Supporting Information

TiO_2 with controllable oxygen vacancy for efficient isopropanol degradation: photoactivity and reaction mechanism

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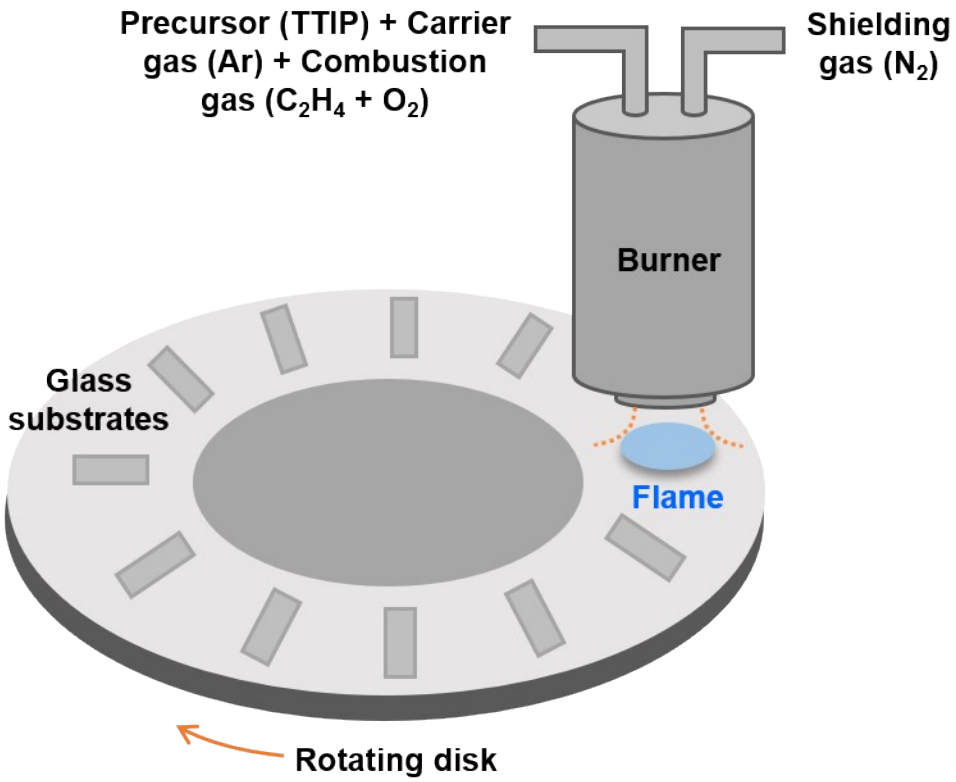

Fig. S1 Schematic illustration of TiO_2 nanoparticles prepared by FSRS method.

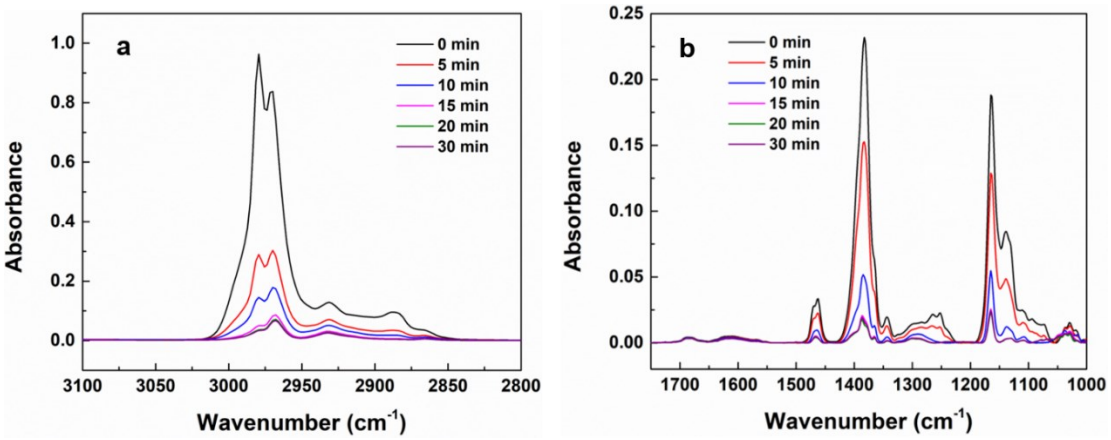

Fig. S2 (a, b) *In situ* DRIFTS spectra for IPA desorption on TiO_{2-x}-20 min under the dark which indicate that the steady-state can be reached at 15 min.

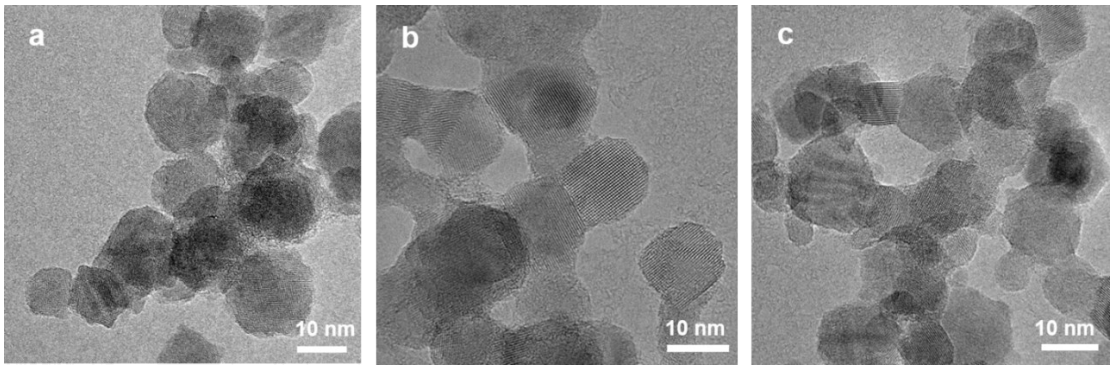

Fig. S3 TEM images of (a) TiO_{2-x}-4 min, (b) TiO_{2-x}-8 min and (c) TiO_{2-x}-35 min.

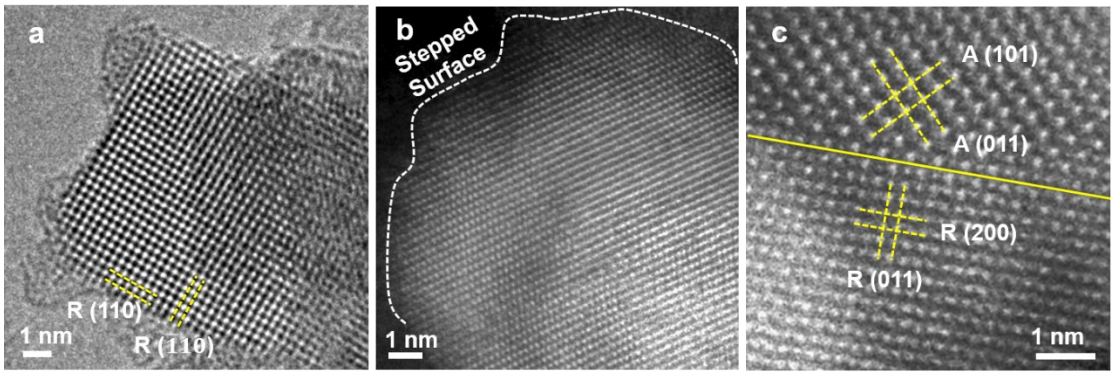

Fig. S4 Atomic-resolution TEM and STEM analysis of TiO_{2-x}-20 min. (a) Atomic-resolution TEM image of TiO_{2-x}-20 min with rutile (110) and ($\bar{1}$10) facets co-present. Aberration-corrected HAADF-STEM images of TiO_{2-x}-20 min (b) with stepped surface, and (c) with anatase-rutile hetero-phase junction.

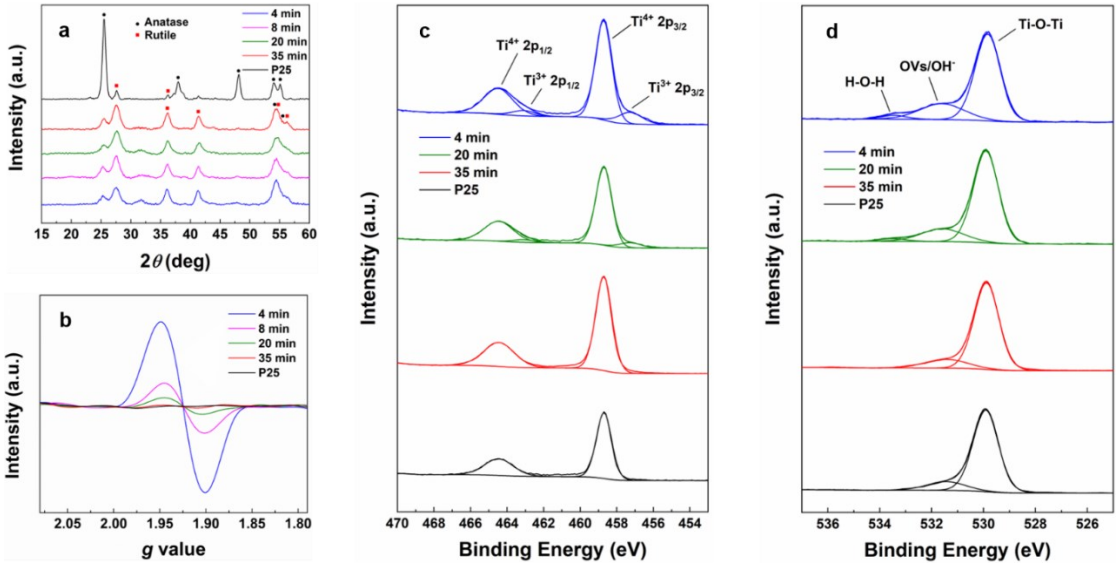

Fig. S5 (a) XRD patterns, (b) EPR spectra. XPS spectra of (c) Ti 2p and (d) O 1s.

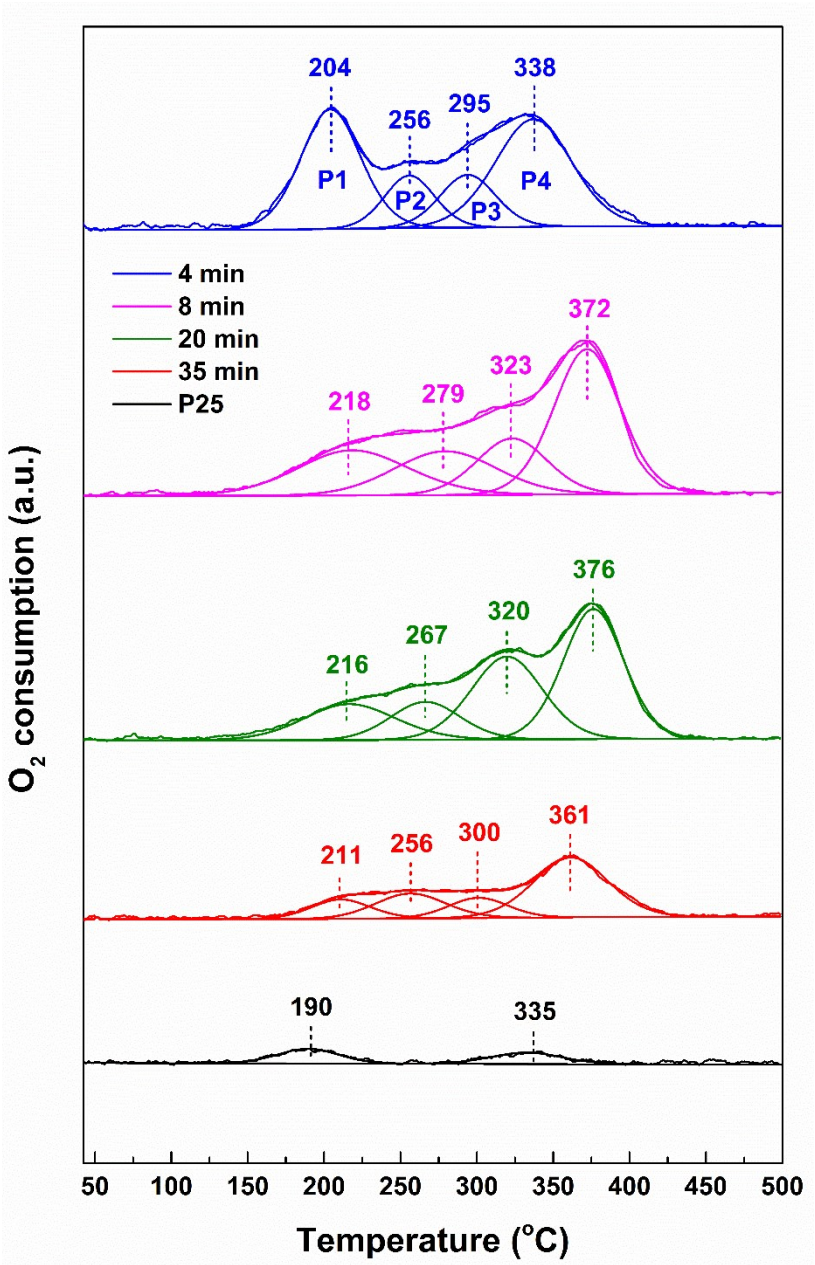

Fig. S6 TPO profiles flame-made TiO_{2-x} and P25 TiO_2.

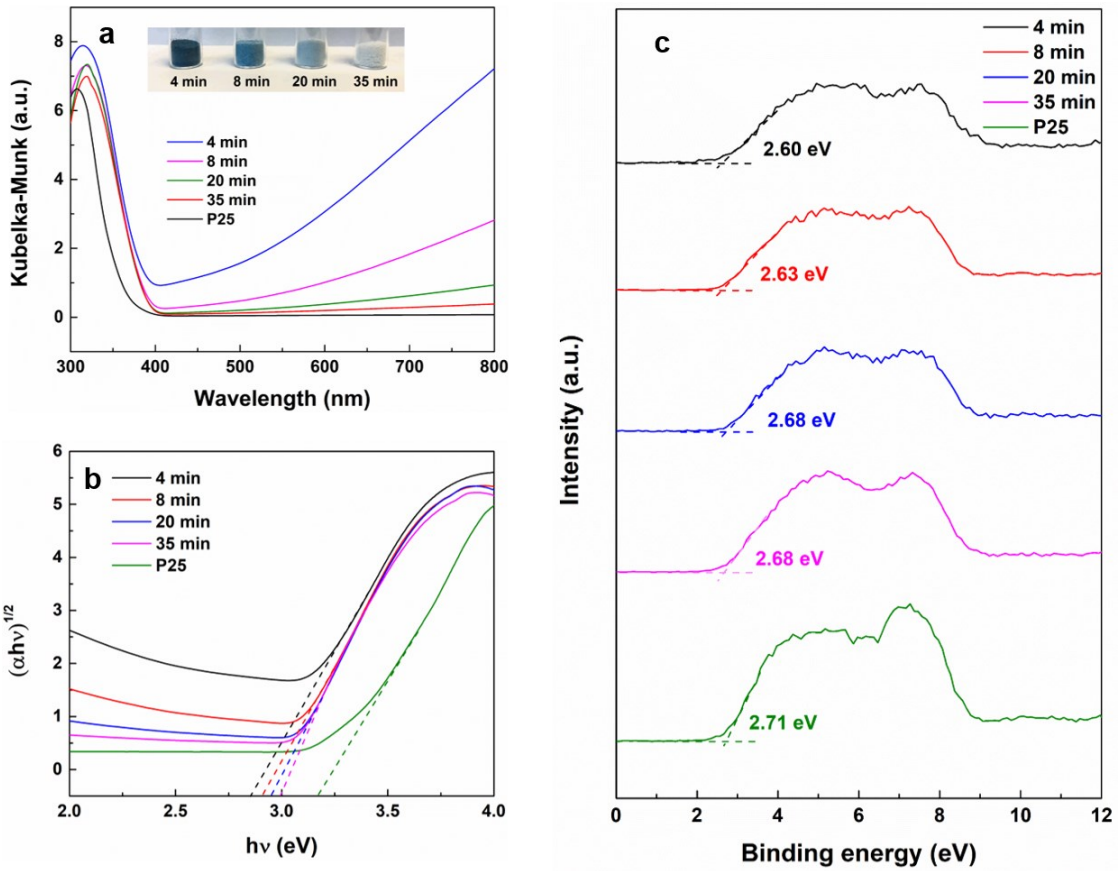

Fig. S7 (a) UV-Vis DRS spectra (inset: picture of flame-made samples), (b) Bandgap analysis and (c) Valence band position of flame-made TiO_{2-x} and P25 TiO_2.

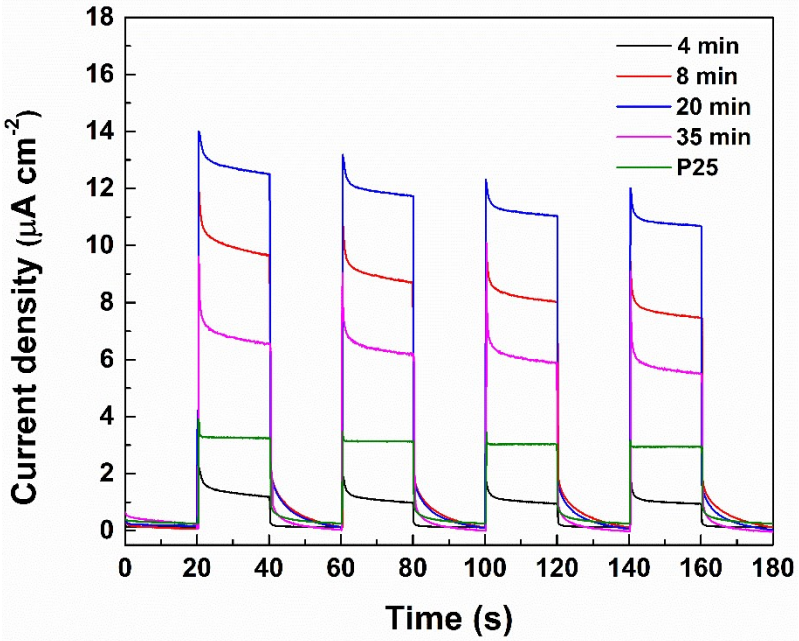

Fig. S8 Transient photocurrent density of flame-made TiO_{2-x} and P25 TiO_2.

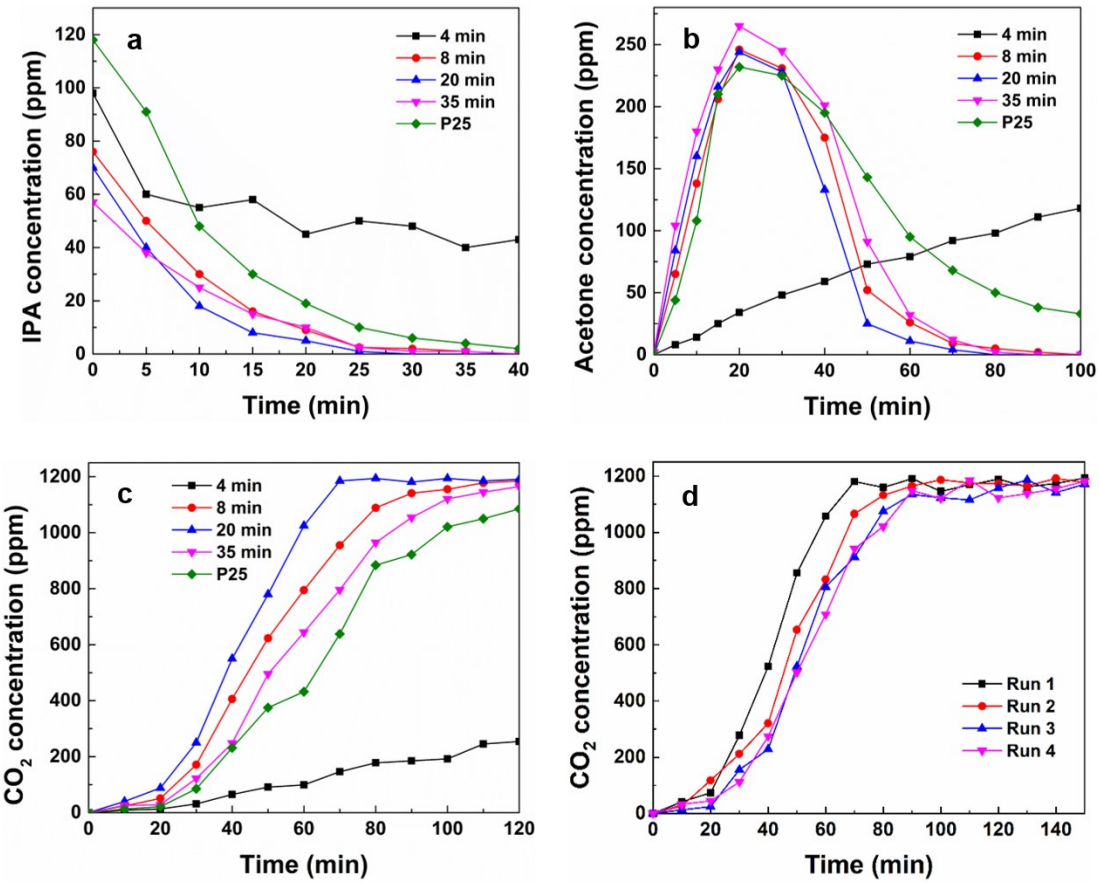

Fig. S9 (a) Photocatalytic IPA degradation, (b) Acetone production, and (c) CO_2 generation over flame-made TiO_{2-x} and P25 TiO_2. (d) Stability test of TiO_{2-x}-20 min (40 mg of TiO_2, 400 ppm initial IPA concentration, 300 W Xe lamp).

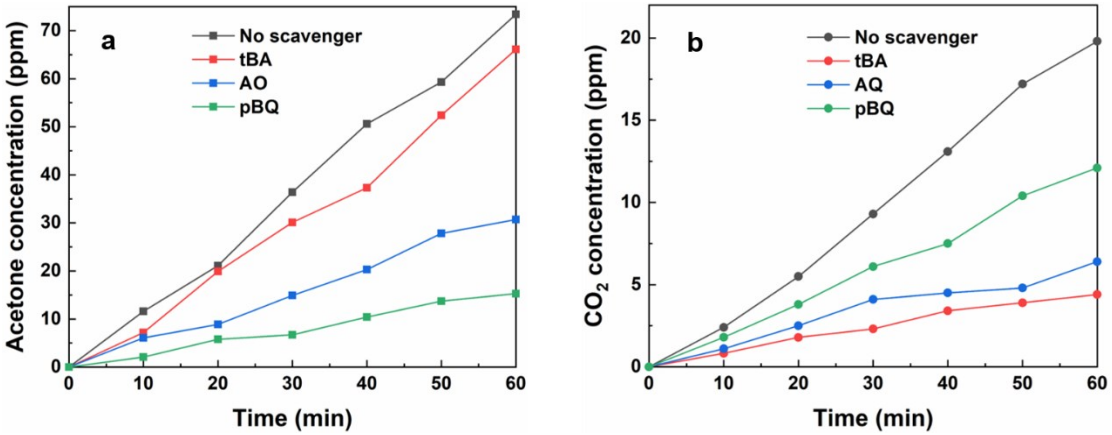

Fig. S10 IPA photodegradation over TiO_{2-x}-20 min with different scavengers. (a) Acetone evolution amount; (b) CO_2 generation amount (40 mg of TiO_2, 400 ppm initial IPA concentration, 20% O_2 concentration, 75% RH, 150 W Xe lamp, > 400 nm).

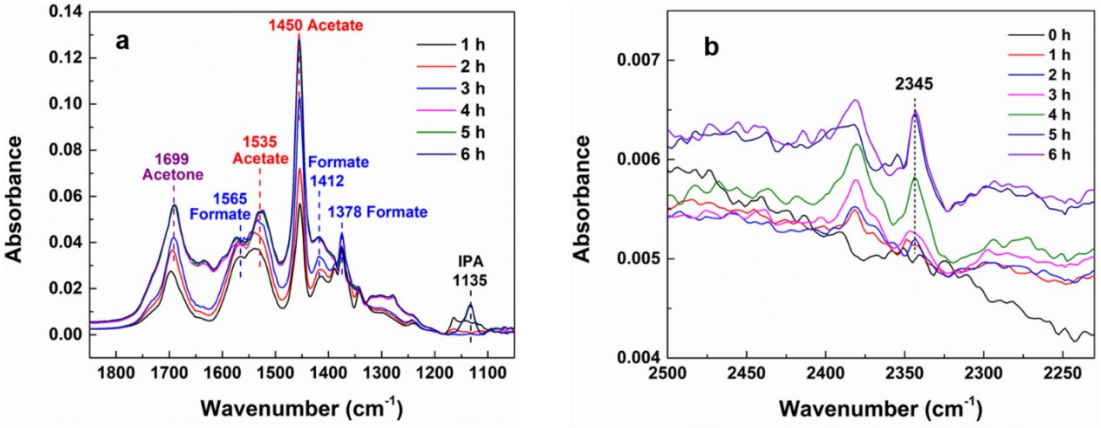

Fig. S11 *In situ* DRIFTS spectra for TiO_{2-x}-20 min under light illumination (300 W Xe lamp, > 400 nm) for 6 h in the range of (a) 1050-1850 cm^{-1} and (b) 2230-2500 cm^{-1}.

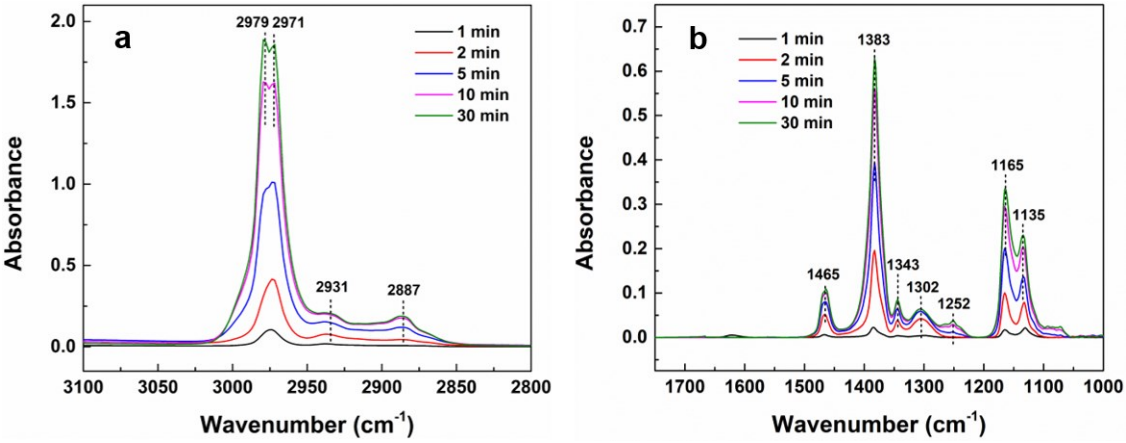

Fig. S12 *In situ* DRIFTS spectra of (a,b) P25 TiO_2 in the dark after purging with IPA

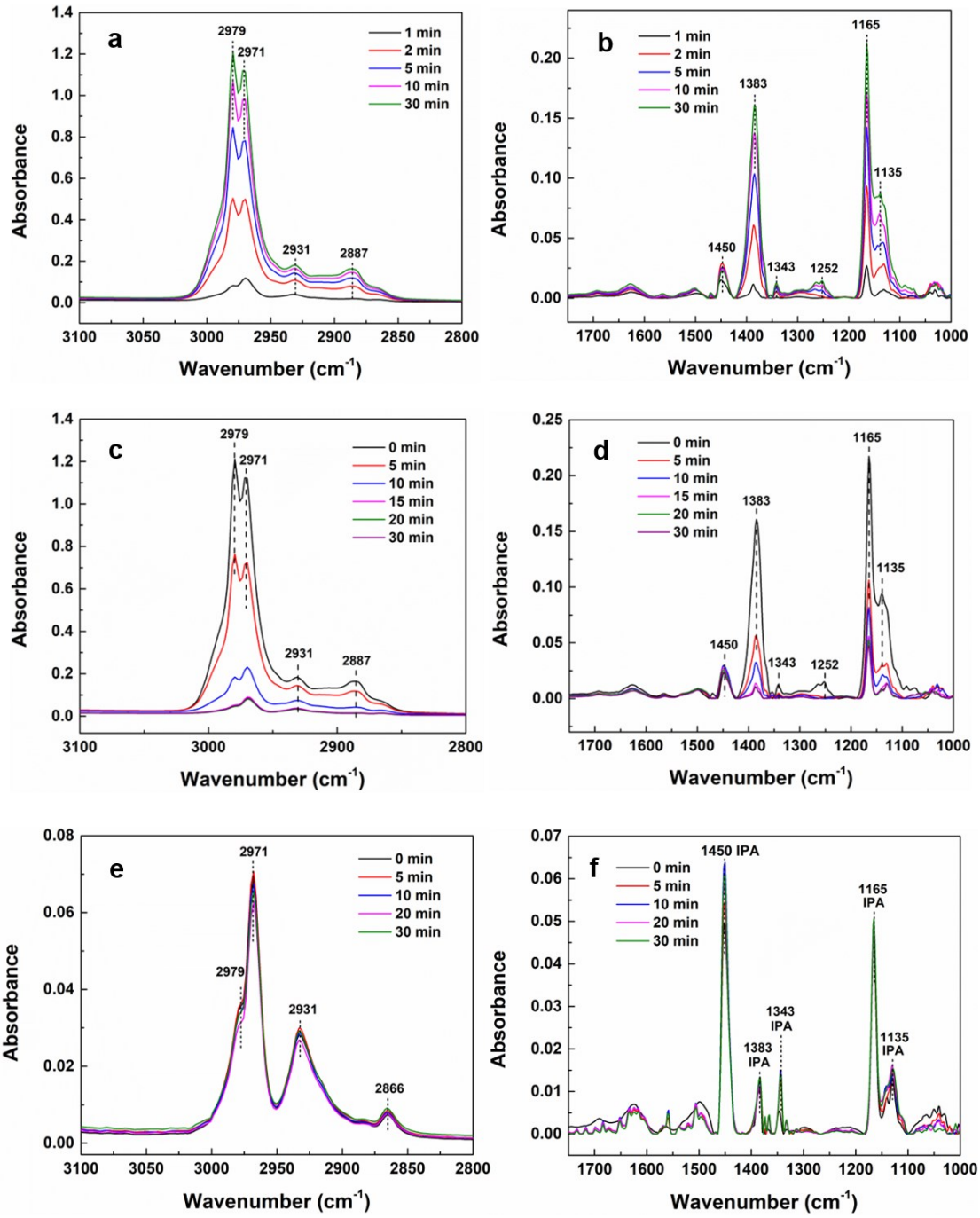

Fig. S13 *In situ* DRIFTS spectra for TiO_{2-x}-4 min under the dark adsorption (a) and (b); dark desorption (c) and (d); light irradiation (300 W Xe lamp, > 400 nm) (e) and (f).

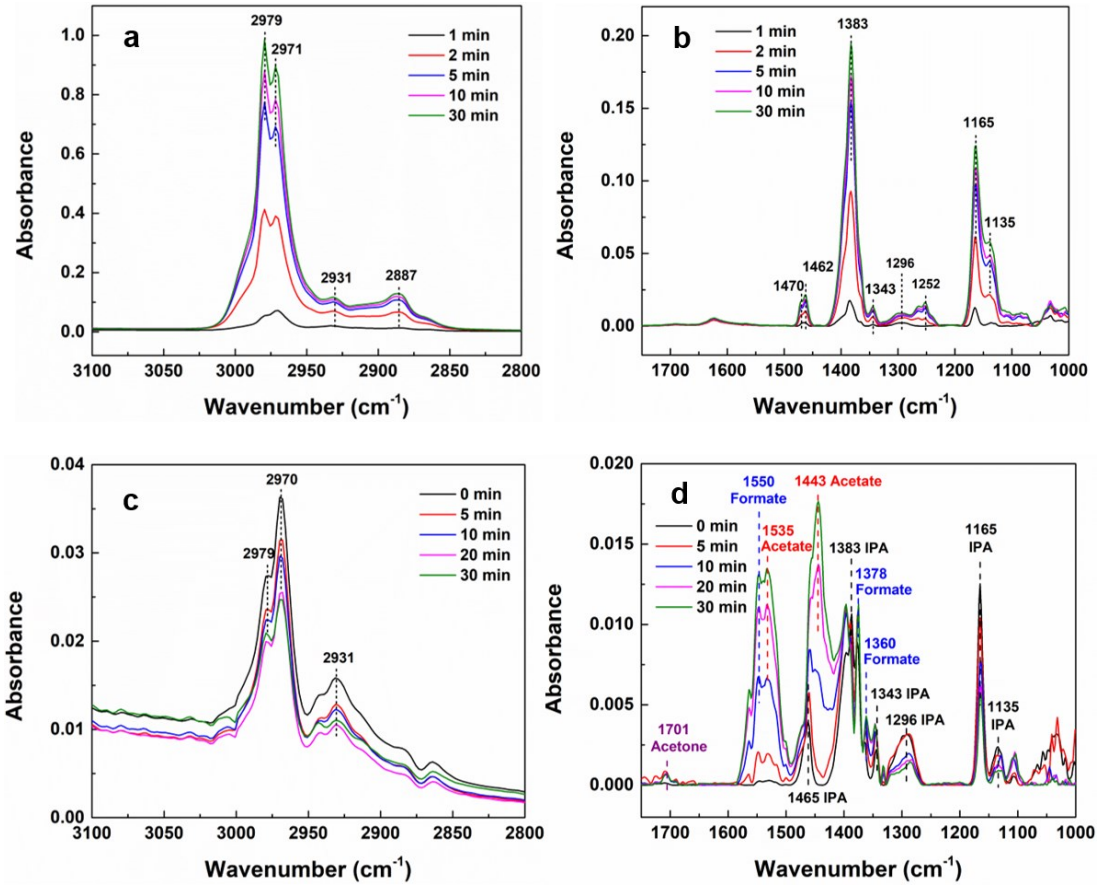

Fig. S14 *In situ* DRIFTS spectra for TiO_{2-x}-35 min in the dark (a) and (b); under light irradiation (300 W Xe lamp, > 400 nm) (c) and (d).

Table S1. The initial IPA, O_2, H_2O amount and their molar ratios under different reaction conditions

Samples and reaction conditions	IPA amount (mmol)	O_2 amount (mmol)	H_2O amount (mmol)	Molar ratio IPA : O_2 : H_2O
TiO_{2-x}-4 min, 20 vol% O_2, RH 0%	18	8929	0	1 : 496 : N/A
TiO_{2-x}-8 min, 20 vol% O_2, RH 0%	18	8929	0	1 : 496 : N/A
TiO_{2-x}-20 min, 20 vol% O_2, RH 0%	18	8929	0	1 : 496 : N/A
TiO_{2-x}-35 min, 20 vol% O_2, RH 0%	18	8929	0	1 : 496 : N/A
P25 TiO_2, 20 vol% O_2, RH 0%	18	8929	0	1 : 496 : N/A
TiO_{2-x}-20 min, 0 vol% O_2, RH 0%	18	0	0	1 : N/A : N/A
TiO_{2-x}-20 min, 5 vol% O_2, RH 0%	18	2232	0	1 : 124 : N/A
TiO_{2-x}-20 min, 35 vol% O_2, RH 0%	18	15625	0	1 : 868 : N/A
TiO_{2-x}-20 min, 50 vol% O_2, RH 0%	18	22322	0	1 : 1240 : N/A
TiO_{2-x}-20 min, 100 vol% O_2, RH 0%	18	44645	0	1 : 2480 : N/A
TiO_{2-x}-20 min, 20 vol% O_2, RH 25%	18	8929	240	1 : 496 : 13
TiO_{2-x}-20 min, 20 vol% O_2, RH 50%	18	8929	480	1 : 868 : 27
TiO_{2-x}-20 min, 20 vol% O_2, RH 75%	18	8929	720	1 : 868 : 40

Table S2. The specific surface area (SSA), phase composition and electronic properties of flame-made TiO_{2-x} samples and P25.

Sample	SSA (m^2 g^{-1})	Rutile content (%)	CB potential (eV)	VB potential (eV)	Bandgap energy (eV)
TiO_{2-x}-4 min	110.7	74.4	-0.25	2.60	2.85
TiO_{2-x}-8 min	127.4	72.3	-0.28	2.63	2.91
TiO_{2-x}-20 min	130.8	78.5	-0.27	2.68	2.95
TiO_{2-x}-35 min	121.3	76.7	-0.32	2.68	3.0
P25 TiO_2	50.0	19.8	-0.49	2.71	3.2

Table S3. Quantitative defects analysis of flame-made TiO_{2-x} using TPO measurement.

Sample	O_2 consumption (μmol g^{-1})				x (TiO_{2-x})
	P1	P2	P3	P4	
4 min	250	89	98	277	0.114
8 min	170	143	125	321	0.121
20 min	107	89	196	259	0.104
35 min	36	54	36	143	0.043
P25	24	0	24	0	0.008

Table S4. Photocatalytic activity of IPA degradation over flame-made TiO_{2-x} and P25 with different light sources.

Sample	Visible light irradiation		UV-Vis irradiation	
	Mineralization in 6 h (%)	CO_2 production rate (ppm h^{-1})	Mineralization in 70 min (%)	CO_2 production rate (ppm h^{-1})
TiO_{2-x}-4 min	4.1	8.2	12.2	125.1
TiO_{2-x}-8 min	20.8	41.7	79.6	818.6
TiO_{2-x}-20 min	22.7	45.4	98.8	990
TiO_{2-x}-35 min	17.9	35.9	66.3	682.3
P25 TiO_2	8.8	17.5	53.2	546.8

Table S5. Assignments of the IR bands in the spectra of the surface species on TiO_2.

Vibration mode	Wavenumber (cm^{-1})	Species
$\nu_{as\ CH_3}$	2979, 2971	IPA
$\nu_{s\ CH_3}$	2931, 2866	
$\nu_{s\ C-H}$	2887	
$\delta_{as\ CH_3}$	1470, 1465, 1462, 1450	
$\delta_{s\ CH_3}$	1383	
γ_{C-H}	1343	
δ_{OH}	1302, 1296, 1252	
ν_{C-C}	1165	
ν_{C-O}	1135	
ν_{C-C}, γ_{CH_3}	1088, 1072	
$\nu_{C=O}$	1701, 1699	Acetone
$\delta_{s\ CH_3}$	1387	
$\nu_{as\ COO}$	1553, 1550, 1565	Formate
ρ_{COO}	1412	
δ_{C-H}	1378	
$\nu_{s\ COO}$	1360	
$\nu_{as\ COO}$	1535	Acetate
$\nu_{s\ COO}$	1443, 1450	