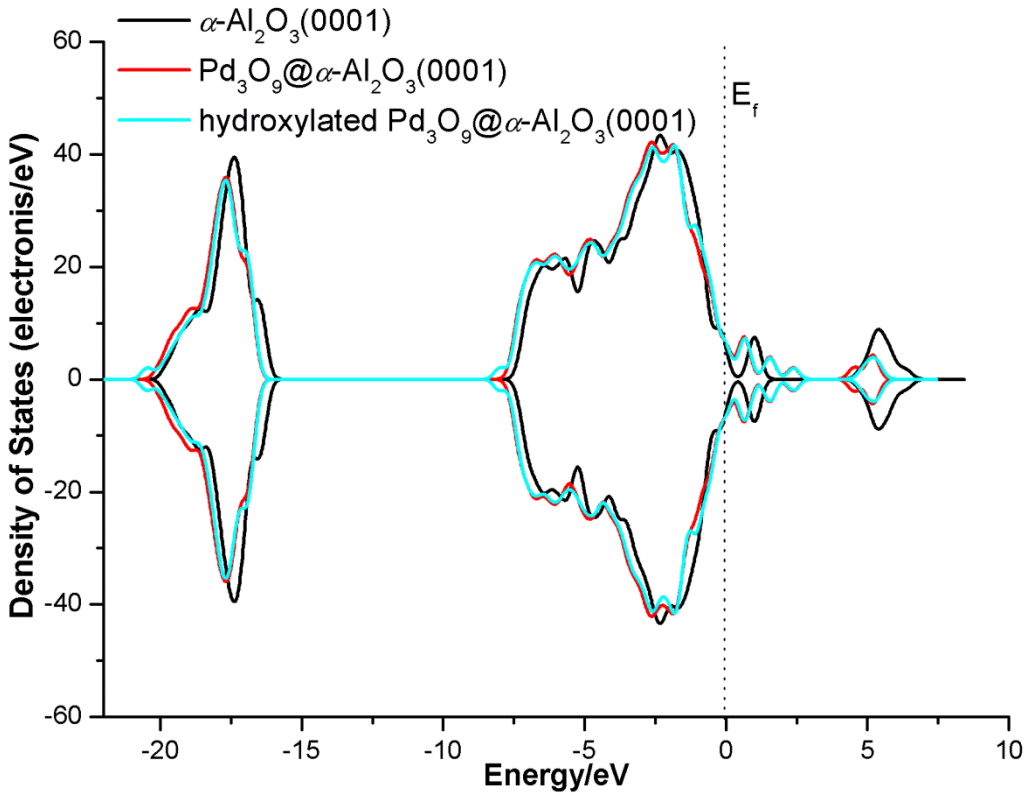

Fig. 2S. A: spin-polarized total density of states (DOS) of the undoped Pd@α-Al_2O_3(0001) and hydroxylated Pd@α-Al_2O_3(0001) surface.