Supplementary Information

Unlocking the chemical environment of nitrogen in perovskite-type oxides

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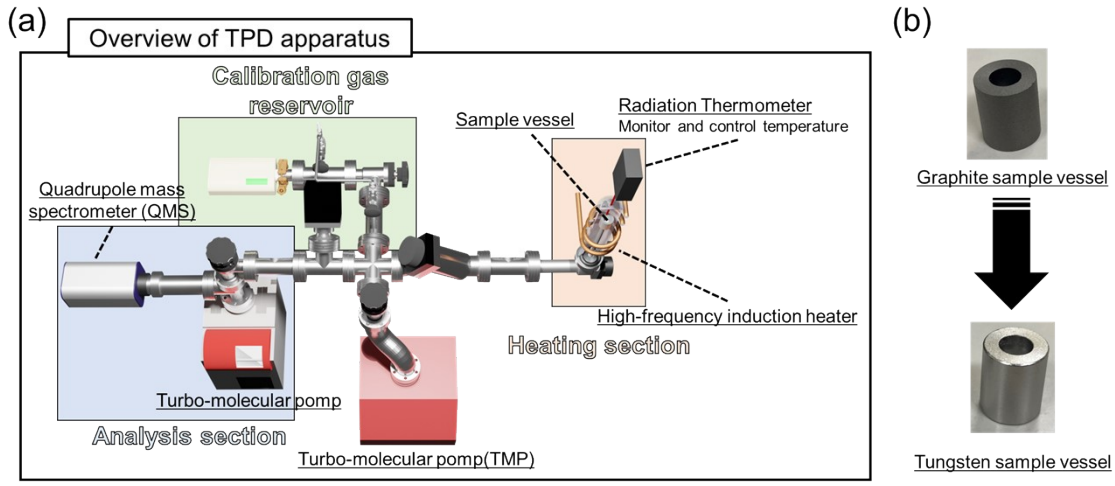

Fig. S1 (a) Schematic illustration of the advanced TPD device. (b) Photograph of graphite and tungsten sample holders.

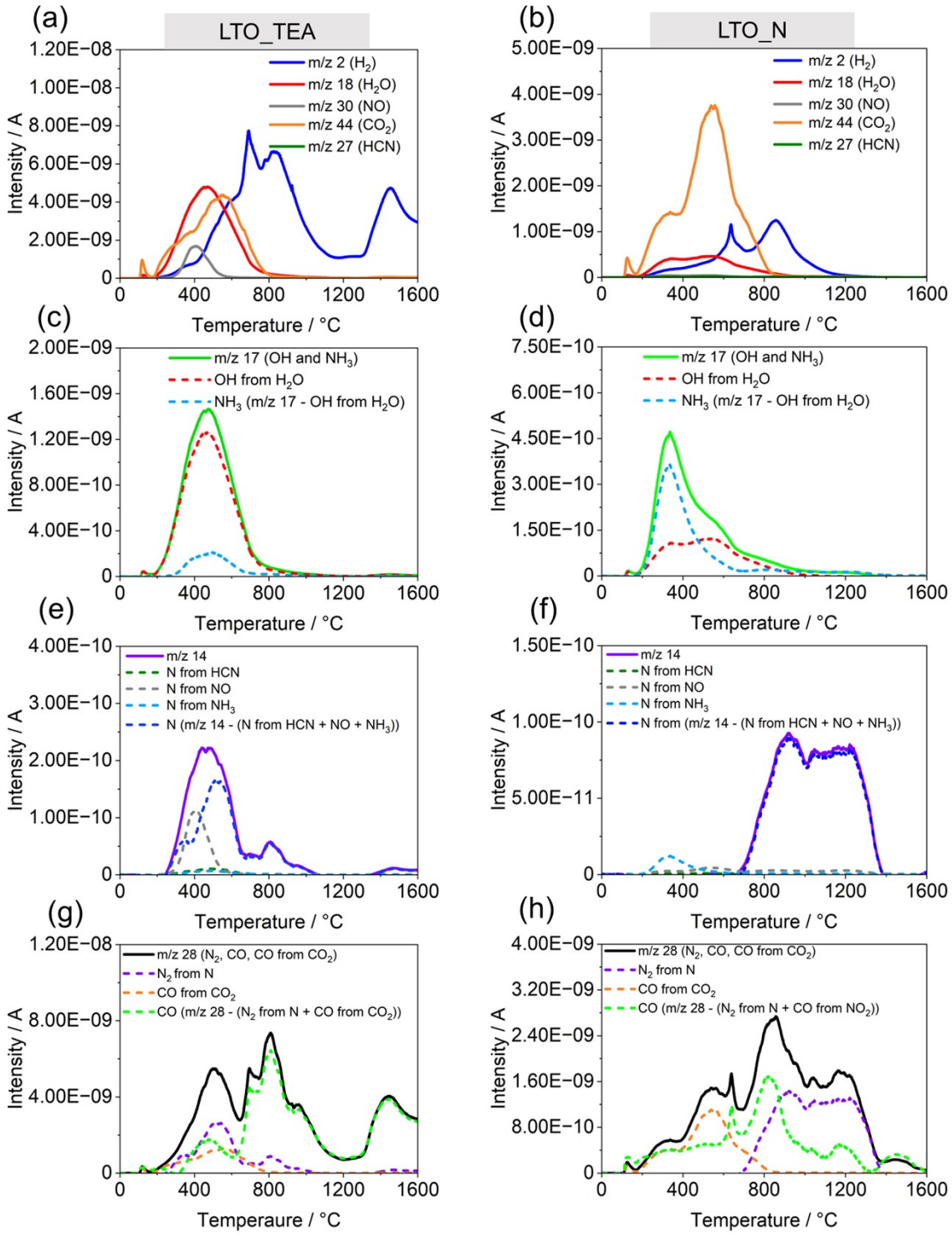

Fig. S2 TPD profiles of (a) LTO_TEA and (b) LTO_N for desorbed species: H_2 (m/z = 2), H_2O (m/z = 18), NO (m/z = 30), CO2 (m/z = 44) HCN (m/z = 27). Extraction of NH_3 component from TPD profile of (c) LTO_TEA and (d) LTO_N. Separation of TPD profile of (e) LTO_TEA and (f) LTO_N. Extraction of CO component from TPD profile of (g) LTO_TEA and (h) LTO_N.

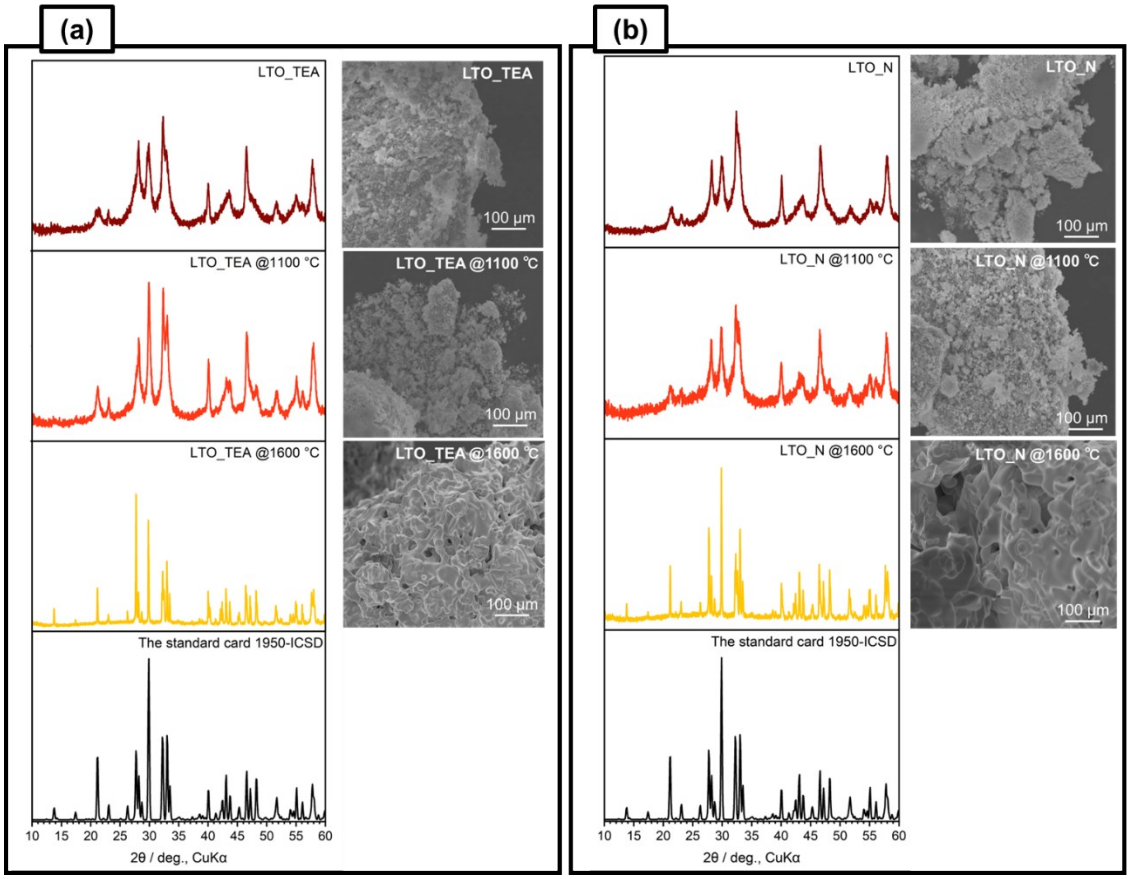

Fig. S3 Changes in PXRD patterns and SEM images of (a) LTO_TEA and (b) LTO_N before and after heat treatment at 1100 °C and 1600 °C, and standard XRD pattern of $La_2Ti_2O_7$ (the standard card 1950-ICSD).

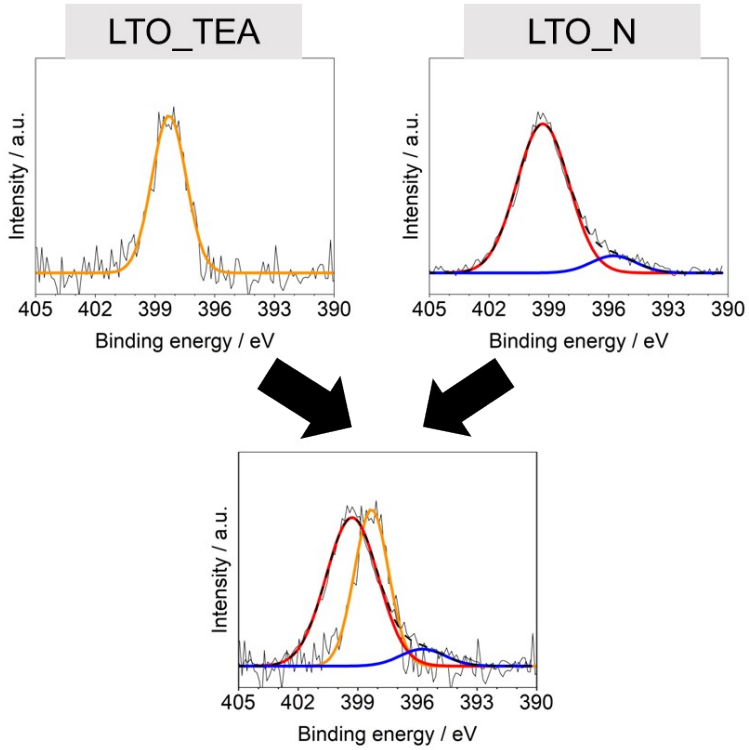

Fig. S4 Overlap of N 1s XPS spectra of LTO_TEA and LTO_N.

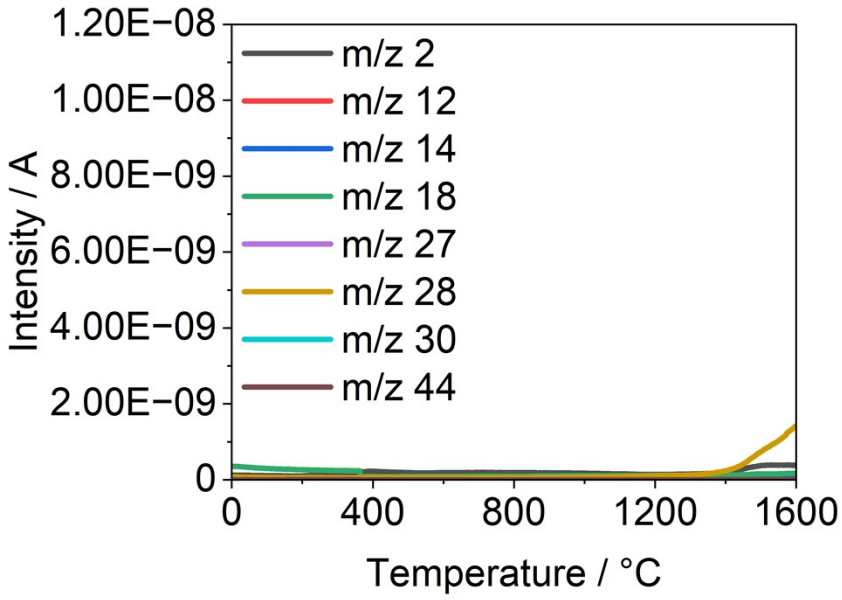

Fig. S5 TPD profiles of blank test with the tungsten holder.

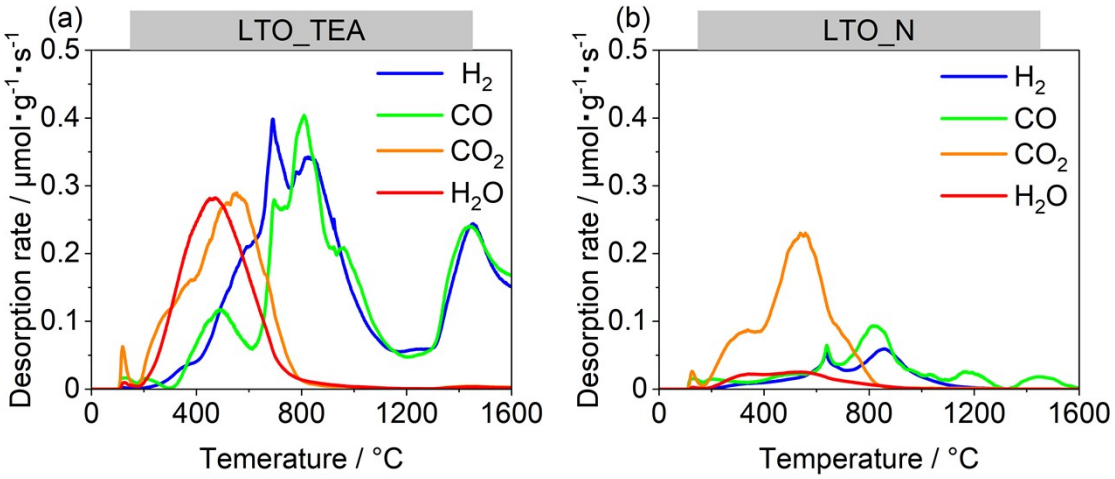

Fig. S6 H_2, CO, CO_2, and H_2O desorption pattern determined by TPD of (a) LTO_TEA and (b) LTO_N.

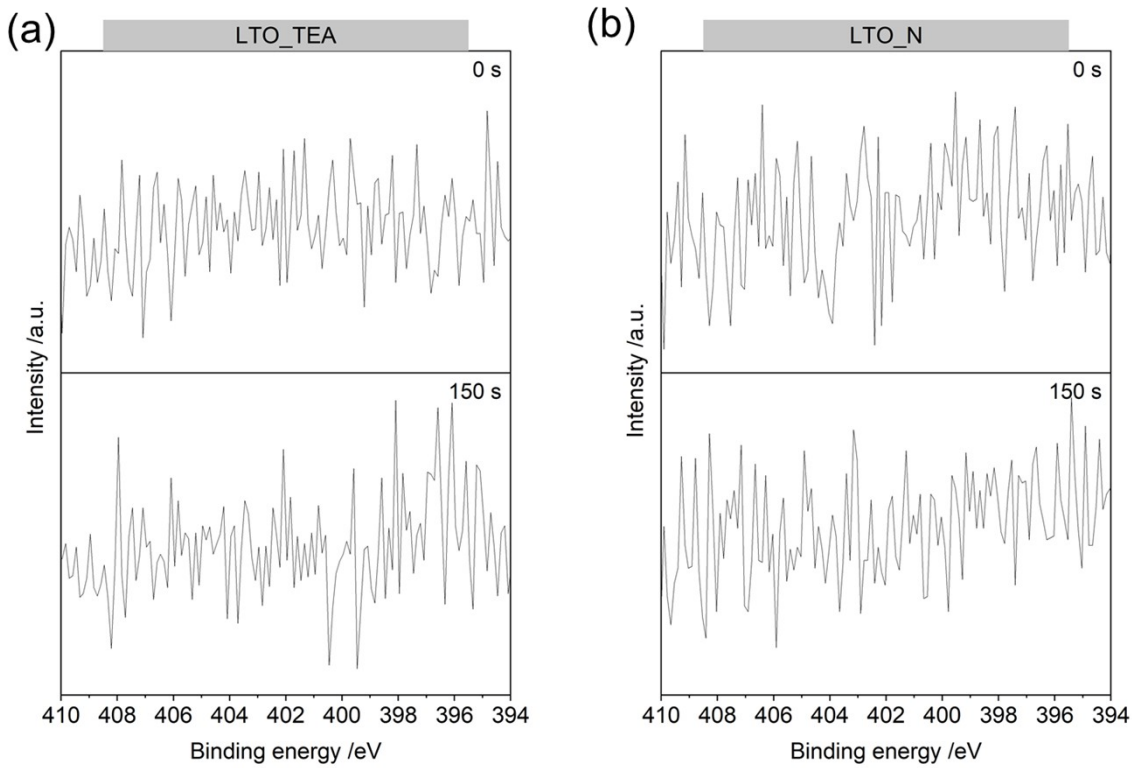

Fig. S7 N 1s XPS spectra of (a) LTO_TEA and (b) LTO_N after TPD measurements up to 1600 °C, before and after Ar^+ sputtering for 150 s.

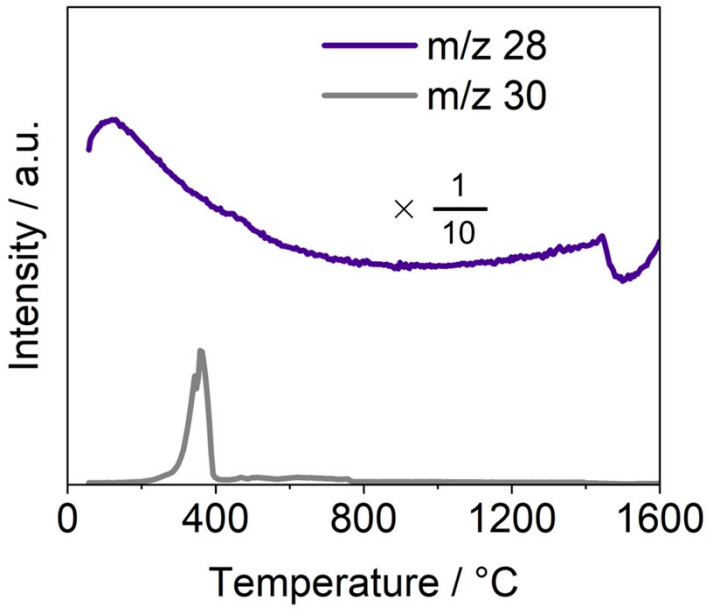

Fig. S8 MS spectra of LTO_TEA using the commercial TG-MS system under a He flow.

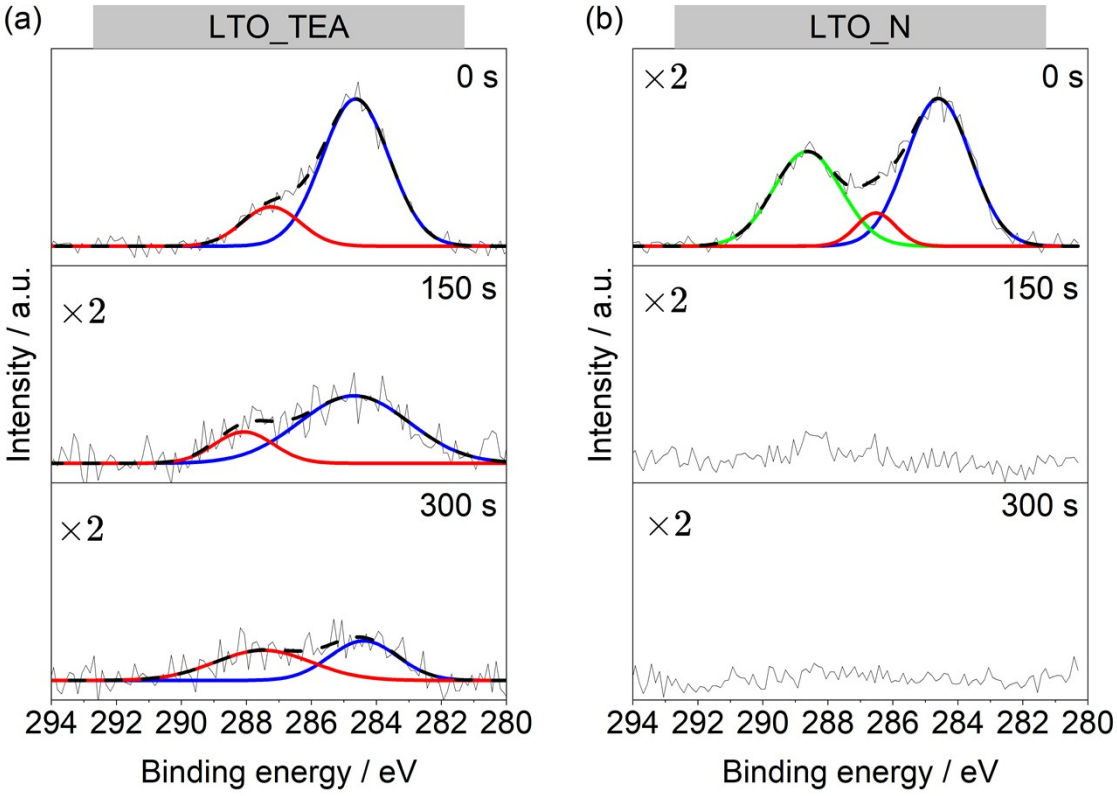

Fig. S9 C 1s XPS spectra of (a) LTO_TEA and (b) LTO_N before and after Ar^+ sputtering for 150 s or 300 s.

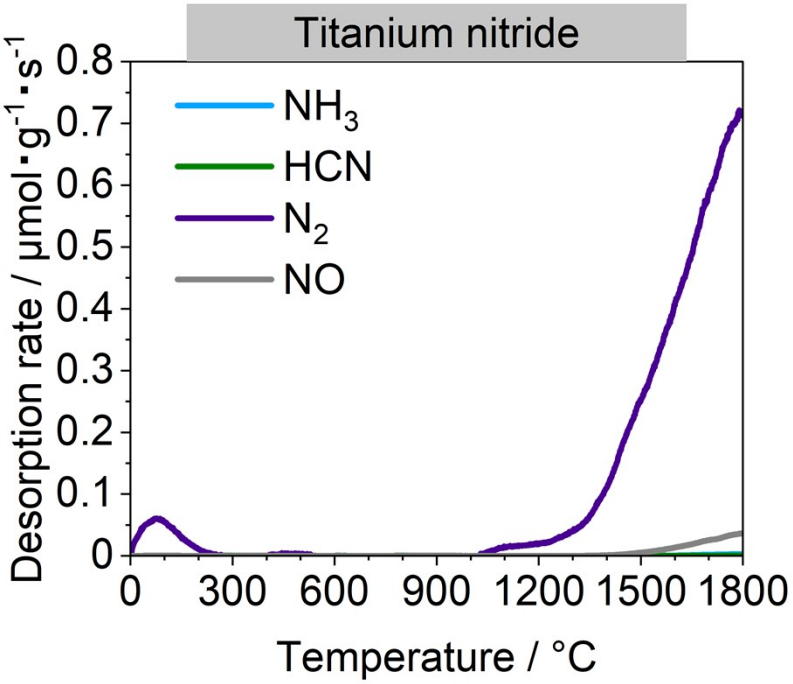

Fig. S10 TPD profile of Titanium nitride.

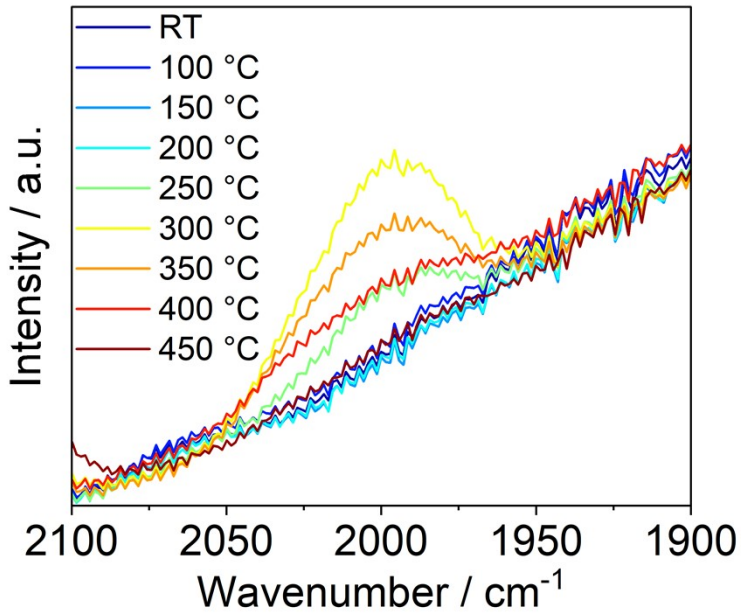

Fig. S11 *In situ* DRIFTS spectra of LTO_TEA in 2100-1900 cm^{-1} region.

Table S1 The slope of calibration curves prepared by introducing each gas into the TPD chamber using a gas reservoir tank of known volume.

	The slope of calibration curves / μmol • s^{-1}
H_2	703300
CO	844300
CO_2	904500
H_2O	803700
N_2	824300
HCN	521800
NH_3	450700
NO	2047800

Table S2 N content before and after TPD measurements determined from CHN elemental analysis.

	Before TPD measurement / wt%	After TPD measurement /wt%
LTO_TEA	1.13	0.14
LTO_N	0.72	0.06