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Supplementary information for

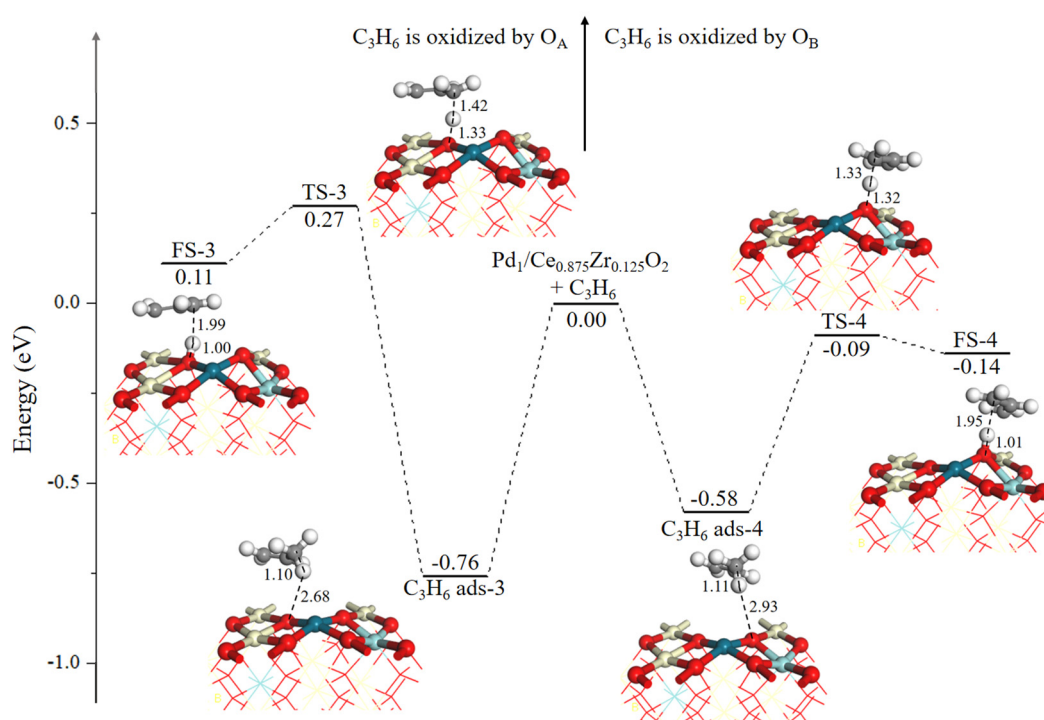
# Carbon Monoxide and Propylene Catalytic Oxidation Activity of Noble Metals (M = Pt, Pd, Ag, and Au) Loaded on the Surface of Ce<sub>0.875</sub>Zr<sub>0.125</sub>O<sub>2</sub> (110)

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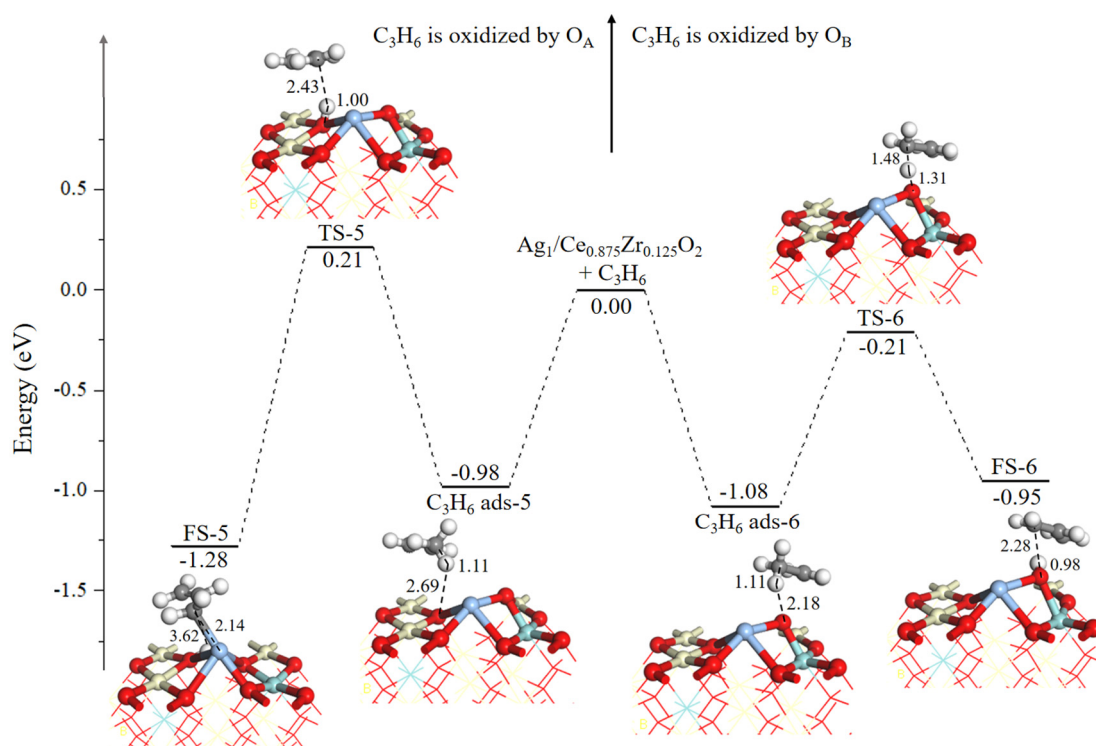
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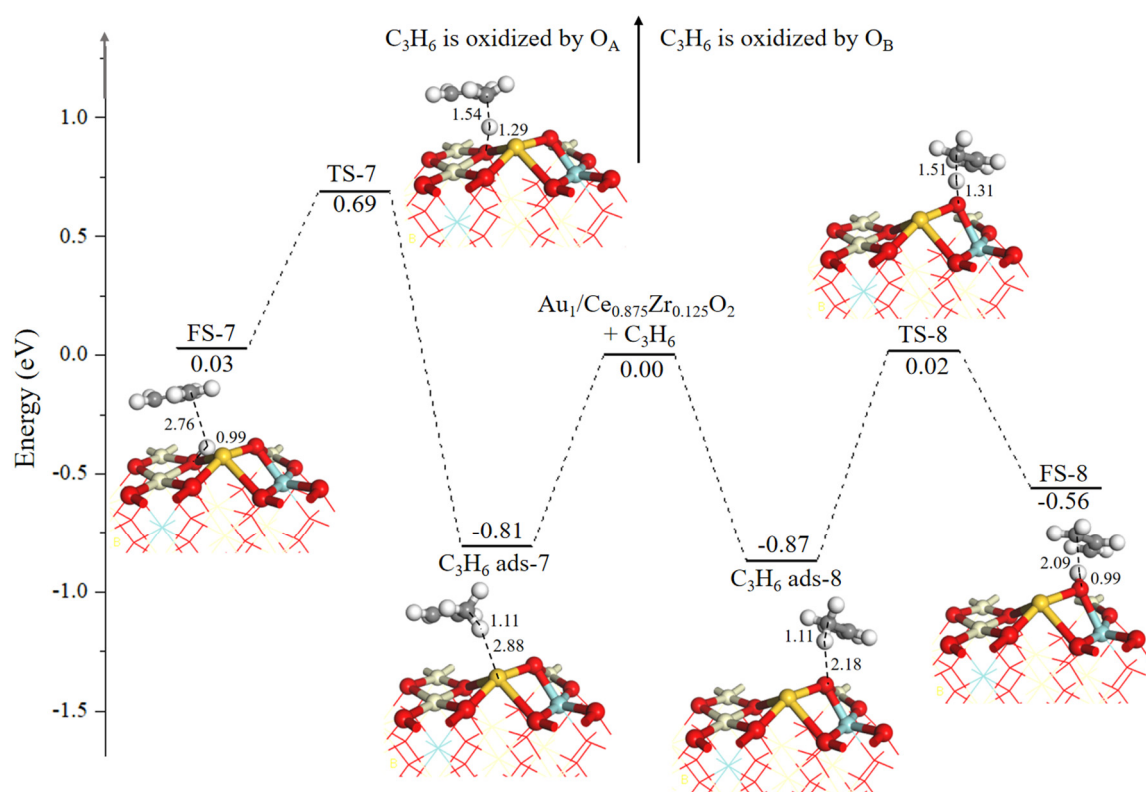
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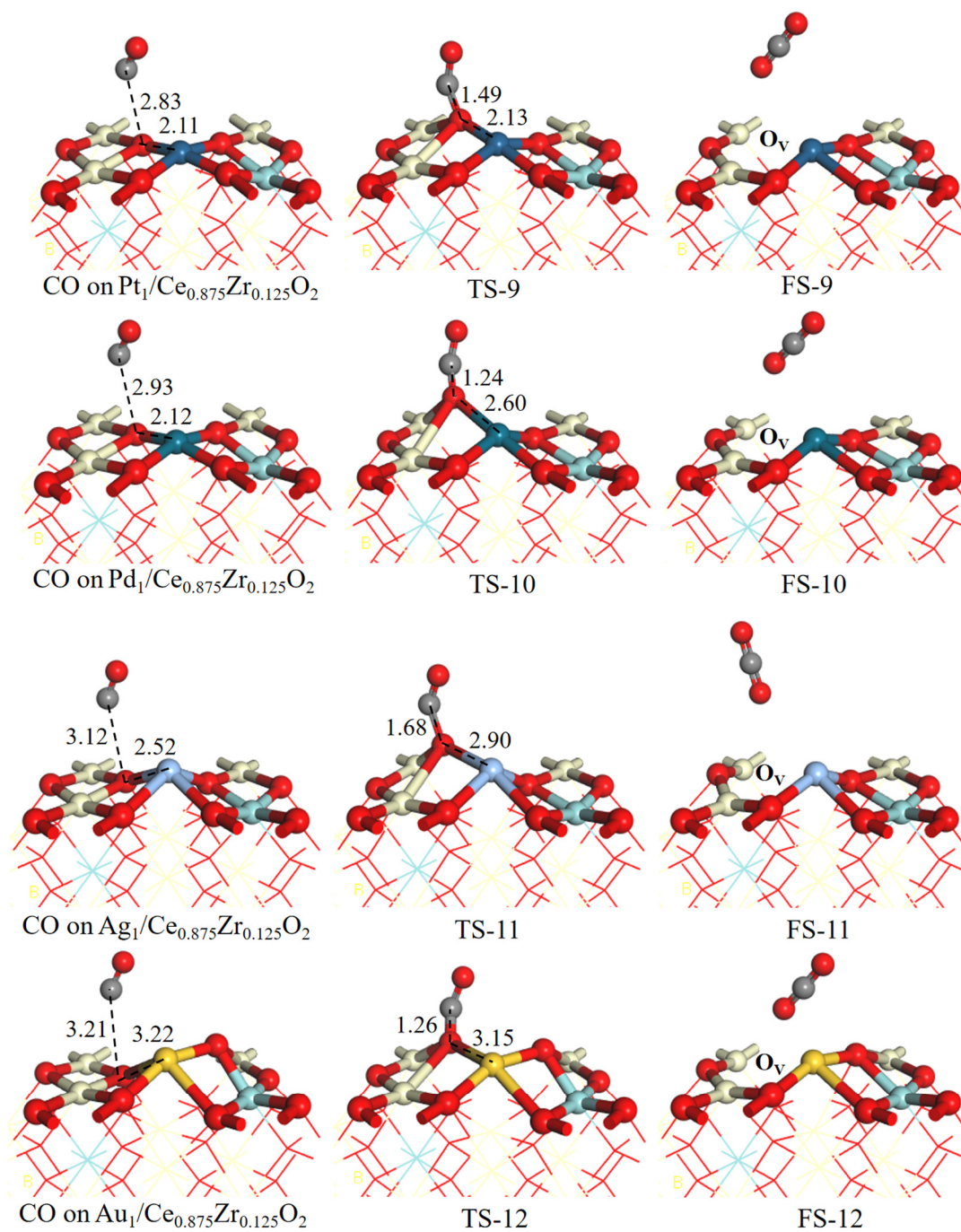
**Figure S1.** Calculated energy profile and corresponding optimized configurations of reactants, transition states and products of the activation of C<sub>sp3</sub>-H bond of C<sub>3</sub>H<sub>6</sub> on the Pd<sub>1</sub>/Ce<sub>0.875</sub>Zr<sub>0.125</sub>O<sub>2</sub> (110) surface.



**Figure S2.** Calculated energy profile and corresponding optimized configurations of reactants, transition states and products of the activation of C<sub>sp3</sub>-H bond of C<sub>3</sub>H<sub>6</sub> on the Ag<sub>1</sub>/Ce<sub>0.875</sub>Zr<sub>0.125</sub>O<sub>2</sub> (110) surface.



**Figure S3.** Calculated energy profile and corresponding optimized configurations of reactants, transition states and products of the activation of C<sub>sp3</sub>-H bond of C<sub>3</sub>H<sub>6</sub> on the Au<sub>1</sub>/Ce<sub>0.875</sub>Zr<sub>0.125</sub>O<sub>2</sub> (110) surface.



**Figure S4.** The reactants, transition states and products of CO oxidation reaction on the  $\text{Pt}_1/\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$ ,  $\text{Pd}_1/\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$ ,  $\text{Ag}_1/\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$  and  $\text{Au}_1/\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$  (110) surfaces.