Supporting Information

Defect dipoles and stable dielectric properties improve Nb-doped Ba$_{0.7}$Sr$_{0.3}$TiO$_3$ photocatalytic H$_2$ evolution activity

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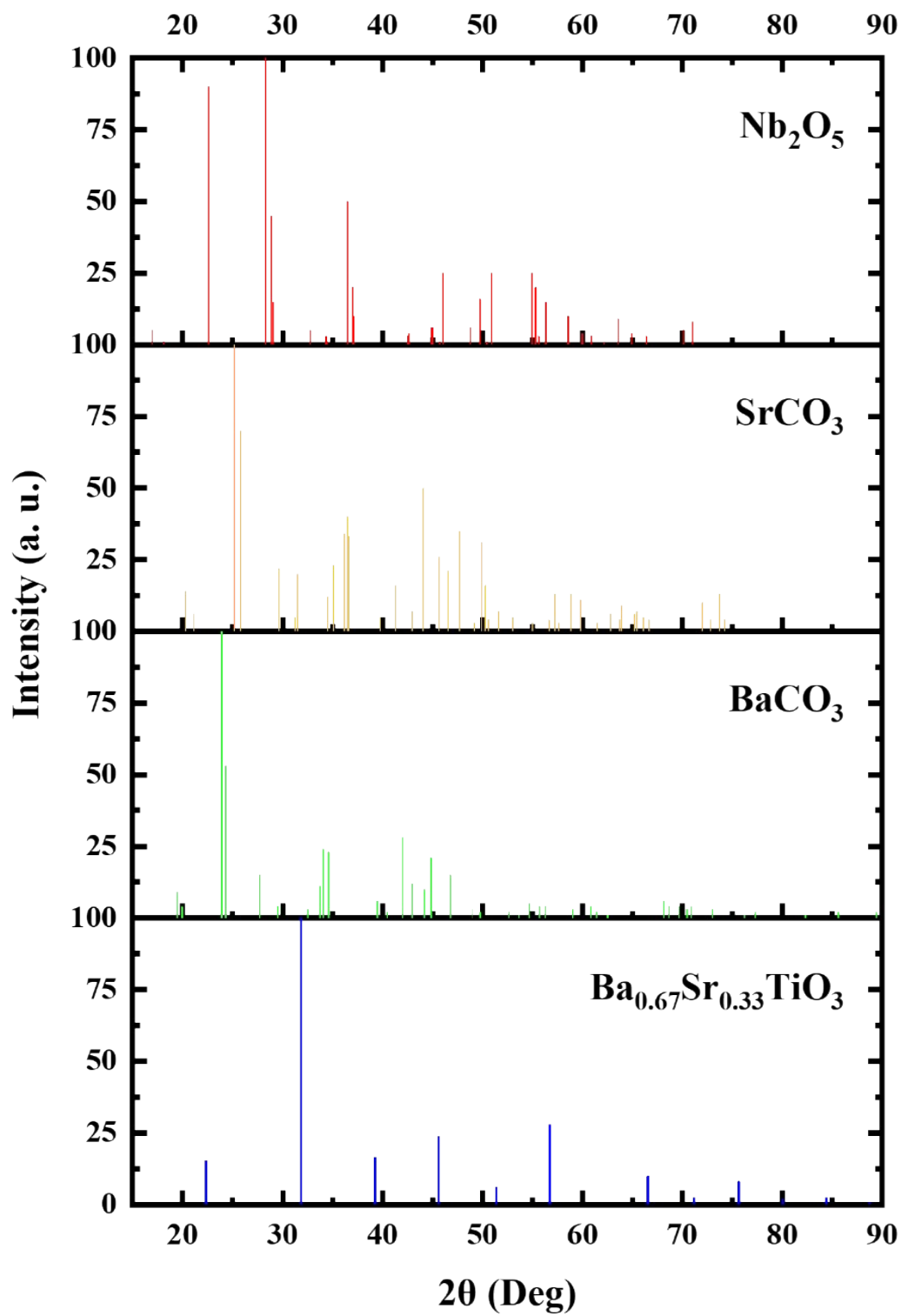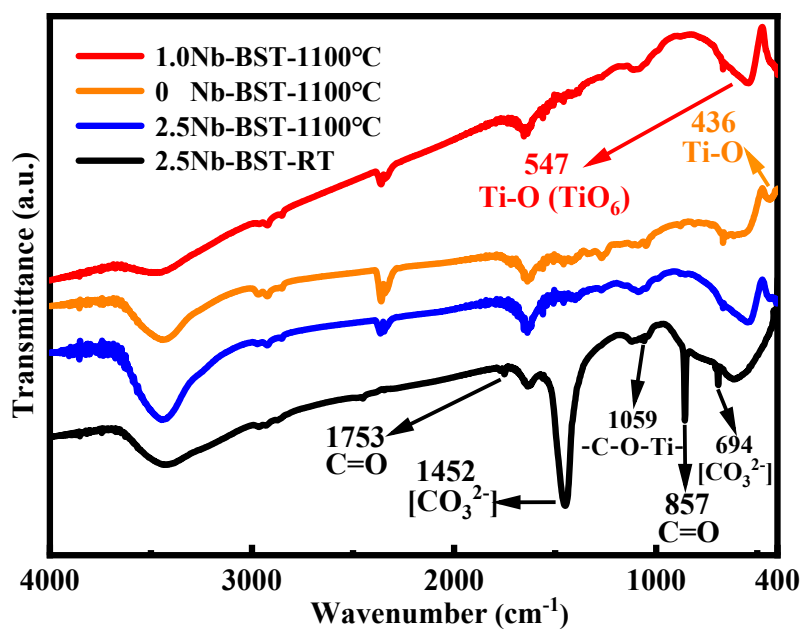
Fig. S1 Standard XRD for each phase

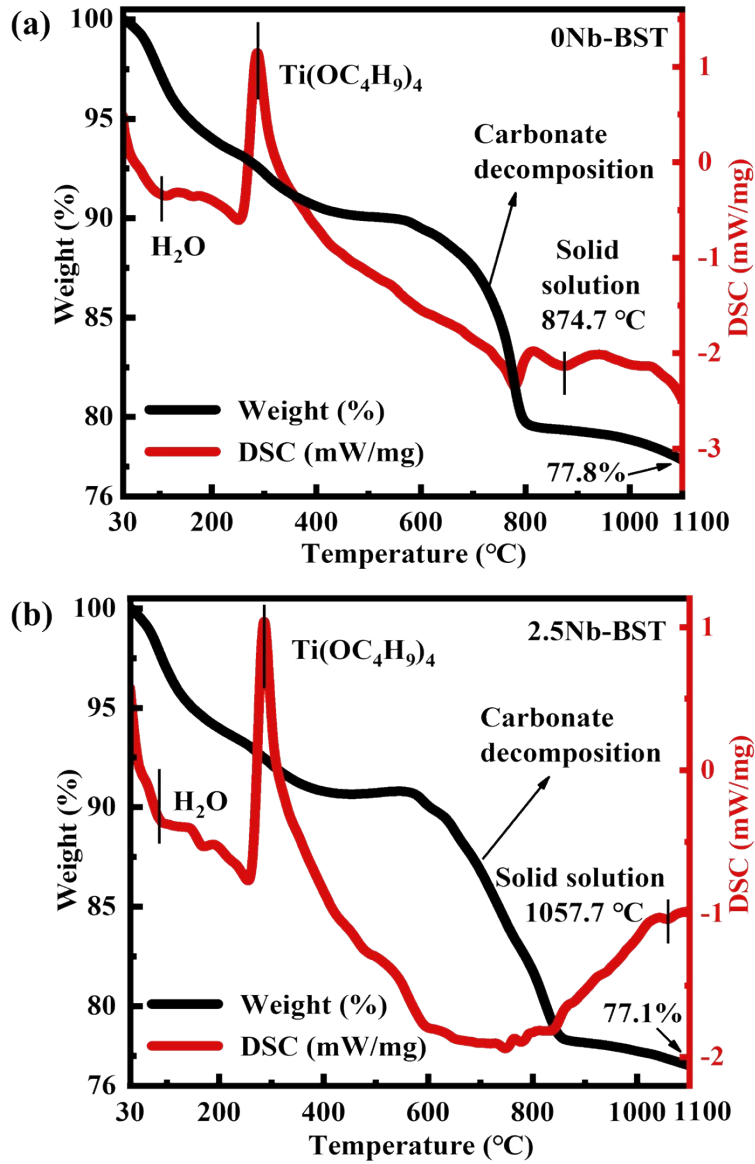Fig. S2 FT-IR of Nb doped BST and precursor xerogel

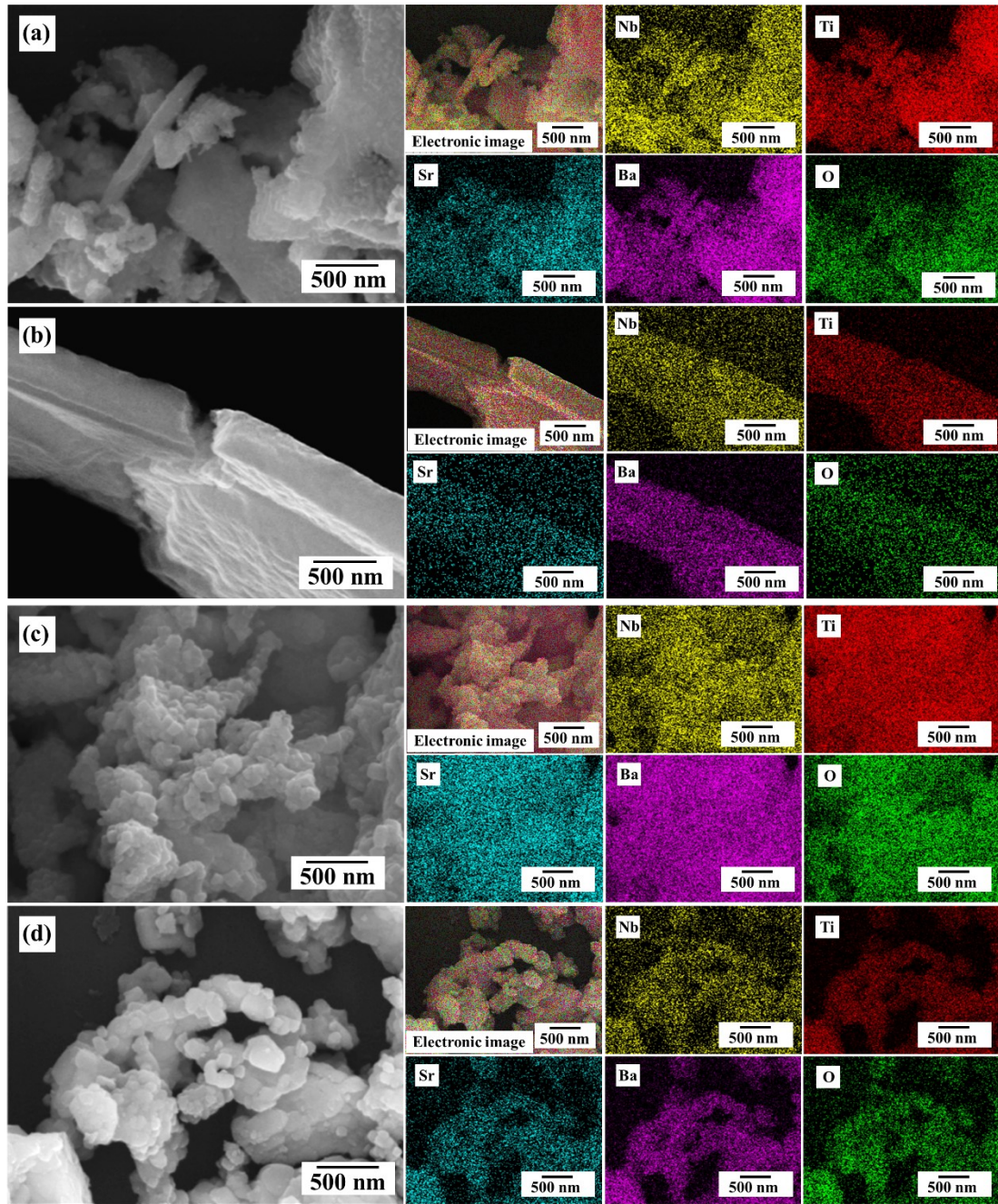Fig. S3 TG-DSC: (a) 0Nb-BST gel, (b) 2.5Nb-BST gel

Fig. S4 EDS elemental distribution of 2.5Nb-BST in different temperature heat treatment: (a) 700 °C, (b) 800 °C, (c) 1000 °C, and (d) 1100 °C
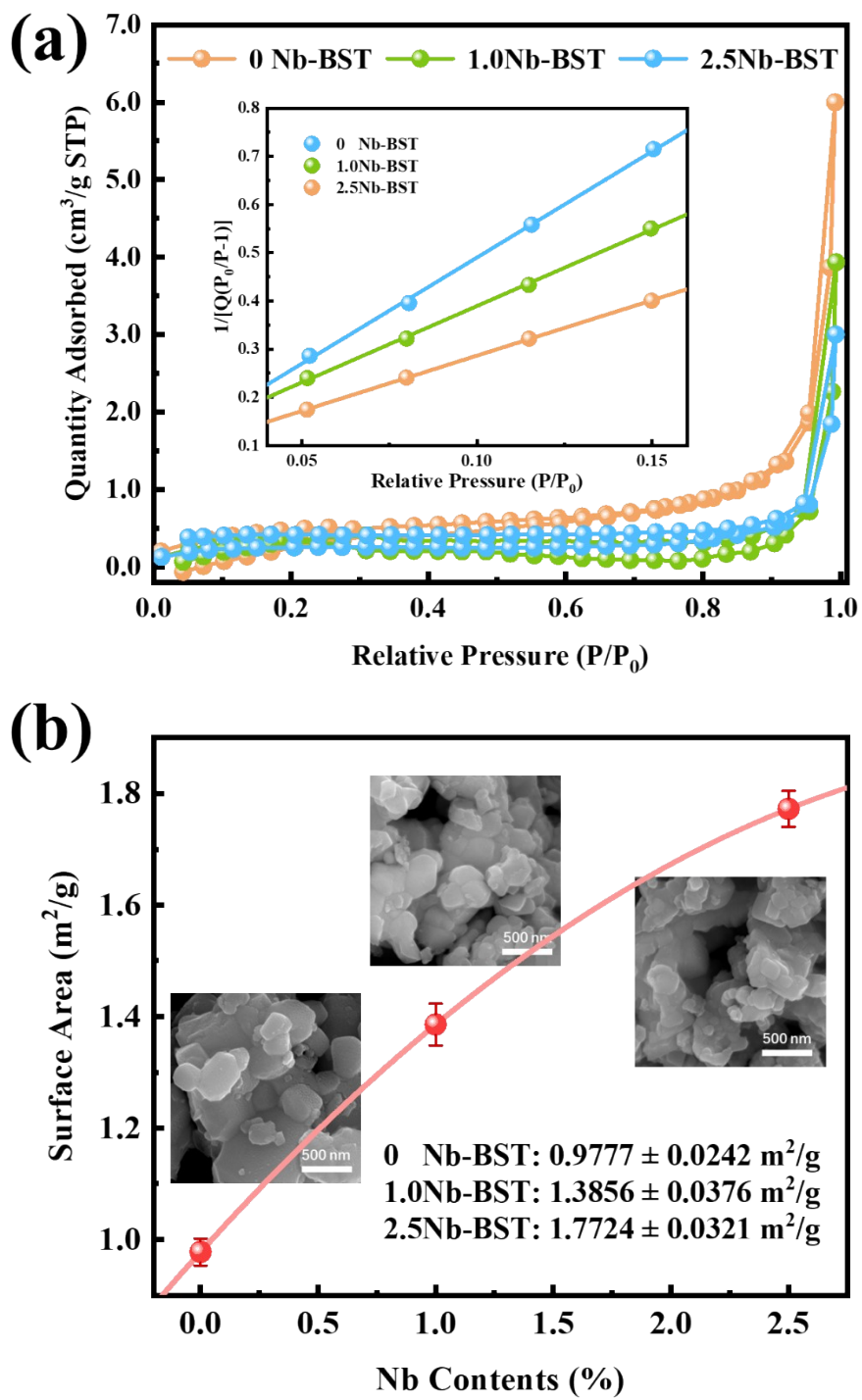
Fig. S5 (a) Adsorption and desorption curves and BET of xNb-BST, (b) specific surface area statistics
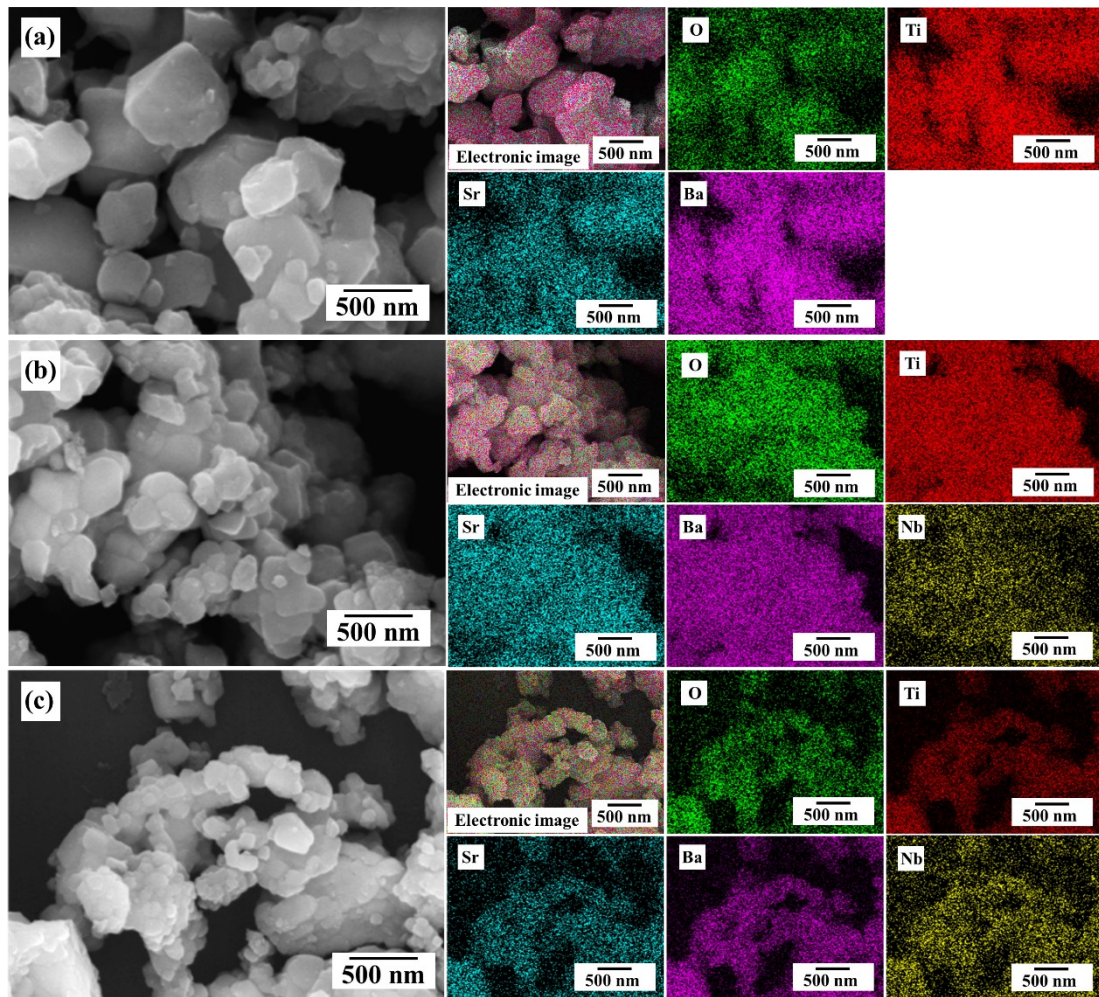
Fig. S6 EDS elemental distribution of xNb-BST-1100 °C.: (a) 0Nb-BST, (b) 1.0Nb-BST, and (c) 2.5Nb-BST
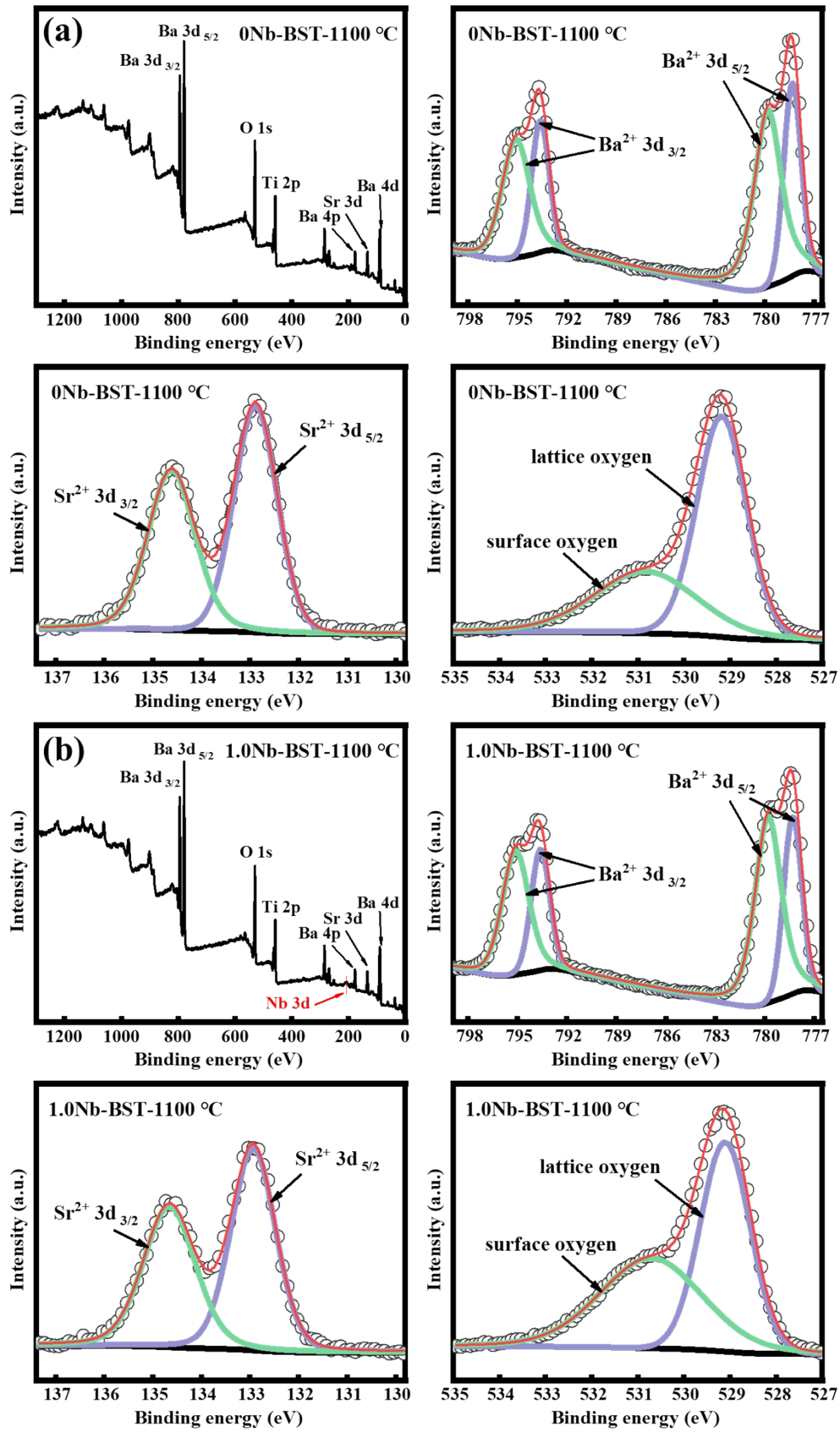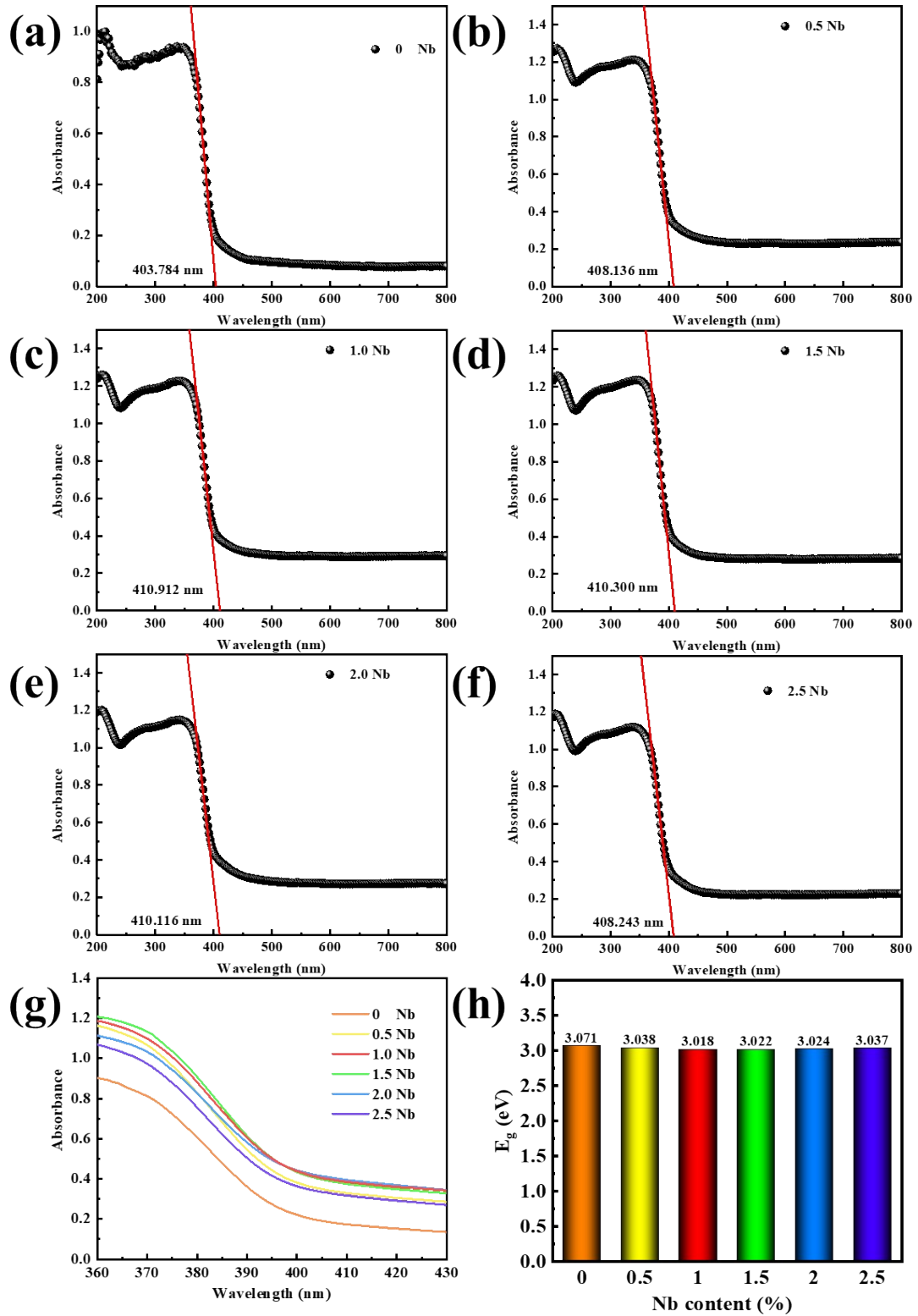
Fig. S7 (a) XPS of 0Nb-BST, (b) XPS of 1.0Nb-BST

Fig. S8 UV-Vis of (a) 0Nb-BST, (b) 0.5Nb-BST, (c) 1.0Nb-BST, (d) 1.5Nb-BST, (e) 2.0Nb-BST, (f) 2.5Nb-BST, (g) partial enlargement (h) energy band gap from UV-Vis
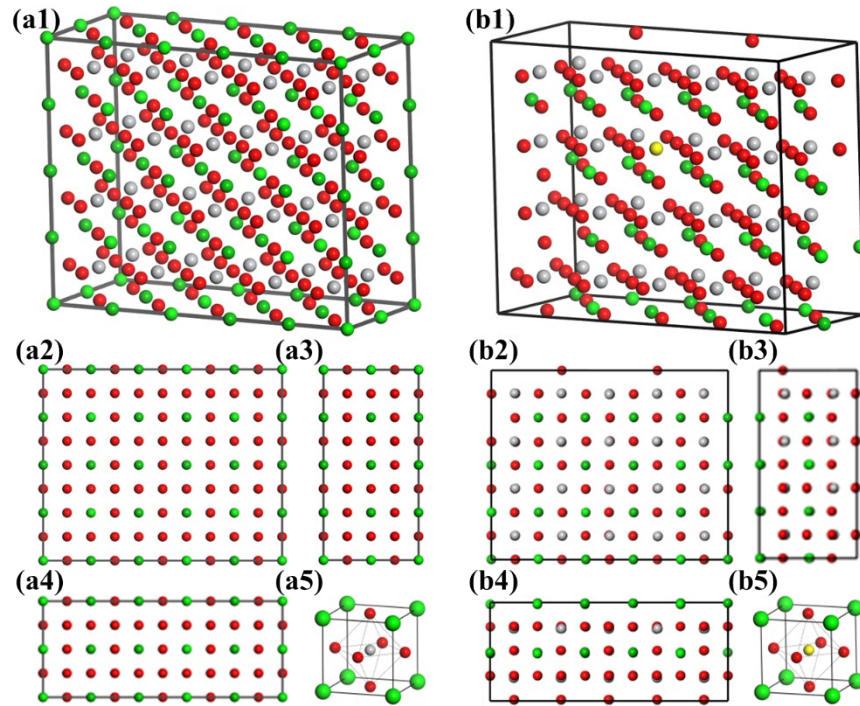
Fig. S9 First principles models: (a1)-(a5) Undoped BST, (b1)-(b5) Nb doped BST.

To simplify the theoretical calculation of the band structure of Nb doped BST, the following approximation is processed for Nb doped BST firstly. As shown in Figure S5:

(1) In 40 original cells, the number of Ba^{2+} and Sr^{2+} in BST are 27 and 13, respectively, which means that the mole fraction of Ba is 67.5% (the actual value is 70 %), the mole fraction of Sr is 32.5% (the actual value is 30%). However, the doped Nb would induce lattice distortion of BST, which changes its symmetry, as shown in Fig. S5 (b).

(2) It is believed that the valence state of the doped Nb^{5+} ions has not changed, and they are all Nb^{5+}.

(3) The doping amount of Nb^{5+} was properly increased. One Ti^{4+} ion was replaced with one Nb^{5+} ion in the 40 original cells. Therefore, the mole fraction of Nb^{5+} is 2.5% (the actual Nb doping range is 0-2.5%).
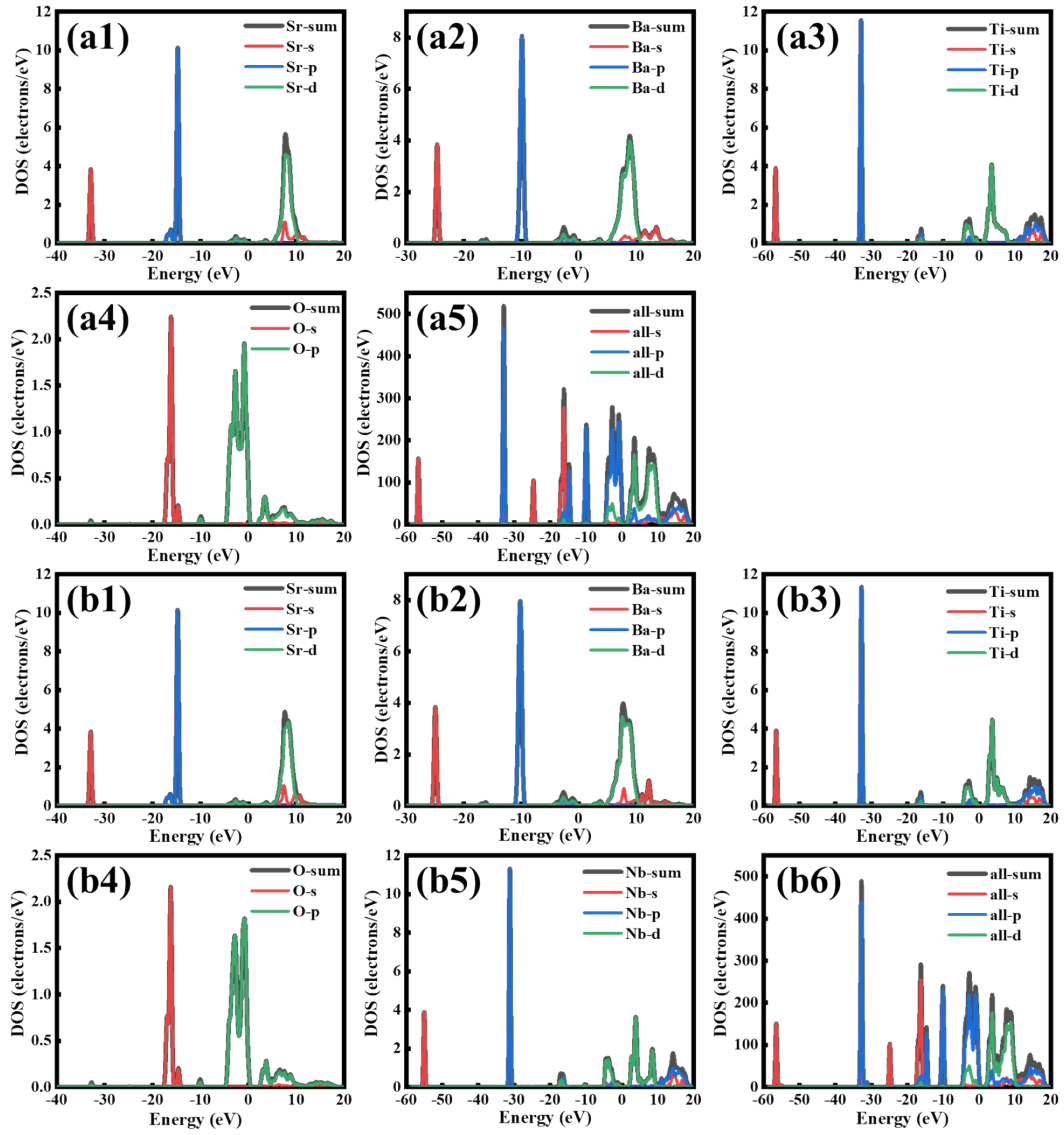
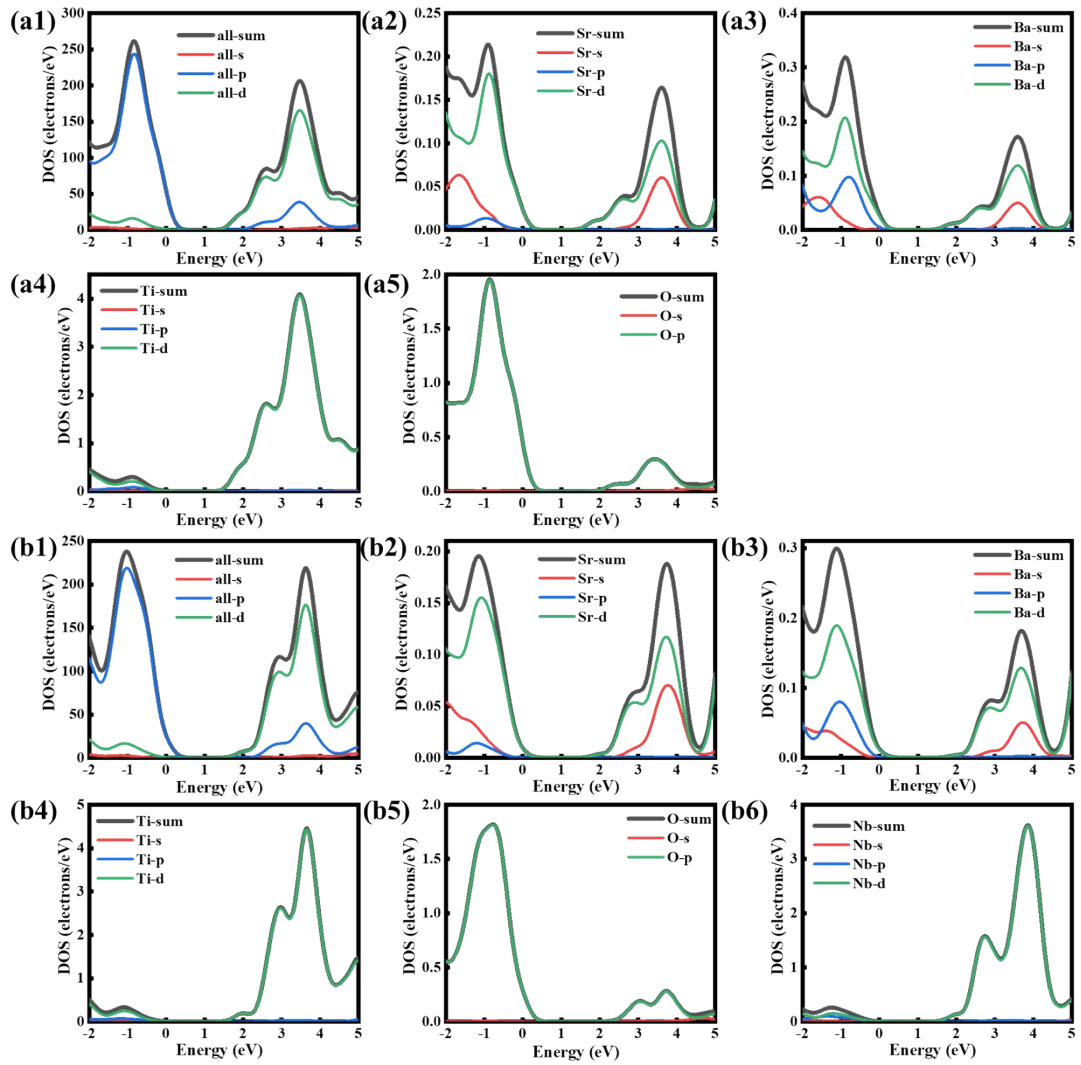Fig. S10 Density of States: (a1)-(a5) Undoped BST, (b1)-(b6) Nb doped BST.

Fig. S11 The DOS around Fermi level: (a1)-(a5) Undoped BST, (b1)-(b6) Nb doped BST.
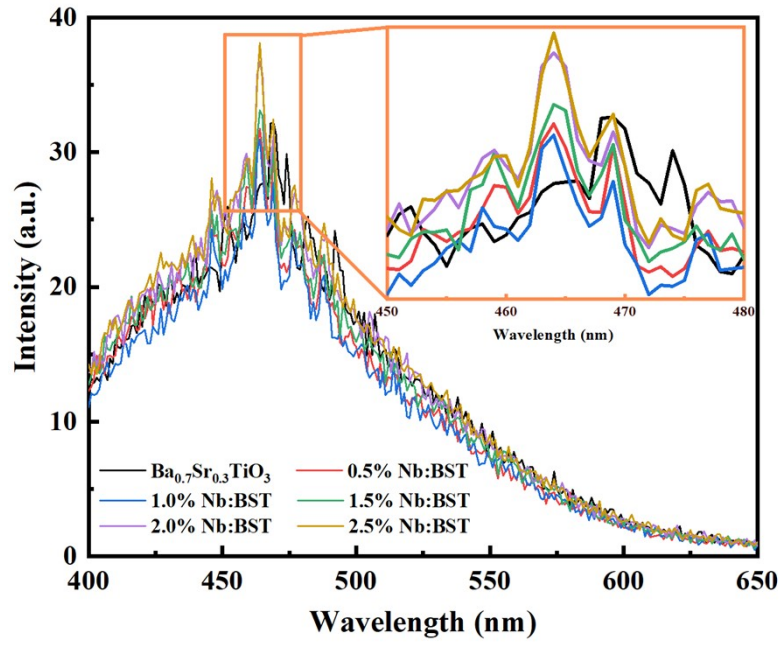
Fig. S12 The photoluminescence spectrum of Nb-doped BST.

Table. S1 Summary of photocatalysts for H$_2$ evolution. (In addition to special notes, numerical values are in units of headings.)

Materials	Light source	Light power (W)	Co-catalyst (wt%)	Coupling field	H$_2$ evolution (μmol·g^{-1}·h^{-1})	Ref.
Nb-Ba$_{0.7}$Sr$_{0.3}$TiO$_3$	Xenon lamp	210	H$_2$PtCl$_6$ (1.0)	None	27.52	This work
Sr$_{0.9}$La$_{0.1}$Ti$_{0.9}$Cr$_{0.1}$O$_3$	Xenon lamp	300	Pt (1.0)	None	28.8	1
BaTiO$_3$/MoS$_x$	Xenon lamp	300	H$_2$PtCl$_6$ (52)	None	1485	2
Ag-Pd-Sn-Ni-BaTiO$_3$	Xenon lamp	300	None	Electric field	156.7 μmol·h^{-1}	3
Pt/BaTiO$_3$	Xenon lamp	300	None	Electric field	4.77 μmol·h^{-1}	4
TiO$_2$/BaTiO$_3$	Xenon lamp	300	None	Ultrasonic	67.7	5
BaTiO$_3$@ZnIn$_2$S$_4$	Xenon lamp	Not mentioned	None	Ultrasonic	8041 μmol·g^{-1}	6
Rh-BaTiO$_3$	Xenon lamp	300	Pt (0.25)	None	30 μmol·h^{-1}	7
Pt/ZnIn$_2$S$_4$/BaTiO$_3$	Xenon lamp	300	None	None	1335.3	8
BaTiO$_3$/CaFe$_2$O$_4$	metal halide lamp	250	None	None	2240	9
Rh-CaTiO$_3$	Xenon lamp	300	H$_2$PtCl$_6$ (0.1)	None	16.6	10

References

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