Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting Information

Controlling the carrier density in niobium oxynitride $BaNbO_2N$ *via* cation doping for efficient photoelectrochemical water splitting under visible light

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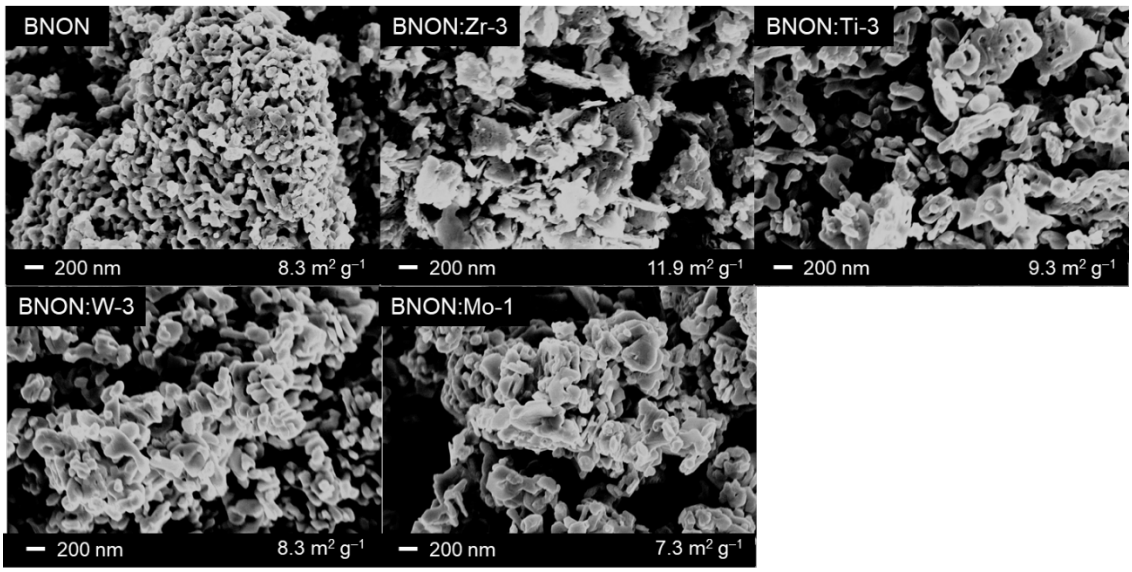

Fig. S1 SEM images of BNON, BNON:Zr-3, BNON:Ti-3, BNON:W-3, and BNON:Mo-1 samples.

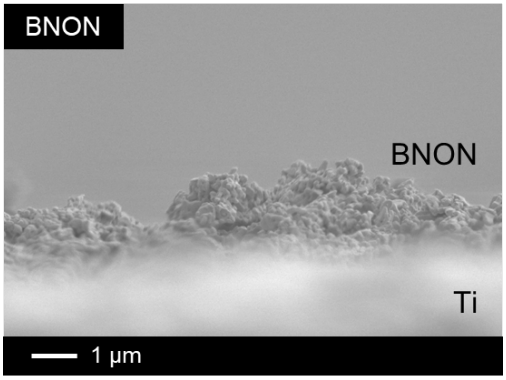

Fig. S2 Cross-sectional SEM image of BNON electrode.

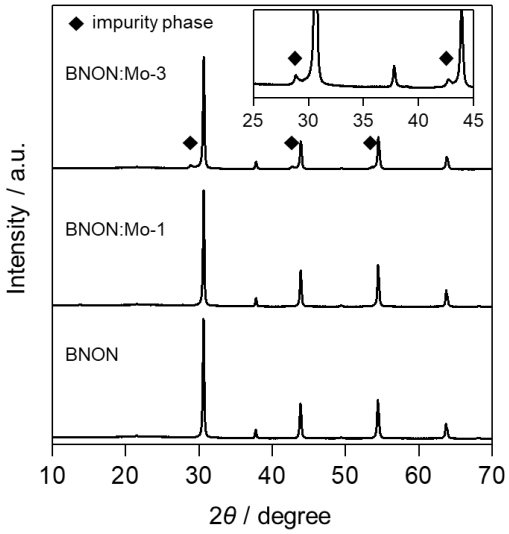

Fig. S3 XRD patterns of BNON, and BNON:Mo-*x* (*x* = 1, 3) samples. The inset shows the enlarged pattern around impurity phases.

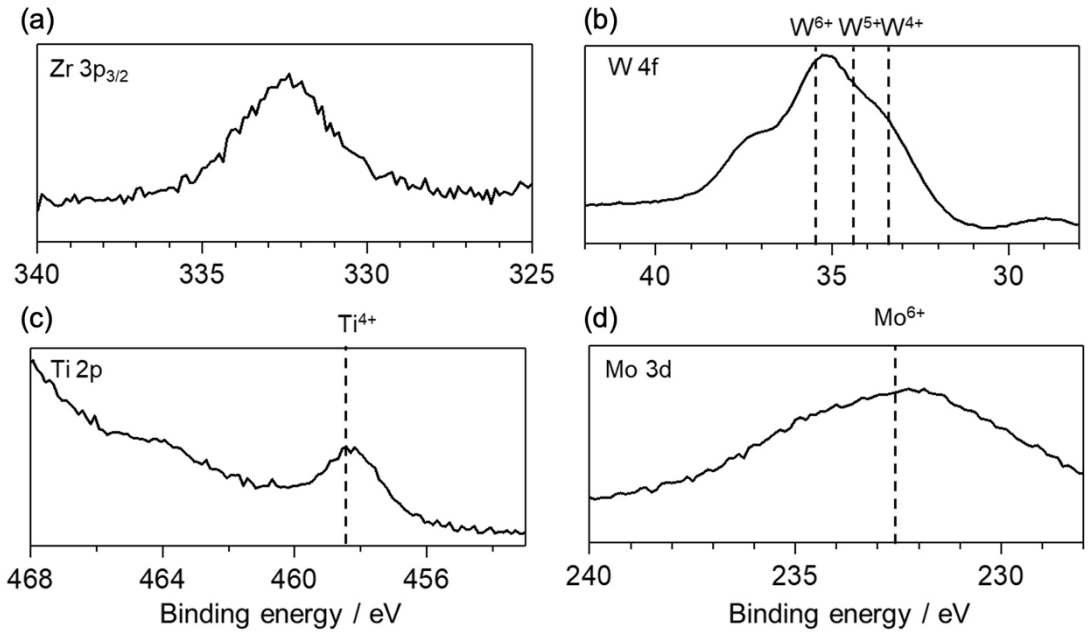

Fig. S4 XP spectra in (a) Zr 3p, (b) W 4f, (c) Ti 2p, and (d) Mo 3d regions of BNON:Zr-3, BNON:W-3, BNON:Ti-3, and BNON:Mo-1 samples.

Table S1 The atomic ratio of the dopant to Nb in BNON samples evaluated by XPS.

Sample	Measured dopant/(Nb+dopant) ratio	Ideal dopant/(Nb+dopant) ratio
BNON:Mo-1	0.01	0.01
BNON:W-3	0.08	0.03
BNON:Zr-3	–[a]	0.03
BNON:Ti-2	0.02	0.02
BNON:Ti-3	0.03	0.03
BNON:Ti-4	0.04	0.04

[a] Unmeasurable due to the overlap of the peaks corresponding to Zr 3d and Ba 4p.

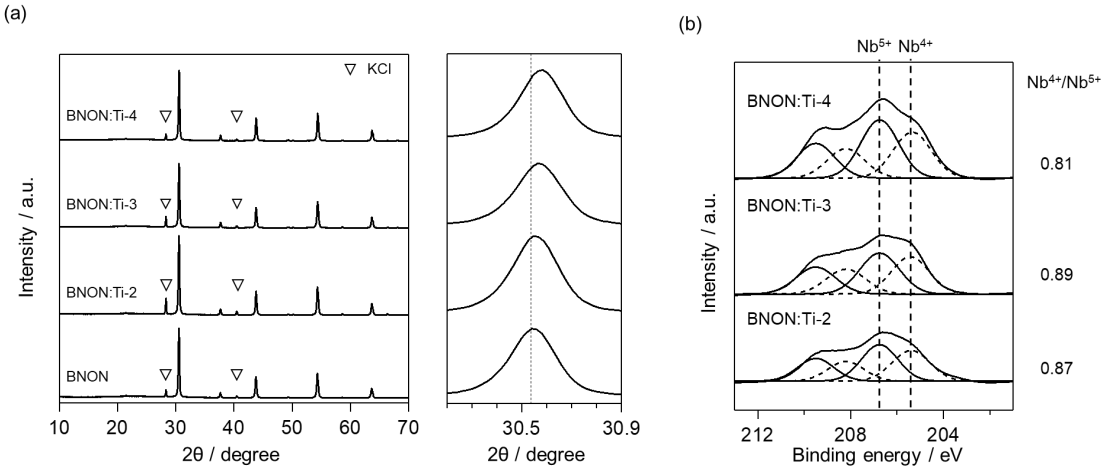

Fig. S5 (a) XRD patterns of BNON, and BNON:Ti-*x* (*x* = 2, 3, 4) samples. KCl (10 wt%) was added as an internal standard sample for the correction of 2θ angles. (b) XP spectra of Nb 3d region for BNON:Ti-*x* (*x* = 2, 3, 4) samples.

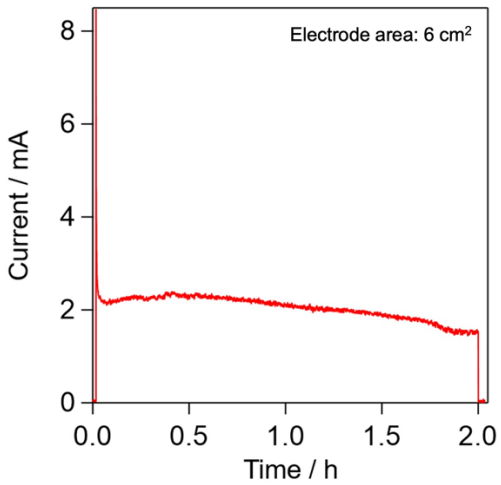

Fig. S6 Time course of photocurrent at +1.02 V (vs. RHE) in an aqueous Na_2SO_4 solution (0.1 M, pH 6) containing H_2O_2 (0.1 M) for unmodified BNON:Ti-4 electrode under visible light ($400 < \lambda < 800$ nm).

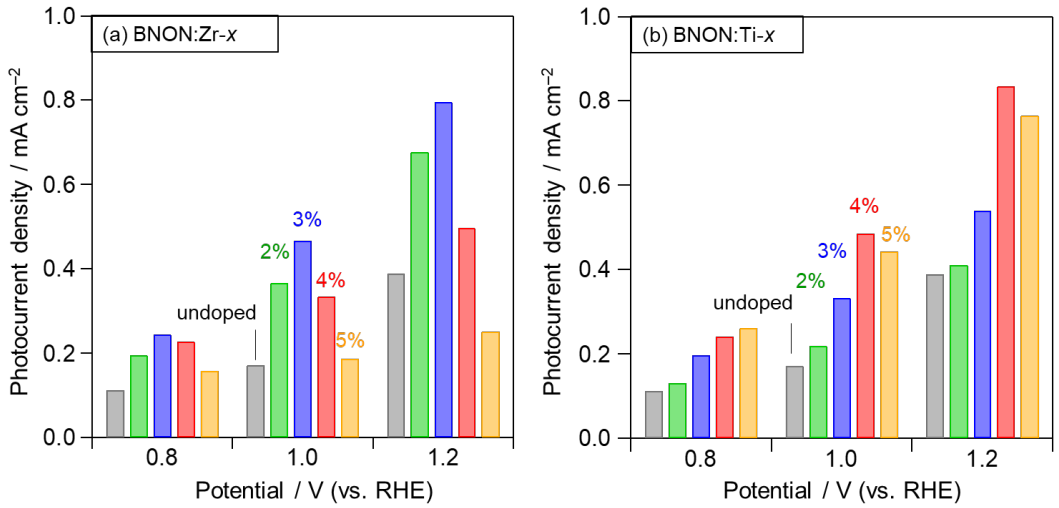

Fig. S7 Dependence of photocurrent density of (a) BNON:Zr-*x* and (b) BNON:Ti-*x* electrodes in an aqueous Na_2SO_4 solution (0.1 M, pH 6) under visible light on the amount of dopant.

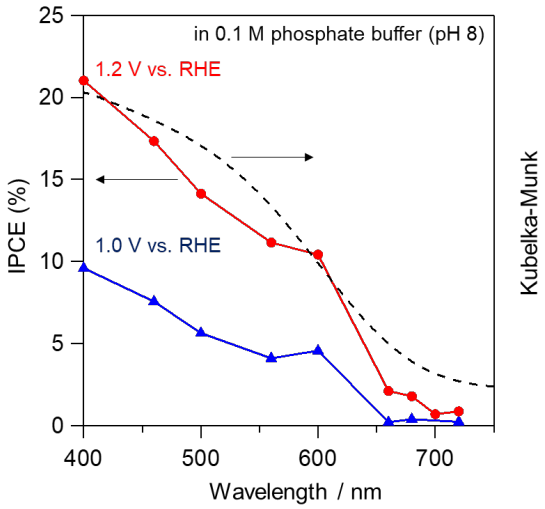

Fig. S8 IPCE spectra of CoO_y/BNON:Ti-4 electrode (phosphate buffer solution, pH 8), and absorption spectrum of BNON:Ti-4.