Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information for:

Tuning electronic structure of $BaTiO_3$ for enhanced photocatalytic performance using cation-anion codoping: A first-principles study

Yumeng Fo[a], Yanxia Ma[a], Hao Dong[b,*] Xin Zhou[a,*]

[a] *College of Environment and Chemical Engineering, Dalian University, Dalian 116622, Liaoning, China*

[b] *School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, Liaoning, China*

* Corresponding authors.

E-mail addresses: zhouxin@dlu.edu.cn (X. Zhou), sinodonghao@gmail.com (H. Dong)

Table S1. Calculated formation energies (in eV) for TM/X monodoped $BaTiO_3$ under O-rich and Ti-rich growth conditions.

E_{form} (2×2×2)	TM/X	Ti-rich	O-rich
TM@Ti	V	2.06	-13.12
	Nb	1.04	-14.14
	Ta	-0.06	-15.24
	Mo	3.45	-11.73
	W	2.63	-12.55
X@O	N	-5.07	-0.01
	C	-4.68	0.38

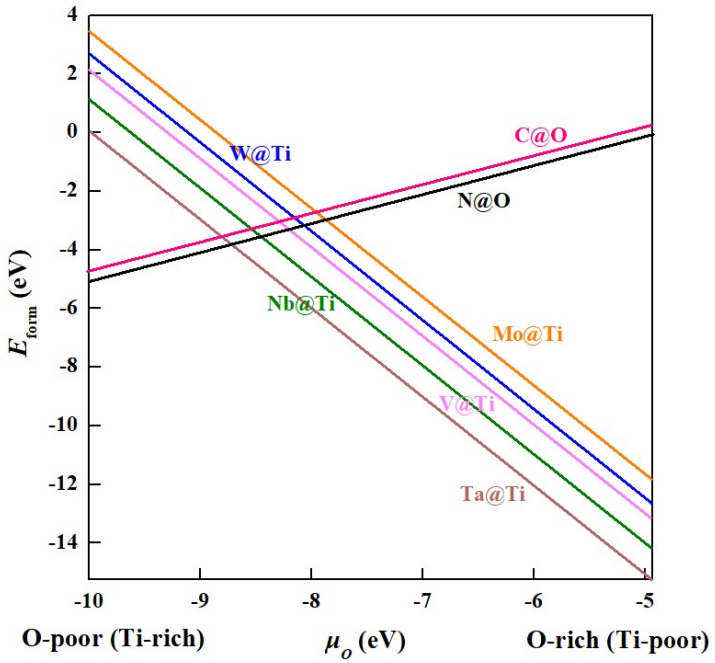

Fig. S1. Formation energies (eV) E_{form} as a function of the oxygen chemical potential for N-, C-, V-, Nb-, Ta-, Mo-, and W-monodoped $BaTiO_3$.

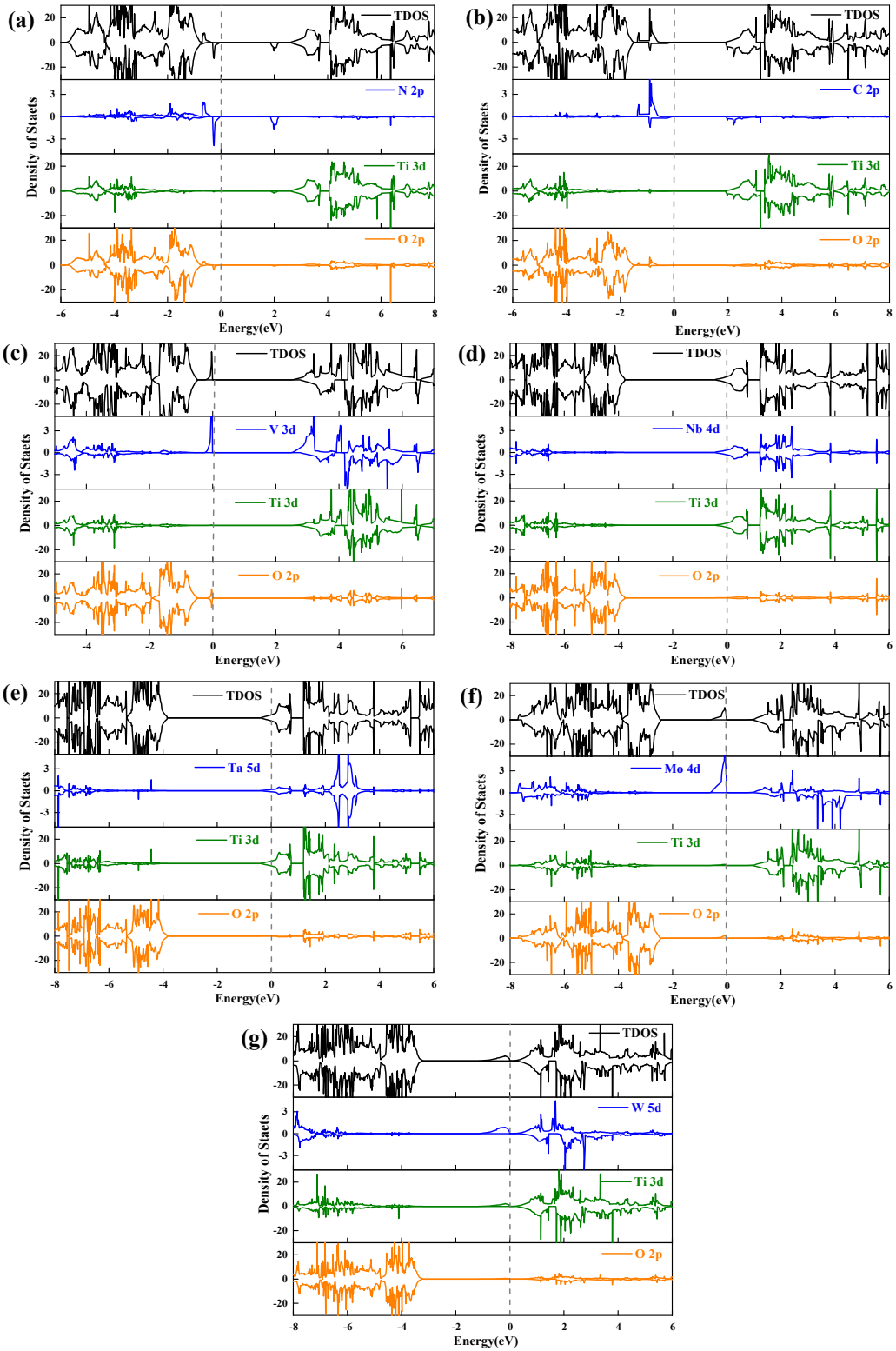

Fig. S2. The calculated density of states for (a) N-doped, (b) C-doped (c) V-doped, (d) Nb-doped, (e) Ta-doped, (f) Mo-doped and (g) W-doped $BaTiO_3$. The dashed line is the Fermi level.

Table S2. The fully optimized crystal parameters and band gaps of (TM+X)-codoped $BaTiO_3$

	Relaxed parameters			Band gap
	a	b	c	
V-N	8.1425	7.9659	7.9659	3.04
Nb-N	8.1437	8.0141	8.0141	3.03
Ta-N	8.1035	8.0163	8.0163	2.79
Mo-N	8.0975	8.0094	8.0094	3.24
W-N	8.0621	8.0142	8.0142	2.88
Mo-C	8.2046	7.9919	7.9919	2.44
W-C	8.1991	7.9899	7.9899	2.18
Mo-2N	8.0193	8.0266	8.0266	1.56
W-2N	8.0230	8.0237	8.0237	1.78

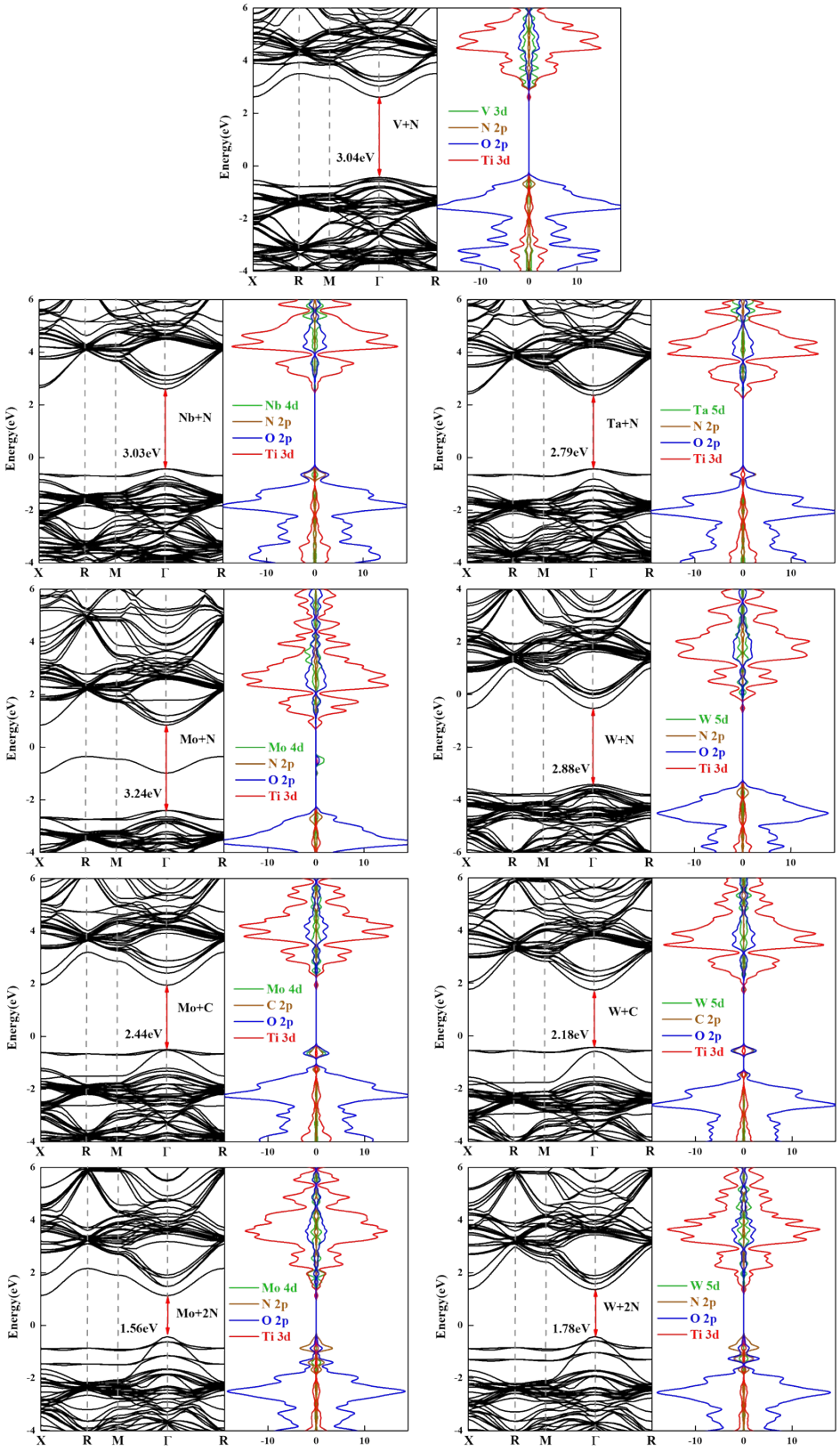

Figure S3. Computed band structure and density of states for fully relaxed (TM+X)-codoped $BaTiO_3$