

**Supplementary material for “Effects of Strong Interactions between
Ti and Ceria on the Structures of Ti/CeO₂ ”**

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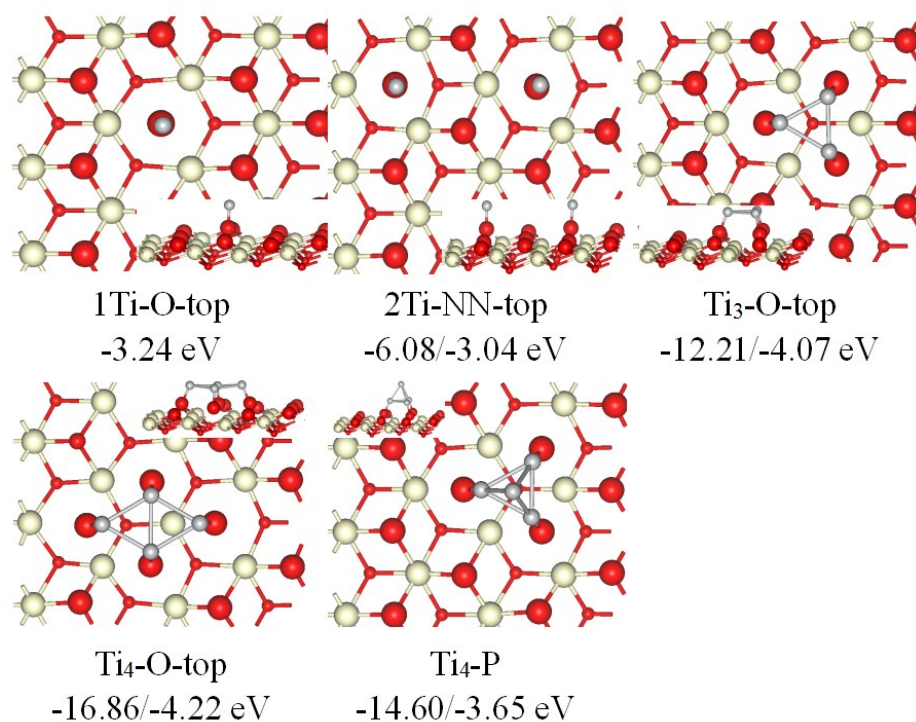


Fig. S1 $x\text{Ti}(x=1-4)$ configurations on $\text{CeO}_2(111)$ and adsorption energies (E_t/E_p). Red, faint yellow and grey balls represent O, Ce and Ti atoms, respectively. Small balls mean subsurface atoms, while big ones mean surface atoms.

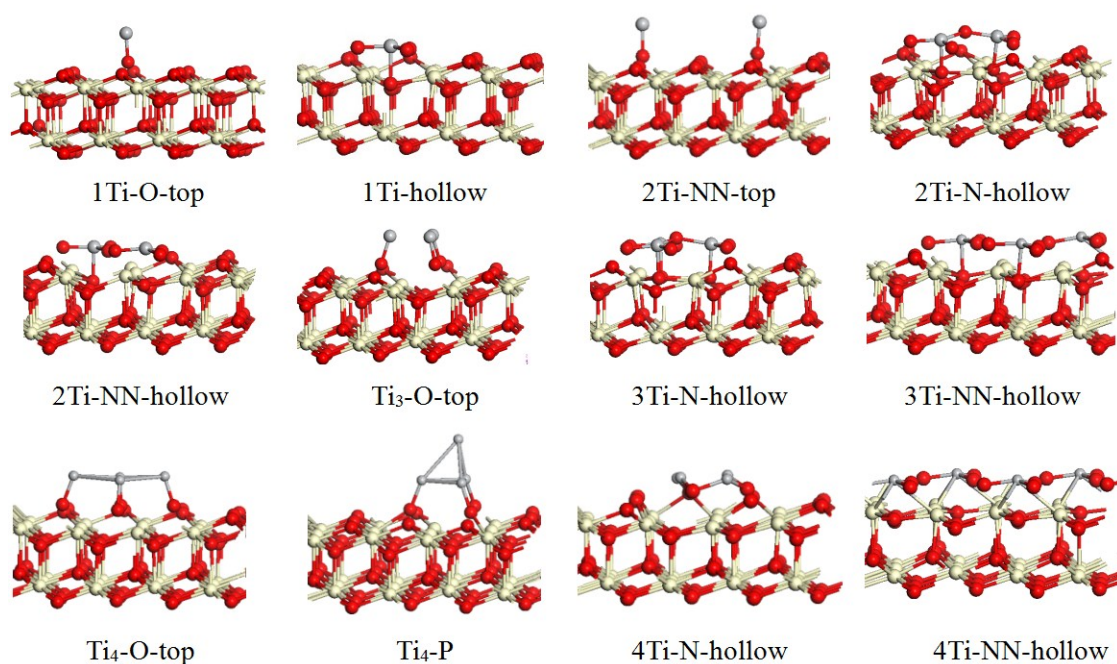


Fig. S2 Side views of $x\text{Ti}(x=1-4)$ configurations on $\text{CeO}_2(111)$.

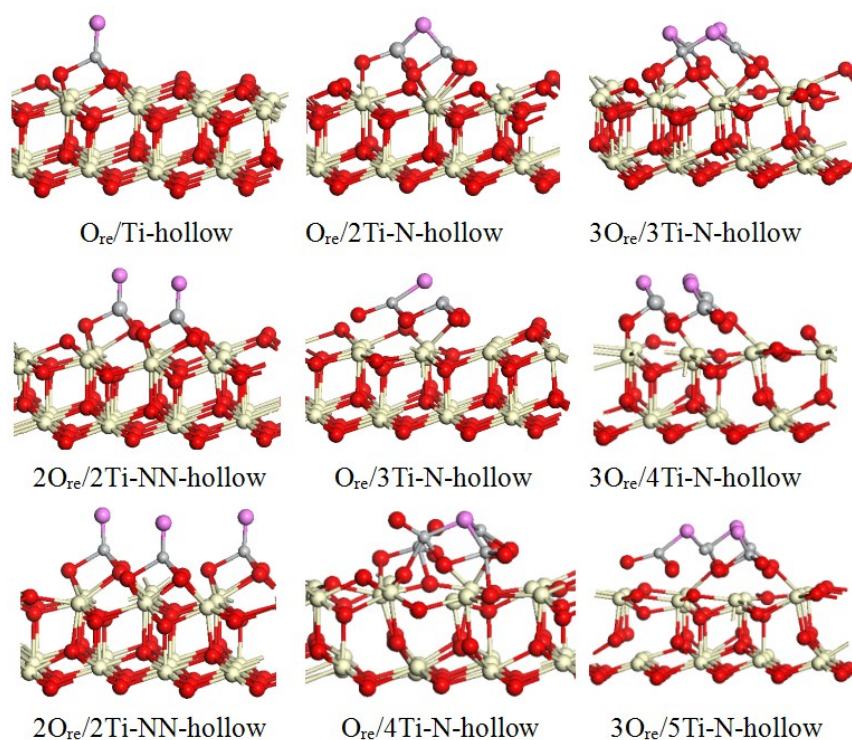


Fig. S3 Side views of $xTi/CeO_2(111)$ configurations with restructuring, Pink balls represent the restructured O atoms.

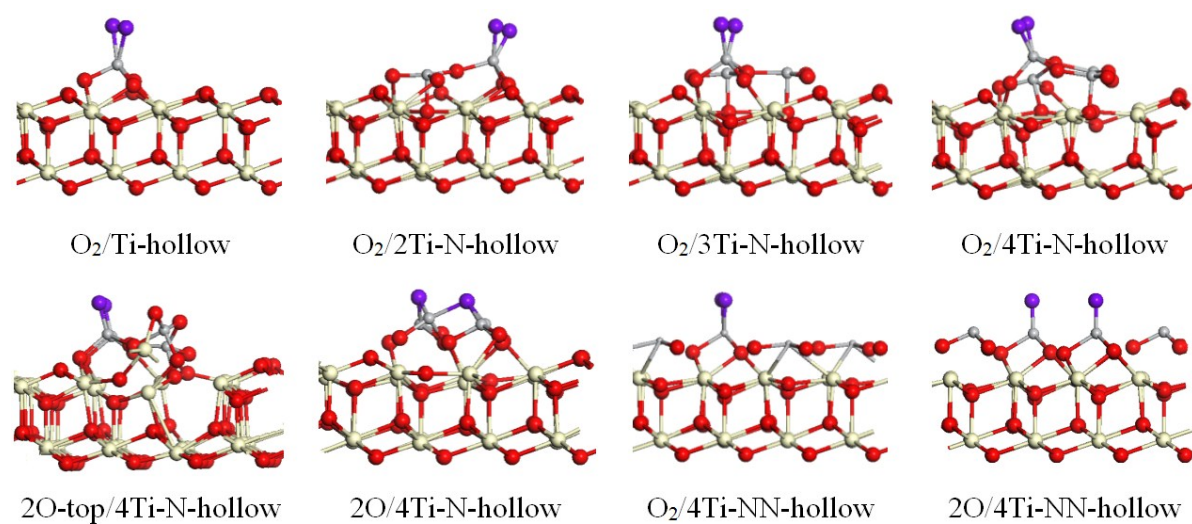


Fig. S4 Side views of O_2 adsorption and dissociation on $Ti_x/CeO_2(111)$. Purple balls represent the adsorbed and dissociated O_2 .

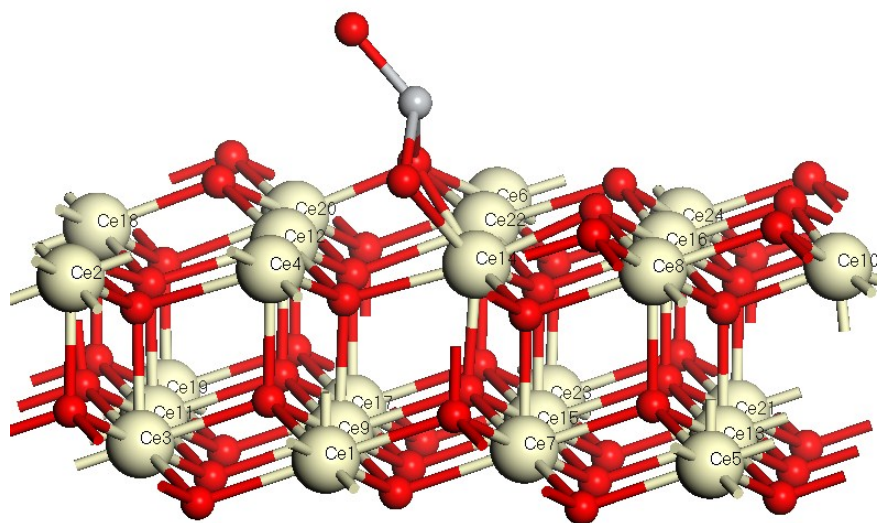


Fig. S5 The atomic number of Ce for $x\text{Ti}/\text{CeO}_2(111)$

Table S1 Binding energies of Ti-Ti and Ti-O bonds with different U values

U value	$E_{\text{bTi-Ti}}$ /eV	$E_{\text{bTi-O}}$ /eV
0	4.08	8.45
1	2.72	7.90
2	1.42	6.85
3	0.05	6.85
4	-1.28	5.22
E_{exp} /eV	1.43	6.93

Table S2 Model tests of thickness and expansion

Configuration	Model	E_{ads} /eV		Lattice fixed / Å			Lattice relaxed / Å		
		Lattice fixed	Lattice relaxed	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>
1Ti-hollow	5/6 Ti/CeO ₂	-7.99	-8.07	13.440	11.640	16.752	13.353	11.563	16.973
	8/9 Ti/CeO ₂	-8.15	-8.11	13.440	11.640	19.920	13.389	11.597	20.068
4Ti-NN-hollow	5/6 Ti/CeO ₂	-29.50	-29.89	13.440	11.640	16.752	13.346	11.548	17.004
	8/9Ti/CeO ₂	-30.09	-30.23	13.440	11.640	19.920	13.379	11.592	20.093
3Ore/4Ti-N-hollow	5/6 Ti/CeO ₂	-32.00	-31.62	13.440	11.640	16.752	13.350	11.567	16.828
	8/9Ti/CeO ₂	-32.81	-32.09	13.440	11.640	19.920	13.374	11.582	20.116

Table S3 Adsorption energies of Ti on Ti(0001)

Configuration	E_{ads} /eV
bridge	-3.28
fcc	-3.21
hcp	-3.26