Supporting Information for

Irreversible Thermochromic $Pb_2Sn_2O_6 \cdot xH_2O$: Competition between Weak Ligand H_2O and Lone-Pair Electrons

Xin Zhang, [a] Chenyang Zhang, *[b] Long Yuan, *[c] and Jiaqi Zhang *[a]

[a] *State Key Laboratory of Integrated Optoelectronics, Key Laboratory of Automobile Materials of MOE, School of Materials Science and Engineering, Jilin University, Changchun 130000, China. Corresponding email: zhangjiaqi@jlu.edu.cn (J.Z.).*
[b] *School of Chemistry and Materials Engineering, Xinxiang University, Xinxiang 453003, China. Email: chenyangz@xxu.edu.cn (C.Z.).*
[c] *Key Laboratory of Functional Materials Physics and Chemistry of the Ministry of Education, Jilin Normal University, Changchun 130103, China. Email: yuanlong@jlnu.edu.cn (L.Y.).*

Table S1. Atomic site parameters of Sample A and Sample B acquired from Rietveld refinement of the PXRD data.

	Atom	Wyckoff	x	y	z	Occ	Uiso
Sample A	Pb1	16c	0.000	0.000	0.000	1.000	0.056
	Sn1	16d	0.500	0.500	0.500	1.000	0.060
	O1	48f	0.404	0.125	0.125	1.000	0.042
Sample B	Pb1	16c	0.000	0.000	0.000	1.000	0.043
	Sn1	16d	0.500	0.500	0.500	1.000	0.033
	O1	48f	0.425	0.125	0.125	1.000	0.015

Table S2. Bond length results of Pb-O and Sn-O in Sample A and Sample B acquired from Rietveld refinement of the PXRD data.

Length (Å)	Pb-O	Sn-O
Sample A	2.522	2.168
Sample B	2.676	2.070

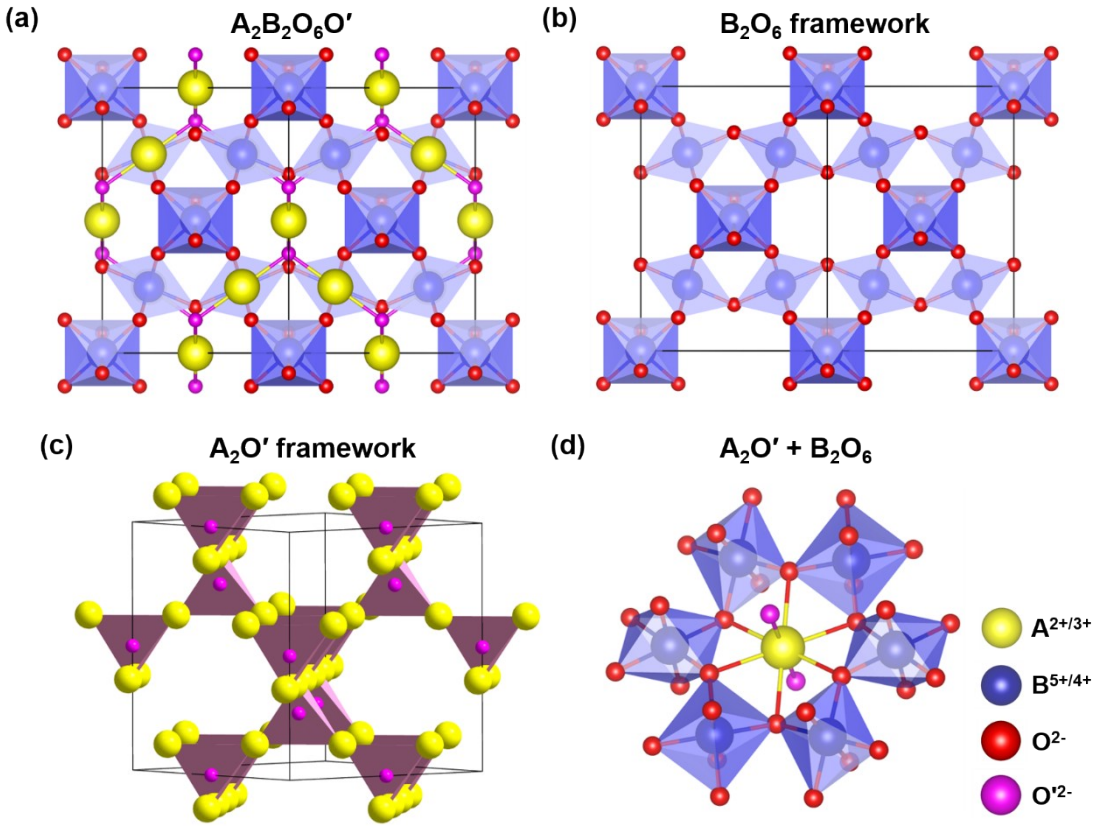

Fig. S1. (a) Ideal pyrochlore $A_2B_2O_6O'$ crystal structure in the $Fd\bar{3}m$ space group. (b) View of the B_2O_6 framework. (c) View of the tetrahedral A_2O' framework. (d) Coordination of Bi atom in the corner-shared SnO6 ring.

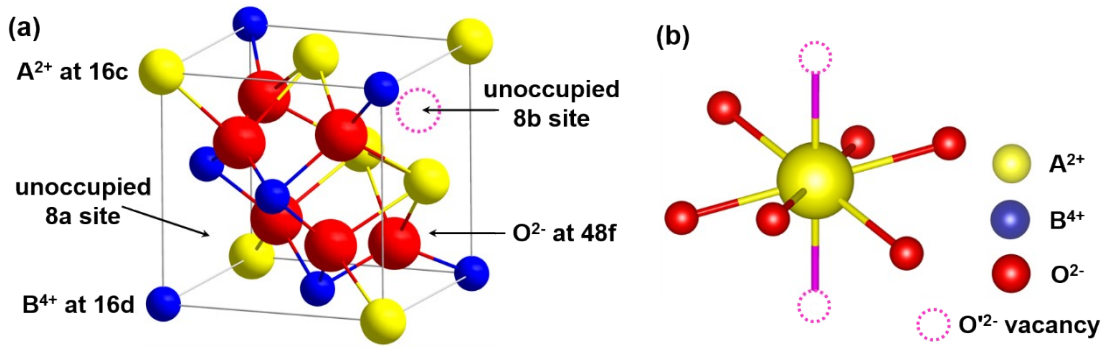

Fig. S2. (a) Local crystal structure of defect pyrochlore $A_2B_2O_6\square'$. (b) The $AO_6\square'_2$ coordination environment of each A^{2+}.

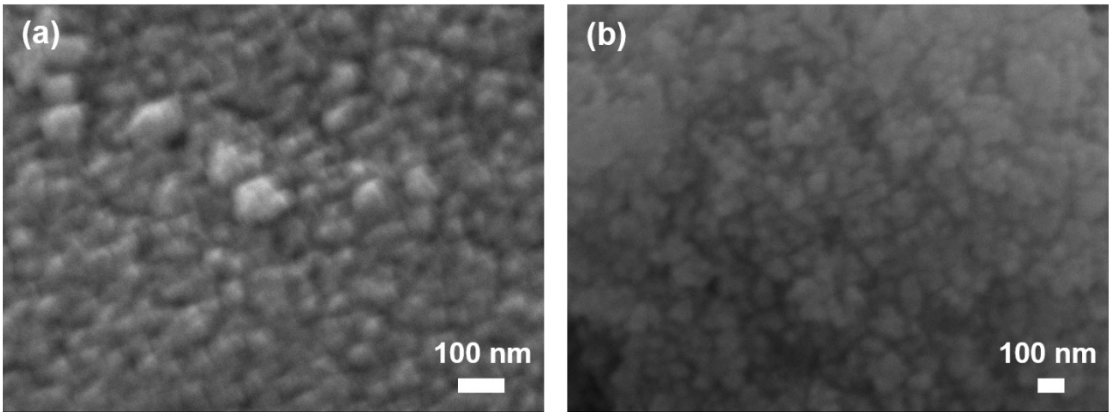

Fig. S3. SEM graphs of the as-synthesized samples (a) Sample A and (b) Sample B.

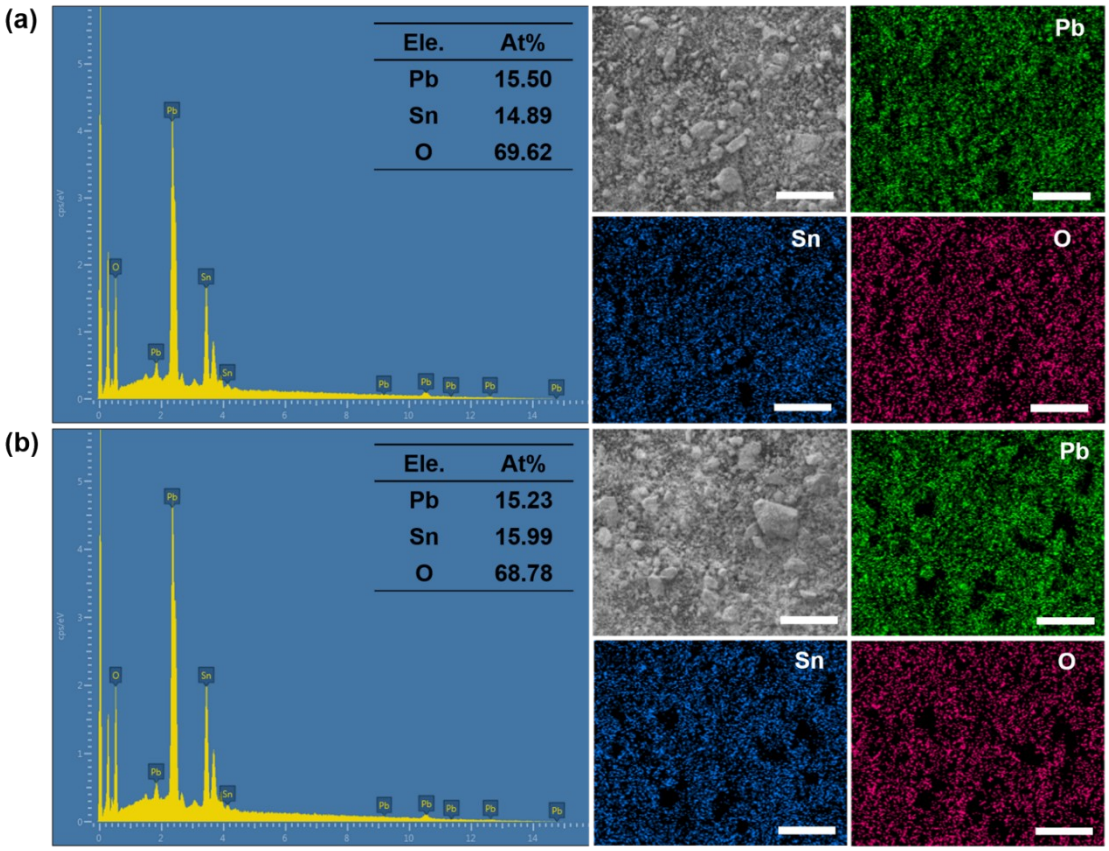

Fig. S4. EDS and element distribution mapping graphs of the samples (a) Sample A, (b) Sample B. Tables in each diagram listed the measured atomic ratio from the integration of the area of each element in the EDS for the samples with varied stoichiometry. Scale: 100 μm.

Table S3. Binding energy values of Pb 4f, Sn 3d and O 1s orbitals for Sample A and Sample B samples.

Element	Pb ($4f_{7/2}$, $4f_{5/2}$)	Sn ($3d_{5/2}$, $3d_{3/2}$)	O (1s)
Sample A	137.5, 142.4	485.8, 494.2	529.7
Sample B	137.8, 142.6	486.1, 494.5	530.0

Table S4. The CIE-L*a*b* parameters at different temperature of Sample A and Sample B samples.

Sample	**A**			**B**		
Tem. (°C)	L*	a*	b*	L*	a*	b*
25	82	5	46	85	7	42
50	81	-4	50	84	-6	44
75	82	-2	53	87	-4	47
100	81	0	53	84	-3	47
125	76	1	53	80	-1	47
150	78	1	55	80	-1	49
175	79	1	58	81	1	51
200	79	0	60	80	1	50
225	77	2	60	77	1	51
250	77	3	61	79	1	52
275	72	6	59	76	3	54
300	67	8	54	78	3	55
325	65	7	54	73	4	58
350	71	9	57	76	7	53
375	69	12	59	67	9	49
400	68	13	61	64	10	48
425	65	14	58	64	9	43
450	64	13	53	61	9	41
475	60	12	46	60	8	37
500	56	12	41	57	9	31
25	63	12	41	65	10	35

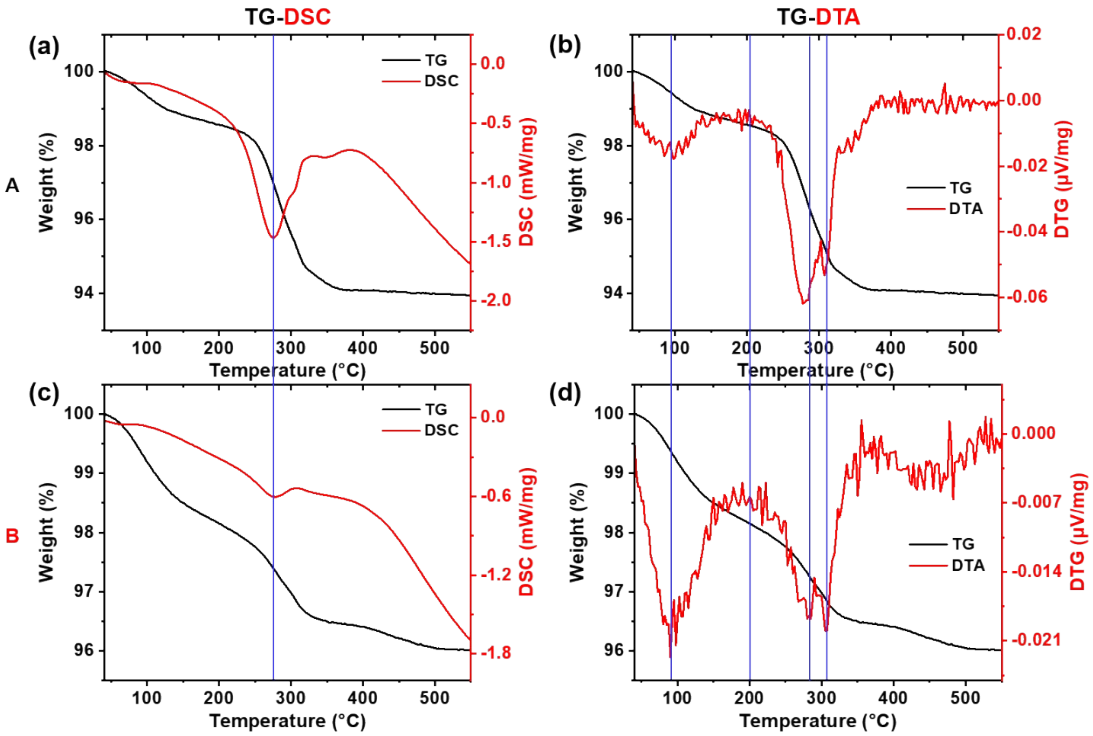

Fig. S5. TG-DTA-DSC of Sample A and Sample B.