Supporting Information

Effects of different exchanging ions on the band structure and photocatalytic activity of defect pyrochlore oxide: A case study in $KNbTeO_6$

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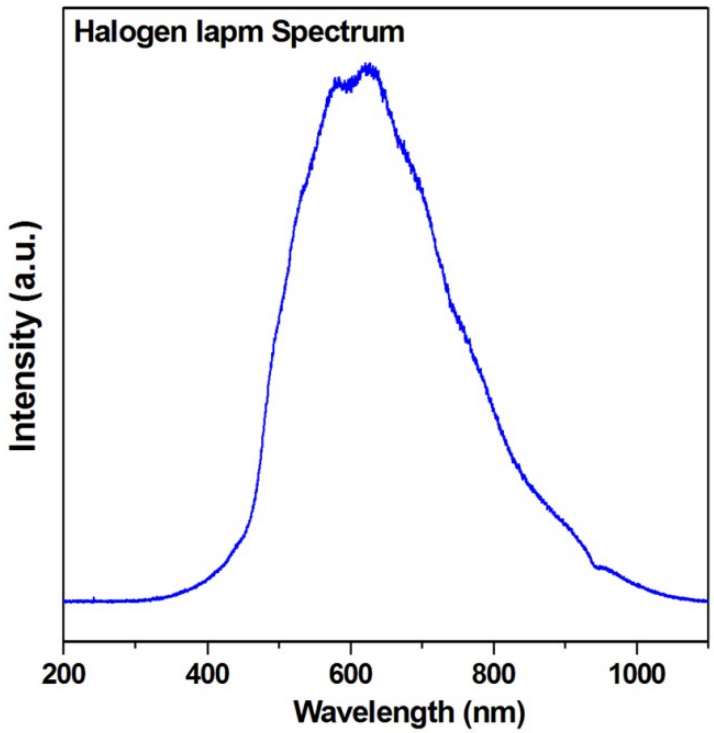

Fig. S1 The spectrum of halogen lamp.

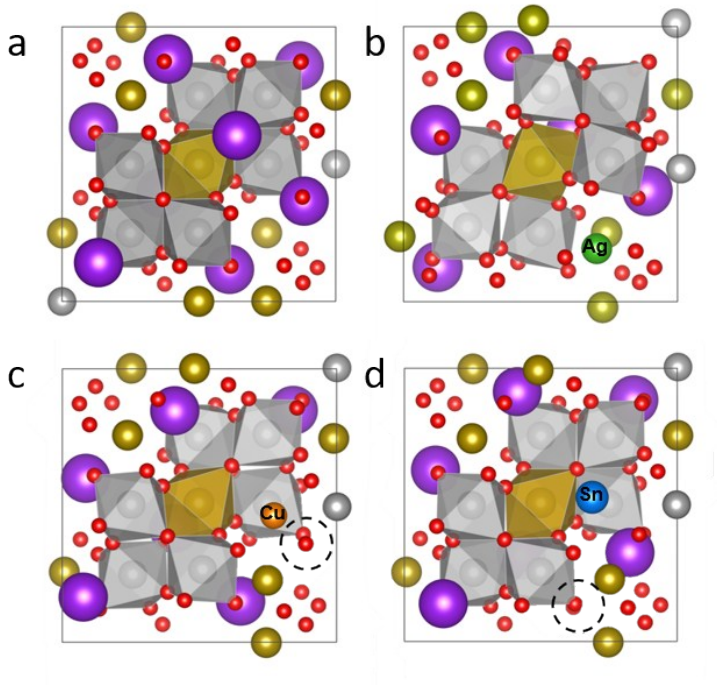

Fig. S2. Schematic structure of a) pristine $KNbTeO_6$ b) Ag doped-$KNbTeO_6$ c) Cu doped-$KNbTeO_6$ d) Sn doped-$KNbTeO_6$. Color legend: K in purple, Nb in yellow, Te in

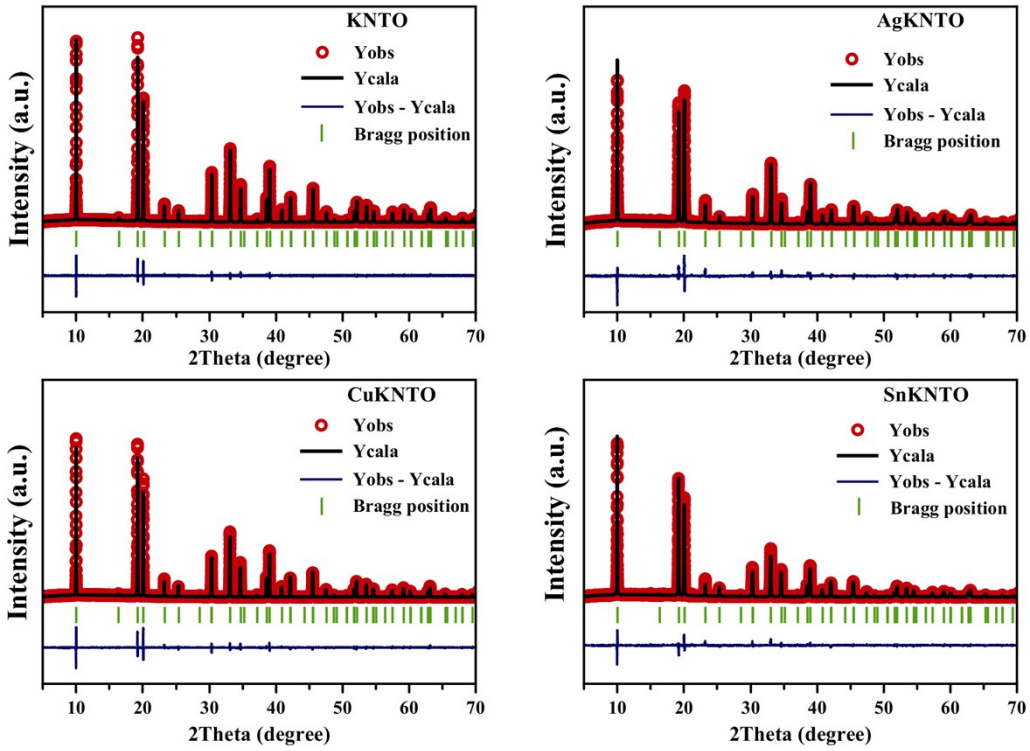

Fig. S3 Rietveld refinement of KNTO, AgKNTO, CuKNTO, and SnKNTO before heating at 300 ^{o}C for 5h

Table S1 Refined parameters and reliability factor of KNTO, AgKNTO, CuKNTO, and SnKNTO after heating at 300 ^{o}C for 5h. according to synchrotron XRD patterns (using 12 keV monochromatic X-ray).

Atom	Site	x	y	z	Occupancy	Beq
KNTO; a= 10.2368(1) Å, Rexp : 5.70 Rwp : 11.96 GOF : 2.10						
K	32e	0.1042(5)	0.1042(5)	0.1042(5)	0.25	4.3(2)
Nb	16c	0.5000	0.5000	0.5000	0.5	2.1(1)
Te	16c	0.5000	0.5000	0.5000	0.5	2.1(1)
O	48f	0.4326(2)	0.1250	0.1250	1	2.6(1)
AgKNTO; a= 10.2526(1)Å, Rexp : 5.39 Rwp : 10.36 GOF : 1.92						
K	32e	0.1008(2)	0.1008(2)	0.1008(2)	0.2	2.4(1)
Ag	16d	0.0000	0.0000	0.0000	0.1	2.4(1)
Nb	16c	0.5000	0.5000	0.5000	0.5	1.1(1)
Te	16c	0.5000	0.5000	0.5000	0.5	1.1(1)
O	48f	0.4259(2)	0.1250	0.1250	1	1.5(1)
CuKNTO; a= 10.2484(1) Å, Rexp : 5.90 Rwp : 12.63 GOF : 2.14						
K	32e	0.1010(4)	0.1010(4)	0.1010(4)	0.2	4.9(2)
Cu	32e	0.1010(4)	0.1010(4)	0.1010(4)	0.025	4.9(2)
Nb	16c	0.5000	0.5000	0.5000	0.5	2.8(2)
Te	16c	0.5000	0.5000	0.5000	0.5	2.8(2)
O	48f	0.4311(2)	0.1250	0.1250	1	3.4(8)
SnKNTO; a= 10.2673(1) Å, Rexp : 5.34 Rwp : 10.48 GOF : 1.96						
K	32e	0.0897(1)	0.0897(1)	0.0897(1)	0.15	7.2(2)
Sn	32e	0.0897(1)	0.0897(1)	0.0897(1)	0.05	7.2(2)
Nb	16c	0.5000	0.5000	0.5000	0.5	0.5(1)
Te	16c	0.5000	0.5000	0.5000	0.5	0.5(1)
O	48f	0.4292(2)	0.1250	0.1250	1	0.6(1)

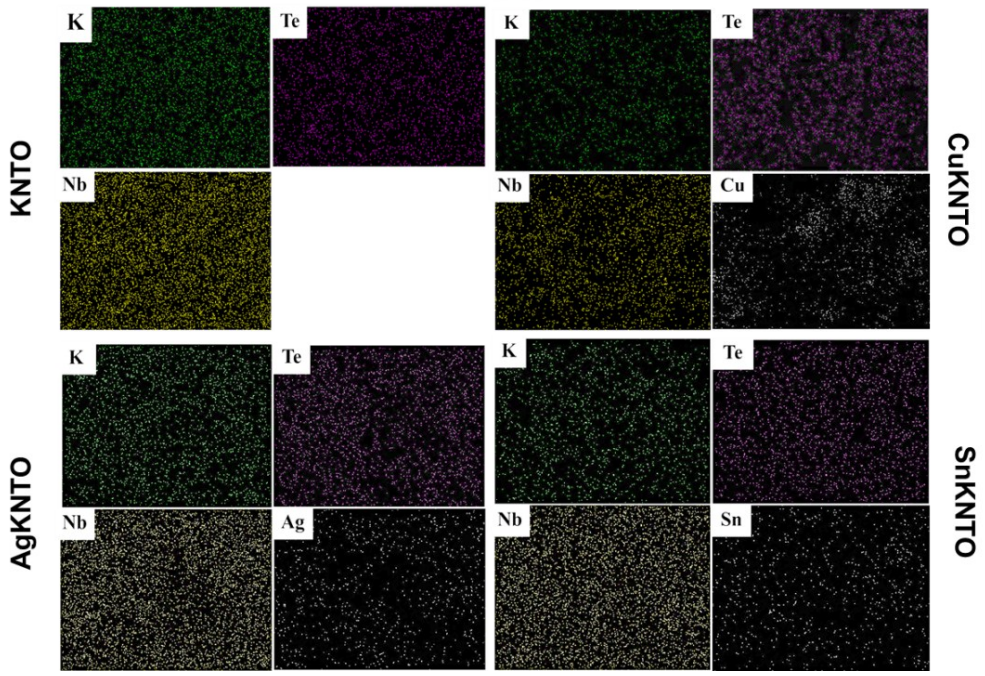

Fig. S4 The energy dispersive X-ray spectroscopy (EDS) elemental mapping images of KNTO, AgKNTO, CuKNTO, and SnKNTO.

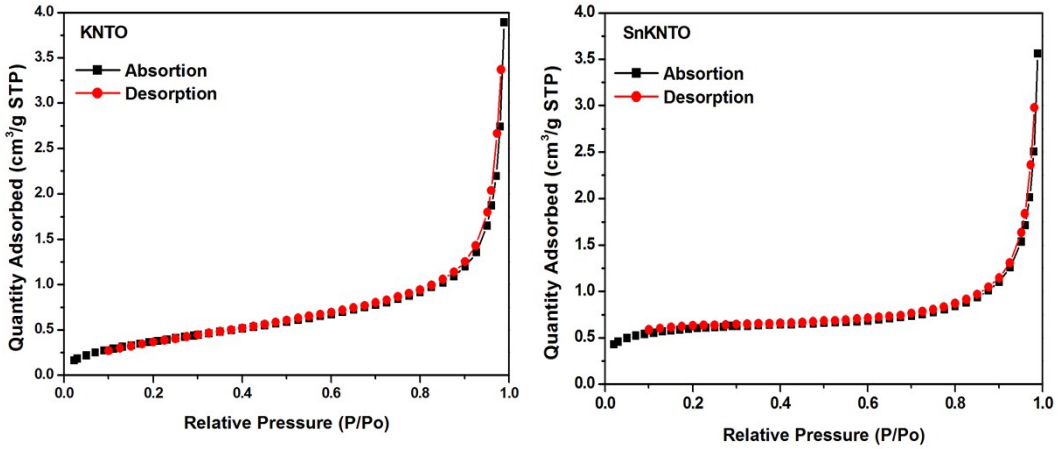

Fig. S5 N_2 adsorption–desorption isotherms of KNTO and SnKNTO

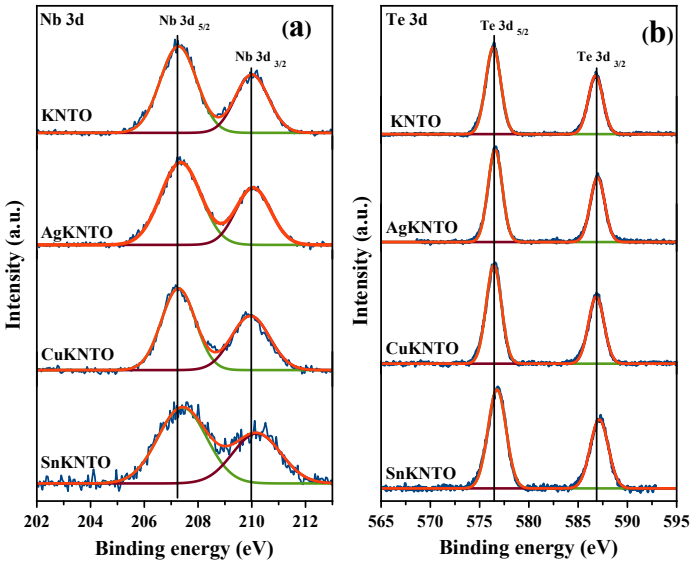

Fig. S6 Nb 3*d* (a) and Te 3*d* (b) XPS spectra of KNTO, AgKNTO, CuKNTO, and SNKNTO.

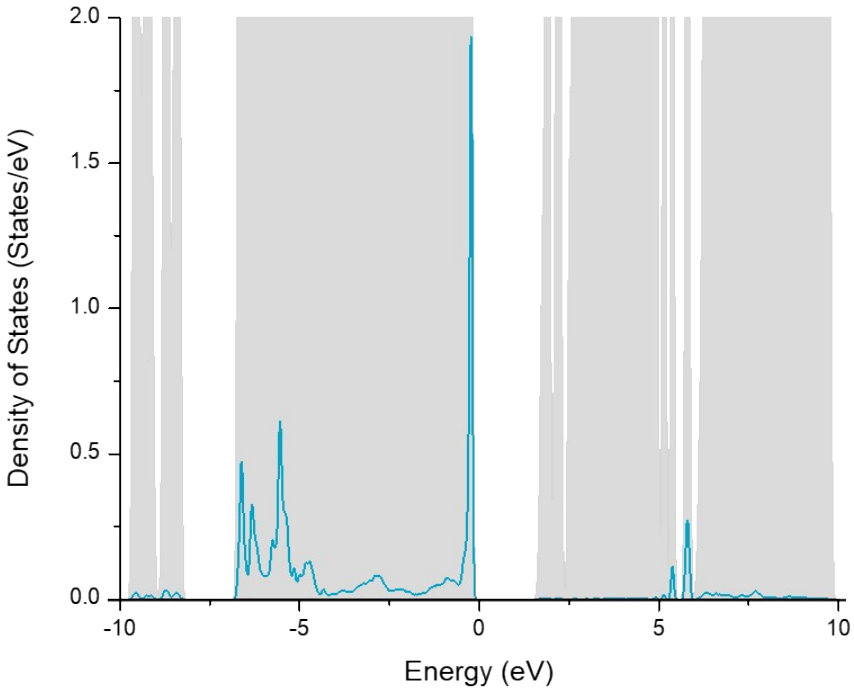

Fig. S7 Projected density of states of Sn 5*s* (blue line) which mainly contribute as bonding interactions (-5.5 eV) and antibonding interactions (-0.5 eV) in the valence band. The grey area illustrates the total DOS.

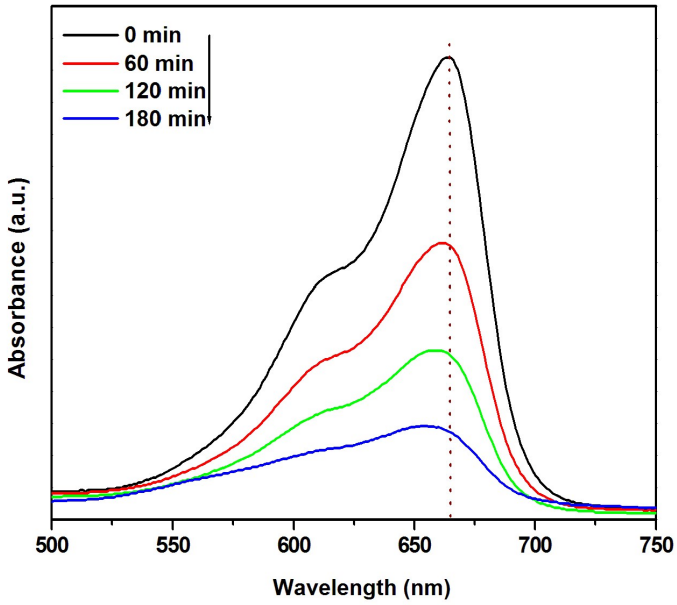

Fig. **S8** The UV-Vis spectra of MB solution degraded with SnKNTO at various times