Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

Synthesis of TiO_xN_y oxynitrides with a tunable nitrogen content

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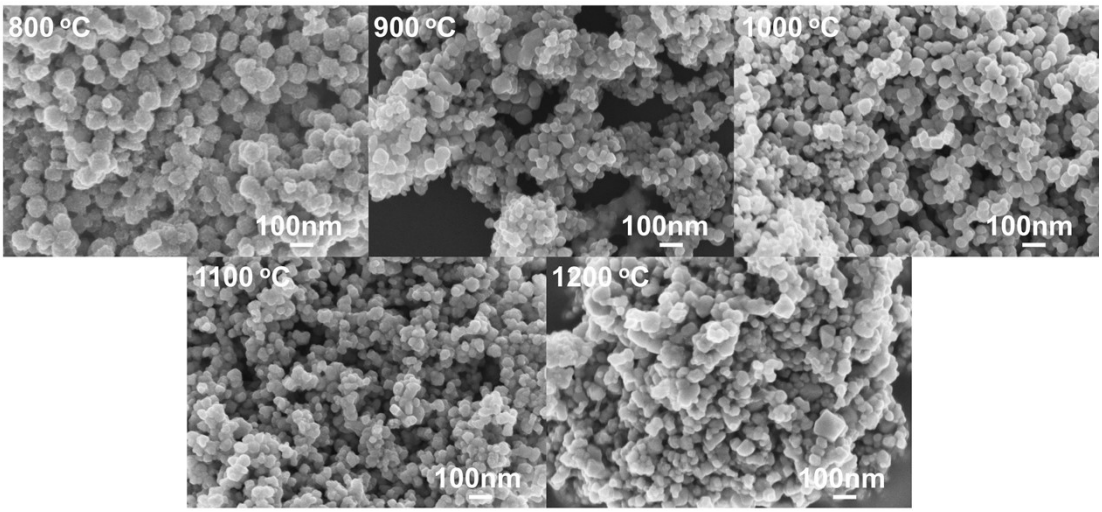

Figure S1. SEM images of oxynitrides TiO_xN_y synthesized at 800-1200 °C**.**

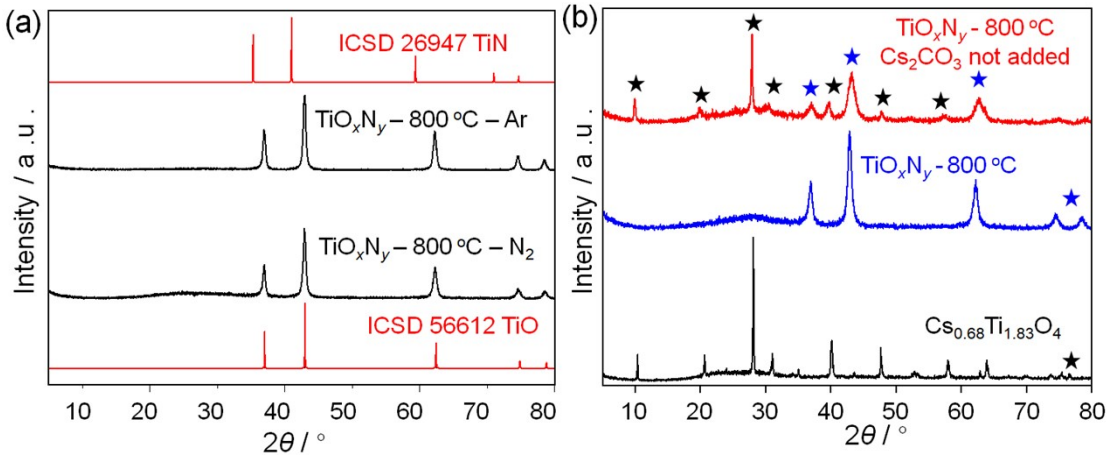

Figure S2. XRD pattern of (a) TiO_xN_y synthesized at 800 °C under N_2, Ar atmosphere, (b) TiO_xN_y synthesized at 800 °C with and without Cs_2CO_3. (★: *$Cs_{0.68}Ti_{1.83}O_4$ phase,* ★: *TiO_xN_y phase*).

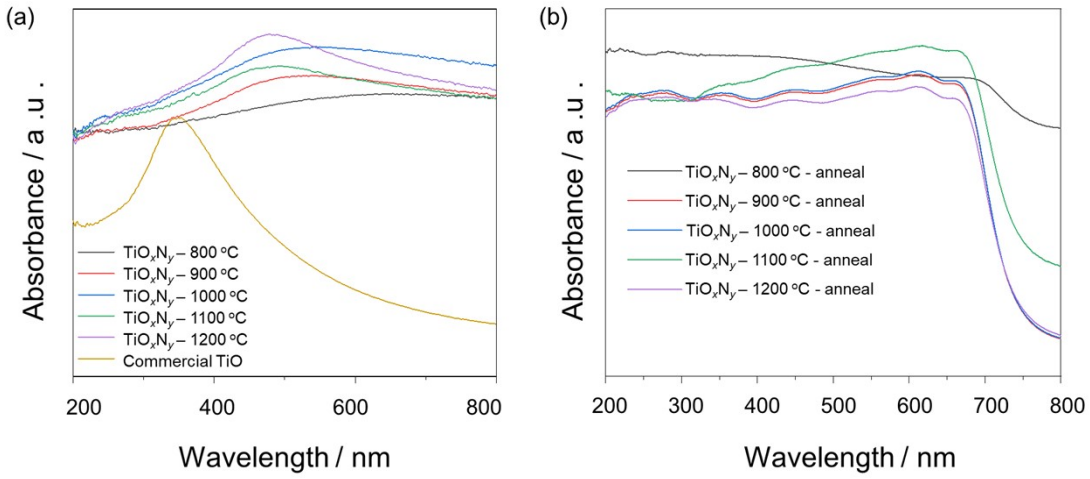

Figure S3. UV-vis spectroscopy. (a) Commercial TiO and TiO_xN_y synthesized at 800-1200 °C. (b) TiO_xN_y annealed at 350°C for 3h.

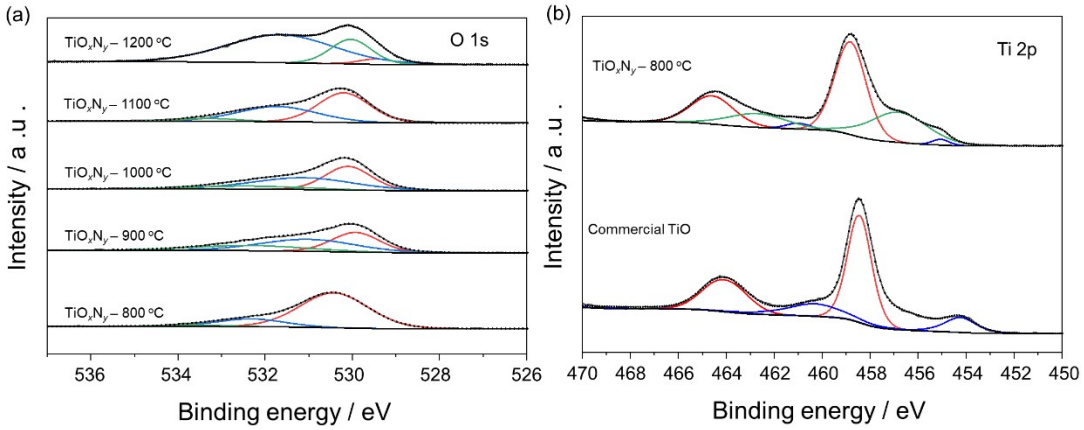

Figure S4. (a) Analysis energy spectrum of TiO_xN_y at different temperatures by XPS (O 1s). (b) Analysis energy spectrum of TiO_xN_y synthesized at 800°C and commercial TiO by XPS (Ti 2p).

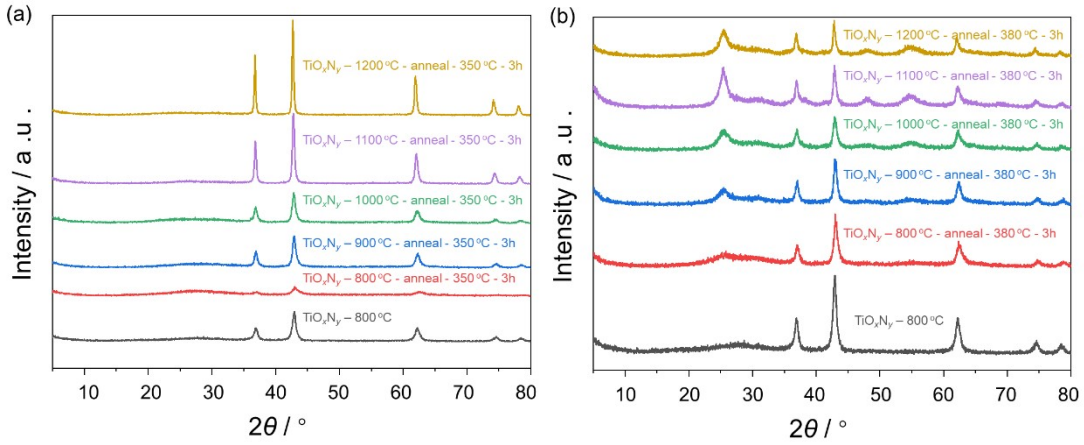

Figure S5. XRD patterns of TiO_xN_y annealed in air at different temperatures (a) 350 °C, (b) 380 °C.

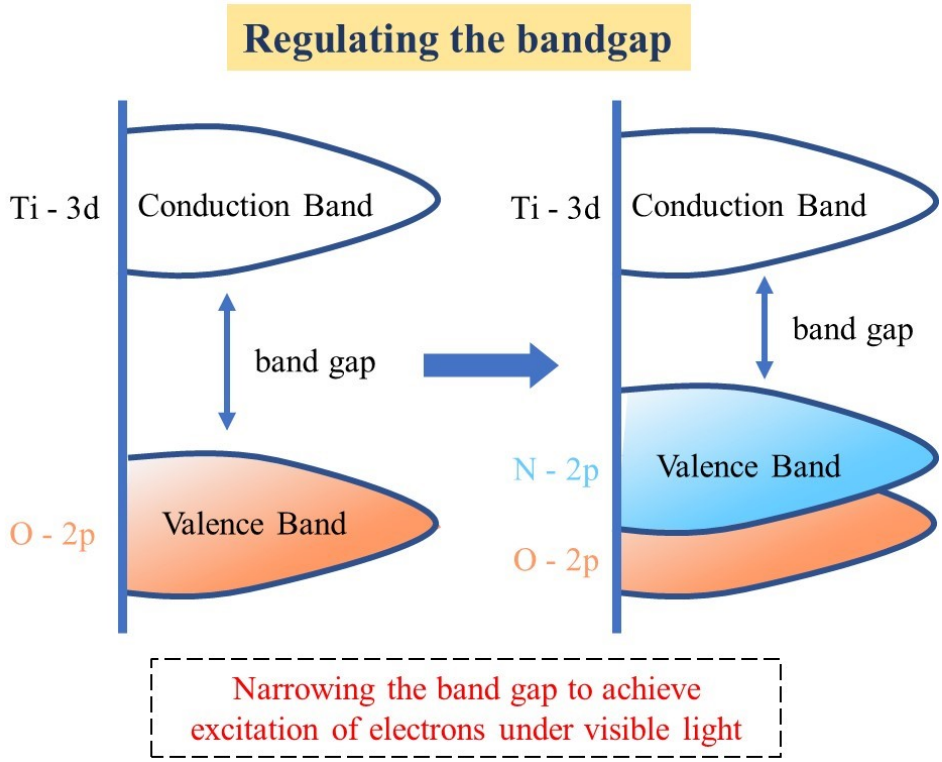

Figure S6. Schematic diagram of TiO_2 and TiO_xN_y energy bands

Table S1. The weight percent of N and C of oxynitride was obtained by elemental analyzer.

	N / wt%	C / wt%
800 °C	13.05	8.02
900 °C	17	6.994
1000 °C	16.3	11.77
1100 °C	19.72	1.92
1200 °C	19.92	2.02

Table S2. Lattice parameters and atomic occupancy of TiO_xN_y synthesized at 800 - 1100 °C determined by Rietveld analysis.

	a (Å)	b (Å)	c (Å)
TiO_xN_y-800 °C	4.2299	4.2299	4.2299
TiO_xN_y-900 °C	4.235	4.235	4.235
TiO_xN_y-1000 °C	4.23489	4.23489	4.23489
TiO_xN_y-1100 °C	4.2363	4.2363	4.2363

Table S3. Refined structural parameters of synchrotron XRD data for TiO_xN_y synthesized at 800 - 1100 °C.

	Atom	Coordinates			Uiso / Å^2	site
		x	y	z		
TiO_xN_y-800 °C	Ti	0.00000	0.00000	0.00000	0.002	4a
	N	0.50000	0.50000	0.50000	0.001	4b
	O	0.50000	0.50000	0.50000	0.001	4b
TiO_xN_y-900 °C	Ti	0.00000	0.00000	0.00000	0.002	4a
	N	0.50000	0.50000	0.50000	0.001	4b
	O	0.50000	0.50000	0.50000	0.001	4b
TiO_xN_y-1000 °C	Ti	0.00000	0.00000	0.00000	0.003	4a
	N	0.50000	0.50000	0.50000	0.001	4b
	O	0.50000	0.50000	0.50000	0.001	4b
TiO_xN_y-1100 °C	Ti	0.00000	0.00000	0.00000	0.003	4a
	N	0.50000	0.50000	0.50000	0.001	4b
	O	0.50000	0.50000	0.50000	0.001	4b