Electronic Supplementary Information (ESI)

High Temperature Hybrid Perovskite Multifunctional Switching Materials Constructed Through Precise Molecular Design

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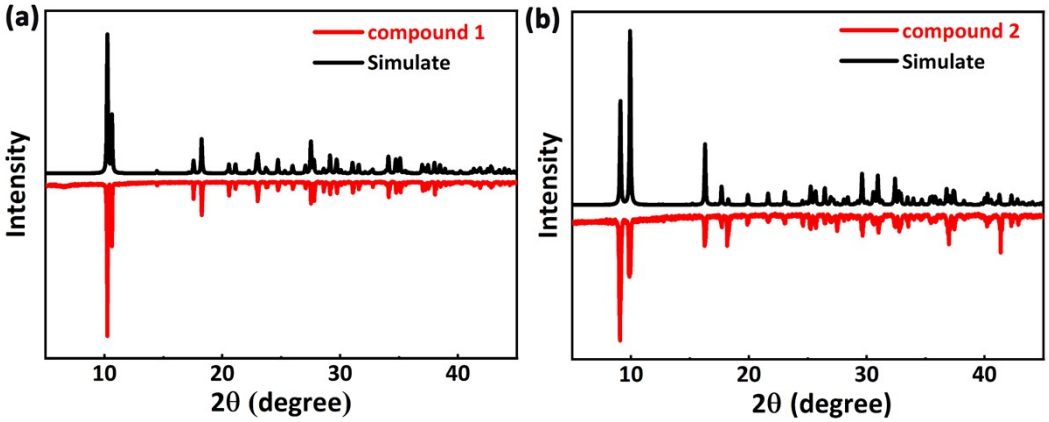

Fig. S1 Experimental and simulated powder x-ray diffractions patterns (PXRD) spectra of compound **1** and **2**.

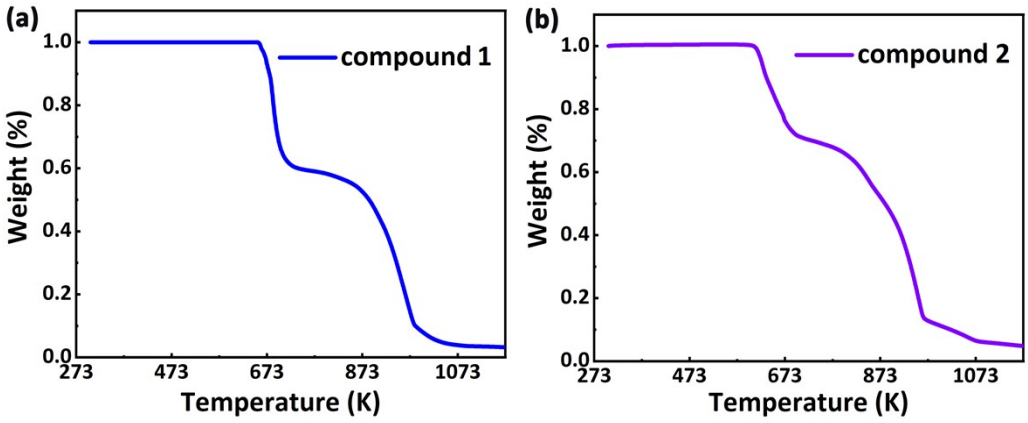

Fig. S2 The TGA of compound **1** (a) and compound **2** (b).

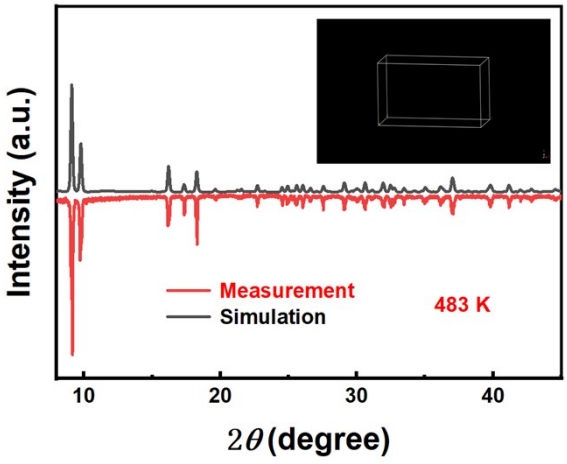

Fig. S3. Pawley refinement of PXRD data of compound **2** at 483 K with an orthorhombic unit cell.

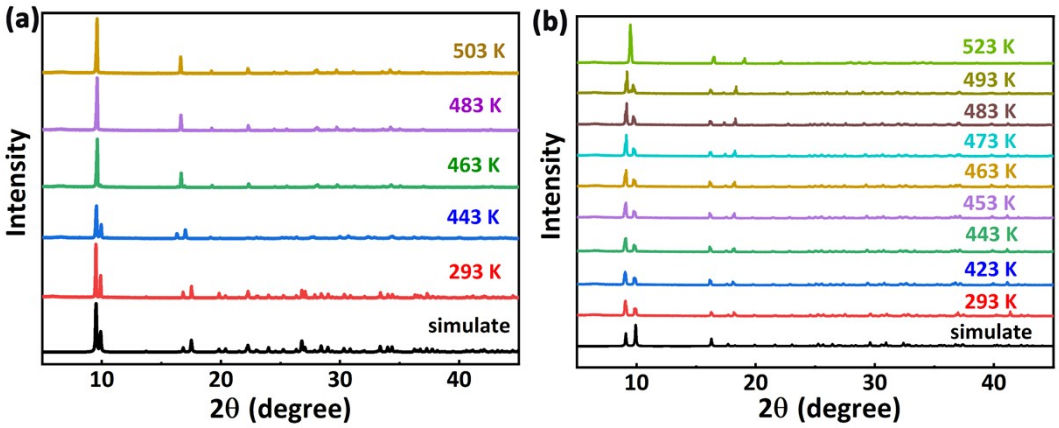

Fig. S4 Variable-temperature PXRD patterns of compound **1** (a) and compound **2** (b).

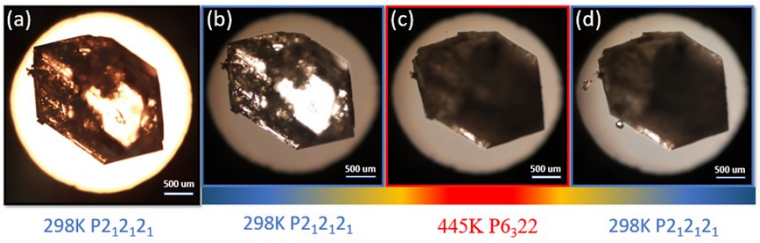

Fig. S5 Ferroelastic domain variation of **1** in the continuous heating and cooling process.

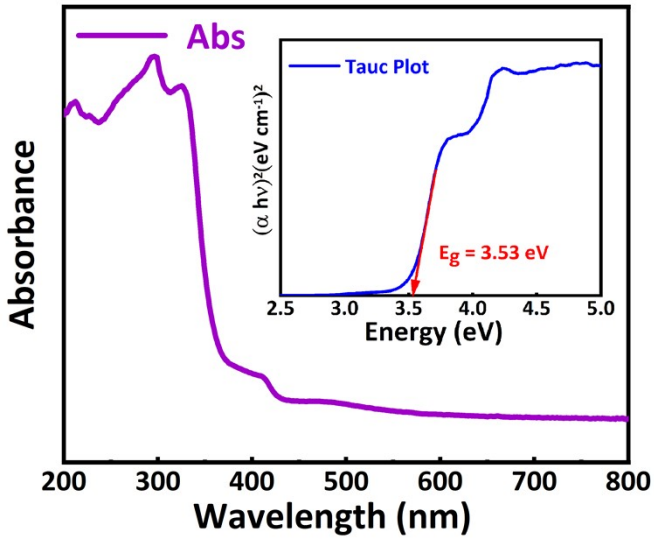

Fig. S6 Absorption spectra and optical bandgap calculated from corresponding Tauc plot of **2** (inset).

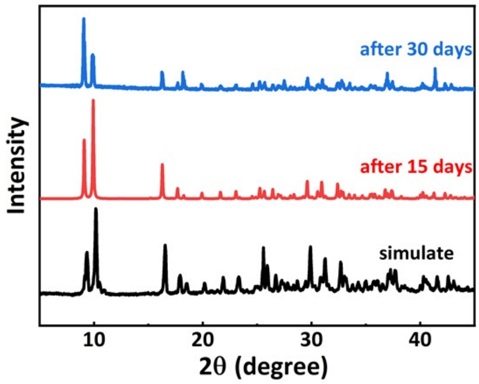

Fig. S7 Stability test of **2** at 45% humidity for 30 days.

α/°	90	90
β/°	90	90
γ/°	90	120
Volume/Å³	1499.14(10)	790.9(5)
Z	4	2
ρ_{calc}g/cm³	2.752	2.406
Index ranges	-9 ≤ h ≤ 10, -12 ≤ k ≤ 12, -24 ≤ l ≤ 24	-15 ≤ h ≤ 13, -10 ≤ k ≤ 13, -9 ≤ l ≤ 11
Reflections collected	8772	4354
Independent reflections	3627 [Rint = 0.0308, Rsigma = 0.0382]	746 [Rint = 0.0822, Rsigma = 0.0596]
Data/restraints/parameters	3627/0/146	746/68/40
Goodness-of-fit on F²	0.993	1.062
Final R indexes [I>=2σ (I)]	R1 = 0.0282, wR2 = 0.0608	R1 = 0.0894, wR2 = 0.1907
Final R indexes [all data]	R1 = 0.0402, wR2 = 0.0636	R1 = 0.2673, wR2 = 0.2561
Largest diff. peak/hole / e Å⁻³	0.91/-1.49	0.21/-0.40

Identification code	**1rt**	**1ht**
Empirical formula	$C_9H_{18}Br_3NOPb$	$C_9H_{18}Br_3NOPb$
Formula weight	603.14	603.14
Temperature/K	300 K	463 K
Crystal system	orthorhombic	hexagonal
Space group	$P2_12_12_1$	$P6_322$
a/Å	8.6914(3)	10.719(3)
b/Å	10.0950(4)	10.719(3)
c/Å	16.6347(6)	7.963(4)
α/°	90	90
β/°	90	90
γ/°	90	120
Volume/Å³	1459.52(9)	792.3(6)
Z	4	2
ρ_{calc}g/cm³	2.745	2.326
Index ranges	-11 ≤ h ≤ 9, -12 ≤ k ≤ 12, -20 ≤ l ≤ 18	-11 ≤ h ≤ 9, -12 ≤ k ≤ 12, -20 ≤ l ≤ 18
Reflections collected	8254	3501
Independent reflections	3449 [Rint = 0.0245, Rsigma = 0.0330]	719 [Rint = 0.0770, Rsigma = 0.0628]
Data/restraints/parameters	3449/9/139	719/103/48
Goodness-of-fit on F²	1.062	1.120
Final R indexes [I>=2σ (I)]	R1 = 0.0333, wR2 = 0.0770	R1 = 0.0532, wR2 = 0.1141
Final R indexes [all data]	R1 = 0.0410, wR2 = 0.0799	R1 = 0.1993, wR2 = 0.1431

Table S1. Crystal Date and Structure Refinement for compound **1.**

Table S2. Crystal Data and Structure Refinement for compound **2**.