High-temperature dielectric switching and photoluminescence in a corrugated lead bromide layer hybrid perovskite semiconductor

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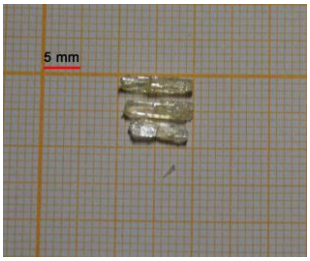

Figure S1. Large crystals of **1,** showing the approximate size of 10mm × 2mm × 2mm.

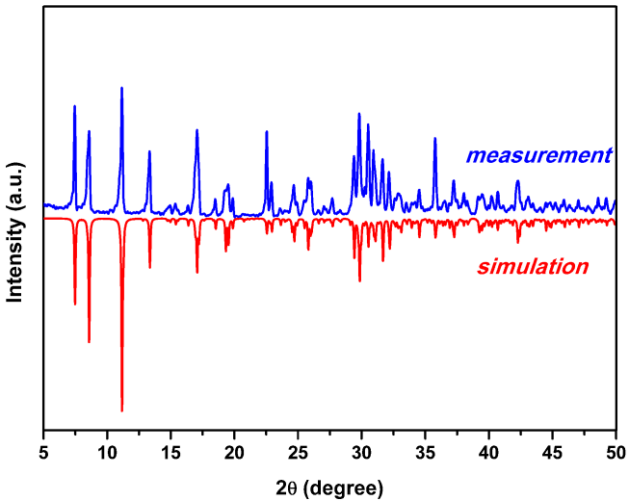

Figure S2. Measurement and simulation pattern of the powder X-ray diffraction (PXRD) for **1**.

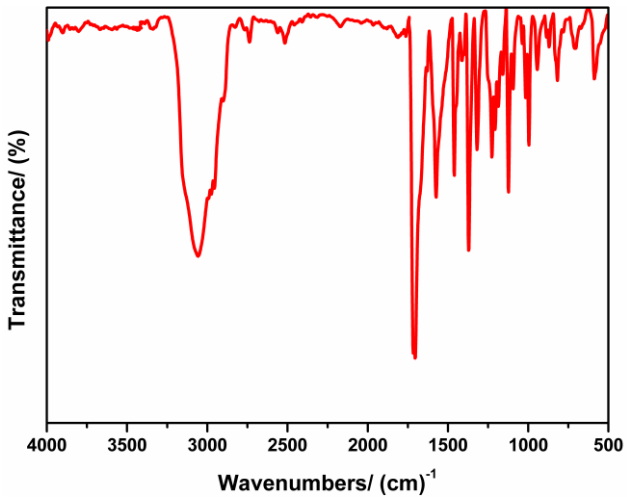

Figure S3. IR spectrum for **1**.

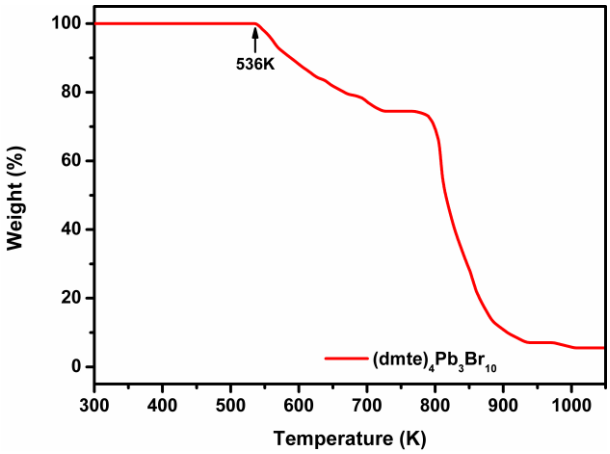

Figure S4. TGA curve of **1**.

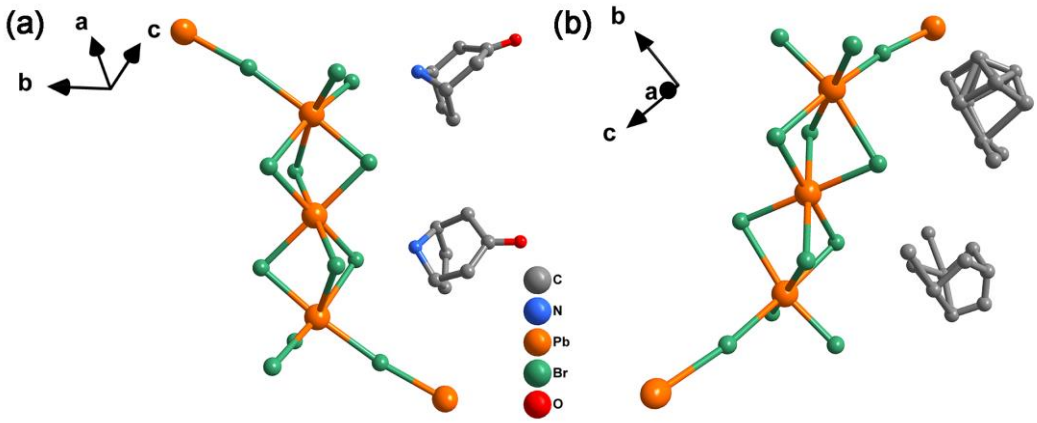

Figure S5. Molecular structures of **1** at 293 K (a) and 443 K (b). All the hydrogen atoms are omitted for clarity.

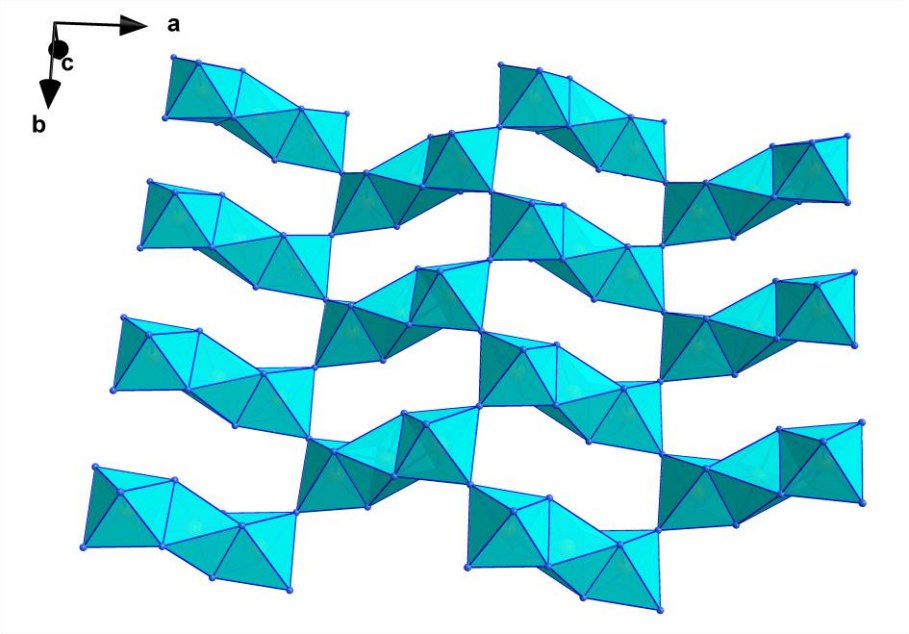

Figure S6. Packing view of inorganic layers in **1**.

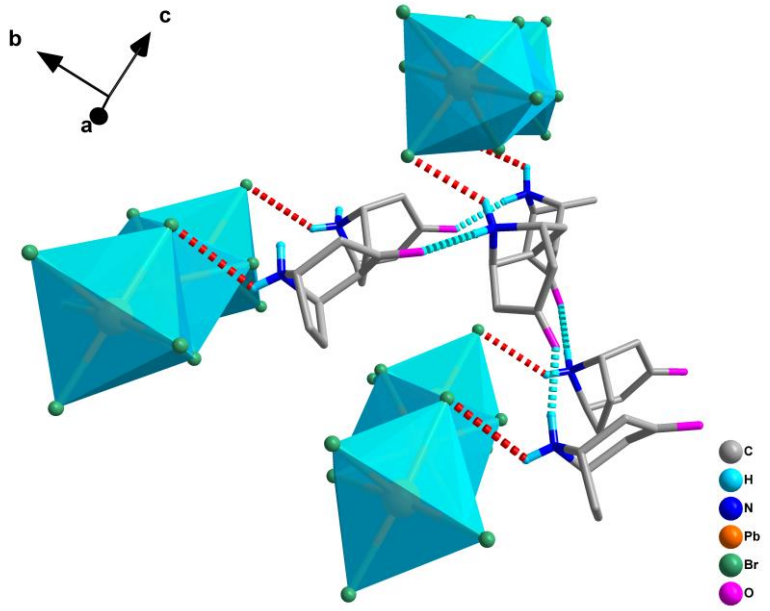

Figure S7. Hydrogen bonding interactions between organic cations (blue) and between the organic cation and inorganic layer (red) at LTP.

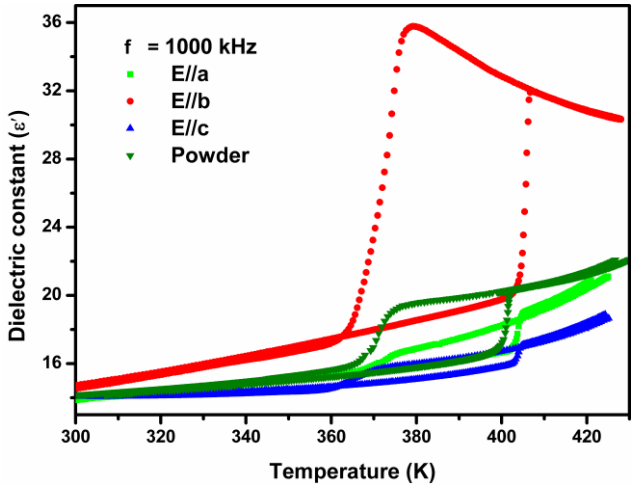

Figure S8. Reversible anisotropic dielectric curves of **1** measured along *a*-, *b*- and *c*-axes under 1000 kHz.

Table S1. Crystal data and refinement details of **1**.

Temperature (K)	293 K	443 K
Crystal system	Orthorhombic	Orthorhombic
Space group	*Pbca*	*Cmca*
a/ Å	20.9220 (5)	9.3779 (3)
b/ Å	9.1743 (2)	23.5404 (9)
c/ Å	23.6345 (6)	21.1914 (8)
Volume/(Å^3)	4536.52 (19)	4678.2 (3)
Z	4	2
Radiation type	Mo-Kα; λ = 0.71073 Å	Mo-Kα; λ = 0.71073 Å
Dcalc / g cm^{-3}	2.819	2.017
F(000)	3488.0	2384
GOF	1.020	1.125
R_1[I > 2σ (I)]	0.0304	0.0557
wR_2 [I > 2σ (I)]	0.0495	0.1675
R_{int}	0.035	0.047

Table S2. Pb-Br bond lengths [Å] and Br−Pb−Br bond angles [°] for **1** in LTP.

Pb1−Br1	3.0120 (4)	Pb2−Br1	3.1187 (4)
Pb1−Br2	3.0008 (4)	Pb2−Br2	3.2131 (5)
Pb1−Br3	3.0435 (5)	Pb2−Br3	3.0179 (5)
		Pb2−Br4	2.9737 (4)
		Pb2−Br5	2.8427 (5)
Br1−Pb1−Br3	83.696 (12)	Br4−Pb2−Br3	90.737 (14)
Br2−Pb1−Br1	81.075 (11)	Br5−Pb2−Br1	94.868 (15)
Br2−Pb1−Br3	83.150 (12)	Br5−Pb2−Br2	164.041 (16)
Br1−Pb2−Br2	76.208 (11)	Br5−Pb2−Br3	85.690 (16)
Br3−Pb2−Br2	80.073 (13)	Br5−Pb2−Br4	94.332 (16)
Br3−Pb2−Br1	82.330 (13)	Pb1−Br1−Pb2	82.697 (10)
Br4−Pb2−Br1	168.023 (15)	Pb1−Br2−Pb2	81.295 (10)
Br4−Pb2−Br2	93.030 (14)	Pb2−Br3−Pb1	83.874 (12)

Table S3. Hydrogen bonds for **1** in LTP (293 K).

D−H···A	D−H	H···A	D···A
N1−H1B···O2^{iv}	0.89	2.06	2.937 (6)
N1−H1A···Br5	0.89	2.70	3.362 (4)
N2−H2A···O1^{iv}	0.89	1.99	2.867 (5)
N2−H2B···Br1^{ii}	0.89	2.69	3.514 (4)
N2−H2B···Br2^{ii}	0.89	2.90	3.386 (3)
C2−H2D···Br3^{vii}	0.97	2.92	3.828 (5)
C4−H4B···Br3	0.97	3.00	3.759 (6)
C6−H6···Br4	0.98	2.86	3.698 (5)
C9−H9B···Br2^{viii}	0.97	2.82	3.625 (4)
C9−H9A···O1^{iv}	0.97	2.57	3.274 (6)
C12−H12A···Br2^{vi}	0.97	2.94	3.863 (4)
C13−H13···Br3	0.98	3.11	3.817 (4)
C14−H14A···Br1^{v}	0.97	3.07	3.788 (4)
Symmetry codes: (ii) −x+1, −y+1, −z; (iv) −x+1, y+1/2, −z+1/2; (v) x, y−1, z; (vi) −x+1, −y, −z; (vii) −x+1, y−1/2, −z+1/2; (viii) x−1/2, −y+1/2, −z.			

Table S4. Pb-Br Bond lengths [Å] and Br−Pb−Br bond angles [°] for **1** in HTP.

Pb1−Br1	3.0933 (3)	Br2−Pb1−Br1	90.80 (6)
Pb1−Br2	2.801 (2)	Br2−Pb1−Br4	91.59 (6)
Pb1−Br4	3.0455 (15)	Br4−Pb1−Br1	89.90 (3)
Pb2−Br3	2.9825 (16)	Br3−Pb2−Br4	82.95 (4)
Pb2−Br4	3.0306 (16)	Pb2−Br4−Pb1	84.26 (3)