

## 理想与还原 $\text{Fe}_2\text{O}_3$ [001]表面上汞吸附协同催化 CO 分解作用

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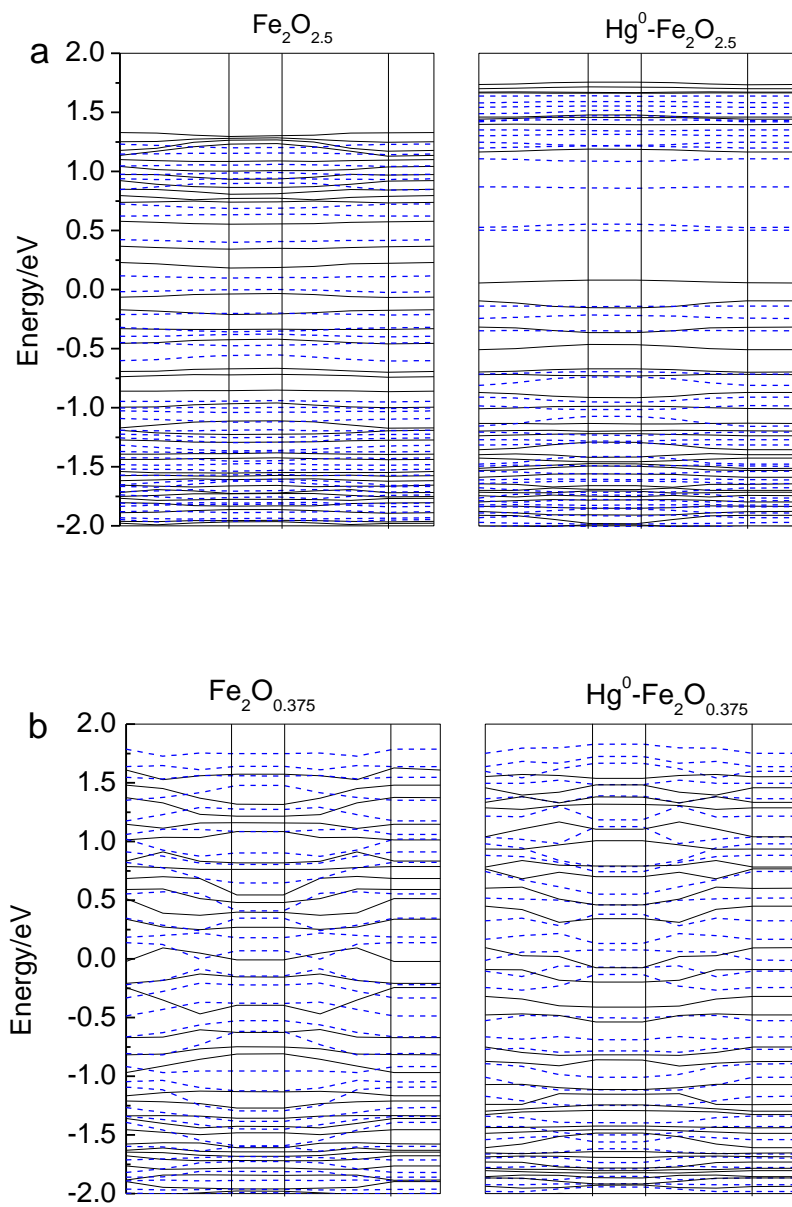
## Synergetic Effect of Mercury Adsorption on the Catalytic Decomposition of CO over Perfect and Reduced $\text{Fe}_2\text{O}_3$ [001] Surface

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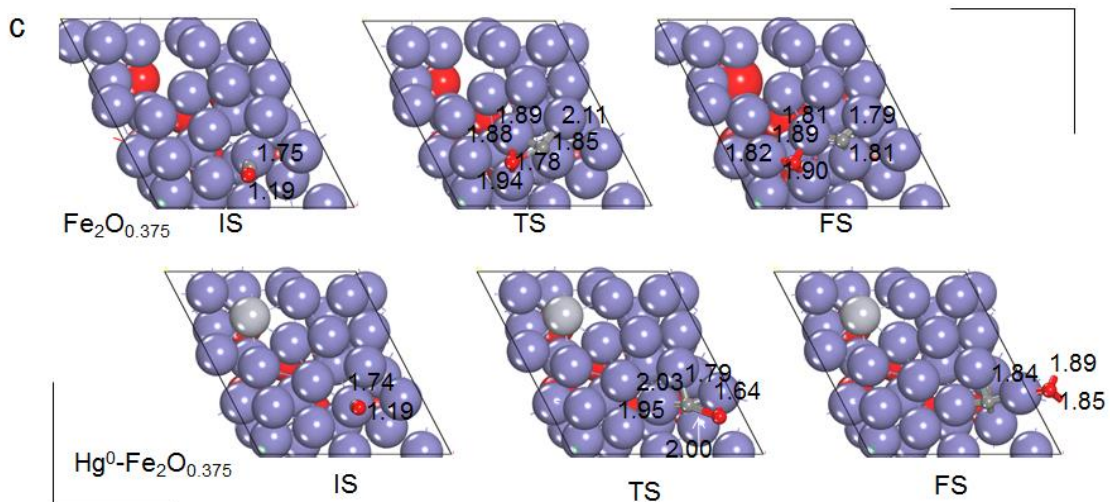
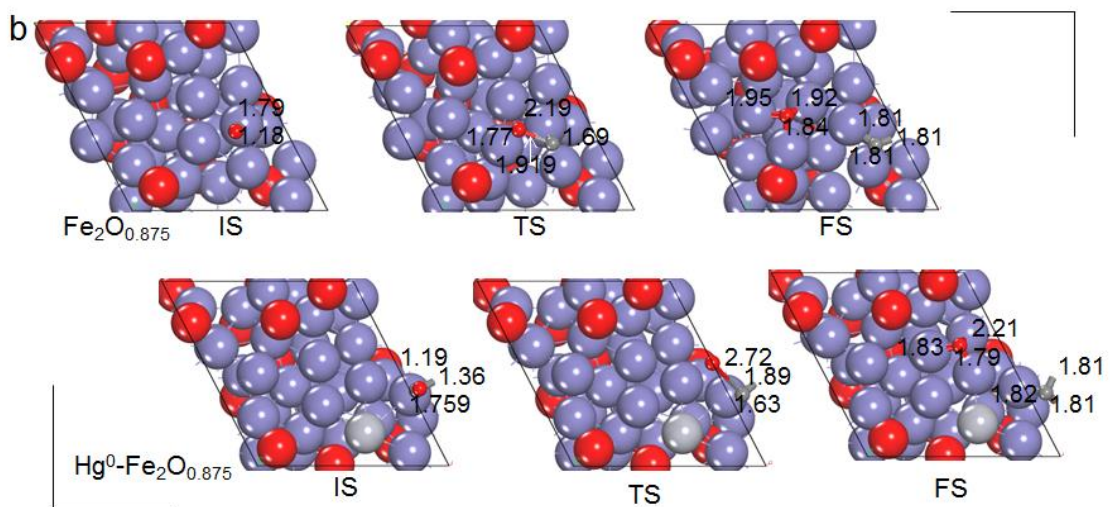
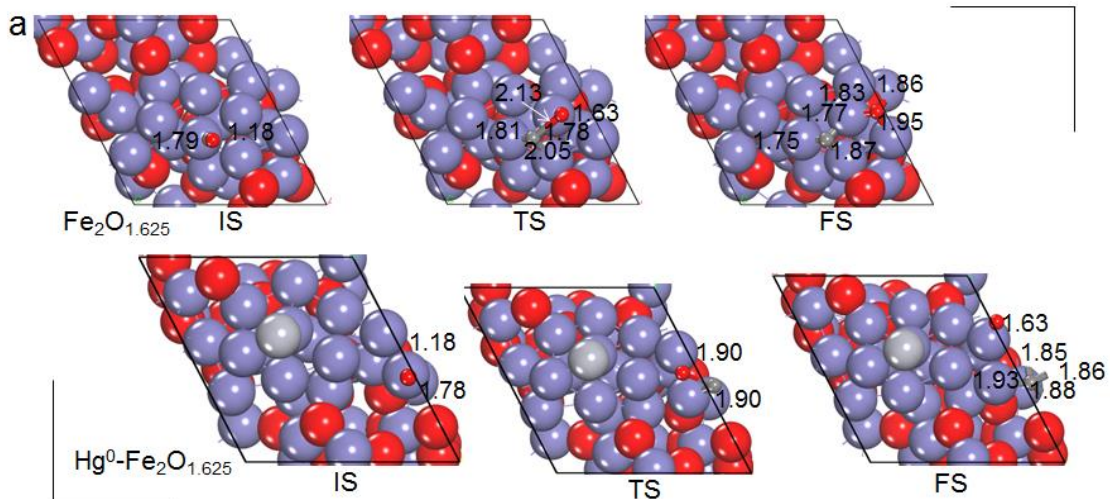
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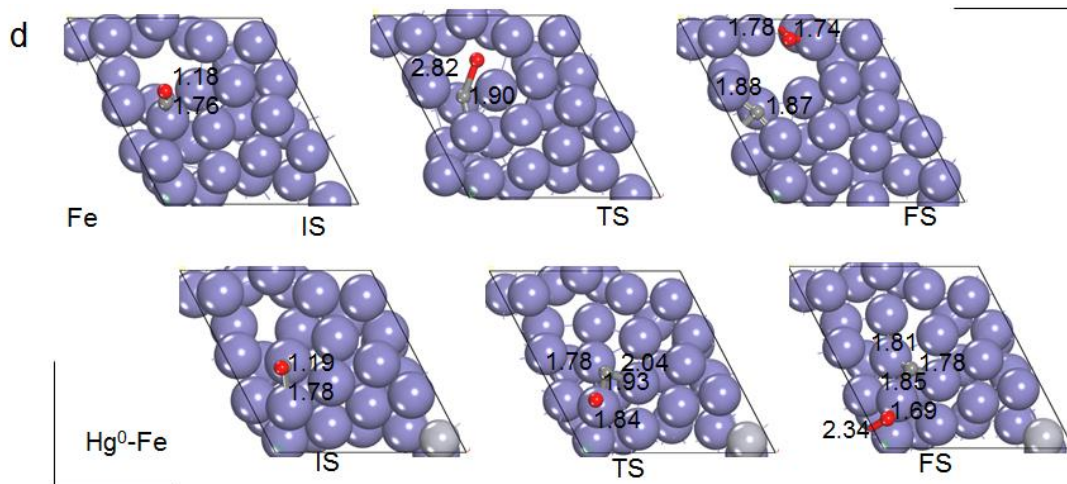
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**Fig.S1 Band structures for (a)  $\text{Fe}_2\text{O}_{2.5}$  and  $\text{Hg}^0\text{-Fe}_2\text{O}_{2.5}$  and (b)  $\text{Fe}_2\text{O}_{0.375}$  and  $\text{Hg}^0\text{-Fe}_2\text{O}_{0.375}$**





**Fig.S2 Geometric structures of initial state (IS), transition state (TS), and final state (FS) for CO decomposition on (a)  $\text{Fe}_2\text{O}_{1.625}$  and  $\text{Hg}^0\text{-Fe}_2\text{O}_{1.625}$ , (b)  $\text{Fe}_2\text{O}_{0.875}$  and  $\text{Hg}^0\text{-Fe}_2\text{O}_{0.875}$ , (c)  $\text{Fe}_2\text{O}_{0.375}$  and  $\text{Hg}^0\text{-Fe}_2\text{O}_{0.375}$ , (d)  $\text{Fe}$  and  $\text{Hg}^0\text{-Fe}$**

The C-O bond length and the distance between C and Fe of the IS are given in Å. And the related bond distances for the TS and FS are also given in Å.