Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Exploiting Two-Dimensional Hybrid Perovskites Incorporating Secondary Amine for High-Performance Array Photodetection

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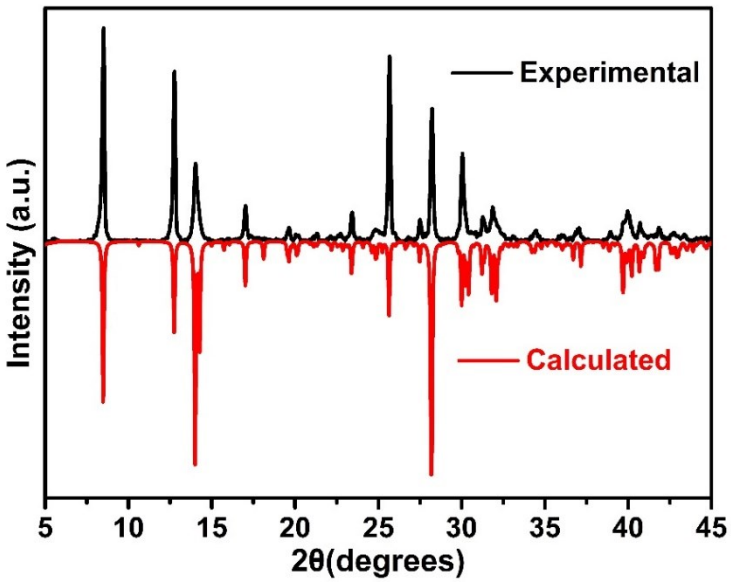

Figure S1. Experimental and calculated powder X-ray diffraction patterns of **1** at room temperature.

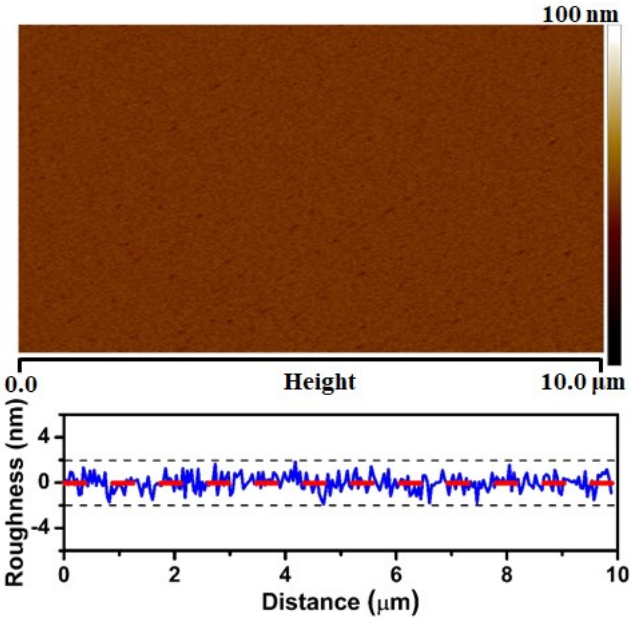

Figure S2. Surface morphology measured by AFM.

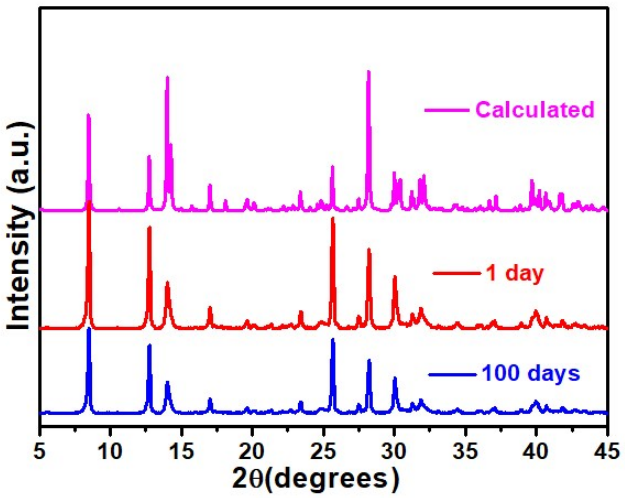

Figure S3. Powder X-ray diffraction patterns of **1** recorded on the sample after 1 day and 100 days, respectively.

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

Empirical formula	$C_{11}H_{33}I_7N_4Pb_2$
Temperature/K	200.00
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	20.857(2)
b/Å	9.1020(7)
c/Å	8.7015(8)
α/°	90
β/°	97.683(9)
γ/°	90
Volume/Å^3	1637.1(3)
Z	2
F(000)	1328.0
Index ranges	$-26 \le h \le 28$, $-12 \le k \le 8$, $-10 \le l \le 11$
Independent reflections	3985 [R_{int} = 0.0671, R_{sigma} = 0.0671]
Final R indexes [I>=2σ (I)]	R_1 = 0.0972, wR_2 = 0.2032
Final R indexes [all data]	R_1 = 0.1253, wR_2 = 0.2163

Table S2. Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I0	Pb01	3.053(5)	C1A	N3	1.49(2)
Pb01	I1	3.049(6)	N1	C40	1.34(2)
Pb01	I002$^{1\#}$	3.1904(19)	C1B	C2	1.40(7)
Pb01	I002	3.2050(19)	C1B	N3	1.39(7)
Pb01	I003	3.170(2)	N2	C40	1.34(2)
Pb01	I003$^{2\#}$	3.156(2)	C2	C3	1.495(18)
Pb01	I005	3.3587(10)	C3	C4	1.496(19)
C1A	C2	1.50(2)	C4	C5B	1.49(5)

$^{1\#}$+X,1/2-Y,1/2+Z; $^{2\#}$+X,3/2-Y,1/2+Z

Table S3. Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
I0	Pb01	I002	84.6(3)	I003$^{1\#}$	Pb01	I002	177.69(8)
I0	Pb01	I003$^{1\#}$	93.5(3)	I003$^{1\#}$	Pb01	I003	86.91(2)
I0	Pb01	I003	83.8(3)	I003$^{1\#}$	Pb01	I005	83.28(6)
I0	Pb01	I005	166.6(2)	I003	Pb01	I005	83.03(6)
I1	Pb01	I002	93.6(3)	N3	C1A	C2	115(3)
I1	Pb01	I002$^{2\#}$	84.6(3)	N3	C1B	C2	129(6)

I1	Pb01	I003[1#]	84.3(3)	C1B	C2	C3	123(4)
I1	Pb01	I003	93.2(4)	C3	C2	C1A	115(3)
I1	Pb01	I005	167.2(2)	Pb01[3#]	I002	Pb01	161.65(9)
I002[2#]	Pb01	I002	85.74(2)	Pb01[4#]	I003	Pb01	166.00(12)
I002[2#]	Pb01	I005	99.18(5)	C2	C3	C4	117(3)
I002	Pb01	I005	98.86(5)	C5B	C4	C3	114(3)
I003[1#]	Pb01	I002[2#]	93.08(6)	Pb01	I005	Pb01[5#]	180.0
I003	Pb01	I002	94.20(6)	N2	C40	N1	118(3)
I003	Pb01	I002[2#]	177.77(8)				

[1#]+X,3/2-Y,1/2+Z; [2#]+X,1/2-Y,1/2+Z; [3#]+X,1/2-Y,-1/2+Z; [4#]+X,3/2-Y,-1/2+Z; [5#]1-X,1-Y,1-Z

Table S4. N-H···I hydrogen bonds of **1.**

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N2-H2BD[b]	0.890	2.992	157.45	3.829	I2 [x, -y+1/2, z-1/2]
N2-H2BE[b]	0.890	2.960	136.70	3.659	I4Bb [x, -y+3/2, z-1/2]
N2-H2BE[b]	0.890	3.159	134.64	3.837	I3 [x, -y+3/2, z-1/2]
N2-H2BF[b]	0.890	3.145	163.79	4.008	I4B[b]
N2-H2AA[a]	0.890	2.890	145.29	3.657	I4A[a] [x, -y+3/2, z-1/2]
N2-H2AA[a]	0.890	3.305	120.72	3.837	I3 [x, -y+3/2, z-1/2]
N2-H2AB[a]	0.890	3.120	132.63	3.780	I2
N2-H2AB[a]	0.890	3.197	125.15	3.780	I3
N2-H2AC[a]	0.890	2.957	167.04	3.829	I2 [x, -y+1/2, z-1/2]
N1[a]-H1D[a]	0.890	2.992	153.91	3.811	I3 [-x+1, y-1/2, -z+1/2]
N1[a]-H1E[a]	0.890	3.080	138.99	3.797	I3 [-x+1, -y+1, -z]