Supplementary Material

A novel Pd$_3$O$_9$@$\alpha$-Al$_2$O$_3$ catalyst under hydroxylated effect: high activity in CO oxidation reaction

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For further investigation of the hy-3Pd@α-Al2O3 model, the total electron density and the charge density difference are dominated in Fig 1S. The results show hydroxylation has litter influence on Pd3O9 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-Pd3O9@α-Al2O3 model.
The total density of states (DOS) of a clean $\alpha$-$\text{Al}_2\text{O}_3$(0001) surface, Pd-doped clean and hydroxylated Pd-doped $\alpha$-$\text{Al}_2\text{O}_3$(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@$\alpha$-$\text{Al}_2\text{O}_3$(0001) and hydroxylated Pd@$\alpha$-$\text{Al}_2\text{O}_3$(0001) surface.