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Supporting Information

Polar 2D Hybrid Perovskite Crystals with Intrinsic Strong Linear Dichroism for Polarization-Sensitive and Self-Powered Detection

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Figure

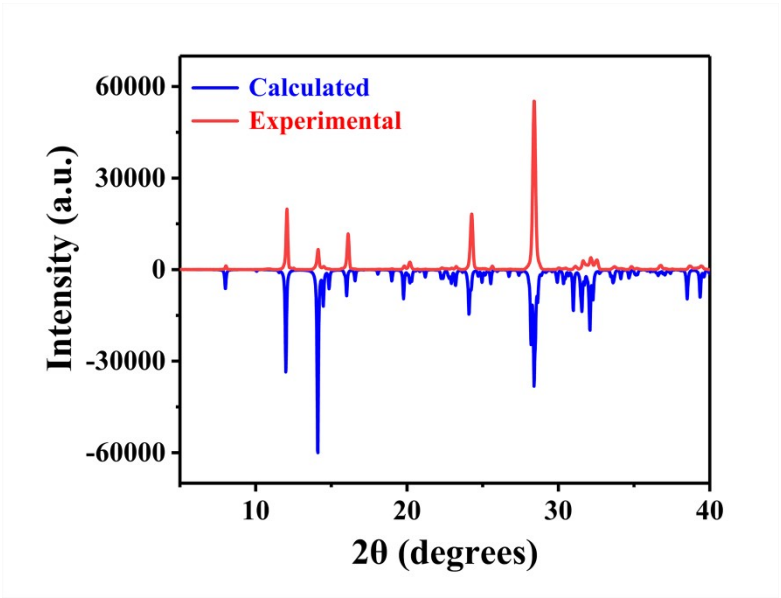

Figure S1. Experimental and calculated powder X-ray diffraction patterns of **1** at 298K.

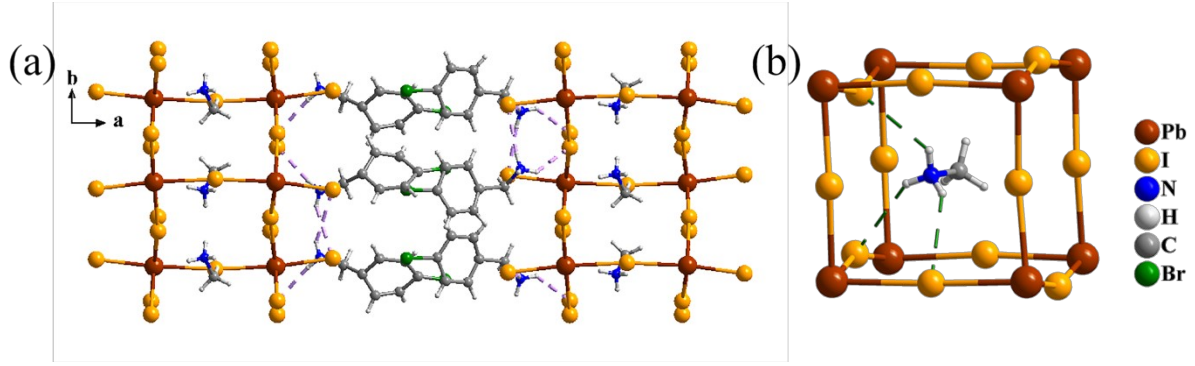

Figure S2. (a) Hydrogen-bonding N-H···I interactions between the organic BBA^+ and inorganic perovskite frameworks. (b) Hydrogen-bonding N-H···I interactions between the organic MA^+ and inorganic perovskite frameworks.

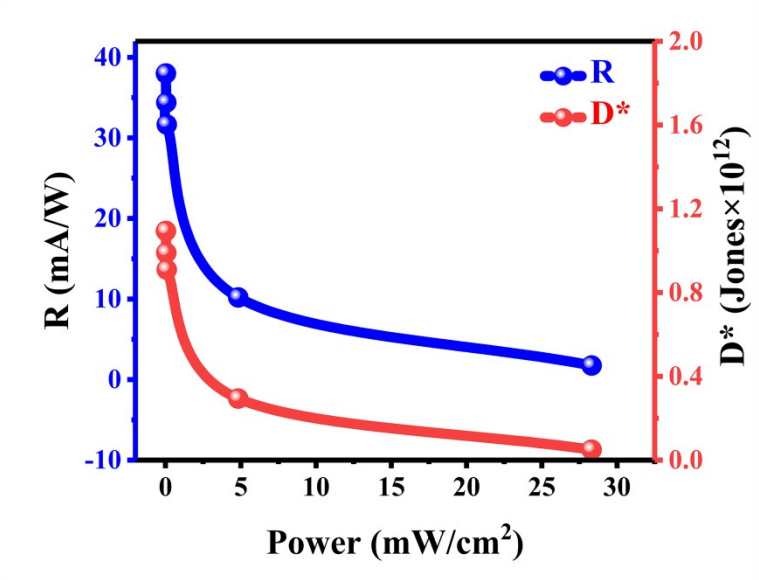

Figure S3. Photoresponsivity and detectivity of **1** under various incident-light power density at 520 nm. The responsivity is defined as $R = \frac{I_{light}}{P}$, where I_{light} is the photocurrent and P is the incident light power.[1] The detectivity is defined as $D^* = \frac{R\sqrt{Af}}{i_n}$, where A is the effective illumination area of the photodetector, f is the electric bandwidth, and i_n is the noise current. The shot noise ($i_{n,s}$) is defined as $i_{n,s} = \sqrt{2qi_d/A}$, where i_d is the dark current, q is the absolute value of electron charge. If, as expected, the shot noise from the dark current is the major contribution, the detectivity can be expressed as $D^* = \frac{R}{\sqrt{2qi_d/A}}$.[1,2]

[1] X. Gong, M. Tong, Y. Xia, W. Cai, J. Moon, Y. Cao, G. Yu, C. Shieh, B. Nilsson and A. Heeger, High-Detectivity Polymer Photodetectors with Spectral Response from 300 nm to 1450 nm, *Science*, 2009, **325**, 1665-1667.

[2] K. Yang, Z. Zhao, M. Liu, L. Niu, X. Zhao, G. Yuan, X. Ma and F. Zhang, Highly sensitive broadband photomultiplication type all-polymer photodetectors and their applications in optical pulse counting, *J. Mater. Chem. C*, 2022, **10**, 10888-10894.

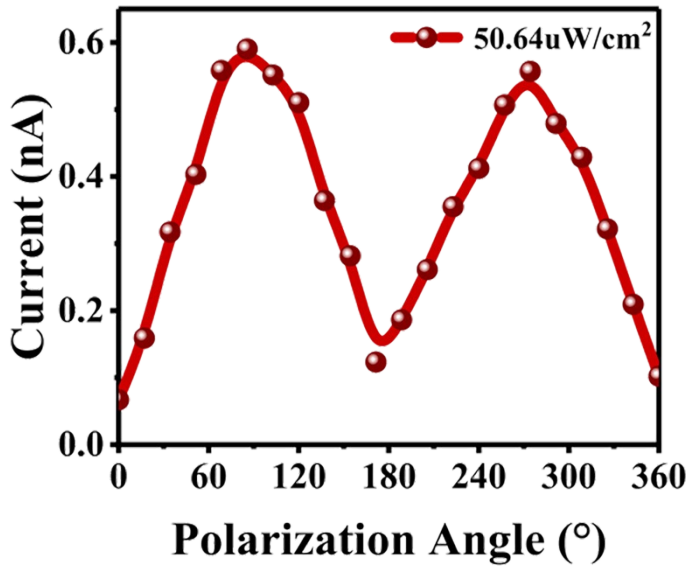

Figure S4. Polarization-dependent photocurrents (V_{bias} = 0 V, at 520 nm).

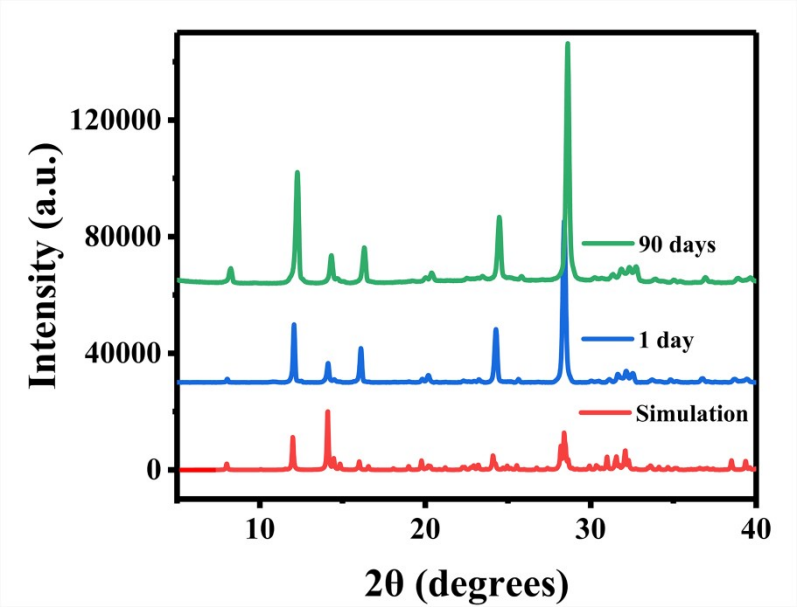

Figure S5. Powder X-ray diffraction patterns of **1** recorded on the sample after 1 day and 90 days, respectively.

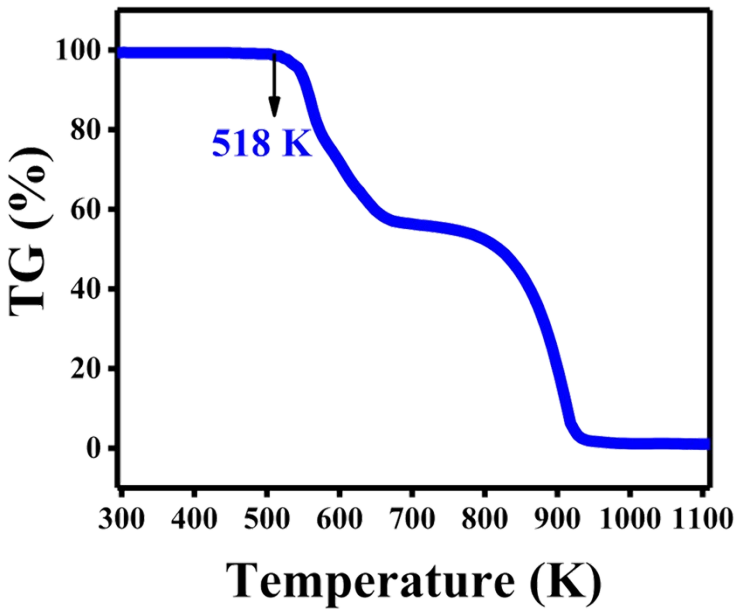

Figure S6. Thermal analysis curve of **1**, showing a thermal stability up to ~518 K.

Table

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

Empirical formula	$C_{15}H_{24}Br_2I_7N_3Pb_2$
Formula weight	1708.87
Temperature/K	298
Crystal system	monoclinic
Space group	*Cc*
a/Å	44.702(8)
b/Å	8.9866(14)
c/Å	8.8252(17)
α/°	90
β/°	97.362(7)
γ/°	90
Volume/Å^3	3516.1(11)
Z	4
ρ_{calc}g/cm^3	3.228
μ/mm^{-1}	17.992
F(000)	2960.0
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	4.624 to 50.05
Index ranges	-52 ≤ *h* ≤ 52, -10 ≤ *k* ≤ 10, -10 ≤ *l* ≤ 10
Reflections collected	14802
Independent reflections	5999 [R_{int} = 0.0916, R_{sigma} = 0.1334]
Data/restraints/parameters	5999/203/232
Goodness-of-fit on F^2	1.091
Final *R* indexes [*I*>=2σ (*I*)]	R_1 = 0.0933, wR_2 = 0.2016
Final *R* indexes [all data]	R_1 = 0.1501, wR_2 = 0.2359

Table S2. Selected bond lengths of **1.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pb2	I7	3.104(7)	C2	C7	1.39(3)
Pb2	I4	3.258(9)	C2	C3	1.41(3)
Pb2	I6	3.238(8)	C7	C6	1.38(3)
Pb2	I6[1]	3.200(8)	C3	C4	1.40(2)
Pb2	I5[2]	3.170(8)	C6	C5	1.39(3)
Pb2	I5	3.176(8)	C4	C5	1.39(3)
I4	Pb[1]	3.300(9)	C5	Br1	2.00(7)
I6	Pb2[3]	3.200(8)	Br2	C12	1.538(19)
I5	Pb2[4]	3.170(8)	C13	C14	1.40(3)
Pb1	I2	3.138(7)	C13	C12	1.43(3)
Pb1	I3	3.213(8)	C14	C9	1.42(3)
Pb1	I3[1]	3.214(7)	C12	C11	1.43(3)
Pb1	I1[4]	3.198(9)	C11	C10	1.40(3)
Pb1	I1	3.170(8)	C10	C9	1.43(3)
I3	Pb1[3]	3.214(7)	C9	C8	1.53(3)
I1	Pb1[2]	3.198(9)	C8	N2	1.49(3)
N3	C1	1.50(2)	N1	C15	1.48(3)
C2	C1	1.70(2)			

[1]+X,1-Y,-1/2+Z; [2]+X,2-Y,1/2+Z; [3]+X,1-Y,1/2+Z; [4]+X,2-Y,-1/2+Z

Table S3. Selected bond angles of **1.**

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
I7	Pb2	I4	174.2(2)	$I1^4$	Pb1	$I3^1$	91.8(3)
I7	Pb2	I6	86.8(2)	I1	Pb1	I3	90.7(2)
I7	Pb2	$I6^1$	92.3(2)	I1	Pb1	$I3^1$	178.7(3)
I7	Pb2	I5	96.6(3)	I1	Pb1	$I1^4$	89.11(9)
I7	Pb2	$I5^2$	91.0(2)	Pb1	I3	$Pb1^3$	158.9(3)
$I6^1$	Pb2	I4	85.6(2)	Pb1	I1	$Pb1^2$	160.6(3)
I6	Pb2	I4	87.8(2)	C7	C2	C1	124(4)
$I6^1$	Pb2	I6	87.96(9)	C7	C2	C3	121(4)
I5	Pb2	I4	88.8(2)	C3	C2	C1	114(3)
$I5^2$	Pb2	I4	91.0(3)	N3	C1	C2	101(2)
I5	Pb2	I6	176.6(3)	C6	C7	C2	121(5)
$I5^2$	Pb2	$I6^1$	176.4(3)	C4	C3	C2	116(4)
I5	Pb2	$I6^1$	91.6(3)	C7	C6	C5	114(6)
$I5^2$	Pb2	I6	90.6(3)	C5	C4	C3	117(6)
$I5^2$	Pb2	I5	89.64(9)	C6	C5	C4	126(6)
Pb2	I4	Pb1	174.6(2)	C6	C5	Br1	118(4)
$Pb2^3$	I6	Pb2	159.7(3)	C4	C5	Br1	114(4)
$Pb2^4$	I5	Pb2	161.0(3)	C14	C13	C12	126(3)
I2	Pb1	I4	174.7(2)	C13	C14	C9	118(5)
I2	Pb1	I3	92.3(2)	C13	C12	Br2	118(3)
I2	Pb1	$I3^1$	86.7(2)	C13	C12	C11	106(2)
I2	Pb1	$I1^4$	88.7(2)	C11	C12	Br2	136(4)
I2	Pb1	I1	94.2(2)	C10	C11	C12	125(3)
I3	Pb1	I4	88.1(2)	C11	C10	C9	123(3)
$I3^1$	Pb1	I4	88.0(2)	C14	C9	C10	109(3)
I3	Pb1	$I3^1$	88.33(9)	C14	C9	C8	110(3)
$I1^4$	Pb1	I4	90.9(3)	C10	C9	C8	125(7)
I1	Pb1	I4	91.0(2)	N2	C8	C9	110(3)
$I1^4$	Pb1	I3	179.0(3)				

^{1}+X,1-Y,-1/2+Z; ^{2}+X,2-Y,1/2+Z; ^{3}+X,1-Y,1/2+Z; ^{4}+X,2-Y,-1/2+Z

Table S4. Hydrogen bonds of **1.**

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N3-H3A	0.890	2.974	132.13	3.631	I3 [x, -y+1, z-1/2]
N3-H3A	0.890	3.287	113.80	3.736	I1 [x, y-1, z]
N3-H3B	0.890	3.073	172.39	3.957	I2 [x, -y+1, z+1/2]
N3-H3C	0.890	2.681	174.14	3.567	I2
N2-H2A	0.890	3.122	134.57	3.800	I7 [x-1/2, y+1/2, z]
N2-H2A	0.890	3.240	132.55	3.898	I6 [x-1/2, -y+3/2, z-1/2]
N2-H2C	0.890	2.583	172.30	3.468	I5 [x-1/2, y-1/2, z]
N1-H1C	0.890	3.191	145.99	3.960	I1 [x, -y+2, z+1/2]
N1-H1D	0.890	3.243	146.31	4.014	I4 [x, y, z+1]
N1-H1E	0.890	3.244	111.83	3.669	I3