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Supporting information for:

First-principles calculations of structural, energetic, electronic, optical, and photocatalytic properties of $BaTaO_2N$ low-index surfaces

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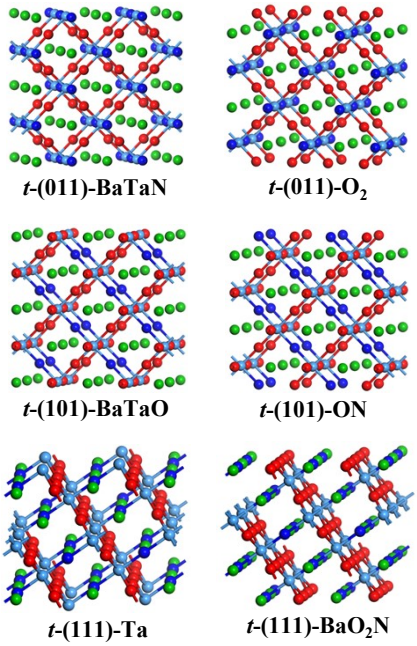

Fig. S1 Slab models of (011), (101) and (111) surfaces for *trans* $BaTaO_2N$. The green, light blue, red, and dark blue balls represent Ba, Ta, O, and N atoms, respectively.

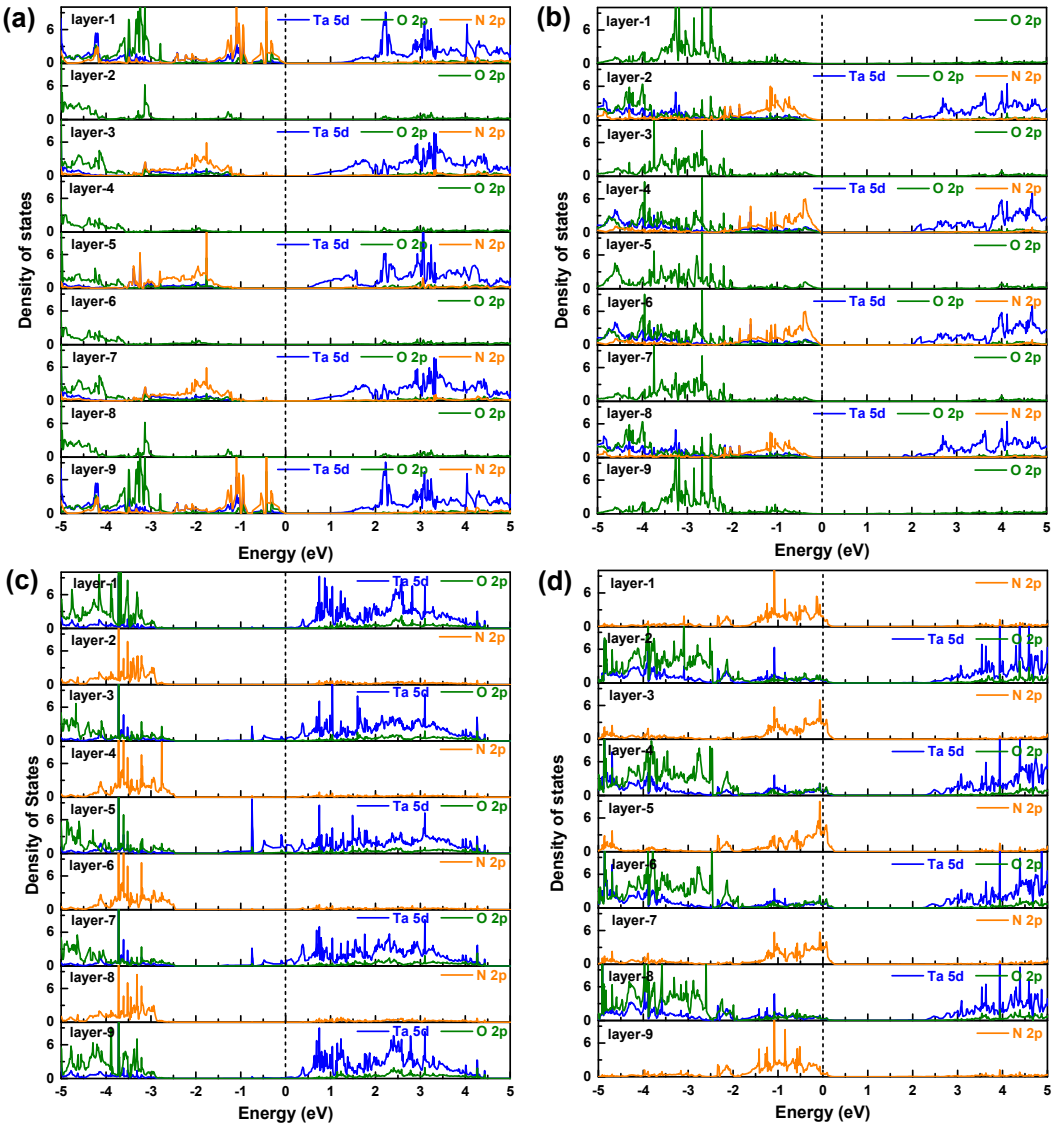

Fig. S2 The layer-resolved spin-up density of states for (a) *t*-(001)-TaON, (b) *t*-(001)-BaO, (c) *t*-(100)-TaO_2, and (d) *t*-(100)-BaN.

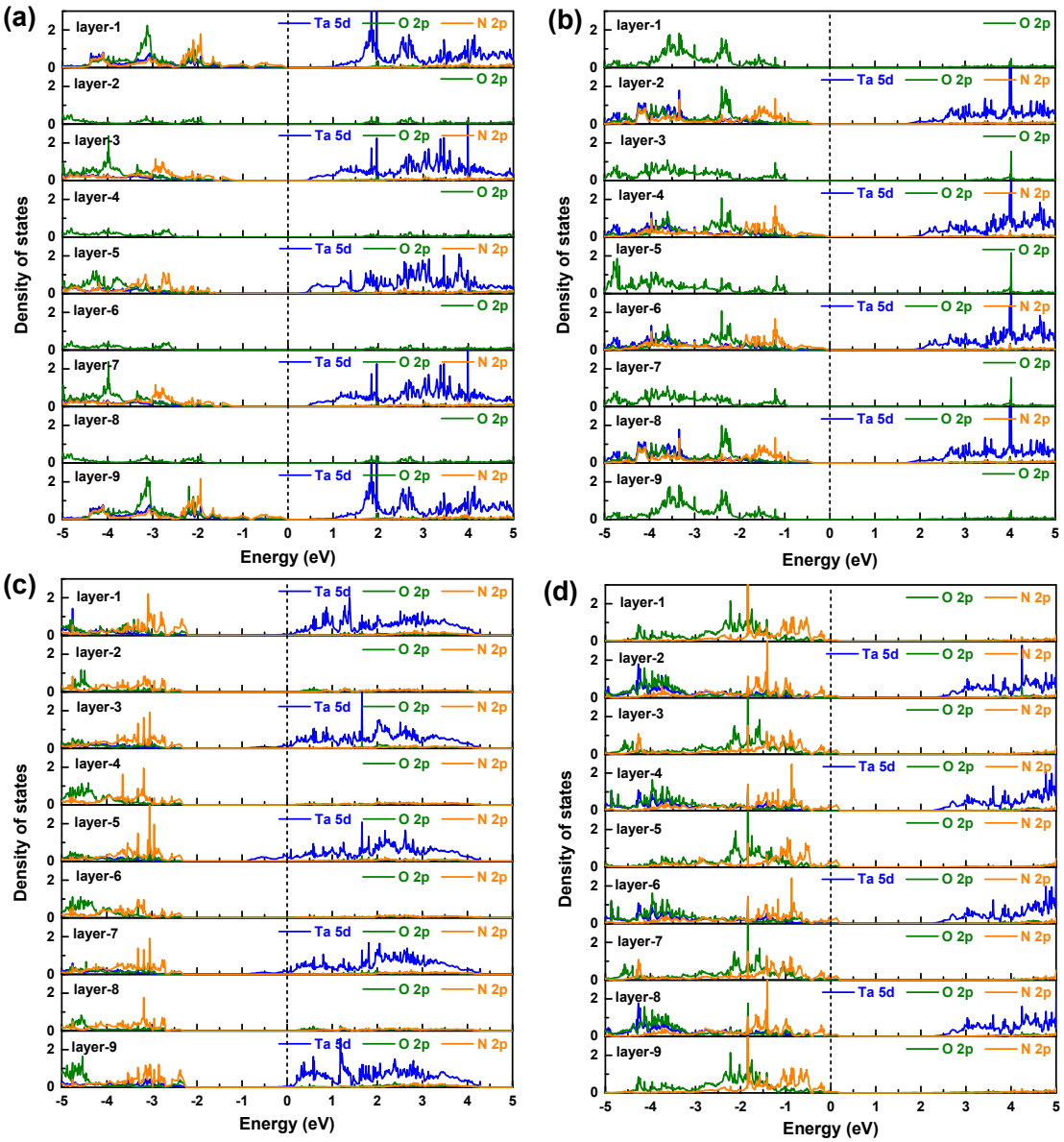

Fig. S3 The layer-resolved spin-up density of states for (a) *c*-(001)-TaON, (b) *c*-(001)-BaO, (c) *c*-(100)-Ta_2O_3N, and (d) *c*-(100)-Ba_2ON.

Table S1 Free energies of every step (in eV) and the overpotential (in V) of OER for (001) and

termination	step 1	step2 to O*/O-O*/N-O*	step3 to HOO*/O-HOO*/N-HOO*	step 4 from HOO*/O-HOO*/N-HOO*	overpotential
t-(001)-TaON	**-0.65**	**1.09**/3.36/0.63	(from O*) 2.79/**2.73**/2.74 (from O-O*) 0.52/0.46/0.47 (from N-O*) 3.25/3.19/3.20	1.69/**1.75**/1.74	1.50
t-(001)-BaO	**0.47**	2.22/**2.05**/—	(from O*) 0.93/0.92/— (from O-O*) **1.10**/1.09/—	**1.29**/1.30/—	0.82
t-(100)-TaO_2	**0.15**	**1.36**/0.23/—	(from O*) 2.45/**2.42**/— (from O-O*) 3.57/3.55/—	0.96/**0.99**/—	1.19
t-(100)-BaN	**1.09**	**2.57**/—/1.67	(from O*) **0.61**/—/0.53 (from N-O*) 4.85/—/3.72	**0.65**/—/1.78	1.34
c-(001)-TaON	**-0.53**	0.94/3.16/**1.80**	(from O*) 3.02/2.91/2.95 (from O-O*) 0.81/0.70/0.74 (from N-O*) 2.17/**2.06**/1.59	1.48/**1.59**/1.56	0.83
c-(001)-BaO	**0.86**	2.53/**2.09**/—	(from O*) 0.64/0.64/— (from O-O*) **1.08**/1.08/—	**0.89**/0.89/—	0.86
c-(100)-Ta_2O_3N	**-0.44**	0.27/0.28/**1.76**	(from O*) 3.56/3.79/3.52 (from O-O*) 3.56/3.79/3.52 (from N-O*) 2.08/2.31/**2.04**	1.52/1.30/**1.57**	0.81
c-(100)-Ba_2ON	**0.64**	2.91/**2.65**/2.65	(from O*) 0.83/0.63/0.63 (from O-O*) 1.08/**0.89**/0.89 (from N-O*) 1.08/0.89/0.89	0.54/**0.74**/0.74	1.42

(100) surfaces of $BaTaO_2N$. The most favorable pathway is highlighted by the numbers in bold.