CsCl−Flux Synthesis of Titanium Oxynitride $Ti_{2.85}O_4N$ for Photocatalysis

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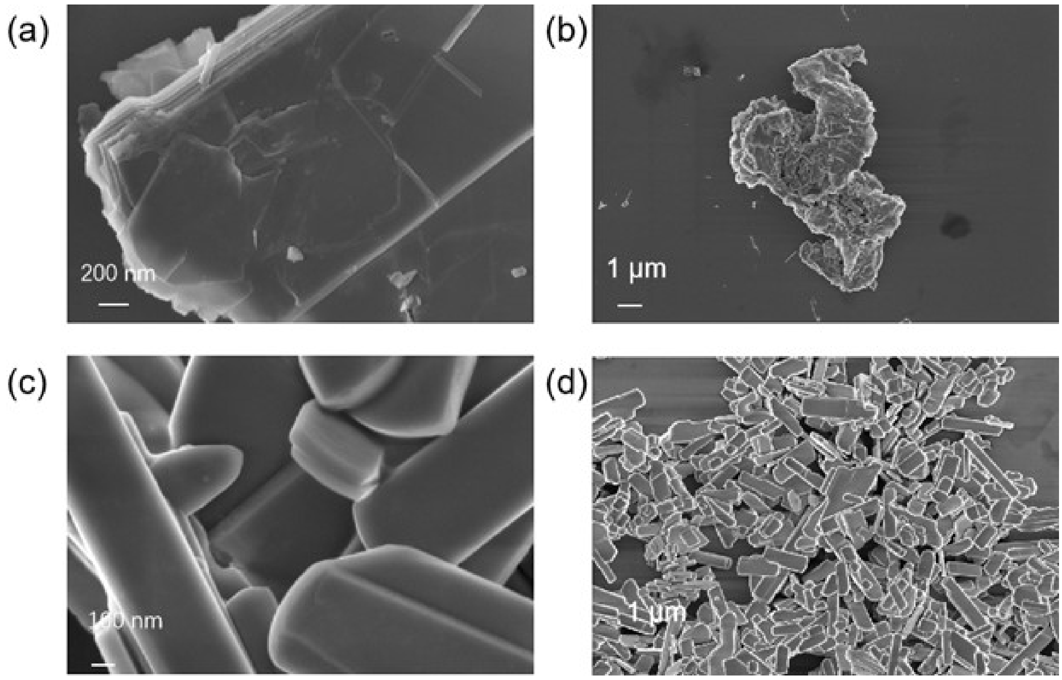

Fig.S1 SEM images of the product (a) and (b) $CsTi_{0.68}O_4$, (c) and (d) $CsTi_{0.68}O_4$-Cl.

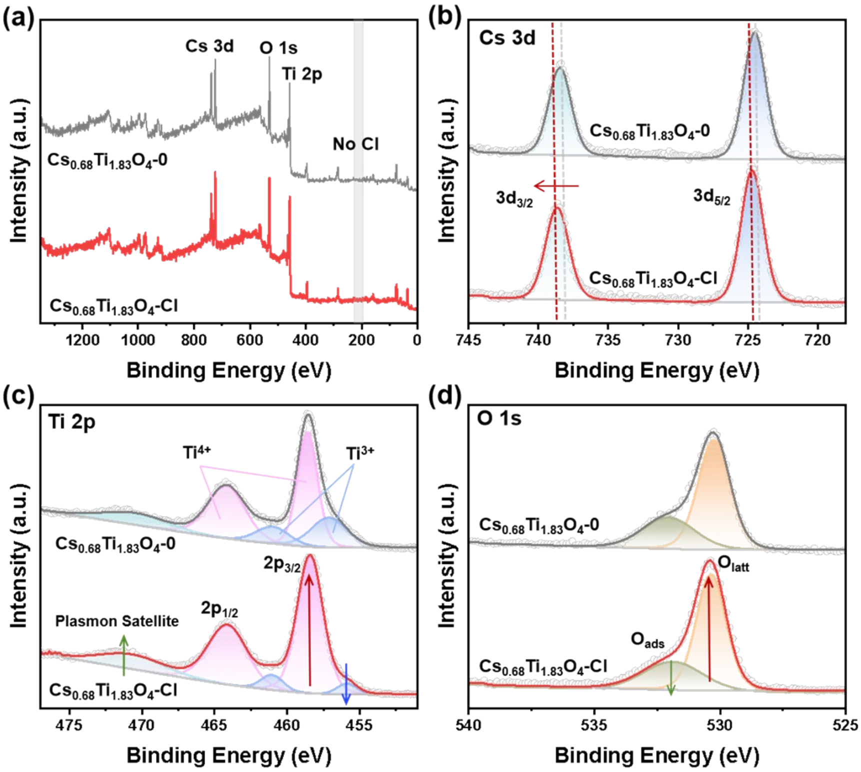

Fig. S2 XPS analysis of pristine and Cl-assisted synthesized $Cs_{0.68}Ti_{1.83}O_4$.

(a) Survey spectra, (b) Cs 3d, (c) Ti 2p, and (d) O 1s. (The suffix "-Cl" denotes samples synthesized via a molten chloride salt method, with no residual Cl detected.)

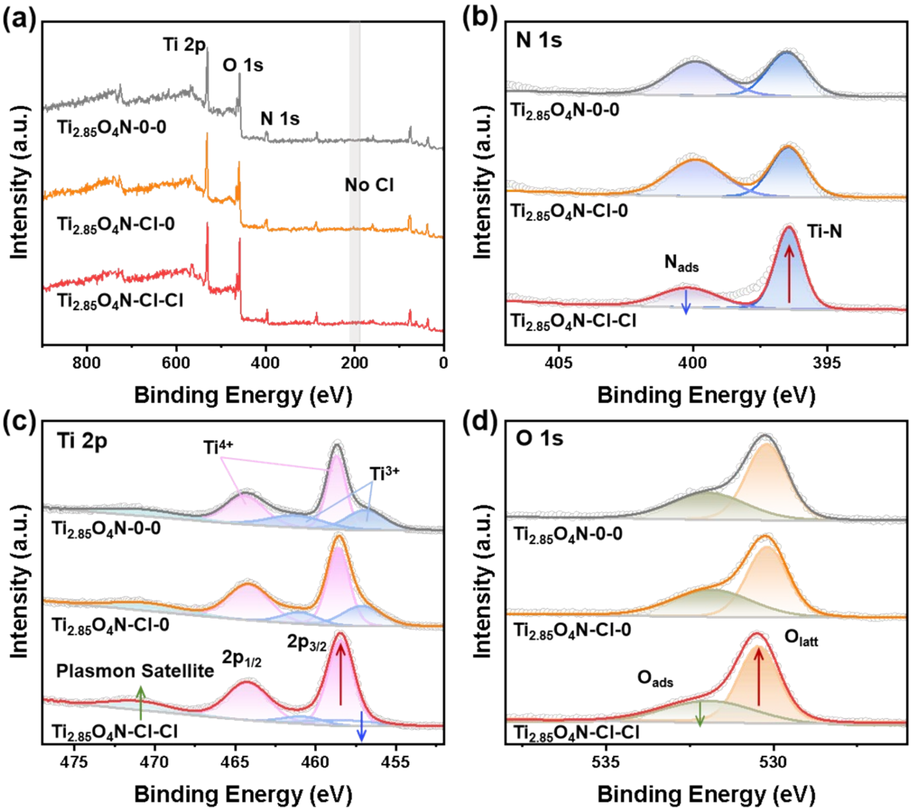

Fig. S3 XPS analysis of $Ti_{2.85}O_4N$ with varying Cl-treatment steps.
(a) Survey spectra, (b) N 1s, (c) Ti 2p, and (d) O 1s. (Labels "-0" and "-Cl" indicate the absence or presence of Cl-assisted processing steps, respectively.)

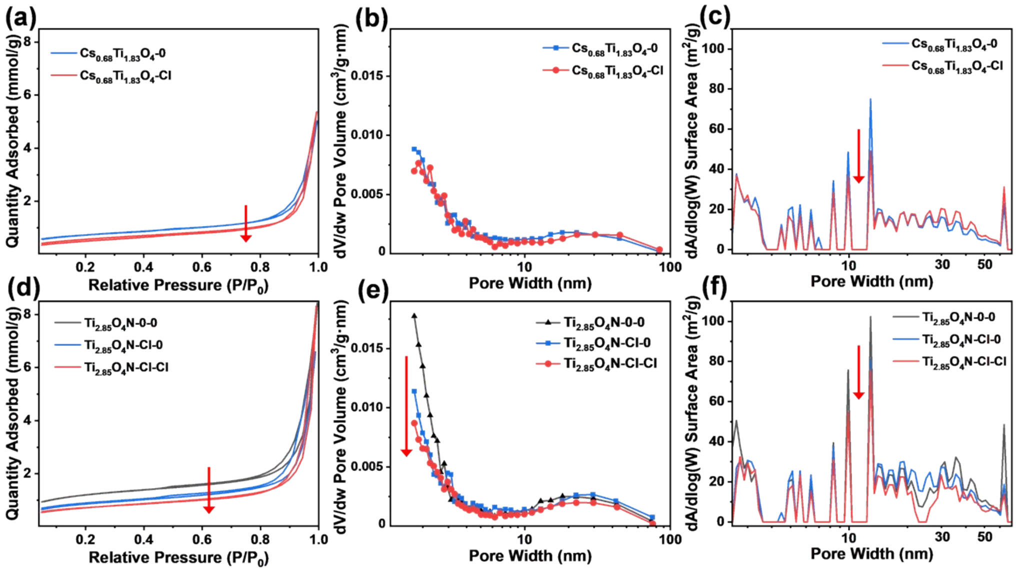

Fig. S4 N_2 adsorption-desorption isotherm test results. (a,d) Isotherm Linear Absolute Plots, (b,e) Barret-Joyner-Halenda Adsorption Pore Volume vs. Pore Width Plots, (c,f) Brunauer-Emmet-Teller Surface Area vs. Pore Width Plots.

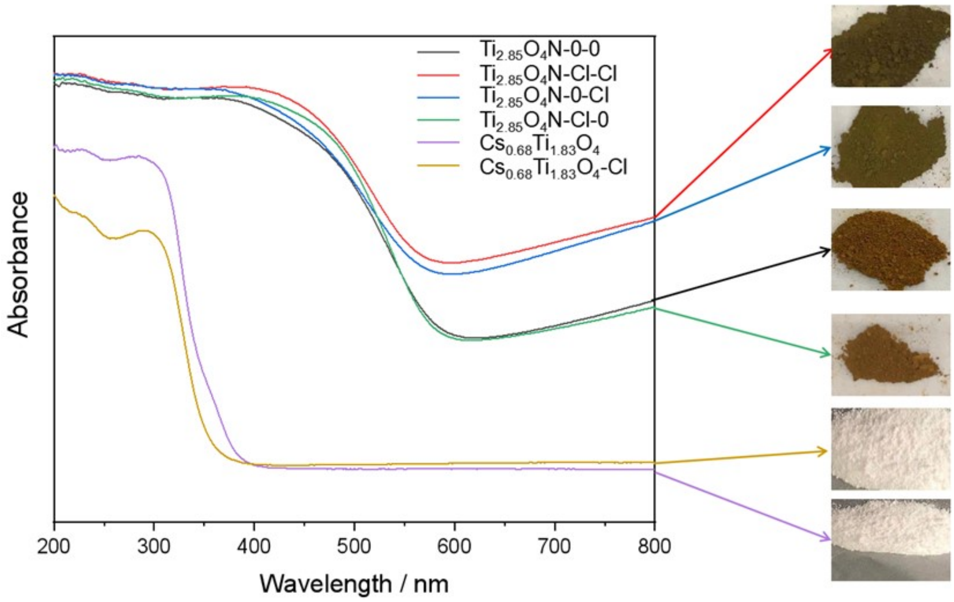

Fig. S5 UV-visible DRS spectra and photographs of the oxides and oxynitrides.

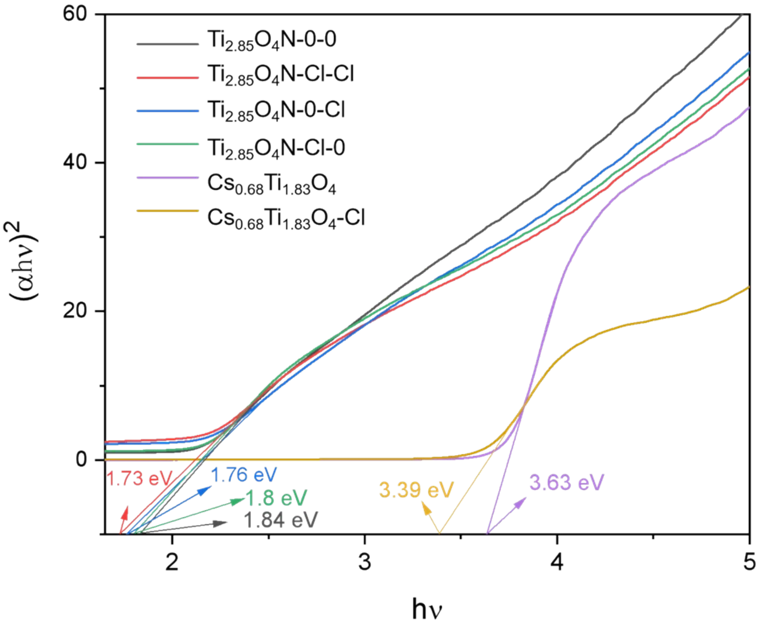

Fig. S6 The band gap obtained by fitting the Tauc-Plot method between oxides and oxynitrides.

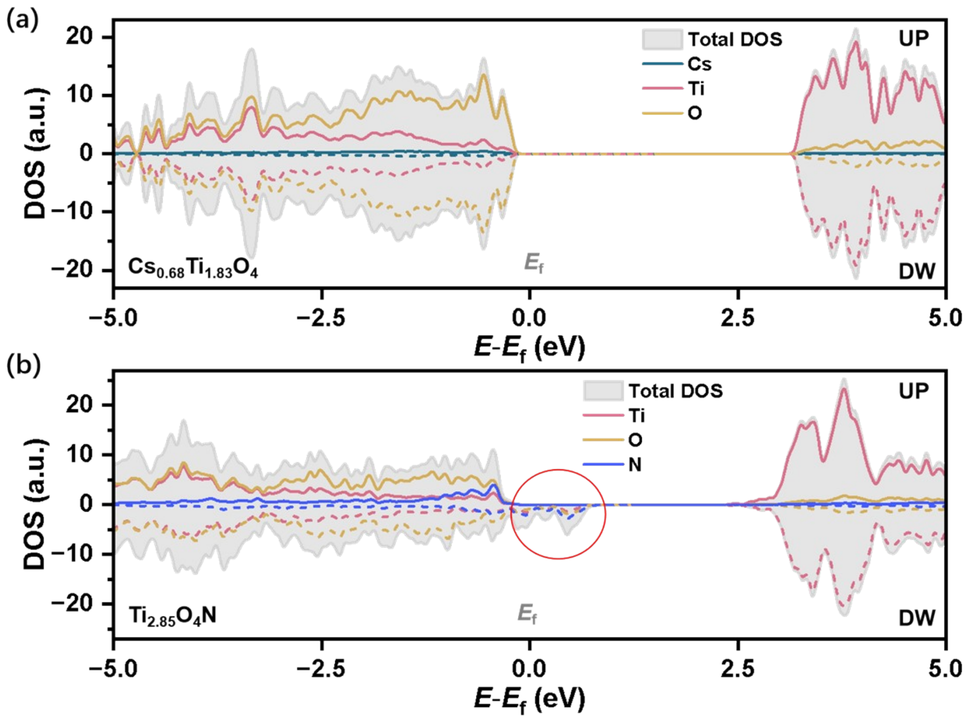

Fig. S7 The density of states (PDOS) of (a) $CsTi_{0.68}O_4$ and (b) $Ti_{2.85}O_4N$.

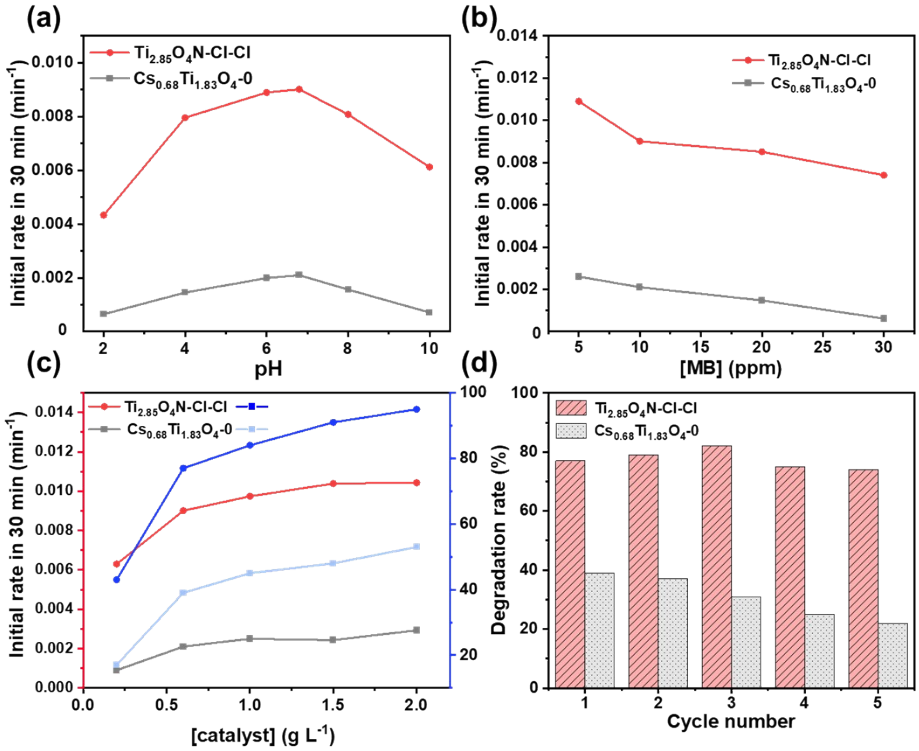

Fig. S8 Influencing factors and stability of photocatalysis. (a) Effect of pH. [Catalyst] = 0.6 g L^{-1}; [MB] = 10 ppm. (b) Effect of MB concentration. [Catalyst] = 0.6 g L^{-1}, pH 6.8. (c) Effect of catalyst concentration. [MB] = 10 ppm; pH 6.8. (d) Recycling stability.

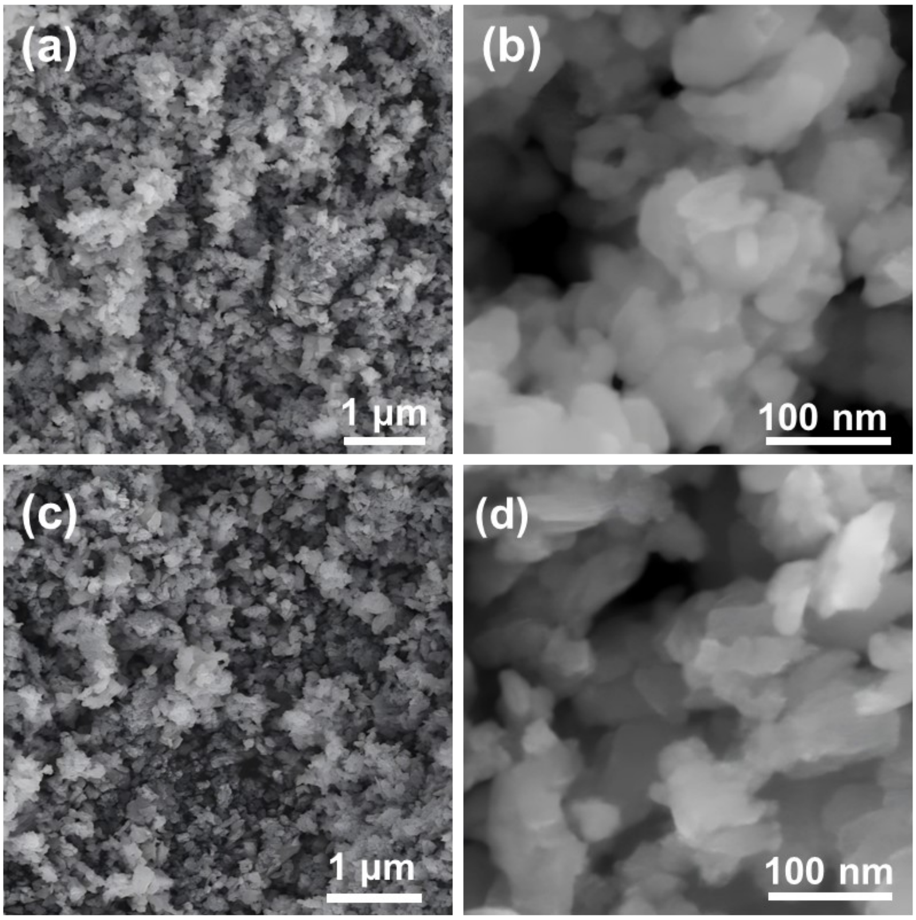

Fig. S9 Recycling stability of $Ti_{2.85}O_4N$-Cl-Cl morphology during photocatalysis. (a-b) SEM of $Ti_{2.85}O_4N$-Cl-Cl after 1 cycle. (c-d) SEM of $Ti_{2.85}O_4N$-Cl-Cl after 5 cycles.

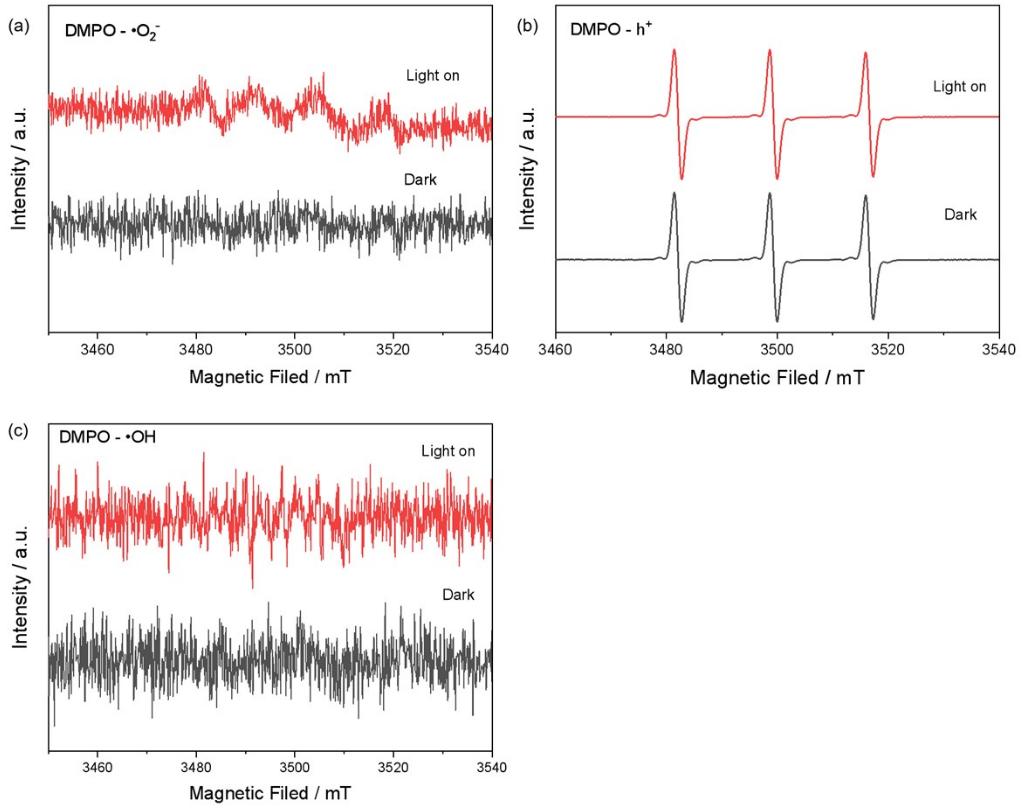

Fig. S10 (a) DMPO-$\bullet O_2^-$, (b) DMPO-h^+, (c) TEMPO-•OH spectrum of the electron spin resonance tested in dark and light conditions.

Table S1 Element content obtained from EDS scanning.

	Cs (wt%)	Ti (wt%)	O (wt%)	N (wt%)
$Ti_{2.85}O_4N$-0-0	11.71	55.495	21.94	5.92
$Ti_{2.85}O_4N$-0-Cl	18.65	50.765	21.84	5.23
$Ti_{2.85}O_4N$-Cl-0	20.445	50.025	19.385	6.43
$Ti_{2.85}O_4N$-Cl-Cl	19.64	50.705	18.905	6.92

Table S2 Specific surface area, pore volume and pore size information

Sample	BET Surface Area m^2/g	t-Plot Micropore Area m^2/g	Single point Total Pore Volume cm^3/g	Average Pore Size nm
$Cs_{0.68}Ti_{1.83}O_4$-0	56.86	10.97	0.0866	17.37
$Cs_{0.68}Ti_{1.83}O_4$-Cl	45.69	2.22	0.0760	20.26
$Ti_{2.85}O_4N$-0-0	92.68	22.40	0.1242	20.13
$Ti_{2.85}O_4N$-Cl-0	67.28	12.63	0.1122	19.67
$Ti_{2.85}O_4N$-Cl-Cl	56.14	6.65	0.0926	26.91

Table S3 Performance Comparison.

	Catalyst amount ($g\ L^{-1}$)	Pollutant Consent ($mg\ L^{-1}$)	Reaction time (min)	Degradation (%)	Ref.
$Ti_{2.85}O_4N$-Cl-Cl	0.6	10	120	77	This work
$Cs_{0.68}Ti_{1.83}O_4$	0.6	10	120	39	This work
Carbon-doped TiO_2	1	10	100	61	S1
Carbon/TiO_2 (T-PVA)	1	10	60	48	S2
0.1 wt% Ag -doped TiO_2	10	10	600	71	S3
5% N/TiO_2	1	20	150	56.5	S4
AlHF-TiO_2	2.5	20	60	65	S5
Hg-doped TiO_2	Thin films	31.985	120	72	S6

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