

Supporting Information

Exploring a layered iodide perovskite crystal with centimetered dimension for extended spectral polarization-sensitive photodetection

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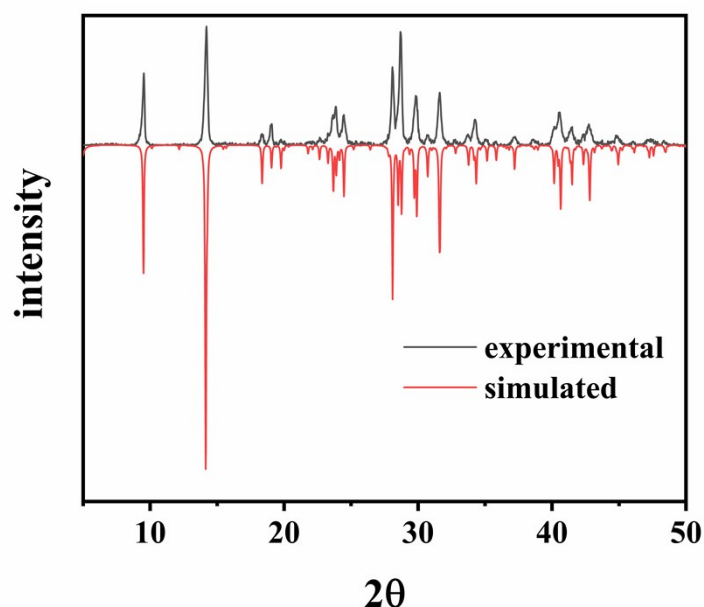


Figure S1. Experimental and calculated powder X-ray diffraction patterns of **1**.

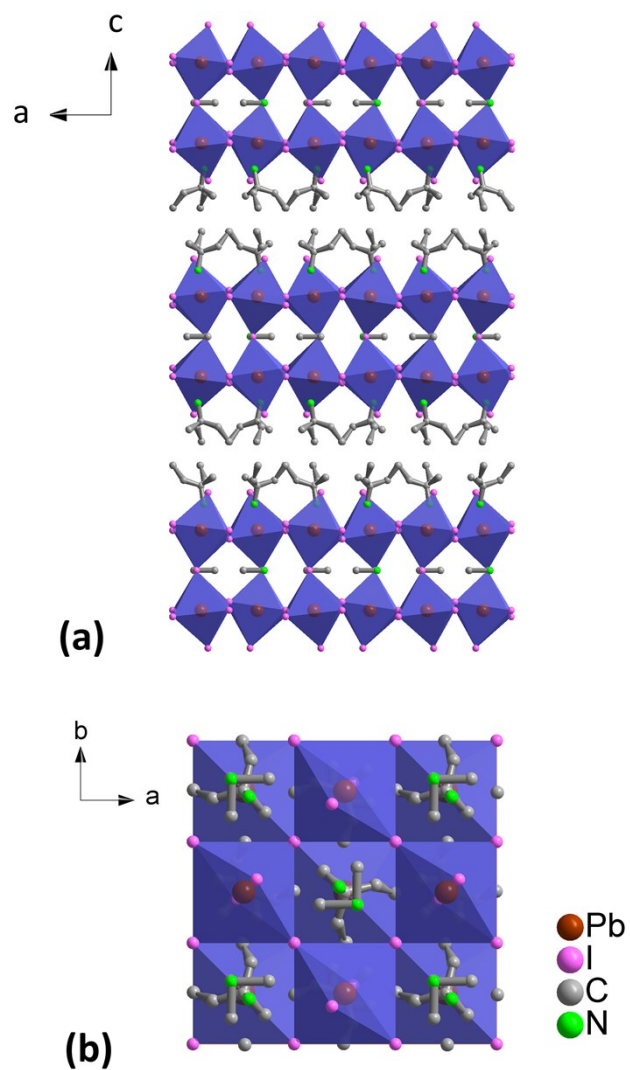


Figure S2. Packing diagram of **1** viewed along b-, and c-axes, respectively.

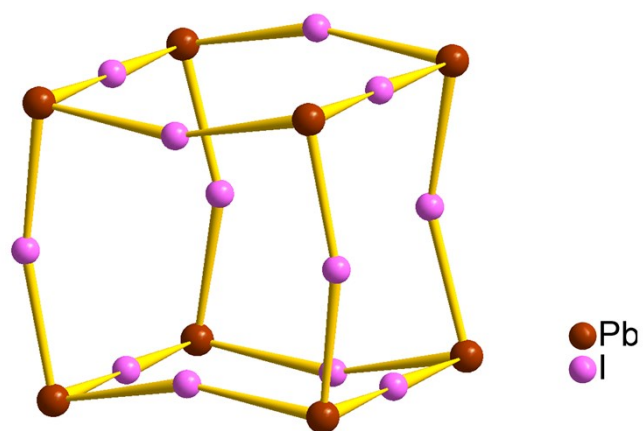


Figure S3. Inorganic layer distortion of **1**.

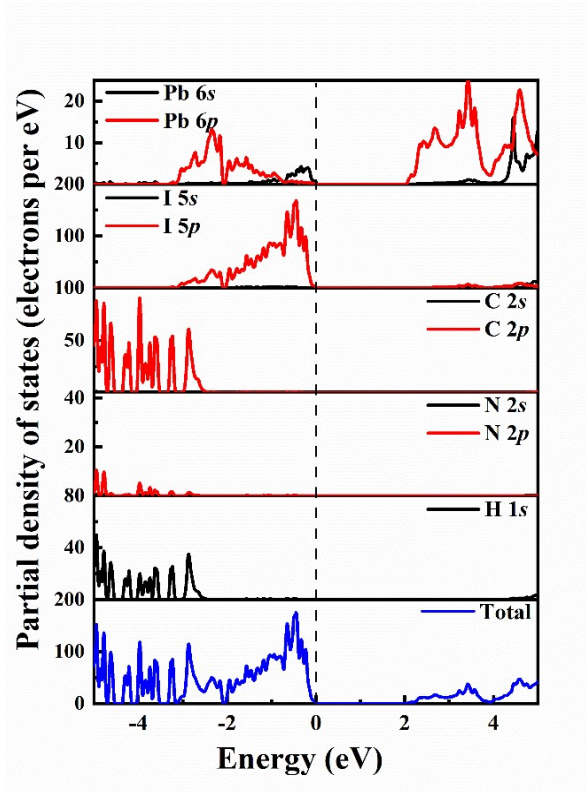


Figure S4. Partial density of states (pDOS) analysis of 1.

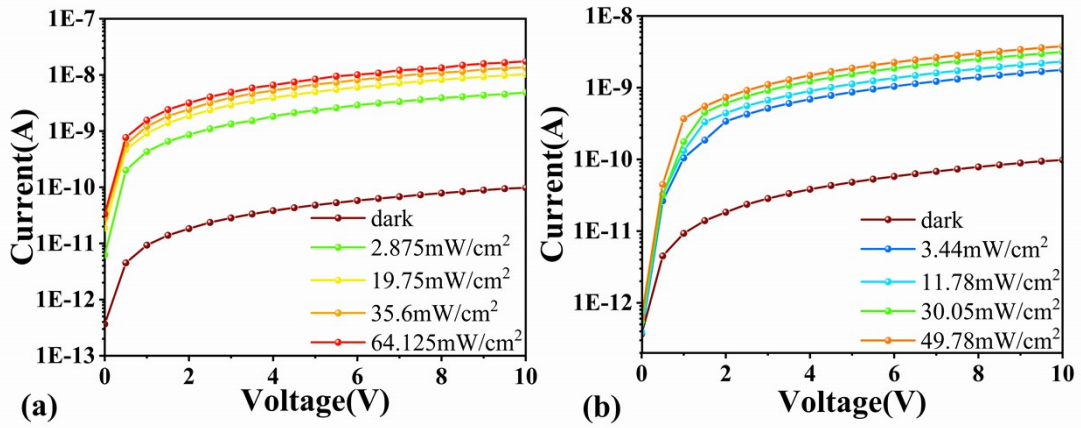


Figure S5. I - V curves under illumination of 405 nm (a) and 637 nm (b).

Table S1 Crystal data for **1** collected at 269 K

Empirical formula	C ₉ H ₃₀ I ₇ N ₃ Pb ₂
Formula weight	1483.04
Temperature/K	269.15
Crystal system	tetragonal
Space group	<i>P4₂/mnm</i>
Cell parameters	$a = 8.9753(7) \text{ \AA}$ $b = 8.9753(7) \text{ \AA}$ $c = 37.215(4) \text{ \AA}$
V(Å ³)	2997.9(6)
Z, ρ _{cal.} (g/cm ³)	4, 3.286
F(000)	2560.0
2Theta range(°)	4.668 to 46.136
Limiting indices	$-9 \leq h \leq 9$ $-9 \leq k \leq 9$ $-39 \leq l \leq 41$
Reflections collected	13302
Independent reflections	1183 [$R_{\text{int}} = 0.0715$, $R_{\text{sigma}} = 0.0291$]
Data/restraints/parameters	1183/51/95
GOF	1.068
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0426$, $wR_2 = 0.1066$
Final R indexes [all data]	$R_1 = 0.0682$, $wR_2 = 0.1225$

Table S2 Bond lengths (Å) for **1** at 269 K

Pb1	I1	3.2400(5)	C2	N2	1.473(9)
Pb1	I2	3.1734(3)	C2	C3	1.463(8)
Pb1	I2 ¹	3.1734(2)	C2	C4	1.463(8)
Pb1	I3	3.2434(5)	C4	C5	1.488(9)
Pb1	I4	3.2218(5)	N1	C1	1.479(14)
Pb1	I5	3.0999(9)			

¹1-Y,1-X,+Z**Table S3** Bond angles for **1** at 269K

I1	Pb1	I3	86.85(3)	I5	Pb1	I2 ¹	90.522(14)
I2 ¹	Pb1	I1	90.084(7)	I5	Pb1	I3	174.53(3)
I2	Pb1	I1	90.084(7)	I5	Pb1	I4	96.09(3)
I2	Pb1	I2 ¹	178.95(3)	Pb1	I1	Pb1 ²	154.89(4)
I2	Pb1	I3	89.488(14)	Pb1	I2	Pb1 ³	179.02(3)
I2 ¹	Pb1	I3	89.487(14)	Pb1	I3	Pb1 ⁴	161.20(5)
I2 ¹	Pb1	I4	89.882(7)	Pb1 ⁵	I4	Pb1	162.45(4)
I2	Pb1	I4	89.882(7)	C3	C2	N2	114.2(6)
I4	Pb1	I1	176.22(3)	C4	C2	N2	114.3(6)
I4	Pb1	I3	89.37(3)	C4	C2	C3	117.4(9)
I5	Pb1	I1	87.68(3)	C2	C4	C5	111.5(7)
I5	Pb1	I2	90.521(14)				

¹1-Y,1-X,+Z; ²2-X,-Y,+Z; ³2-X,1-Y,+Z; ⁴+X,+Y,1-Z; ⁵1-X,1-Y,+Z**Table S4** Polarization-sensitive photodetection performance compared with the reported.

	Wavelength nm	Dichroic ratio	R (mA/W)	D* (Jones)	Ref.
GeSe	532	1.09			1
	638	1.44			
	808	2.16			
GeSe ₂	450	3.4			2
p-BP/n-ReS ₂	1064	6.44			3
(BPA) ₂ PbBr ₄	377	6.8	0.1	10 ⁷	4
(n-BA) ₂ CsPb ₂ Br ₇	405	1.5	39.5	1.2×10 ¹²	5
(CMA) ₂ CsPb ₂ Br ₇	405	2.1	1.42	7.45 × 10 ¹⁰	6
(FPEA) ₂ PbI ₄	520	2.1	0.0032	3.8 × 10 ¹¹	7
(s-BA) ₂ (MA)Pb ₂ I ₇	405	1.1	39.19	1.12×10 ¹¹	this
	520	1.16	97.22	2.79×10 ¹¹	work

Herein, BPA is 3-bromopropylammonium; n-BA is n-butylammonium; CMA is (carboxy)cyclohexylmethylammonium; FPEA is p-fluorophenethylammonium;

References:

1. X. Wang, Y. Li, L. Huang, X. W. Jiang, L. Jiang, H. Dong, Z. Wei, J. Li and W. Hu, *J. Am. Chem. Soc.*, 2017, **139**, 14976-14982.
2. Y. Yang, S. C. Liu, W. Yang, Z. Li, Y. Wang, X. Wang, S. Zhang, Y. Zhang, M. Long, G. Zhang, D. J. Xue, J. S. Hu and L. J. Wan, *J. Am. Chem. Soc.*, 2018, **140**, 4150-4156.
3. W. Zhu, X. Wei, F. Yan, Q. Lv, C. Hu and K. Wang, *J. Semicond.*, 2019, **40**, 092001.
4. C. Ji, D. Dey, Y. Peng, X. Liu, L. Li and J. Luo, *Angew. Chem. Int. Ed.*, 2020, **59**, 18933-18937.
5. J. Wang, Y. Liu, S. Han, Y. Ma, Y. Li, Z. Xu, J. Luo, M. Hong and Z. Sun, *Sci. Bull.*, 2021, **66**, 158-163.
6. Y. Liu, J. Wang, S. Han, X. Liu, M. Li, Z. Xu, W. Guo, M. Hong, J. Luo and Z. Sun, *Eur. J. Chem.*, 2020, **26**, 3494-3498.
7. M. Li, S. Han, B. Teng, Y. Li, Y. Liu, X. Liu, J. Luo, M. Hong and Z. Sun, *Adv. Opt. Mater.*, 2020, **8**, 2000149.