

Supplementary information

Room temperature ferroelectricity and blue photoluminescence in zero dimensional organic lead iodine perovskites

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Table S1. Xprep information of the DMAPbI₃ single crystal XRD data measured at room temperature.

Option	Space Group	No.	Type	Axes	CSD	R(sym)	N(eq)	Syst. Abs.	CFOM
[A]	<i>Cmca</i>	#64	centro	2	113	0.060	4617	0.9 / 5.2	4.79
[B]	<i>Aba2</i>	#41	non-cen	5	69	0.060	4617	0.9 / 5.2	4.89

Table S2 Crystallographic data

Temperature	293 K
Formula	C ₈ N ₄ H ₃₂ PbI ₆
Formula weight	1152.71
Crystal system	Orthorhombic
Space group	<i>Aba2</i>
<i>a</i> / Å	11.5704(9)
<i>b</i> / Å	15.1216(14)
<i>c</i> / Å	16.3060(14)
α / °	90
β / °	90
γ / °	90
<i>V</i> / Å ³	2852.9(4)
<i>Z</i>	4
<i>D</i> _c / g·cm ⁻³	2.684
<i>F</i> (000)	1904
GOF on <i>F</i> ²	1.043
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0486, 0.1022
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0870, 0.1158
Flack parameter	0.44(4)
CCDC	2016638

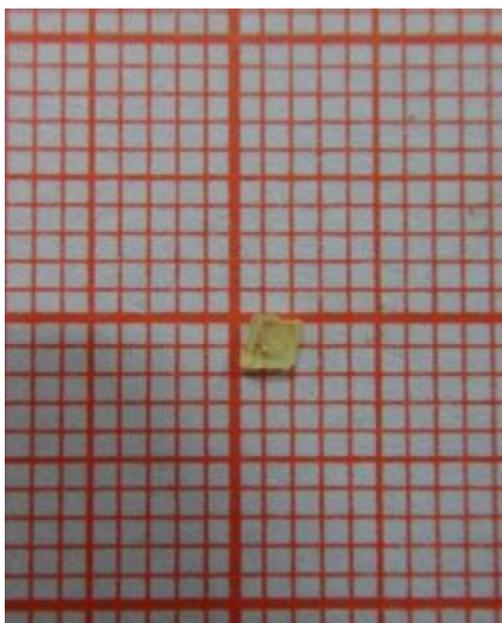


Fig. S1 Digital photo of the grown single crystal of 0D (DMA)₄PbI₆.

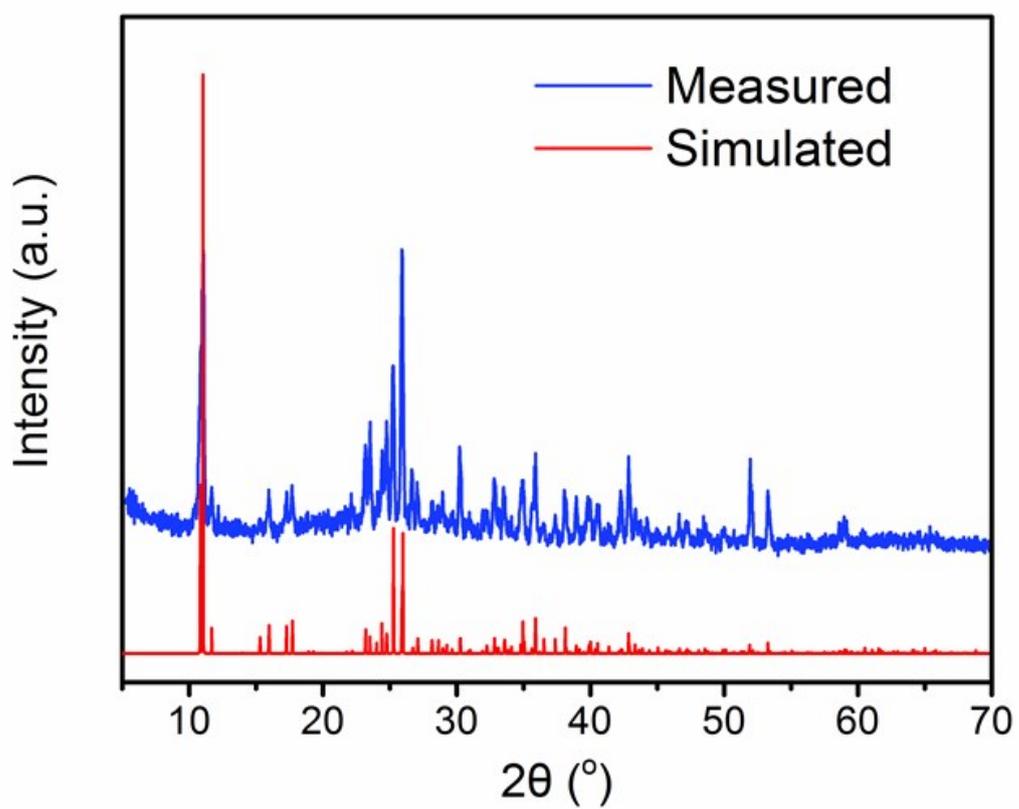


Fig. S2 Powder X-ray diffraction pattern of 0D DMA₄PbI₆ powder and its single crystal X-ray diffraction simulate result

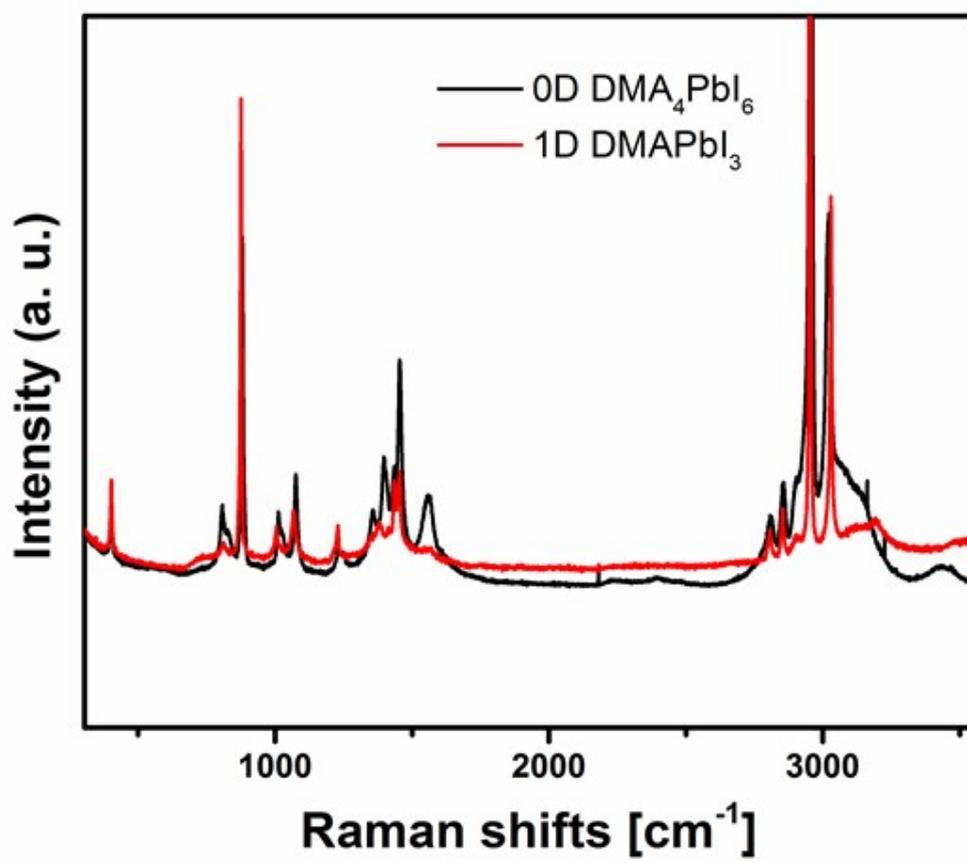


Fig. S3 Raman spectra of (DMA)₄PbI₆ measured at room temperature compared with 1D DMAPbI₃.

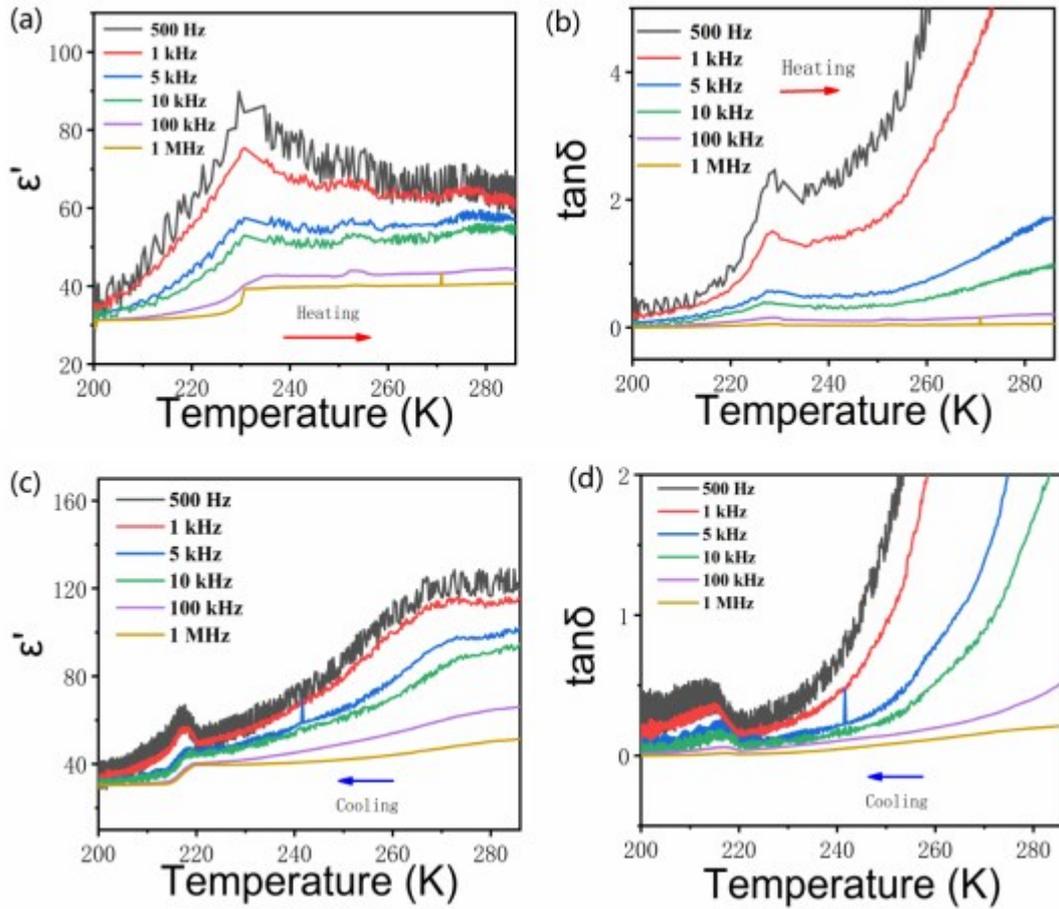


Fig. S4 Temperature dependent dielectric constant and dielectric loss of single crystal $(\text{DMA})_4\text{PbI}_6$ in the heating process and cooling process. (a) Dielectric constant in the heating process, (b) dielectric loss in the heating process, (c) Dielectric constant in the cooling process, (d) dielectric loss in the cooling process.

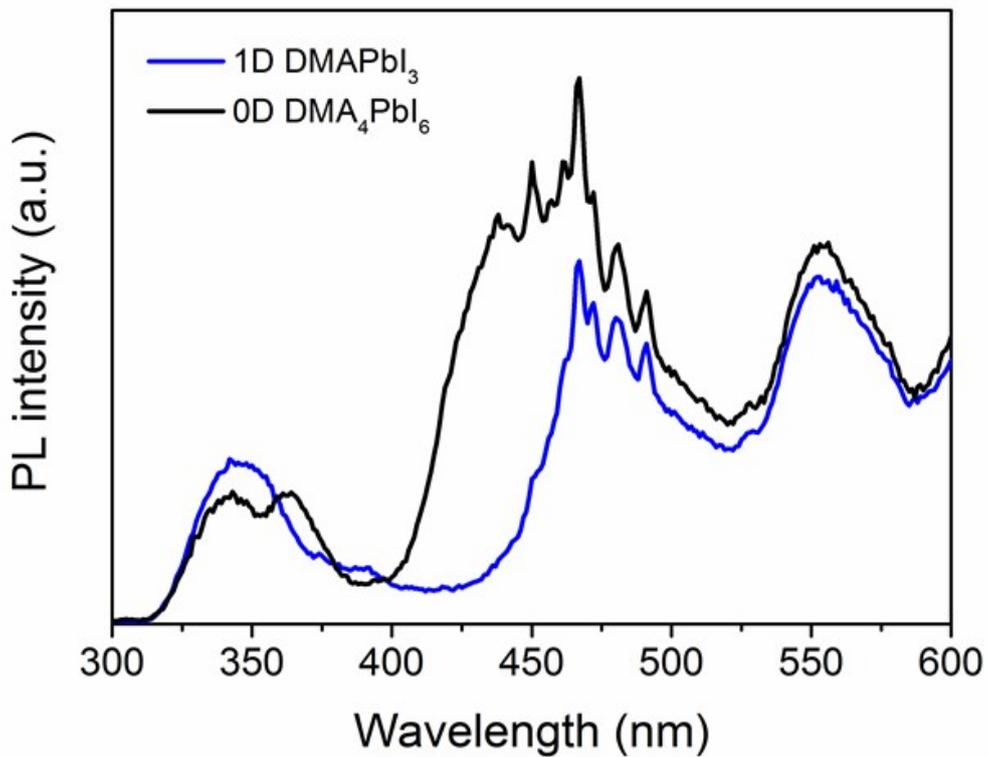


Fig. S5 Photoluminescence of 0D (DMA)₄PbI₆ and 1D DMAPbI₃ excited by 200 nm UV light.

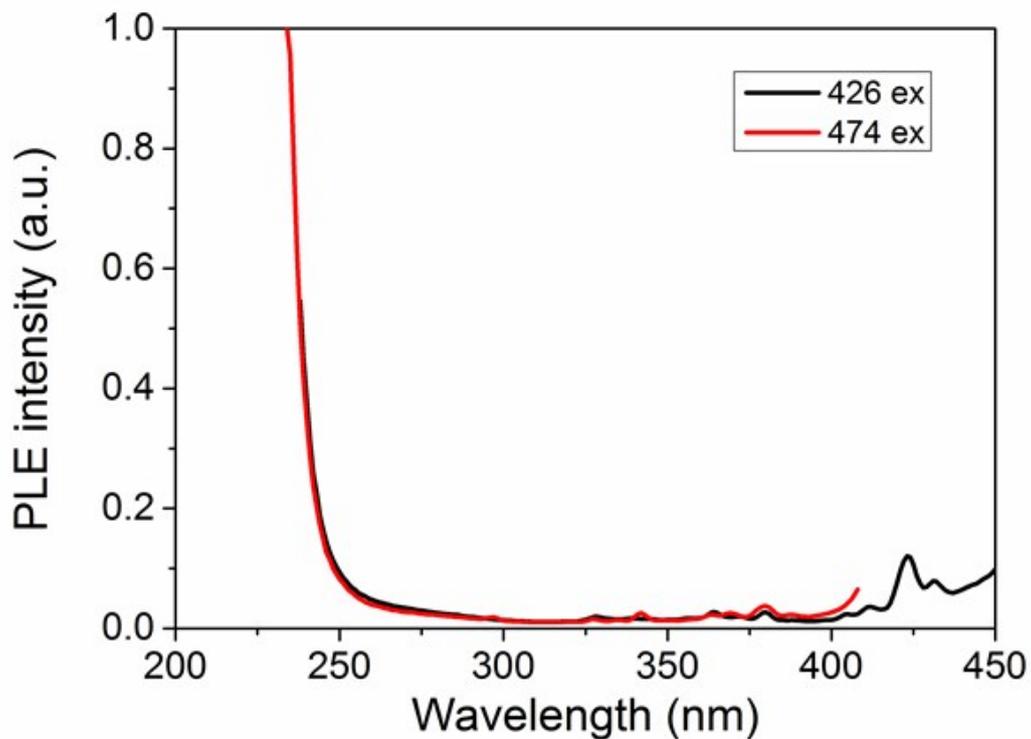


Fig. S6 Photoluminescence excitation spectra of blue 426 nm emission (black line) and blue 474 nm emission (red line) from the powder of 0D (DMA)₄PbI₆.

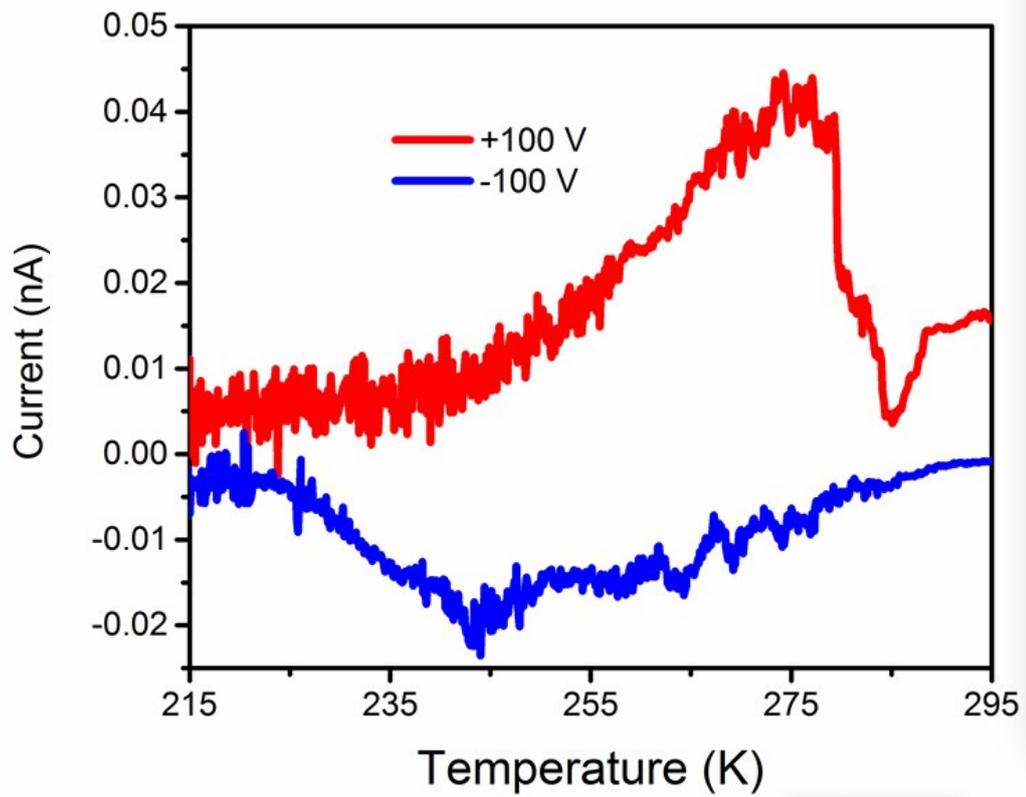


Fig. S7 Pyroelectric current measured on 0D (DMA)₄PbI₆ single crystal.

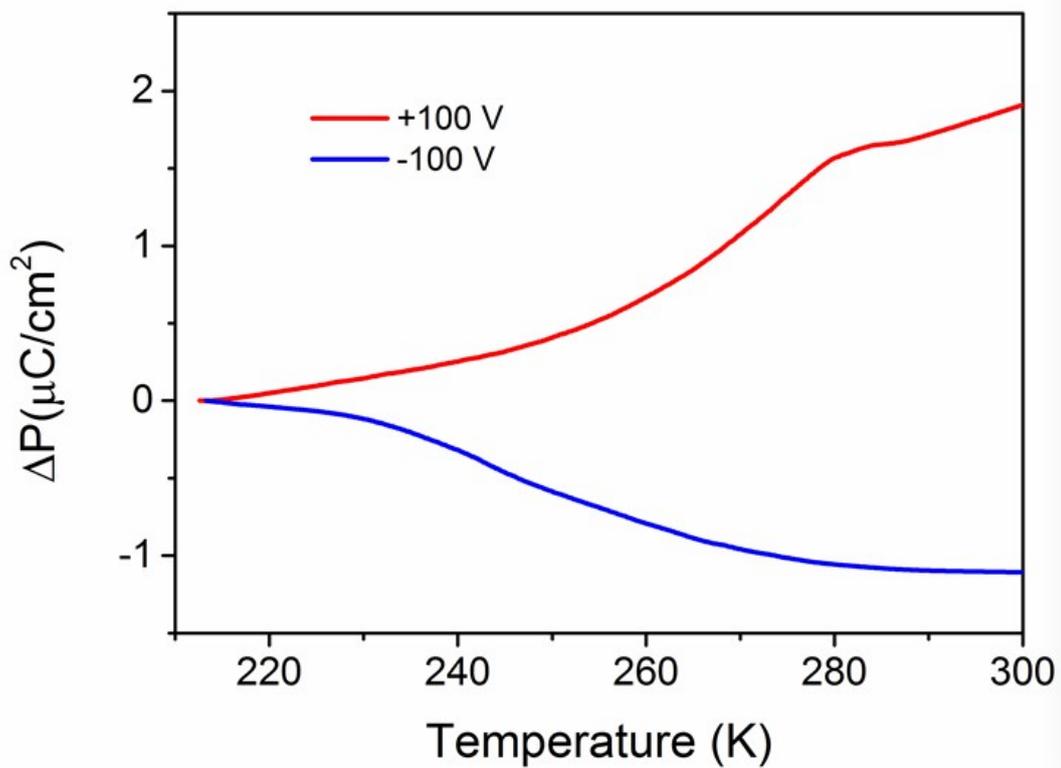


Fig. S8 Polarization change acquired from the pyroelectric current.

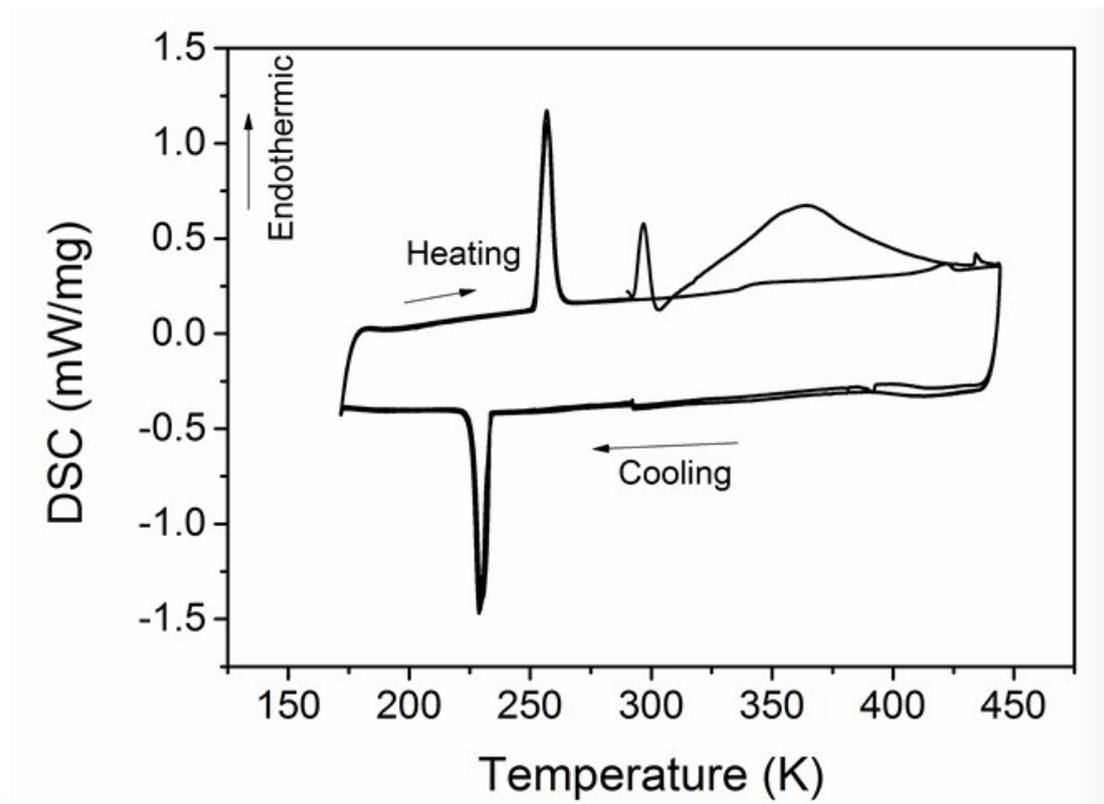


Fig. S9 DSC of OD (DMA)₄PbI₆ measured with 10 K/min.

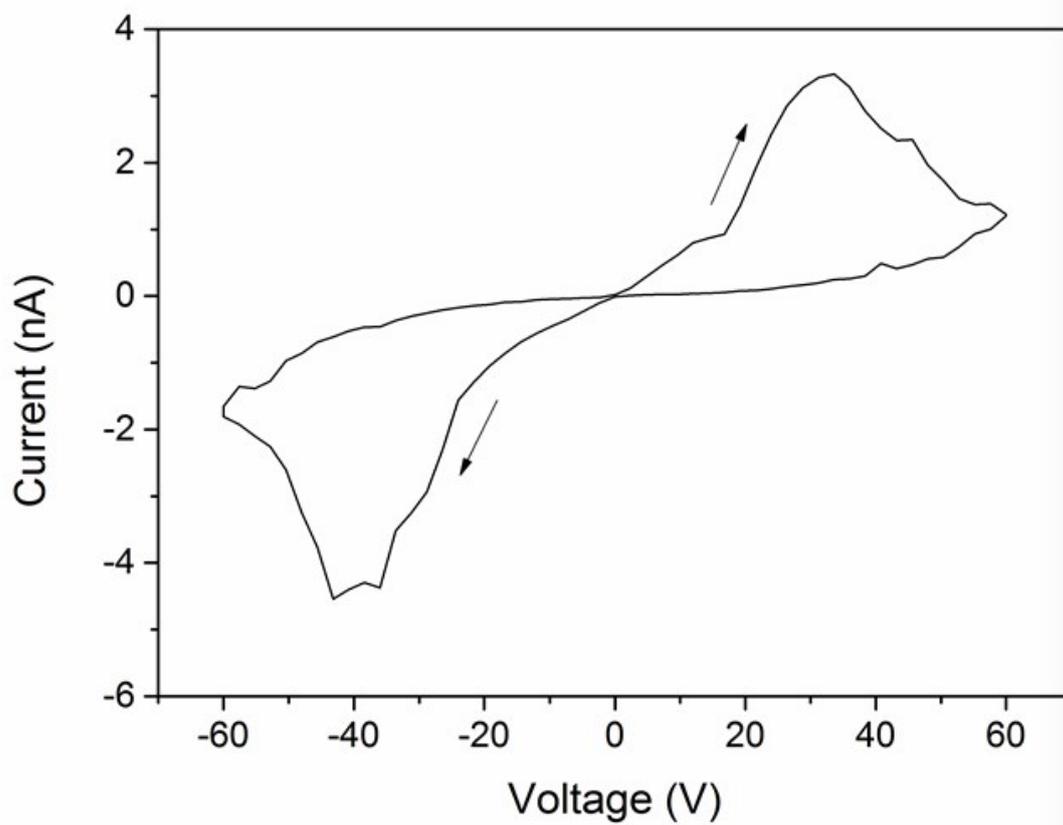


Fig. S10 The IV characteristic curve of OD DMA₄PbI₆.