Supporting Information

Hyper Oxygen Incorporation in CeF_3: A New Intermediate-Band Photocatalyst for Antibiotic Degradation under Visible/NIR Light

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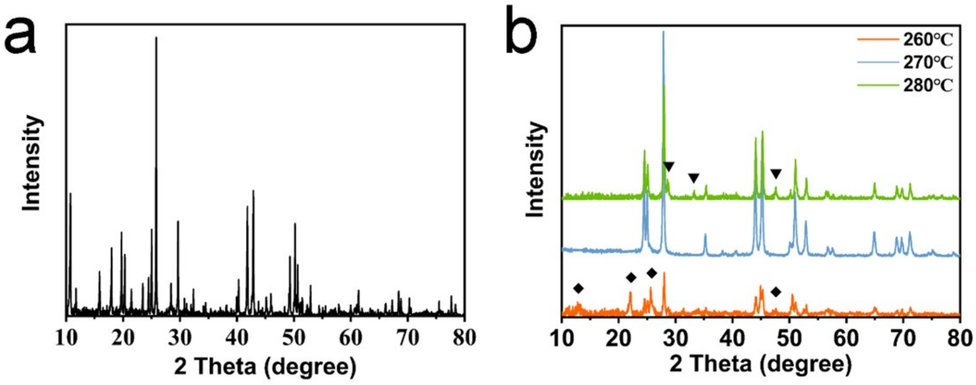

Figure S1. the typical XRD patterns of the precursor JCPDS NO.70-4378(a); samples calcined at different temperature(b). ◆ sign is the precursor ;▼ sign is CeO_2 (JCPDS NO. 08-0045).

Table S1. The element content of CeF_3-O

Element	Ce	F	O
Atomic %	21.45	62.82	15.73

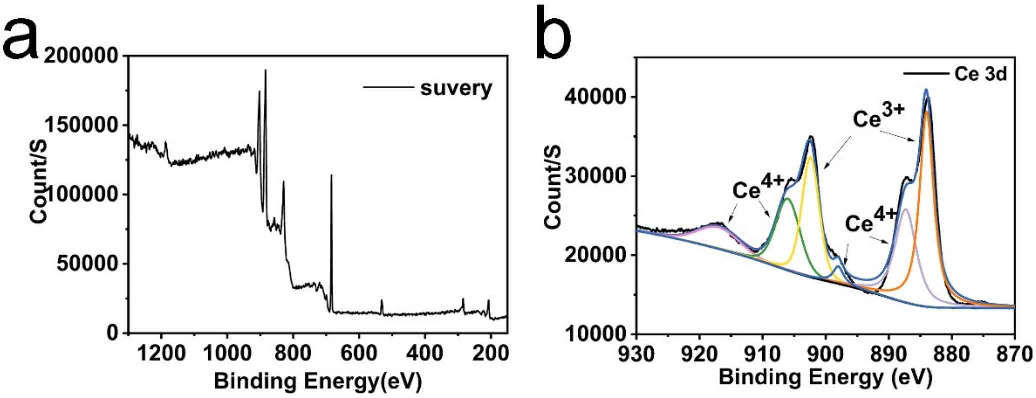

Figure S2. The survey spectrum of CeF_3-O XPS: Ce 3d5 (884.1 eV), F 1s (684.4 eV), O 1s (531.7 eV), Ce Auger (830.0 eV), and Ce 3d3 (902.4 eV) (a); The spectrum of Ce 3d (b).

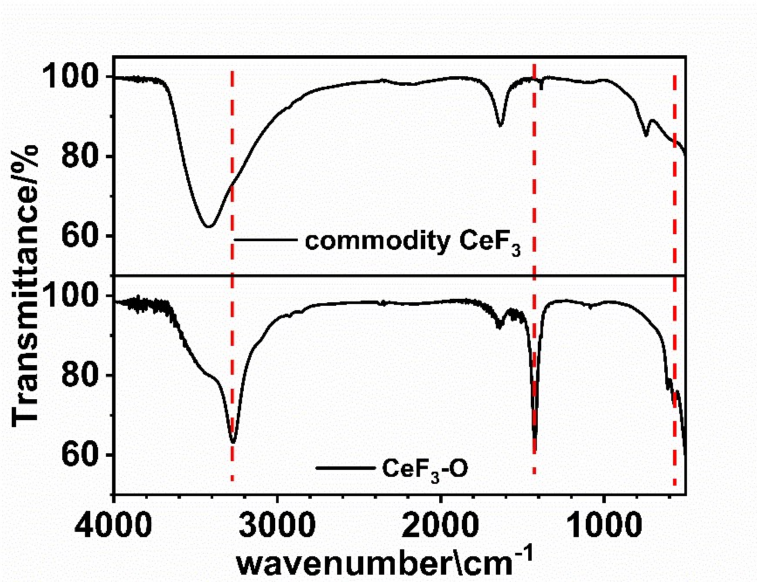

Figure S3. FTIR spectra of commercial CeF_3 and CeF_3-O. The peak at 750 cm^{-1} of commercial CeF_3 is attributed to-CH_2-, and it maybe from organ impurity.

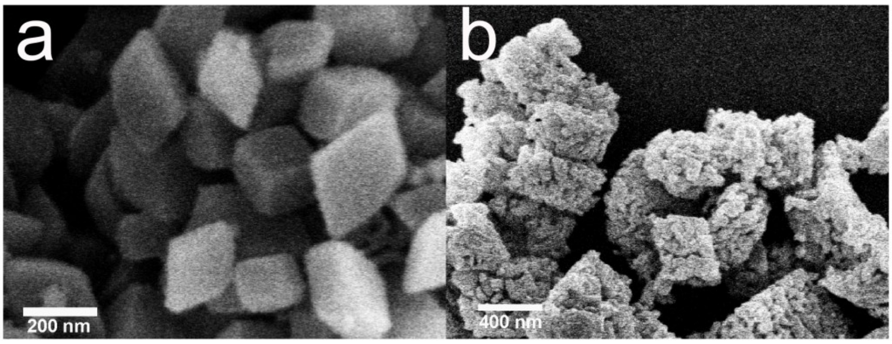

Figure S4. SEM of the precursor $H_{25.5}(NH_4)_{10.5}Ce_9O_{27}F_{18}$ (a) and CeF_3-O(b)

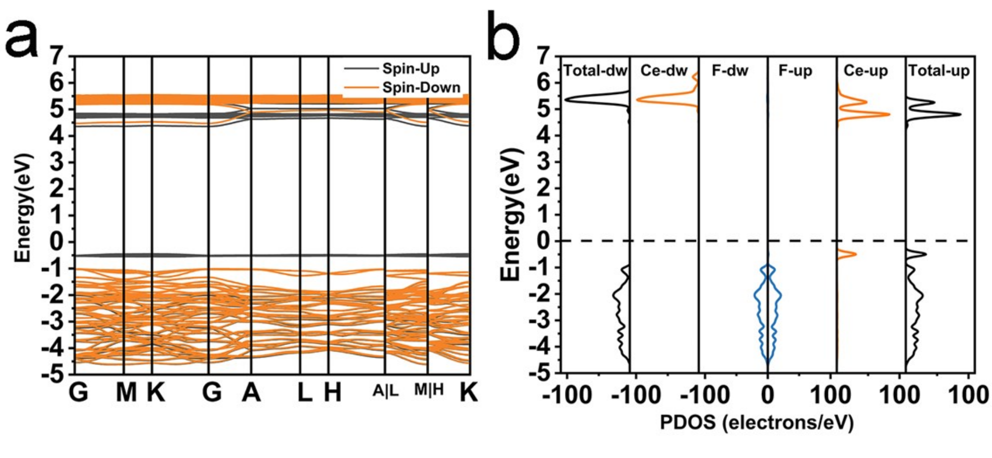

Figure S5. The calculated band structure and DOS of pristine CeF_3.

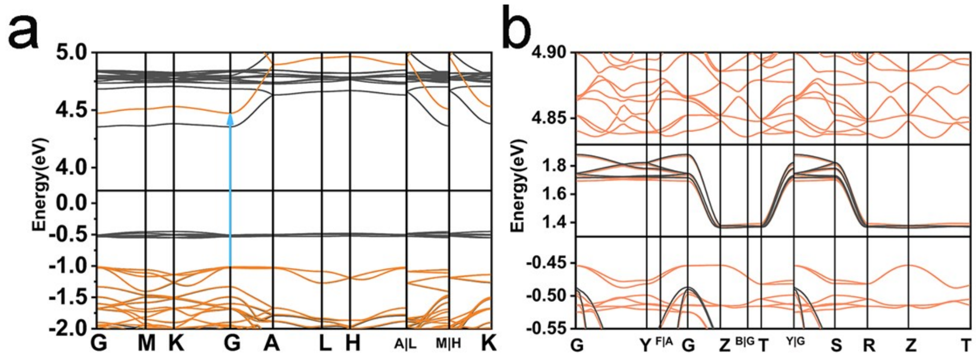

Figure S6. partial enlargement of DFT calculated band structure of pristine CeF_3 and CeF_3-O.

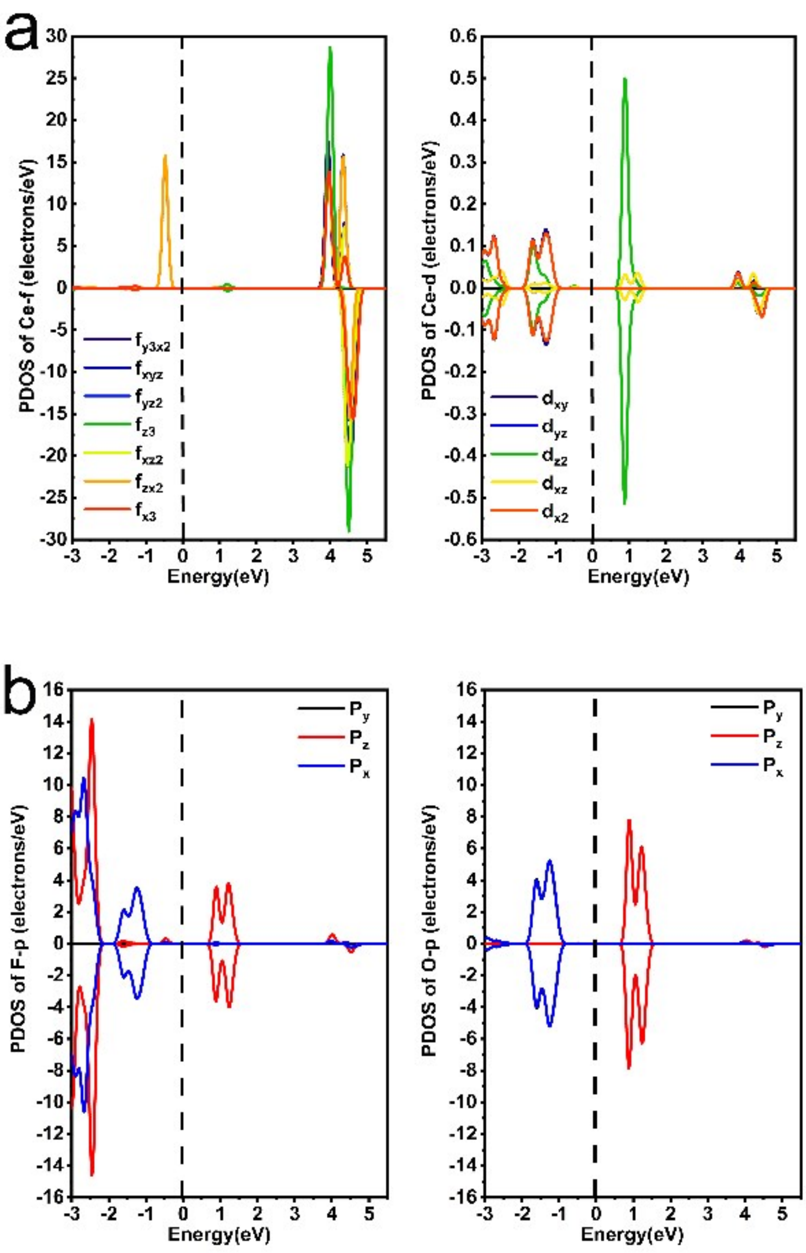

Figure S7. PDOS of Ce(a), O and F(b).

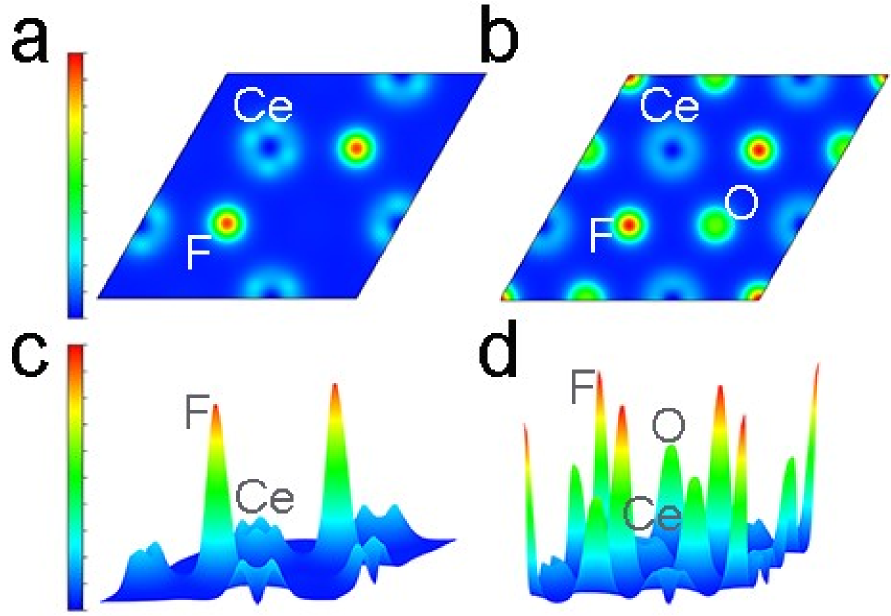

Figure S8. Two dimensional charge density distribution plots of pristine CeF_3 (a,c) and CeF_3-O (b,d) on [001] plane.

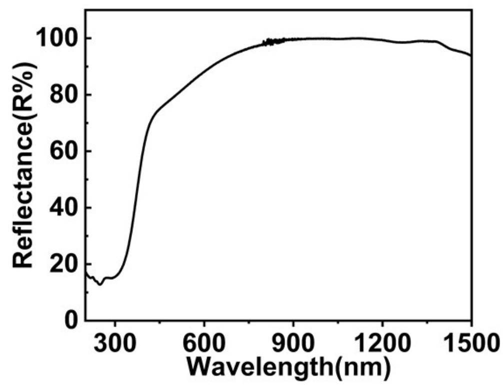

Figure S9. UV−Vis−NIR diffuse reflectance absorption (DRS) spectrum of CeF_3-O.

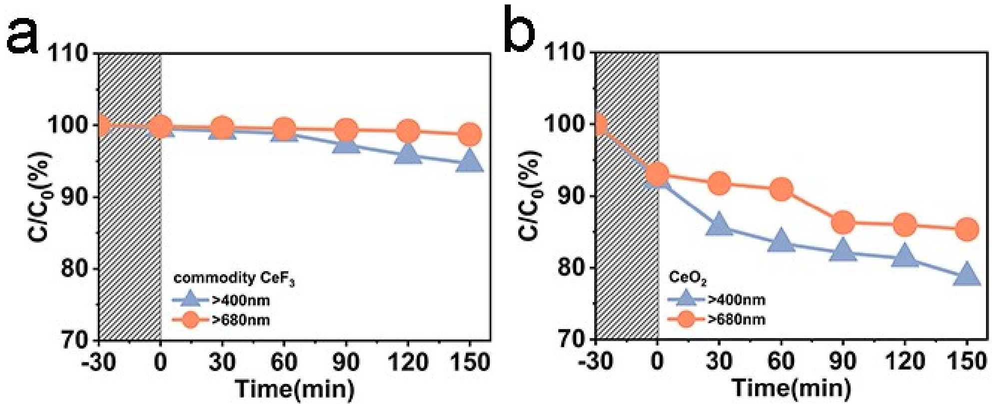

Figure S10. Photodegradation of TC-HCl by CeF_3(a) and CeO_2(b) under different cutoff filters (λ>400 nm and λ>680 nm). the photodegradation of TC-HCl by CeO_2 is is because the filter (cutoff 400nm) has an optical edge extending to about 380nm. Compared with both of commercial CeF_3 and CeO_2 under visible and NIR light, the CeF_3-O has excellent photocatalysis activity under visible light. CeO_2 was synthesized by the similar calcination of precursor $H_{25.5}(NH_4)_{10.5}Ce_9O_{27}F_{18}$ at 600℃ for 1h.

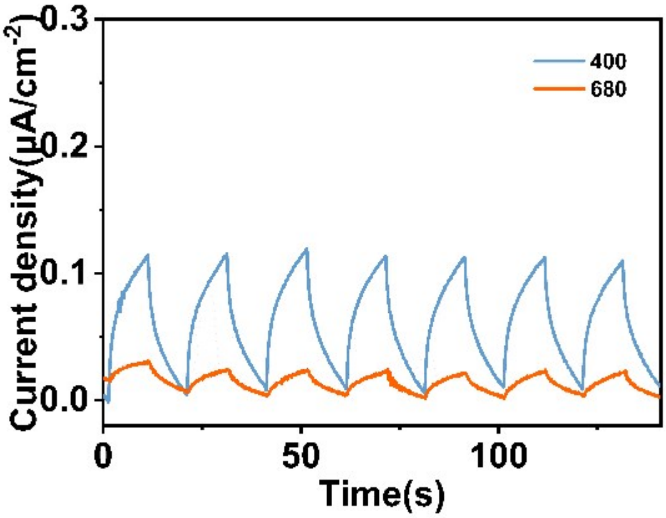

Figure S11. Photocurrent responses of the CeF_3-O under visible light irradiation(λ>400 nm) and near-infrared light irradiation(λ>680 nm). The CeF_3-O under visible light showed the stronger photocurrent transient response in comparison to that of near-infrared light, indicating the higher charge separation efficiency.

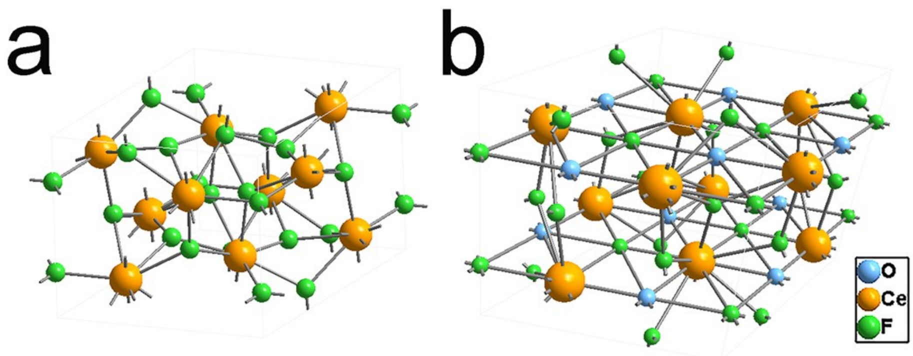

Figure S12 the structure of pristine CeF_3 (a) and CeF_3-O (b)

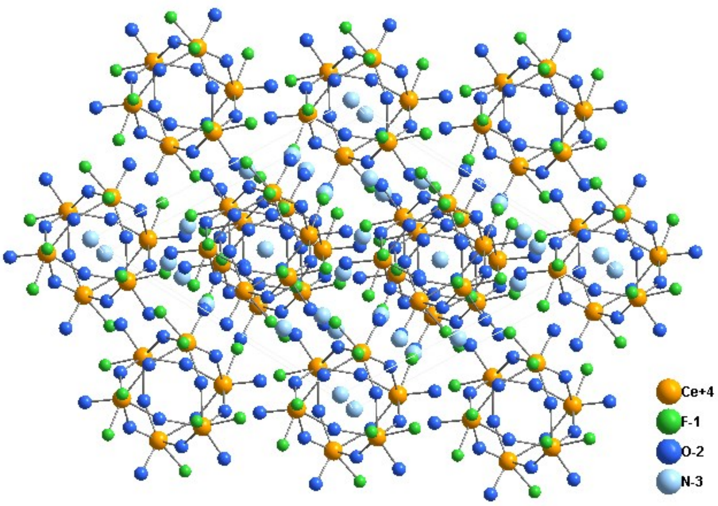

Figure S13 the structure of precursor $H_{25.5}(NH_4)_{10.5}Ce_9O_{27}F_{18}$

Table S2. Details of calculate structure for CeF_3-O.

Configuration		**CeF_3-O**	
Lattice parameter (Aº)	a 7.128	b 7.128	c 7.288
Cell angle	α 90º	β 90 º	γ 120 º
Ce1	0.33333	0.33333	0.00000
F1	0.38000	0.04600	0.16000
F2	0.33333	0.66667	0.08330
F3	0.00000	0.00000	0.25000
O	0.33333	0.33333	0.25000

Table S3. The location and number of k-points

Number	**Label**			
1	GAMMA	0	0	0
2	Y	0.5	0.5	0
3	T	0.5	0.5	0.5
4	T_2	0.5	0.5	-0.5
5	Z	0	0	0.5
6	Z_2	0	0	-0.5
7	S	0	0.5	0
8	R	0	0.5	0.5
9	R_2	0	0.5	-0.5
10	DELTA_0	-0.33321	0.333207	0
11	F_0	0.333207	0.666793	0
12	B_0	-0.33321	0.333207	0.5
13	B_2	-0.33321	0.333207	-0.5
14	G_0	0.333207	0.666793	0.5
15	G_2	0.333207	0.666793	-0.5