

Smart and efficient opto-electronic dual response material based on two-dimensional perovskite crystal/thin film

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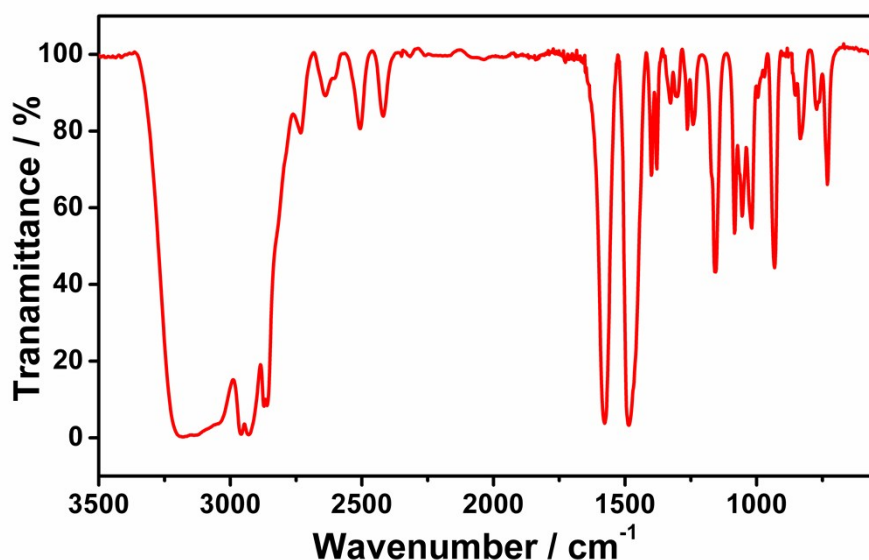


Fig. S1 Infrared spectrum of **1**. Description: the IR spectrum of **1** displayed the existence of typical strong stretching vibration peaks (C-N at 1000-1200 cm⁻¹, C-H/N-H at 2500-3300 cm⁻¹), which could consider as a indirect proof to the crystalline structure we have obtained.

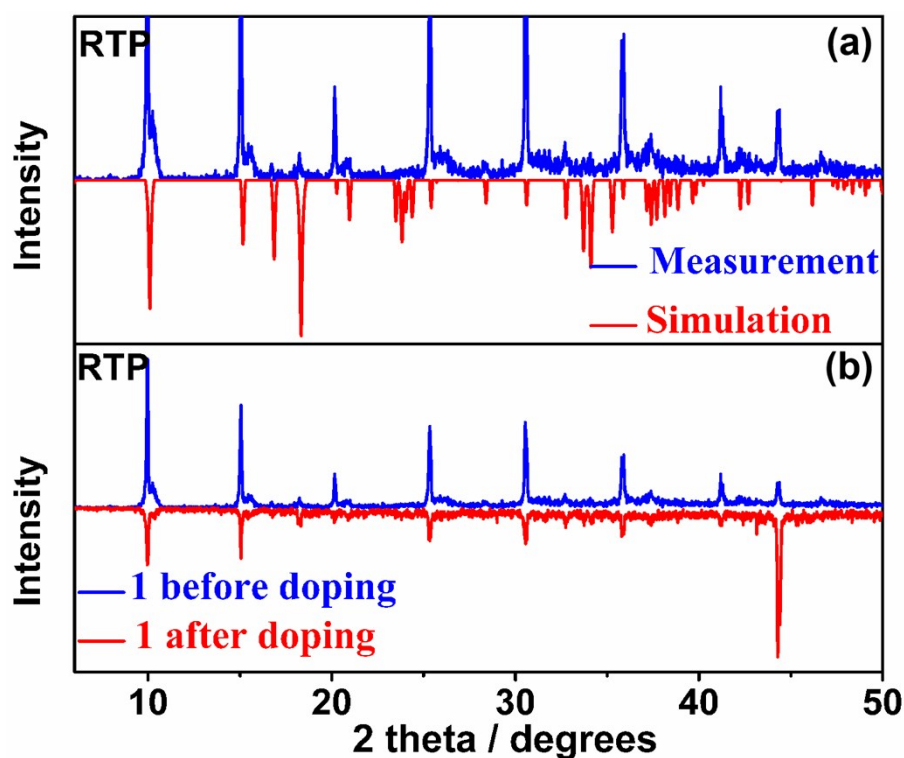


Fig. S2 (a) PXRD pattern of **1** at RTP, verifying the purity of the bulk phase. (b) PXRD pattern of Mn-doped **1**, indicating that the crystal structure nearly no change after doping.

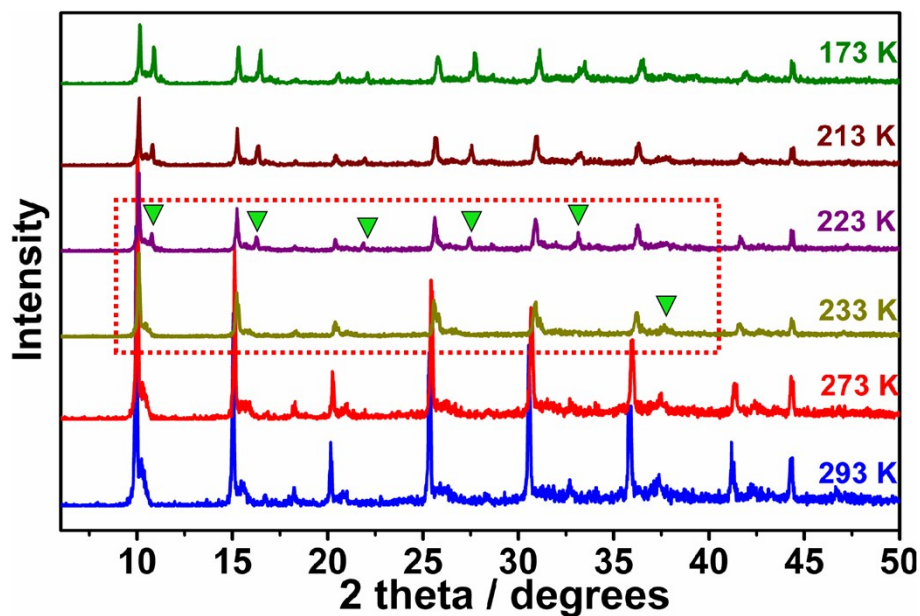


Fig. S3 Variable-temperature PXRD patterns of **1**, the green triangle labeled the changes of diffraction peak near the phase transition point.

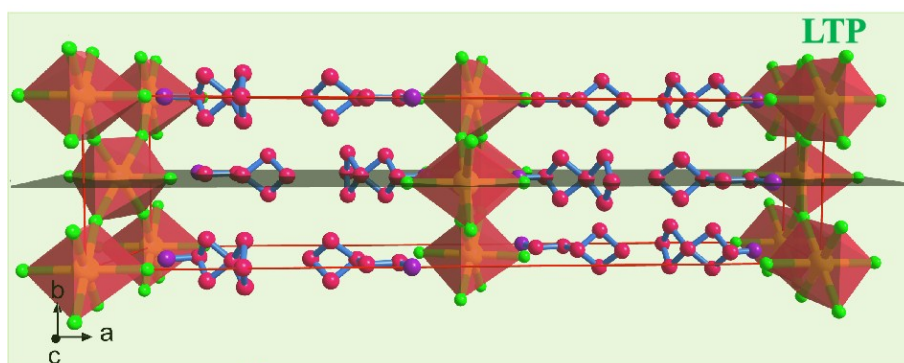


Fig. S4 Crystal-packing views of compound **1** along a-axis at LTP (173 K). Besides, the H atoms had been omitted for clarity.

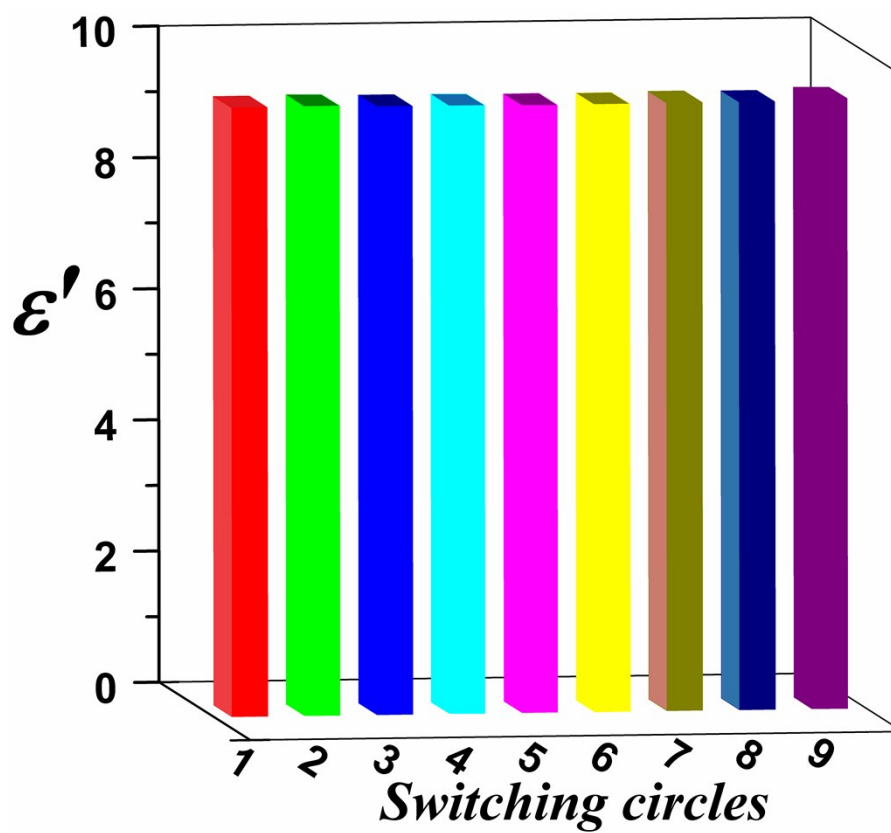


Fig. S5 The real part (ϵ') of the dielectric permittivity at around phase transition point in the top nine cycles.

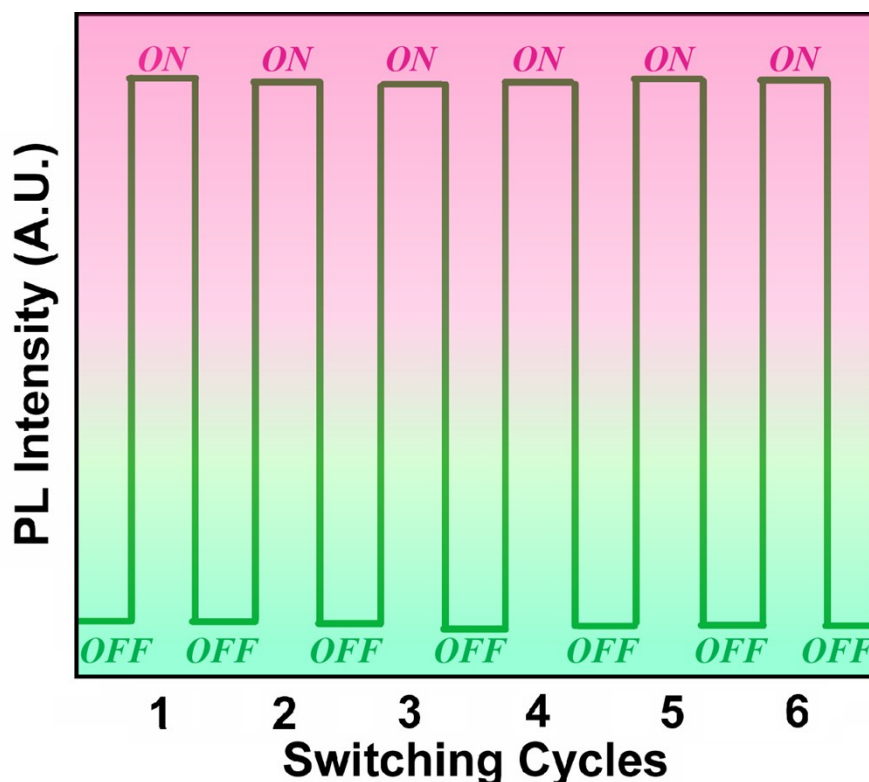


Fig. S6 Schematic diagram of PL "ON"/"OFF" cycles based on **1**, which revealed the rapid recovery of photoluminescent intensity after continuous several cycles without any obvious fatigue.

Table S1. Crystal data and structure refinements for **1** at 173 K and 293 K.

	LTP (173 K)	HTP (293 K)
Empirical formula	[C ₅ H ₁₄ N] ₂ ·[CdCl ₄]	[C ₅ H ₁₄ N] ₂ ·[CdCl ₄]
Formula weight	430.54	1063.64
Crystal system	monoclinic	orthorhombic
Space group	<i>C2/m</i>	<i>Cccm</i>
<i>a</i> /Å	32.62(8)	35.017(2)
<i>b</i> /Å	7.442(16)	7.5656(15)
<i>c</i> /Å	7.618(16)	7.4627(15)
Volume (Å ³)	1825(7)	1977.1(6)
<i>F</i> (000)	872	876
Collected reflections	2902	5300
Unique reflections	1429	948
Absorption correction	Multi-scan	Multi-scan
<i>Z</i> , Calculated density	4, 1.567 Mg/m ³	4, 1.450 Mg/m ³
Goodness-of-fit on <i>F</i> ²	1.034	1.105
<i>R</i> ₁ / <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.121/0.342	0.091/0.275

Table S2 Selected structural data for 1 under 173 K

<i>Bond lengths / Å and bond angles / °</i>			
Cd1-Cl1	2.575(7)	Cd1-Cl1#1	2.575(7)
Cd1-Cl2	2.697(5)	Cd1-Cl2#1	2.697(5)
Cd1-Cl2#2	2.697(5)	Cd1-Cl2#3	2.697(5)
Cd2-Cl2	2.674 (4)	Cd2-Cl2#5	2.674 (4)
Cd2-Cl2#6	2.674 (4)	Cd2-Cl2#7	2.674 (4)
Cd2-Cl3	2.572(6)	Cd2-Cl3#4	2.572(6)
Cl1#1-Cd1-Cl1	180.0	Cl1#1-Cd1-Cl2#1	89.38(8)
Cl1-Cd1-Cl2#1	90.62(8)	Cl1#1-Cd1-Cl2	90.62(8)
Cl1-Cd1-Cl2	89.38(8)	Cl2#1-Cd1-Cl2	180.0
Cl1#1-Cd1-Cl2#2	89.38(8)	Cl1-Cd1-Cl2#2	90.62(8)
Cl2#1-Cd1-Cl2#2	88.2(2)	Cl2-Cd1-Cl2#2	91.8(2)
Cl1#1-Cd1-Cl2#3	90.62(8)	Cl1-Cd1-Cl2#3	89.38(8)
Cl2#1-Cd1-Cl2#3	91.8(2)	Cl2-Cd1-Cl2#3	88.2(2)
Cl2#2-Cd1-Cl2#3	180.00(6)	Cl3-Cd2-Cl3#4	180.00(3)
Cl3-Cd2-Cl2	89.33(10)	Cl3#4-Cd2-Cl2	90.67(10)
Cl3-Cd2-Cl2#5	89.33(10)	Cl3#4-Cd2-Cl2#5	90.67(10)
Cl2-Cd2-Cl2#5	87.17(19)	Cl3-Cd2-Cl2#4	90.67(10)
Cl3#4-Cd2-Cl2#4	89.33(10)	Cl2-Cd2-Cl2#4	180.00(11)
Cl2#5-Cd2-Cl2#4	92.83(19)	Cl3-Cd2-Cl2#6	90.67(10)
Cl3#4-Cd2-Cl2#5	89.33(10)	Cl2-Cd2-Cl2#6	92.83(19)
Cl2#5-Cd2-Cl2#6	180.00(11)	Cl2#4-Cd2-Cl2#6	87.17(19)
Cd2-Cl2-Cd1	109.0(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z; #2 -x, y, -z; #3 x, -y, z; #4 -x, -y+1, -z+1; #5 x, -y+1, z; #6 -x, y, -z+1.

Table S3 Selected structural data for 1 under 293 K

<i>Bond lengths / Å and bond angles / °</i>			
Cd1-Cl1	2.6710(4)	Cd1-Cl1#1	2.6710(4)
Cd1-Cl1#2	2.6710(4)	Cd1-Cl1#3	2.6710(4)
Cl1-Cd1#4	2.6710(4)	Cd1-Cl2	2.526(2)
Cd1-Cl2#1	2.526(2)		
Cl2#1-Cd1-Cl2	180.000(15)	Cl2#1-Cd1-Cl1#2	89.78(6)
Cl2-Cd1-Cl1#2	90.22(6)	Cl2#1-Cd1-Cl1#3	90.22(6)
Cl2-Cd1-Cl1#3	89.78(6)	Cl1#2-Cd1-Cl1#3	180.0
Cl2#1-Cd1-Cl1	89.78(6)	Cl2-Cd1-Cl1	90.22(6)
Cl1#2-Cd1-Cl1	88.612(19)	Cl1#3-Cd1-Cl1	91.388(19)
Cl2#1-Cd1-Cl1#1	90.22(6)	Cl2-Cd1-Cl1#1	89.78(6)

Cl1#2-Cd1-Cl1#1	91.388(19)	Cl1#3-Cd1-Cl1#1	88.612(19)
Cl1-Cd1-Cl1#1	180.00(9)	Cd1-Cl1-Cd1#4	168.14(9)

Symmetry transformations used to generate equivalent atoms: #1 $-x+1/2, -y+1/2, -z$; #2 $x, y, -z$; #3 $-x+1/2, -y+1/2, z$; #4 $x, -y, -z+1/2$.

Table S4 Comparison between 1 and other structurally similar thermal-responsive materials

Empirical formula	Response speed (K)	Reversibility (K)	Reference
$[\text{C}_5\text{H}_{14}\text{N}]_2 \cdot [\text{CdCl}_4]$	<8 K	Around 8 K	This work
$[\text{C}_4\text{H}_{11}\text{NBr}] \cdot [\text{MnBr}_3]$	Around 15 K	Around 23 K	56
$[\text{C}_4\text{H}_{11}\text{NCl}] \cdot [\text{PbI}_3]$	Around 10 K	Around 20 K	57
$[\text{C}_4\text{H}_{11}\text{NBr}] \cdot [\text{PbI}_3]$	Around 9 K	Around 10 K	57
$[\text{C}_6\text{H}_{14}\text{N}_2] \cdot [\text{RbCl}_3]$	Around 15 K	Around 10 K	49
$[\text{C}_3\text{H}_5\text{NH}_3]_2 \cdot [\text{CdCl}_4]$	Around 10 K	Around 5 K	58

Notes: the thermal response speed of compounds is justified by the response temperature range at around phase transition point while reversibility of compounds is justified by the thermal hysteresis between endothermic peak upon heating processes and exothermic peak upon cooling processes.