Supporting Information

Highly Efficient Broadband White-light Emission in Two-dimensional Semi-conductive Hybrid Lead–Chlorine Halide

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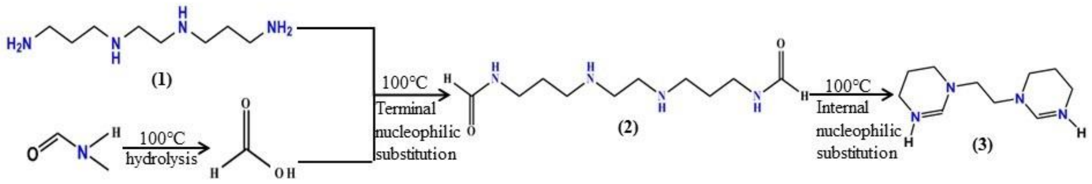


Scheme S1. The possible generation route of DTHPE molecule in the preparation process of [DTHPE]Pb_4Cl_{10}.

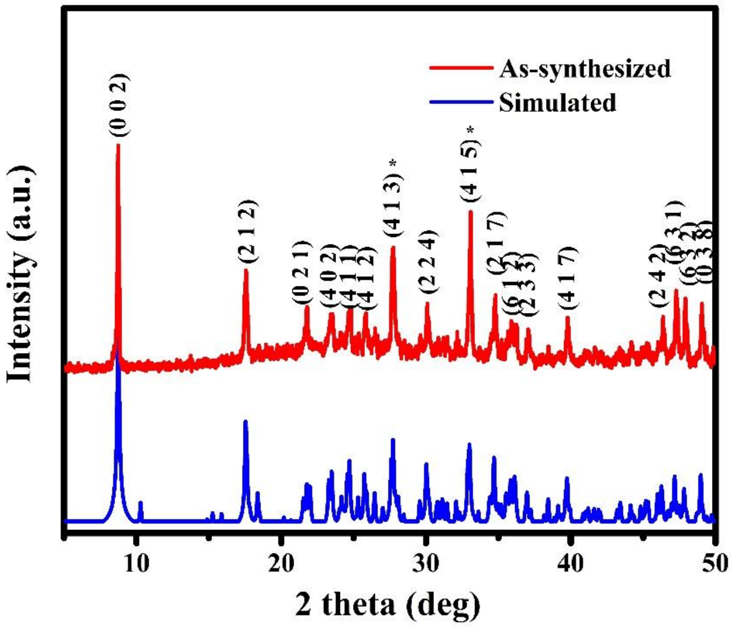


Fig. S1. The simulated and experimental XRD patterns of [DTHPE]Pb_4Cl_{10}. *****stands for the peaks which related with tetranuclear structure of [Pb_3Cl_{20}] clusters.

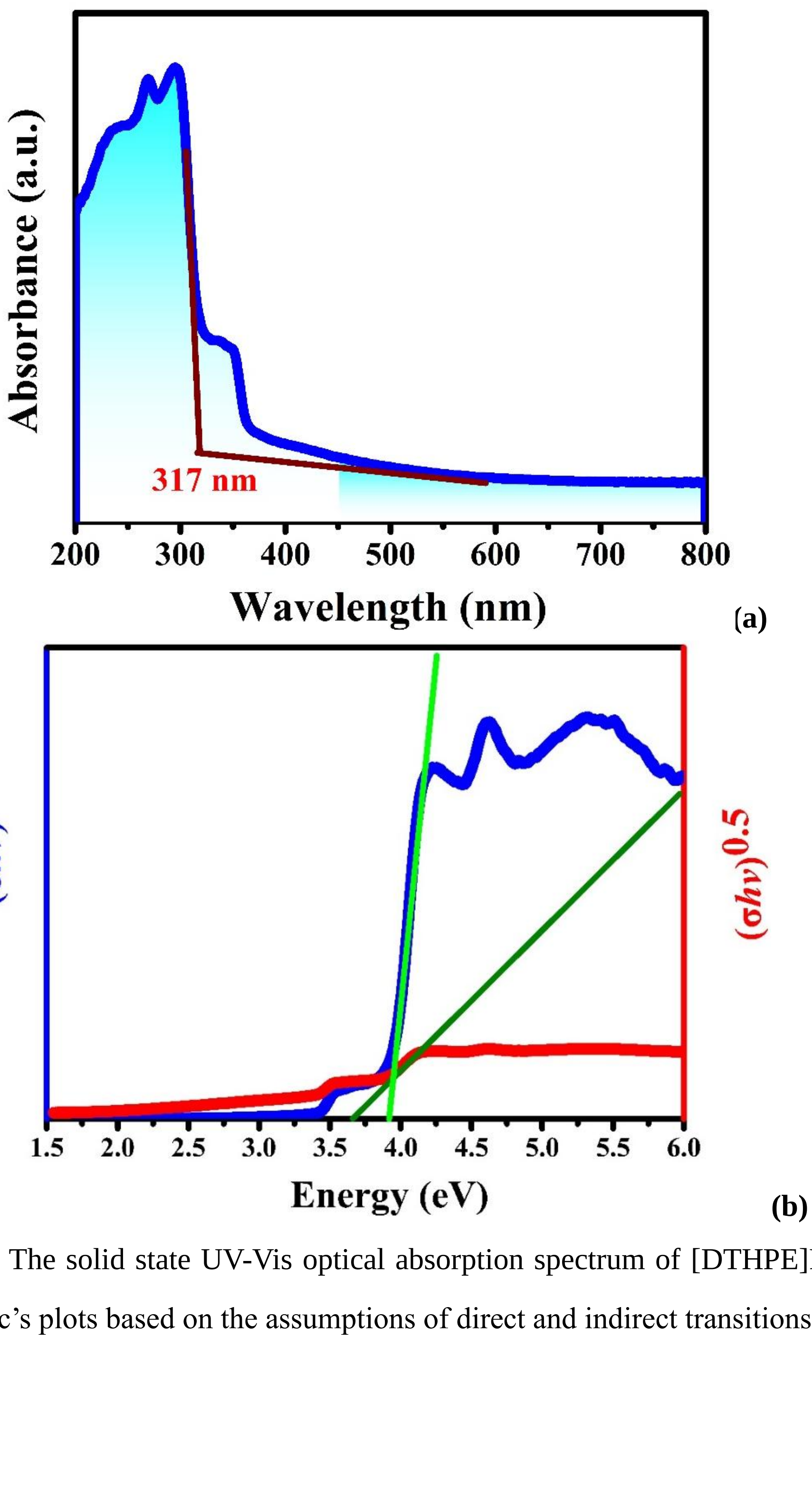


Fig. S2. (a) The solid state UV-Vis optical absorption spectrum of [DTHPE]Pb_4Cl_{10}; (b) The Tauc's plots based on the assumptions of direct and indirect transitions.

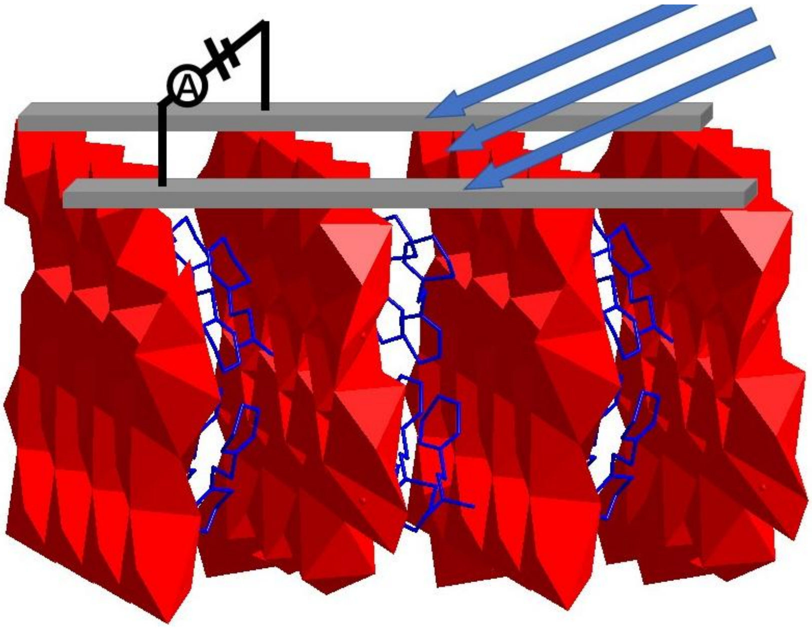


Fig. S3. The schematic diagram of the photoconductive device based on the crystal of $[DTHPE]Pb_4Cl_{10}$.

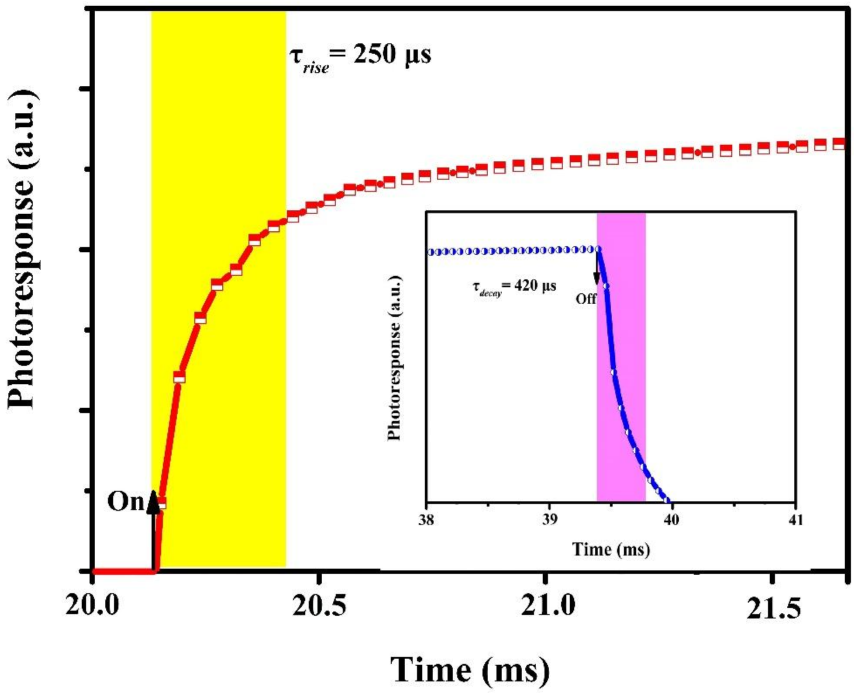


Fig. S4. Temporal measurements of photocurrents, affording the t_{rise}/t_{fall} values of the photoelectric device**.**

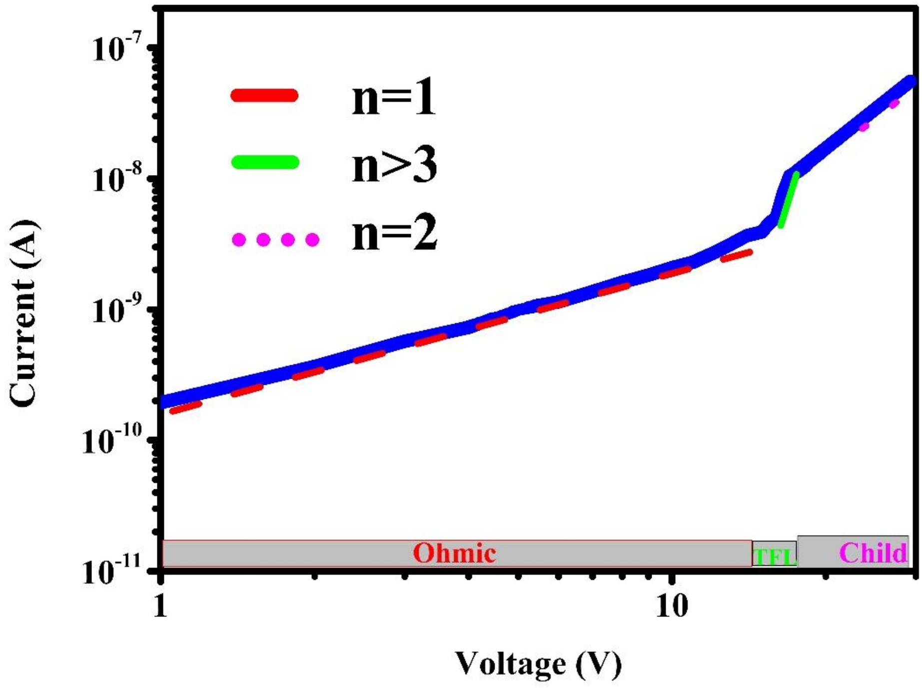


Fig. S5. Logarithmic I-V characteristics of [DTHPE]Pb_4Cl_{10} on the basis of the SCLC method.

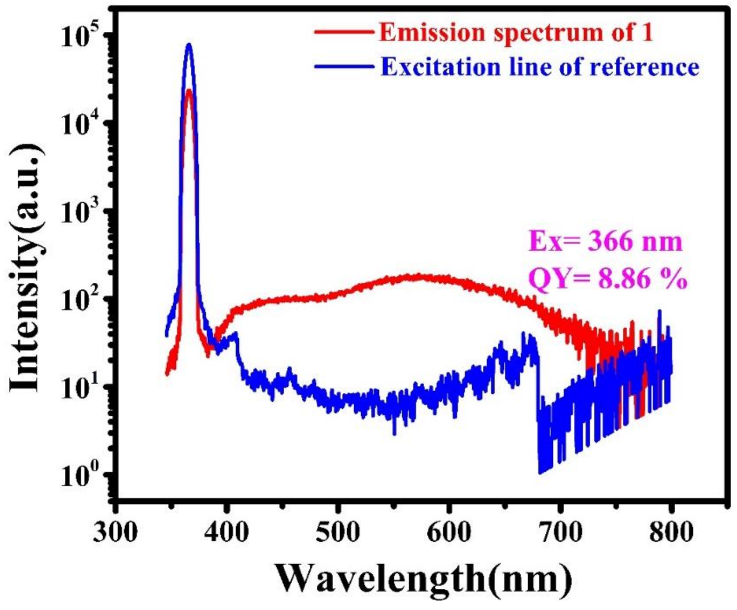


Fig. S6. The PLQY of bulk crystals for [DTHPE]Pb_4Cl_{10}**.**

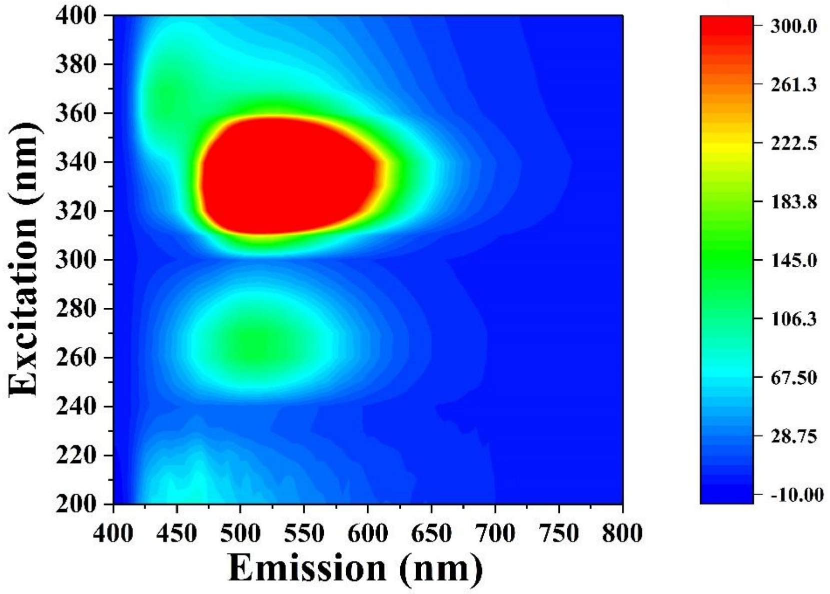
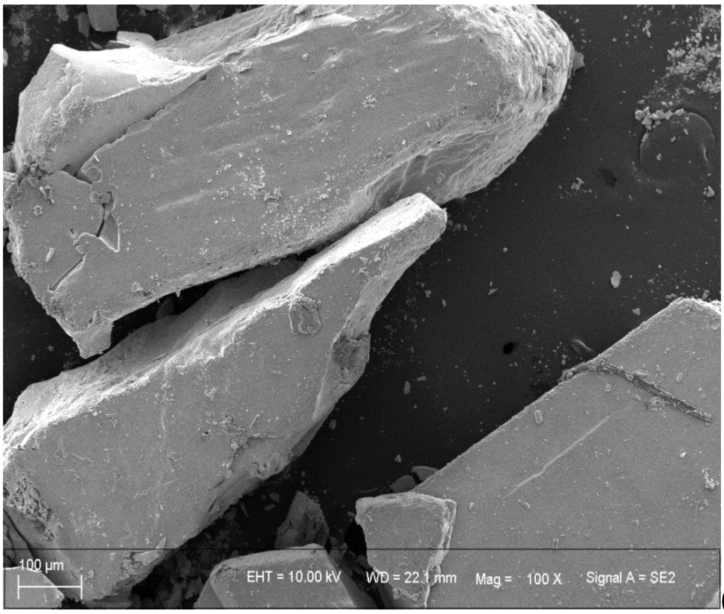
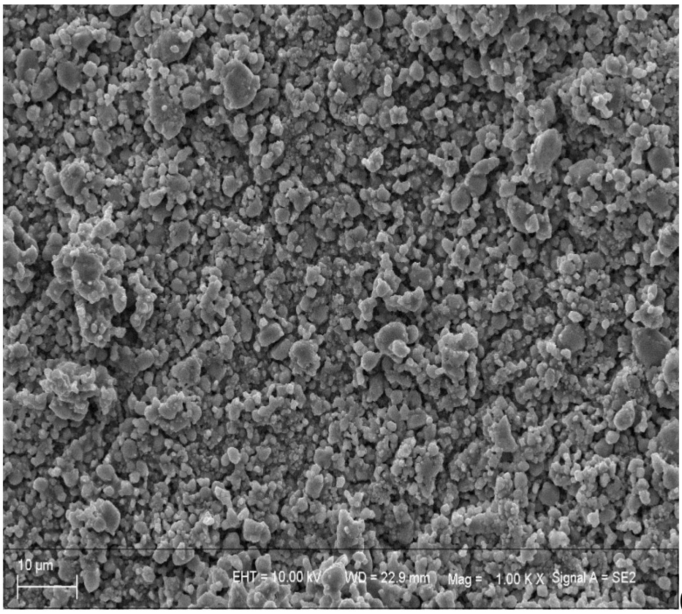


Fig. S7. 3D PL excitation and emission correlation map.



(a)



(b)

Fig. S8. The SEM images of bulk crystals (a) and hand-grinded microscale crystals (b) of [DTHPE]Pb_4Cl_{10}.

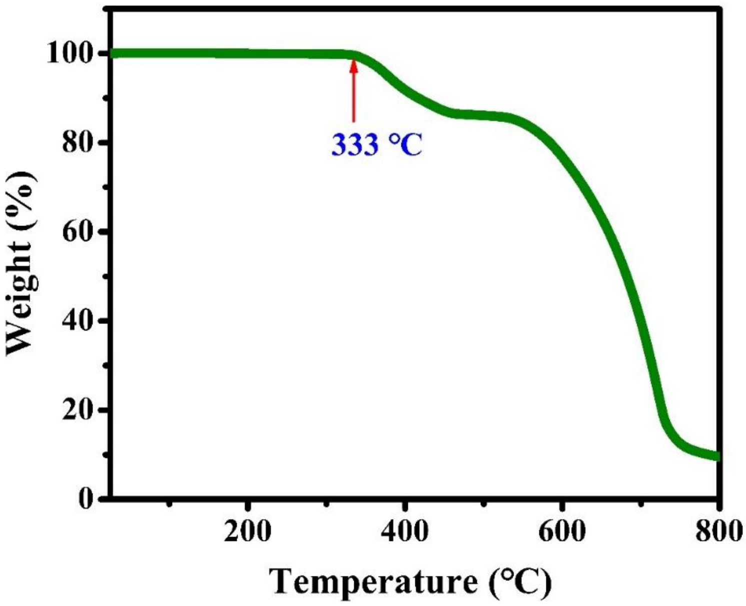


Fig. S9. The thermogravimetric (TG) analyses curves for [DTHPE]Pb_4Cl_{10}**.**

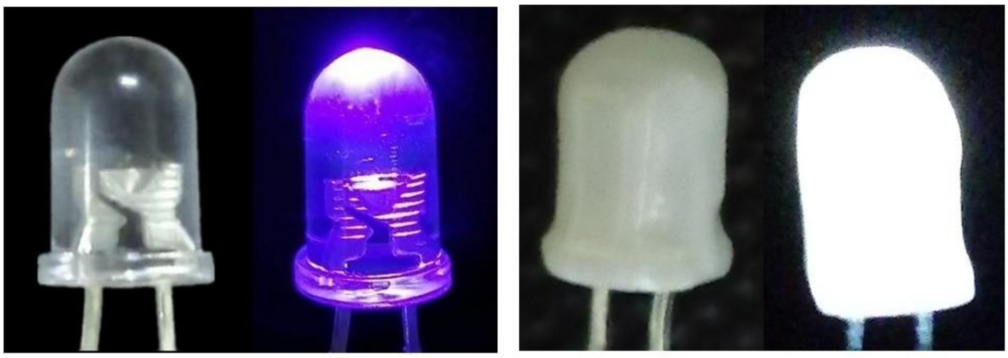


Fig. S10. Photographs of UV-LED lamps (left) and the LED coated with a thin layer of [DTHPE]Pb_4Cl_{10} (right), in the states of turn off and on.

Table S1. Crystal Data and Structural Refinements for $[DTHPE]Pb_4Cl_{10}$.

Compound	$[DTHPE]Pb_4Cl_{10}$
chemical formula	$C_5N_2H_{10}Pb_2Cl_5$
fw	689.80
Space group	*Pbca*
a/Å	16.358(19)
b/Å	8.262(10)
c/Å	20.20(2)
$\beta/^o$	90
V(Å^3)	2730(5)
Z	8
D_{calcd} (g·cm^{-3})	3.357
Temp (K)	296(2)
μ (mm^{-1})	25.580
F (000)	2423
Reflections collected	32913
Unique reflections	3538
Reflections (I>2σ(I))	2496
GOF on F^2	1.061
R_1,wR_2 ($I > 2\sigma(I)$)[a]	0.0368/ 0.0820
R_1,wR_2 (all data)	0.0652/ 0.0938

[a] $R_1 = \Sigma\left\|F_0\right| - \left|F_c\right\| / \Sigma\left|F_0\right|$, $wR_2 = [\Sigma(F_o^2 - F_c^2) / \Sigma w(F_0)^2]^{1/2}$

Table S2. Selected bond lengths (Å) for [DTHPE]Pb_4Cl_{10}.

Pb(1)-Cl(2)	2.752(3)	Pb(2)-Cl(4)#4	2.711(3)
Pb(1)-Cl(7)	2.755(3)	Pb(2)-Cl(3)#4	2.803(3)
Pb(1)-Cl(1)	3.054(4)	Pb(2)-Cl(1)	3.042(4)
Pb(1)-Cl(1)#1	3.065(4)	Pb(2)-Cl(1)#5	3.051(4)
Pb(1)-Cl(7)#2	3.187(4)	Pb(2)-Cl(2)	3.114(4)
Pb(1)-Cl(3)	3.193(3)	Pb(2)-Cl(3)#1	3.190(4)
Pb(1)-Cl(4)	3.254(4)	Pb(2)-Cl(4)#1	3.327(4)
Pb(1)-Cl(2)#2	3.315(4)	Pb(2)-Cl(7)	3.348(4)

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

Table S3. Selected bond angles (°) for [DTHPE]Pb_4Cl_{10}.

Cl(2)-Pb(1)-Cl(7)	83.38(10)	Cl(4)#4-Pb(2)-Cl(3)#4	83.36(10)
Cl(2)-Pb(1)-Cl(1)	77.40(9)	Cl(4)#4-Pb(2)-Cl(1)	79.29(10)
Cl(7)-Pb(1)-Cl(1)	76.74(10)	Cl(3)#4-Pb(2)-Cl(1)	75.71(10)
Cl(2)-Pb(1)-Cl(1)#1	75.29(9)	Cl(4)#4-Pb(2)-Cl(1)#5	77.45(9)
Cl(7)-Pb(1)-Cl(1)#1	78.91(10)	Cl(3)#4-Pb(2)-Cl(1)#5	77.17(10)
Cl(1)-Pb(1)-Cl(1)#1	145.11(6)	Cl(1)-Pb(2)-Cl(1)#5	145.93(6)
Cl(2)-Pb(1)-Cl(7)#2	148.78(7)	Cl(4)#4-Pb(2)-Cl(2)	94.57(10)
Cl(7)-Pb(1)-Cl(7)#2	98.59(10)	Cl(3)#4-Pb(2)-Cl(2)	147.88(7)
Cl(1)-Pb(1)-Cl(7)#2	72.85(8)	Cl(1)-Pb(2)-Cl(2)	72.43(8)
Cl(1)#1-Pb(1)-Cl(7)#2	135.82(8)	Cl(1)#5-Pb(2)-Cl(2)	133.82(9)
Cl(2)-Pb(1)-Cl(3)	86.39(10)	Cl(4)#4-Pb(2)-Cl(3)#1	97.40(10)
Cl(7)-Pb(1)-Cl(3)	150.24(8)	Cl(3)#4-Pb(2)-Cl(3)#1	146.30(6)
Cl(1)-Pb(1)-Cl(3)	127.90(8)	Cl(1)-Pb(2)-Cl(3)#1	137.74(8)
Cl(1)#1-Pb(1)-Cl(3)	71.46(8)	Cl(1)#5-Pb(2)-Cl(3)#1	70.22(8)
Cl(7)#2-Pb(1)-Cl(3)	104.51(8)	Cl(2)-Pb(2)-Cl(3)#1	65.82(7)
Cl(2)-Pb(1)-Cl(4)	142.12(7)	Cl(4)#4-Pb(2)-Cl(4)#1	147.54(6)
Cl(7)-Pb(1)-Cl(4)	103.25(10)	Cl(3)#4-Pb(2)-Cl(4)#1	92.97(9)
Cl(1)-Pb(1)-Cl(4)	140.48(8)	Cl(1)-Pb(2)-Cl(4)#1	131.12(9)
Cl(1)#1-Pb(1)-Cl(4)	69.70(8)	Cl(1)#5-Pb(2)-Cl(4)#1	70.31(8)
Cl(7)#2-Pb(1)-Cl(4)	68.06(7)	Cl(2)-Pb(2)-Cl(4)#1	104.82(7)
Cl(3)-Pb(1)-Cl(4)	69.33(10)	Cl(3)#1-Pb(2)-Cl(4)#1	68.46(10)
Cl(2)-Pb(1)-Cl(2)#2	91.76(10)	Cl(4)#4-Pb(2)-Cl(7)	147.02(7)
Cl(7)-Pb(1)-Cl(2)#2	144.48(8)	Cl(3)#4-Pb(2)-Cl(7)	95.78(10)
Cl(1)-Pb(1)-Cl(2)#2	67.88(8)	Cl(1)-Pb(2)-Cl(7)	68.68(8)
Cl(1)#1-Pb(1)-Cl(2)#2	133.81(8)	Cl(1)#5-Pb(2)-Cl(7)	134.69(8)
Cl(7)#2-Pb(1)-Cl(2)#2	68.55(10)	Cl(2)-Pb(2)-Cl(7)	68.95(10)
Cl(3)-Pb(1)-Cl(2)#2	63.49(7)	Cl(3)#1-Pb(2)-Cl(7)	100.97(7)
Cl(4)-Pb(1)-Cl(2)#2	101.99(7)	Cl(4)#1-Pb(2)-Cl(7)	65.38(7)

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

Table S4. Hydrogen bonds data for [DTHPE]Pb_4Cl_{10}..

D-H ···A	d(D-H)	d(H ···A)	d(D ···A)	<(DHA)
N(2)-H(2)···Cl(2)	0.86	2.53	3.3171	152
C(1)-H(1)···Cl(3)	0.93	2.67	3.5598	160

Table S5. Comparison of the broadband white light emission properties of [DTHPE]Pb_4Cl_{10} and previously reported hybrid lead chlorine halide.

Hybrid halides	**Dimension**	**PLQE**	**Ref.**
$(BZA)_2PbCl_4$	2D	3.57%	1
$(H_2DABCO)(Pb_2Cl_6)$	3D	2.5%	2
$(EDBE)PbCl_4$	2D	2%	3
$(2meptH_2)PbCl_4$	2D	1.05%	4
$(C_4H_9NH_3)_2PbCl_4$	2D	1%	5
$(PEA)_2PbCl_4$	2D	----	6
[DTHPE]Pb_4Cl_{10}	**2D**	**8.86%**	**This work**

Reference

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