

ESI

## What is the Effect of Sn and Mo oxides on Gold Catalyst for Selective Oxidation of Benzyl Alcohol ?

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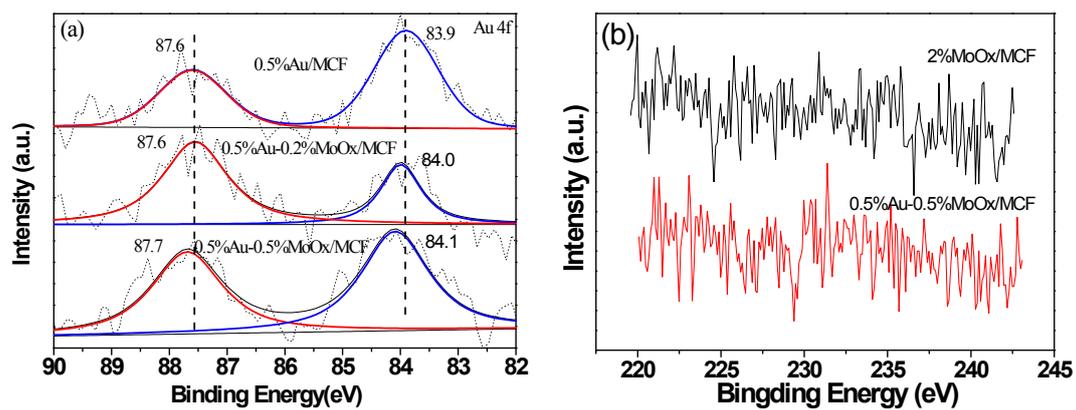
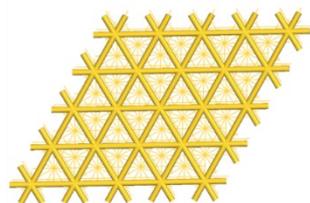
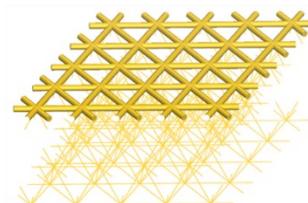


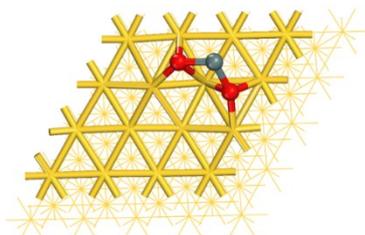
Fig. S1 (a) Au 4f and (b) Mo 3d XPS spectra of samples 0.5%Au/MCF, 0.5%Au-0.2%MoO<sub>x</sub>/MCF, 0.5%Au-0.5%MoO<sub>x</sub>/MCF and 2%MoO<sub>x</sub>/MCF.



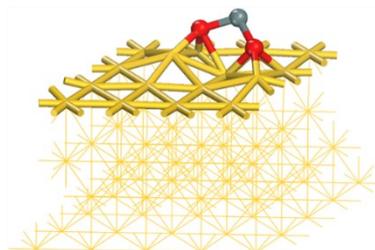
Au(111) (top view)



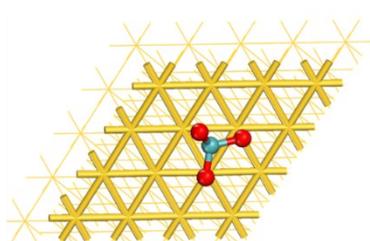
Au (111) (side view)



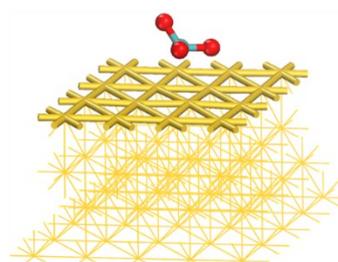
SnO<sub>2</sub>/Au(111) (top view)



SnO<sub>2</sub>/Au (111) (side view)



MoO<sub>3</sub>/Au(111) (top view)



MnO<sub>3</sub>/Au (111) (side view)

Fig. S2 Optimized geometries of Au(111), SnO<sub>2</sub>/Au(111), and MoO<sub>3</sub>/Au(111). Yellow, gray, cambridge blue, and red denote Au, Sn, Mo, and O atoms, respectively.

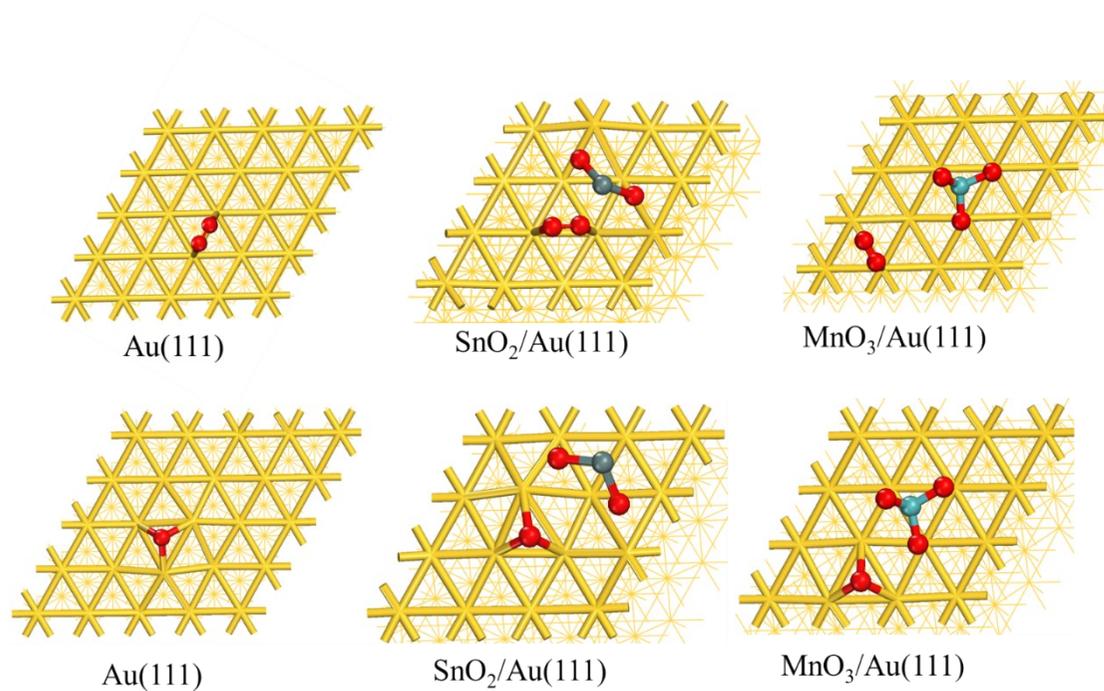


Fig. S3 The most stable adsorption configurations of  $\text{O}_2$  and  $\text{O}$  on Au(111),  $\text{SnO}_2/\text{Au}(111)$ , and  $\text{MoO}_3/\text{Au}(111)$ . Yellow, gray, cambridge blue, and red denote Au, Sn, Mo, and O atoms, respectively.

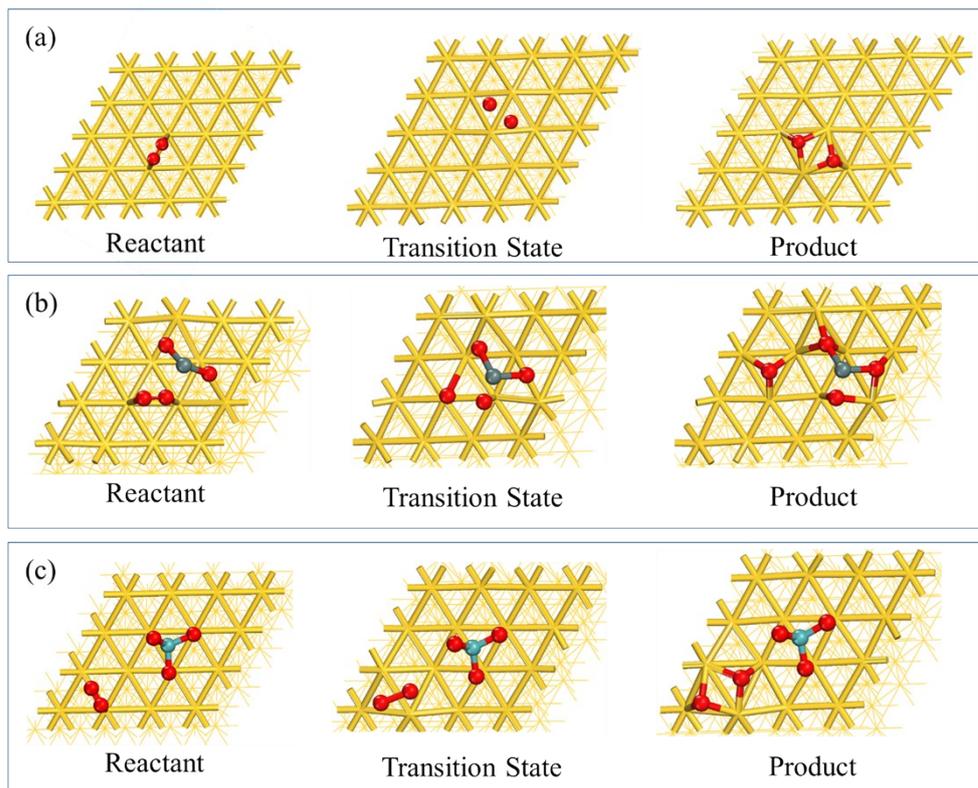


Fig. S4 Dissociation of  $O_2$  on (a) Au(111), (b)  $SnO_2/Au(111)$ , and (c)  $MoO_3/Au(111)$ . Yellow, gray, cambridge blue, and red denote Au, Sn, Mo, and O atoms, respectively.