

Supplementary Information for

“Surface reduction properties of ceria-zirconia solid solutions: A first-principles study”

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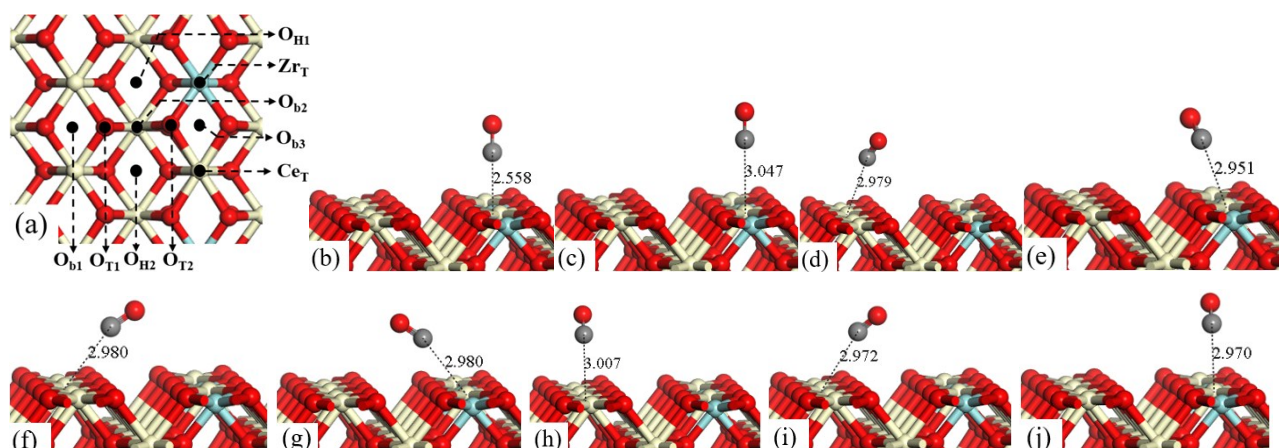


Fig. S1. Structure models of (a) the top view of $\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$ (110) surface and nine possible adsorption sites for CO gas molecule are labeled. Optimized configurations of CO adsorbed at (b) Zr_T site, (c) Ce_T site, (d) O_{T1} site, (e) O_{T2} site, (f) O_{H1} site, (g) O_{H2} site, (h) O_{b1} site, (i) O_{b2} site and (j) O_{b3} site on $\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$ (110) surface. Gray, Red, ivory and cyan spheres represent the C, O, Ce and Zr atoms, respectively.

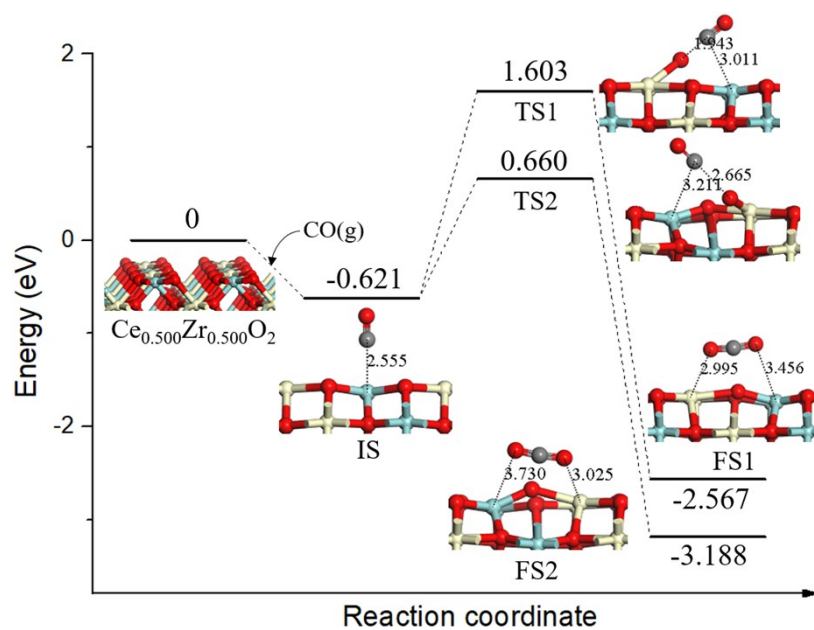


Fig. S2. Calculated energy profile and structures of key states of CO oxidation by lattice oxygen on $\text{Ce}_{0.500}\text{Zr}_{0.500}\text{O}_2$ (110) surface.

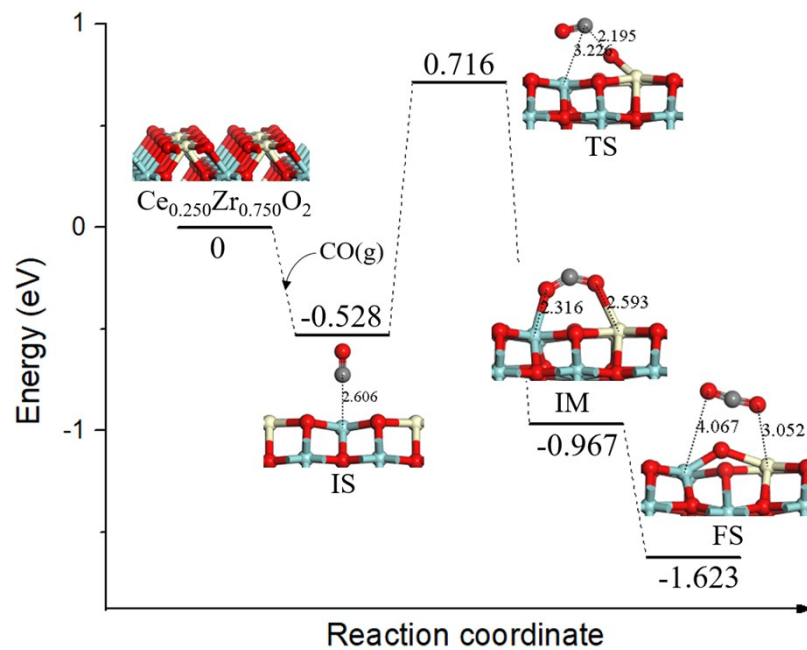


Fig. S3. Calculated energy profile and structures of key states of CO oxidation by lattice oxygen on $\text{Ce}_{0.250}\text{Zr}_{0.750}\text{O}_2$ (110) surface.

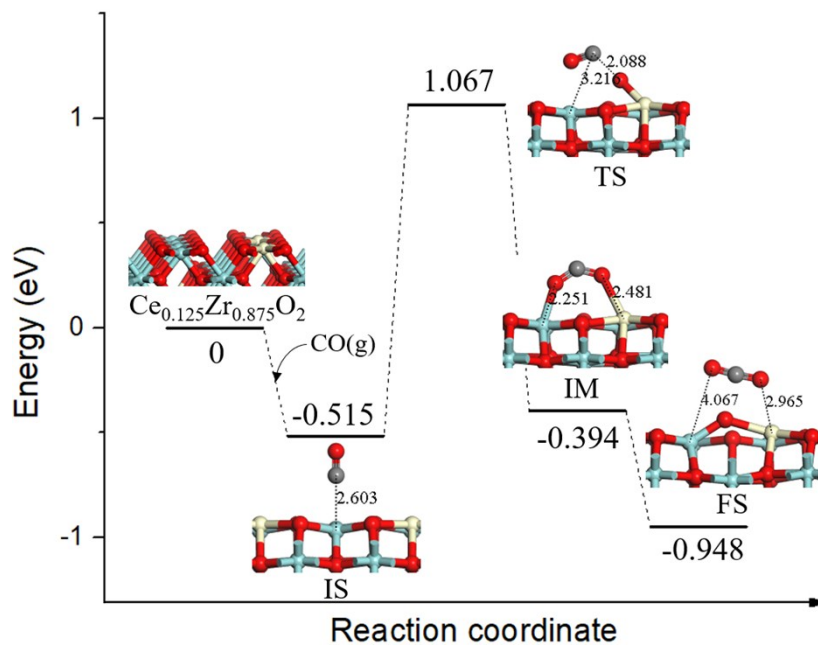


Fig. S4. Calculated energy profile and structures of key states of CO oxidation by lattice oxygen on $\text{Ce}_{0.125}\text{Zr}_{0.875}\text{O}_2$ (110) surface.

Table S1 Calculated adsorption energies (E_{ads}) of CO gas molecule at the different adsorption sites of $\text{Ce}_{0.875}\text{Zr}_{0.125}\text{O}_2$ (110) surface.

Adsorption site	E_{ads} (eV)	Figure
Zr _T	-0.569	S1(b)
Ce _T	-0.408	S1(c)
O _{T1}	-0.417	S1(d)
O _{T2}	-0.434	S1(e)
O _{H1}	-0.462	S1(f)
O _{H2}	-0.470	S1(g)
O _{b1}	-0.389	S1(h)
O _{b2}	-0.446	S1(i)
O _{b3}	-0.421	S1(j)