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## **Supporting Information**

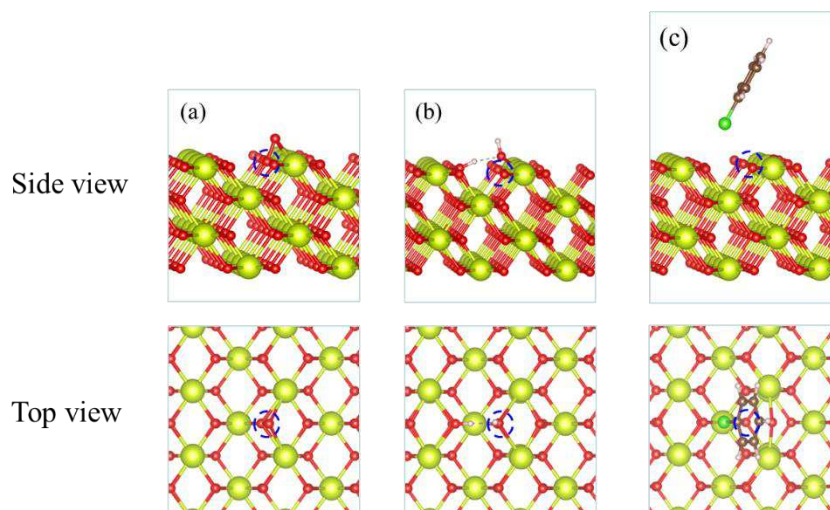
### **Efficient Elimination of Chlorinated Organics on A Phosphoric Acid Modified CeO<sub>2</sub> Catalyst: A Hydrolytic Destruction Route**

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James H. Carter\*, Graham J. Hutchings, Xiaole Weng\*, Zhongbiao Wu

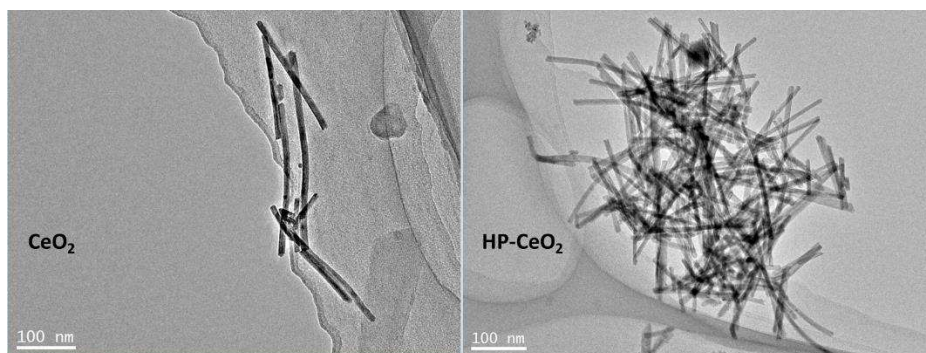
Number of Pages: 5

Number of Figures: 4

Number of Tables: 3



**Figure S1.** Optimized model of CeO<sub>2</sub> (110) with oxygen vacancy. The models were constructed by removing single oxygen atom from CeO<sub>2</sub>(110) supercell to introduce oxygen vacancies. During geometry optimization, the atoms in the top two layers of CeO<sub>2</sub> slab were allowed to relax while atoms in the bottom two layers were fixed in their optimized bulk positions.

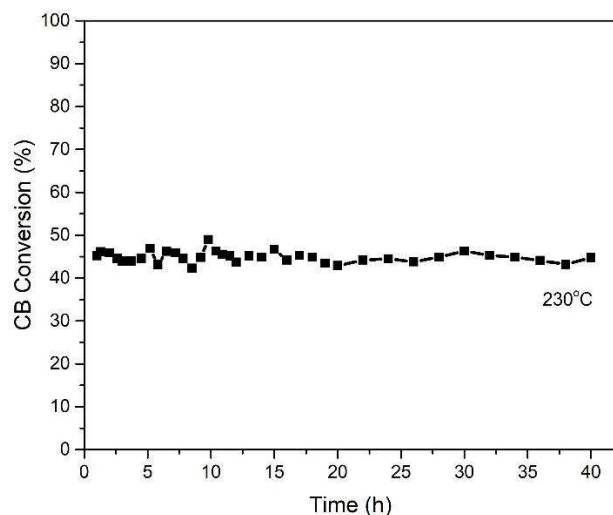


**Figure S2.** TEM images of CeO<sub>2</sub> and HP-CeO<sub>2</sub>

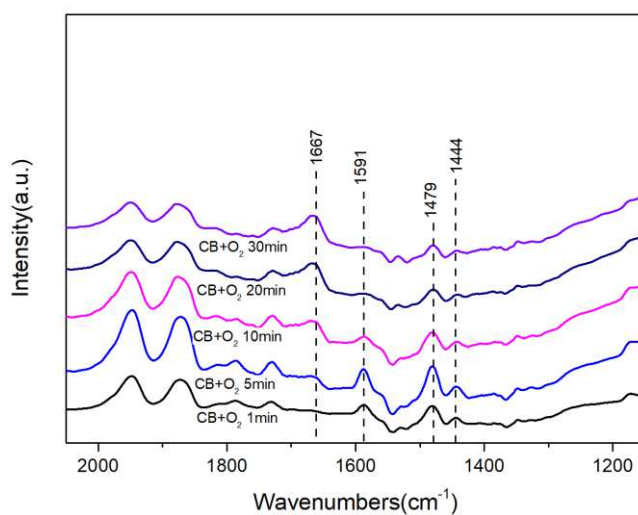
**Table S1.** Physical properties of HP-CeO<sub>2</sub> and CeO<sub>2</sub>

sample	p loading		surface area (m <sup>2</sup> g <sup>-1</sup> )	lattice parameter (Å)	Ce <sup>3+</sup> /Ce <sub>total</sub> <sup>a</sup>
	(mmol g <sup>-1</sup> )	(nm <sup>-2</sup> )			
<b>CeO<sub>2</sub></b>	0	0	96	5.411	29%
<b>HP-CeO<sub>2</sub></b>	0.21	1.18	108	5.413	26%

Note: (a) caculated from XPS results



**Figure S3.** Stability test of CB oxidation over HP-CeO<sub>2</sub> at 230 °C. Reaction condition: GHSV at 10,000 mL/(g h), chlorobenzene at ca. 500 ppm, H<sub>2</sub>O at 5000 ppm, N<sub>2</sub> flow rate at ca. 145 mL/min, O<sub>2</sub> flow rate at ca. 15 mL/min.



**Figure S4.** *in-situ* FTIR spectra of CB oxidation at 150 °C over CeO<sub>2</sub> catalyst in dry condition.

**Table S2.** Adsorption energies on various active sites

Species	Adsorption energy (eV)
O <sub>2</sub> /O <sub>vac</sub>	2.20
H <sub>2</sub> O/O <sub>vac</sub>	1.57
O <sub>2</sub> +H <sub>2</sub> O/O <sub>vac</sub>	2.82
C <sub>6</sub> H <sub>5</sub> Cl/O <sub>vac</sub>	0.39
C <sub>6</sub> H <sub>5</sub> Cl+O <sub>2</sub> /O <sub>vac</sub>	2.37

C <sub>6</sub> H <sub>5</sub> Cl+H <sub>2</sub> O/O <sub>vac</sub>	1.21
O <sub>2</sub> /Ce	0.20
H <sub>2</sub> O/Ce	0.62
O <sub>2</sub> +H <sub>2</sub> O/Ce	0.72
C <sub>6</sub> H <sub>5</sub> Cl/Ce	0.48
C <sub>6</sub> H <sub>5</sub> Cl+H <sub>2</sub> O/Ce	1.81
O <sub>2</sub> /P group	-1.59
H <sub>2</sub> O/P group	0.63
O <sub>2</sub> +H <sub>2</sub> O/P group	-0.94
C <sub>6</sub> H <sub>5</sub> Cl/P group	0.50
C <sub>6</sub> H <sub>5</sub> Cl+O <sub>2</sub> /P group	-0.56
C <sub>6</sub> H <sub>5</sub> Cl+H <sub>2</sub> O/P group	2.77
HCl/P group	0.74
C <sub>6</sub> H <sub>5</sub> OH/P group	0.76

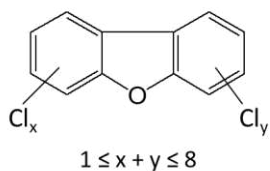
**Table S3.** Ingredients of 17 toxic dioxins in the off-gas of CeO<sub>2</sub> and HP-CeO<sub>2</sub> at 250 °C test with H<sub>2</sub>O stream

Compound	Detection limit (pg)	TEF	CeO <sub>2</sub>		HP-Ce	
			Cout (pg)	I-TEQ (ng/m <sup>3</sup> )	Cout (pg)	I-TEQ (ng/m <sup>3</sup> )
<b>2378TCDD</b>	0.5627	1	<0.5627	ND	<0.5627	ND
<b>12378PeCDD</b>	0.6234	0.5	<0.6234	ND	<0.6234	ND
<b>123478HxCDD</b>	0.6574	0.1	<0.6574	ND	<0.6574	ND

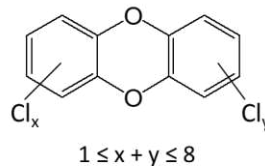
<b>123678HxCDD</b>	0.625	0.1	1.4879	0.00155	<0.625	ND
<b>123789HxCDD</b>	0.6931	0.1	<0.6931	ND	<0.6931	ND
<b>1234678HpCDD</b>	0.5632	0.01	6.2856	0.000655	<0.5632	ND
<b>OCDD</b>	0.7633	0.001	4.2767	4.45E-05	<0.7633	ND
<b>2378TCDF</b>	0.4675	0.1	0.9775	0.001018	<0.4675	ND
<b>12378PeCDF</b>	0.642	0.05	1.2645	0.000659	<0.642	ND
<b>23478PeCDF</b>	0.6132	0.5	1.04855	0.005461	<0.6132	ND
<b>123478HxCDF</b>	0.6015	0.1	2.3201	0.002417	<0.6015	ND
<b>123678HxCDF</b>	0.6329	0.1	2.5632	0.00267	<0.6329	ND
<b>123789HxCDF</b>	0.6512	0.1	0.57475	0.000599	<0.6512	ND
<b>234678HxCDF</b>	0.6877	0.1	2.3671	0.002466	<0.6877	ND
<b>1234678HpCDF</b>	0.7022	0.01	5.3266	0.000555	<0.7022	ND
<b>1234789HpCDF</b>	0.6934	0.01	<0.6934	ND	<0.6934	ND
<b>OCDF</b>	0.7142	0.001	3.3276	3.47E-05	<0.7142	ND
<b>Total</b>				0.01813		ND

Note: (1) CDD/CDF: chlorinated dibenzo-*p*-dioxin/dibenzofuran, structural formula represents as Fig S10 ; (2) ND: not detectable; (3) I-TEQ = Cout × TEF; (4) TEF: Toxic Equivalent Factors, toxic factors relative to the most toxic congener, 2,3,7,8-tetrachlorodibenzo-dioxin; (5) I-TEQ: International Toxicity Equivalence Quotient, the weighted value of the concentrations of 17 PCDD and PCDF congeners with chlorine in the 2, 3, 7 and 8 positions on the dibenzo skeleton, weighted according their Toxic Equivalent Factors (TEF) relative to the most toxic congener, 2,3,7,8-tetrachlorodibenzo-dioxin.

Polychlorinated dibenzofurans



Polychlorinated dibenzo-*p*-dioxins



Structure diagrams of chlorinated dibenzo-*p*-dioxin/dibenzofuran