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

Supporting Information

Pressure enables high-standard white light emission and significant emission enhancement in a 2D halide perovskite

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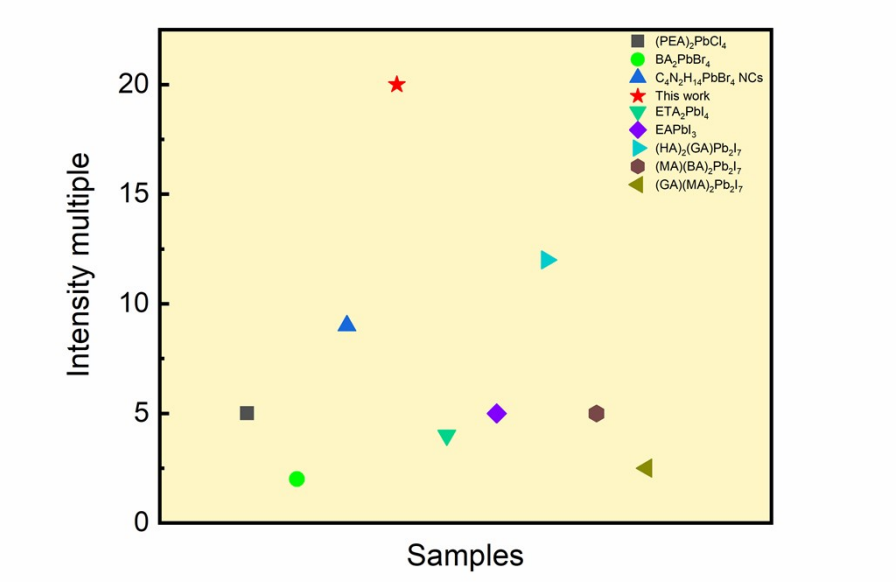


Figure S1. $(PEA)_2PbCl_4$:$(C_6H_5CH_2CH_2NH_3)_2PbCl_4$; BA_2PbBr_4: $[CH_3(CH_2)_3NH_3\ ]_2PbBr_4$; $ETAPbBr_4$: $[(HO)(CH_2)_2NH_3]_2PbI_4$; EA=Ethylammonium; HA=n-hexylammonium, GA=guanidinium; MA=methylammonium

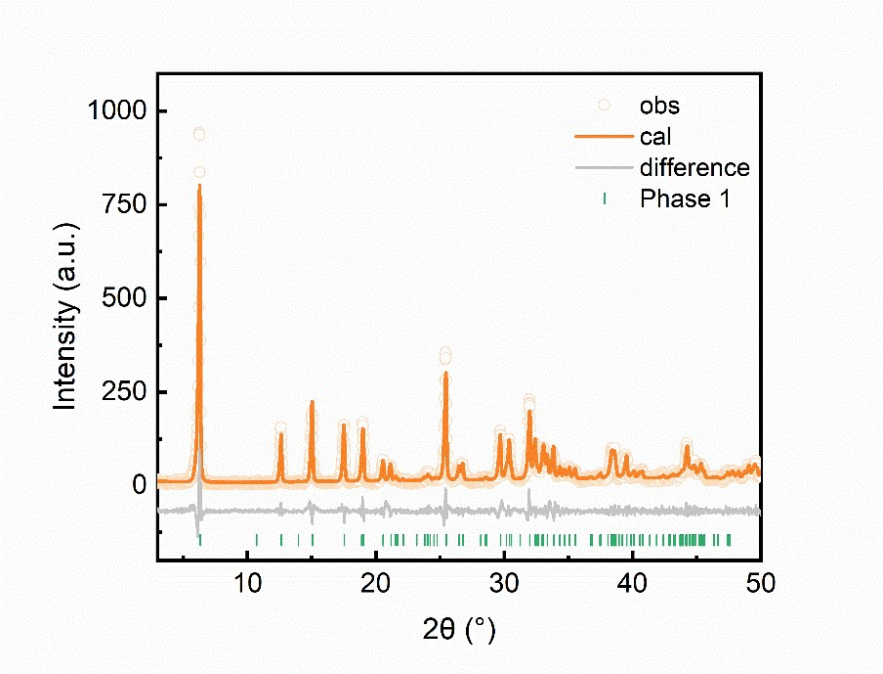


Figure S2. The Le Bail refinements of PXRD patterns of $(CHA)_2PbBr_4$ at ambient conditions. The yellow circles, orange and gray continuous line are experimental, calculated and difference profiles, respectively, and the vertical green markers indicate the allowed Bragg reflections.

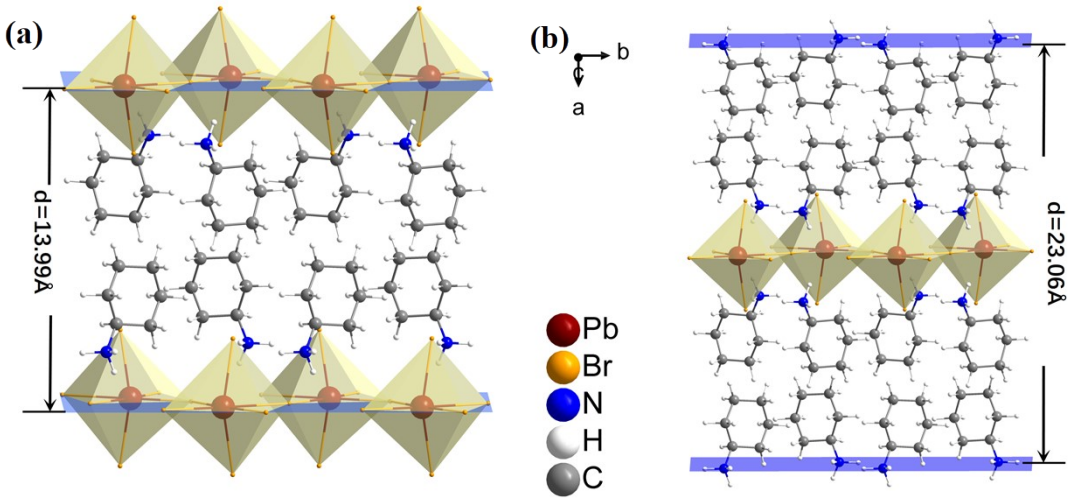


Figure S3. The thickness of the adjacent monolayer in $(CHA)_2PbBr_4$ at 1 atm.

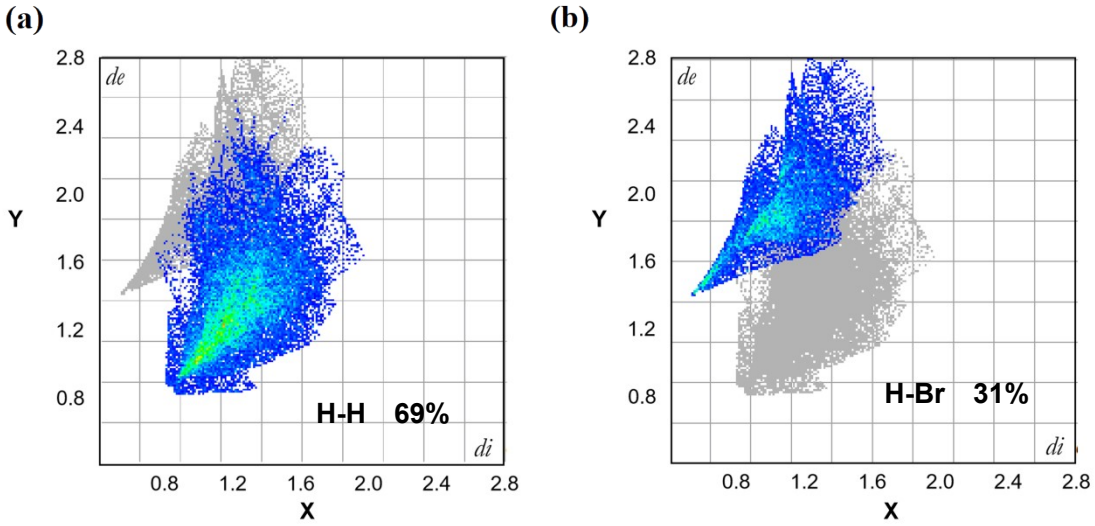


Figure S4. The 2D fingerprint plots of $(CHA)_2PbBr_4$ by element.

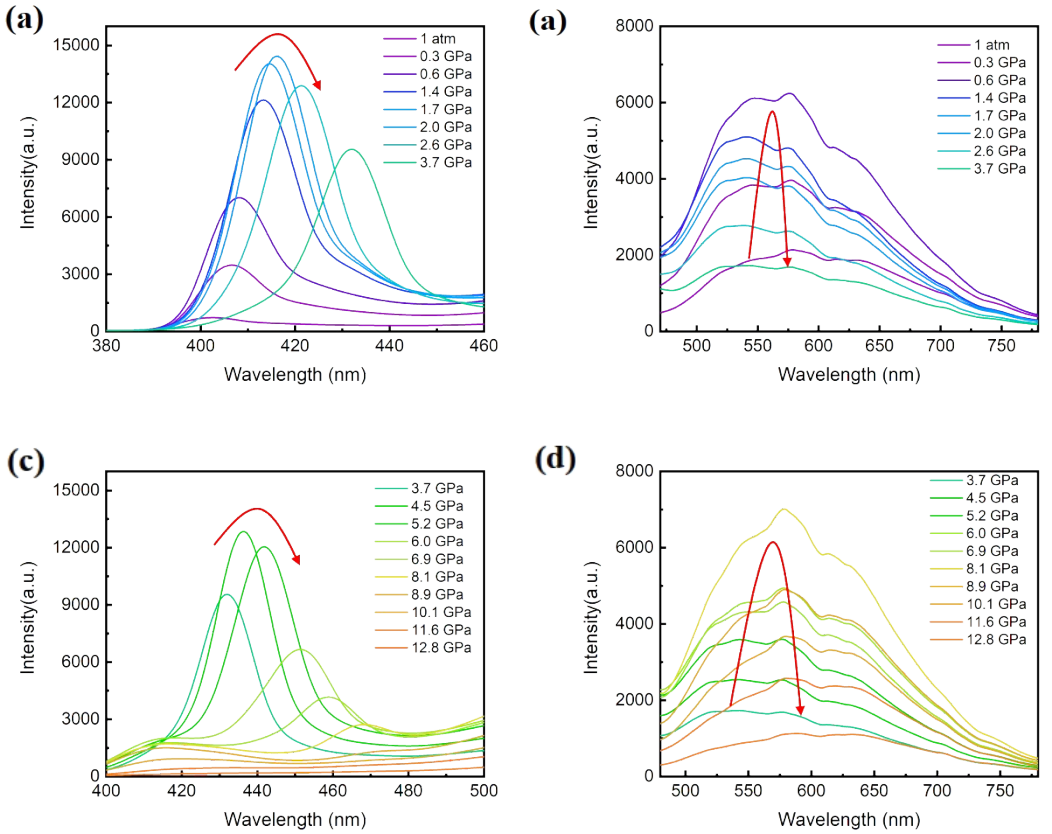


Figure S5. Pressure-induced PL intensity evolution of $(CHA)_2PbBr_4$ ranging from 0.1 MPa (1 atm) to 12.8 GPa.

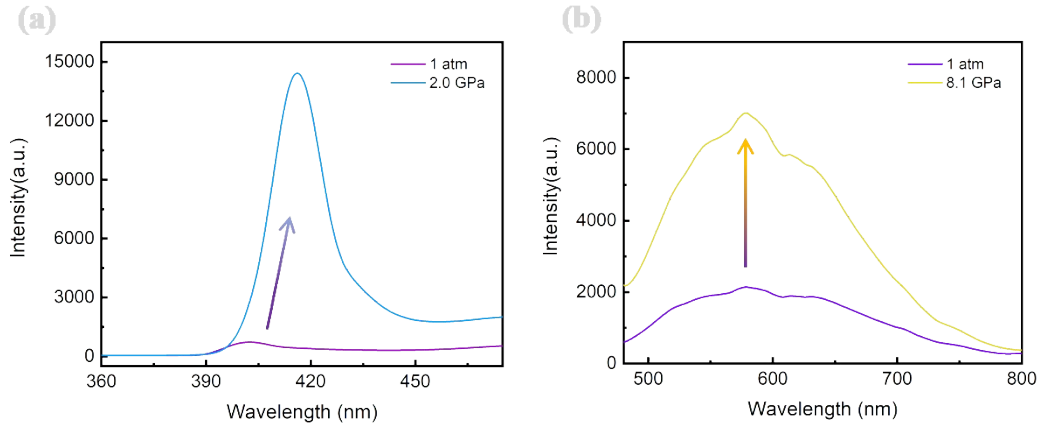


Figure S6. (a). Pressure-induced emission enhancement (PIEE) of FEs emission at 2 GPa. (b). Pressure-induced emission enhancement (PIEE) of STEs emission at 8.1 GPa.

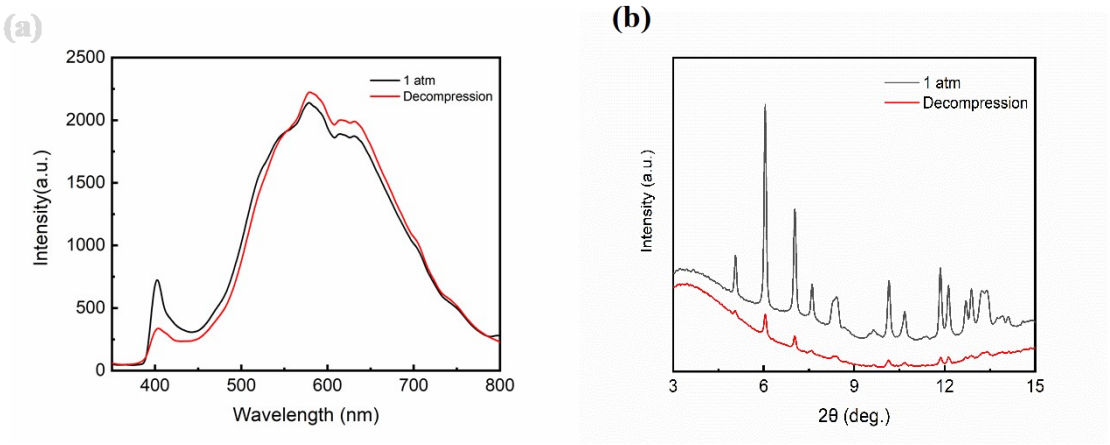


Figure S7. (a) PL spectra of $(CHA)_2PbBr_4$ at 0.1 MPa (1 atm) and decompression condition. (b) XRDs at 1 atm and full decompression.

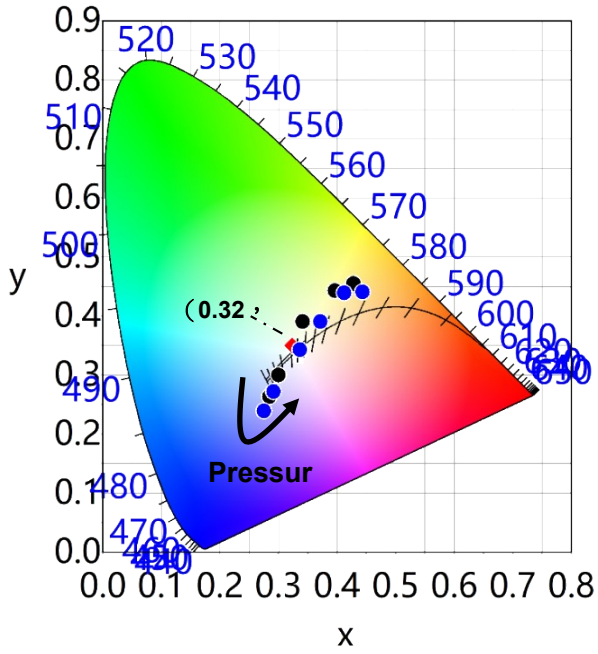


Figure S8. Evolution of the illumination chromaticity coordinates upon compression. The pressure ranged from 1 atm to 2.56 GPa is denoted as black circles, while the range of 3.73-12.78 GPa is denated as blue circles. The red circle is 2 GPa.

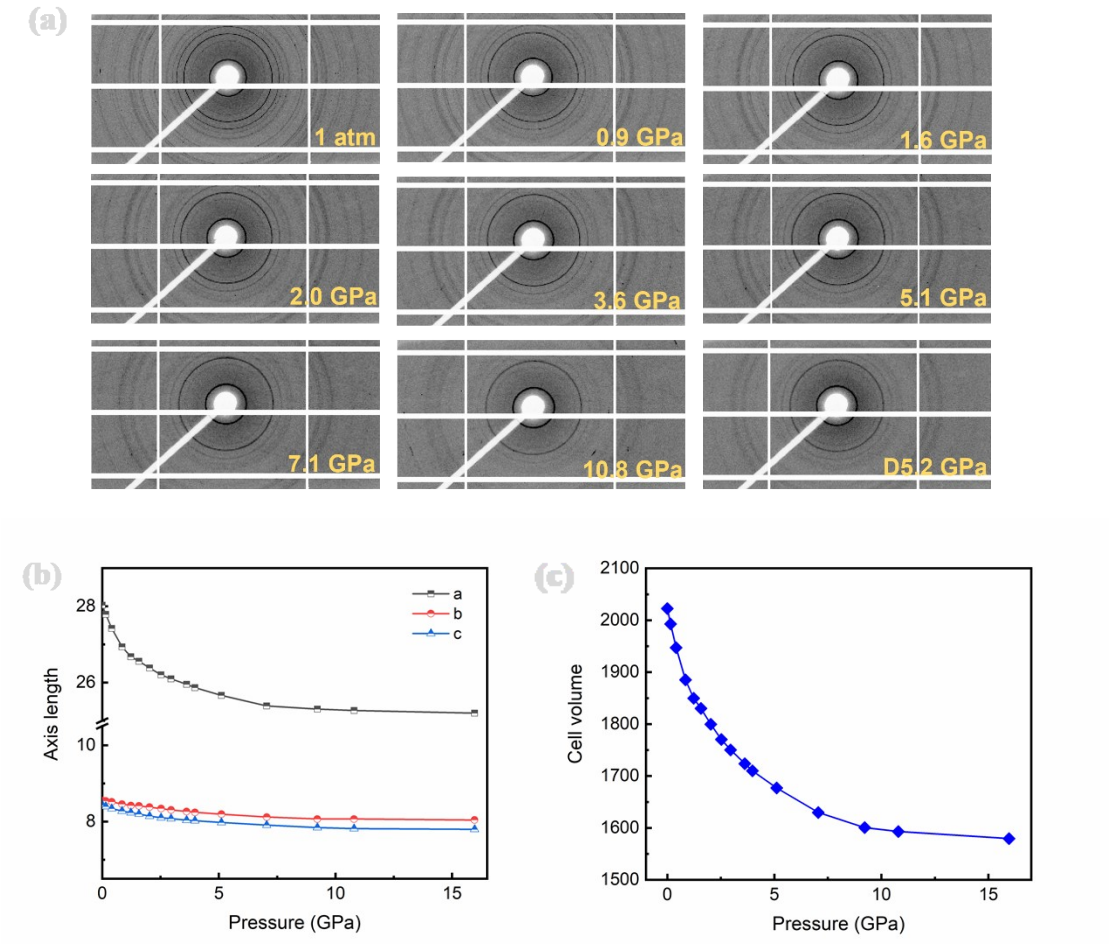
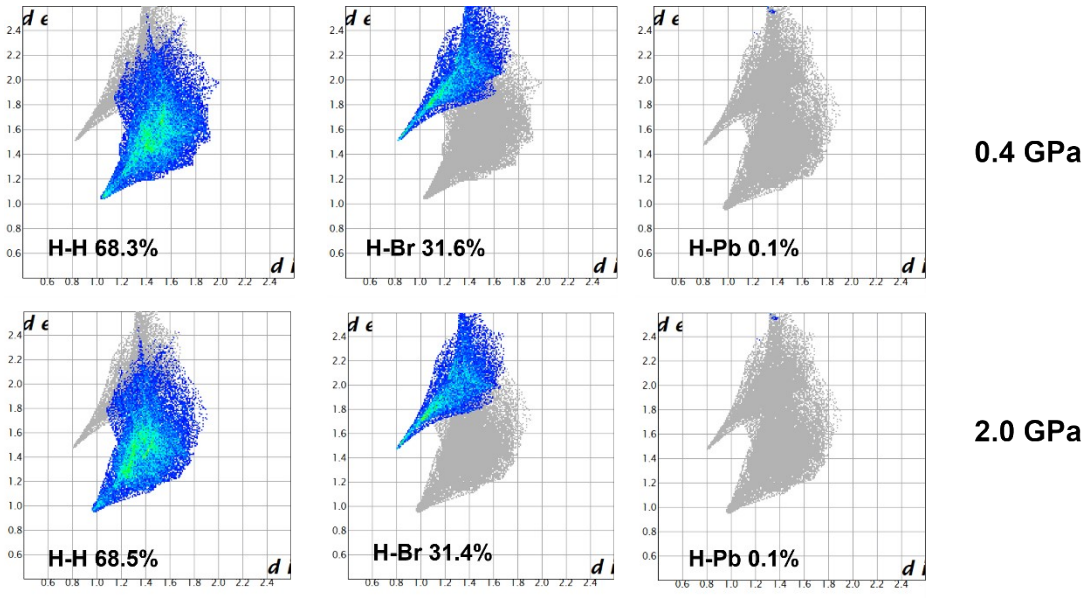


Figure S9. (a) Representative 2D XRD images at specific pressures. (b) (c)The evolution of lattice parameters under different pressure conditions, axis length and unit cell volume respectively.



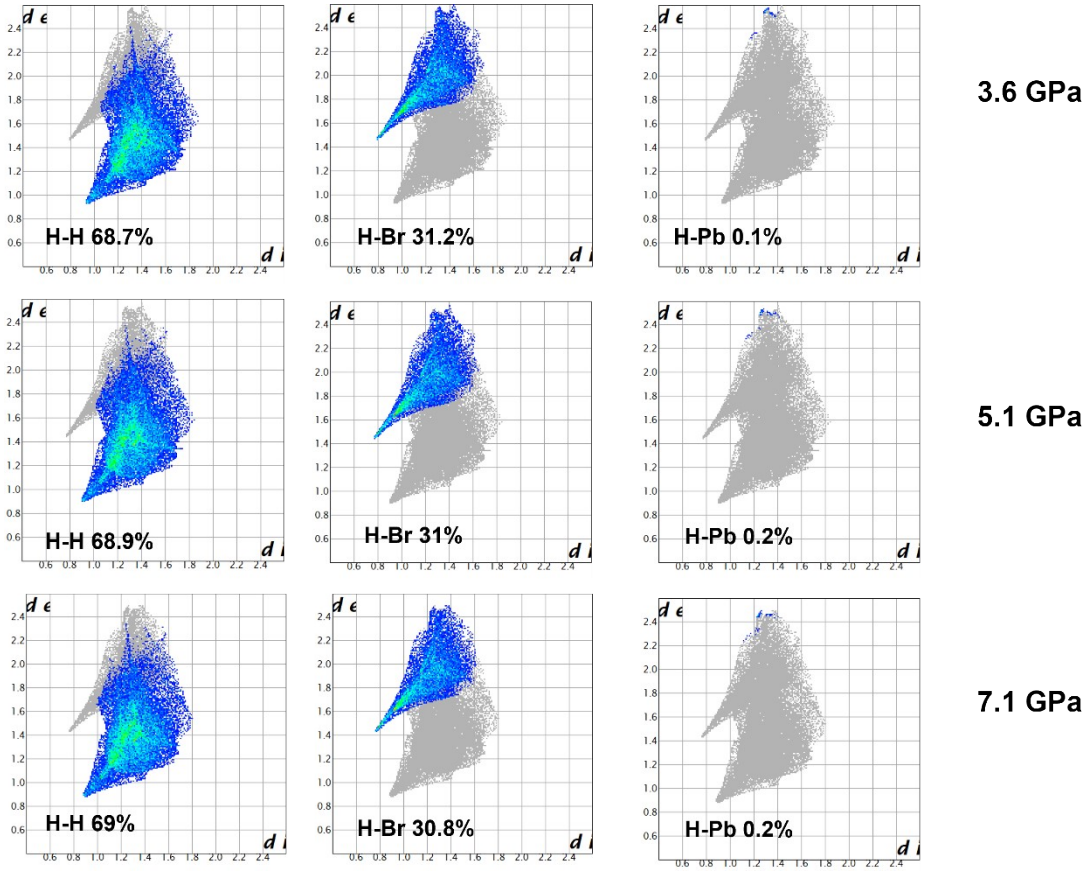


Figure S10. Change of the 2D fingerprint plots of $(CHA)_2PbBr_4$ by element with pressure.

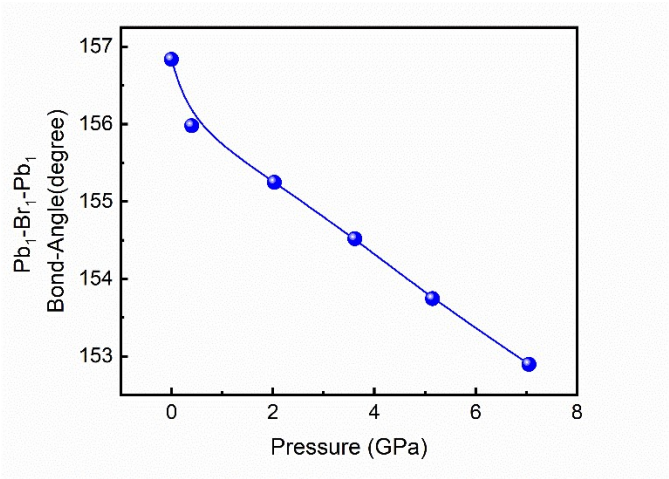


Figure S11. The angle between adjacent octahedra θ (Pb_1–Br_1–Pb_1) as a function of pressure.

Table S1. The CIE coordinate of $(CHA)_2PbBr_4$ under pressure.

Pressure (GPa)	x	y
0.0001	0.4283	0.4550
0.3	0.3963	0.4430
0.6	0.3866	0.4386
1.4	0.3411	0.3902
1.7	0.3331	0.3669
2.0	0.3230	0.3418
2.6	0.2997	0.2997
3.1	0.2846	0.2632
3.7	0.2771	0.2402
4.5	0.2751	0.2391
5.2	0.2912	0.2718
6.0	0.3366	0.3430
6.9	0.3715	0.3905
8.1	0.4124	0.4393
8.9	0.4218	0.4415
10.1	0.4310	0.4379
11.6	0.4389	0.4406
12.8	0.4434	0.4409

Table S2. The variation of crystal structure with pressure.

Pressure (GPa)	Distance of the adjacent inorganic layers (nm)	Organic cation penetration(Å)	Thickness of the organic layer(Å)	Out-plane distortion
0.0001	13.9995	1.3990	23.0592	9.6198°
0.4	13.7104	1.4312	22.5352	8.7556°
2.0	13.1910	1.4821	21.6046	8.0999°
3.6	12.9770	1.5130	21.2618	7.6724°
5.1	12.8335	1.5315	21.0238	7.5678°
7.1	12.6950	1.5518	20.8024	7.2965°

Table S3. The Δd and σ^2 of some known 2D OIHPs

Compound	Δd	σ^2	Ref.
BA_2PbBr_4	0.07	10.01	1
2-NEA_2PbBr_4	0.09	13.80	2

PMA_2PbBr_4	0.11	0.10	2
NMA_2PbBr_4	1.56	13.57	2
Rac-NEA_2PbBr_4	3.10	19.80	3
R/S/-NEA_2PbBr_4	6.00	40.26	3
$(C_6H_{11}NH_3)_2PbBr_4$	6.95	27.01	4
PEA_2PbBr_4	9.77	16.35	5
$C_7H_{12}N_2PbBr_4$	13.66	30.09	6
α-$(DMEN)_2PbBr_4$	17.38	17.35	7
This work	19.38	45.86	/
S-4MeOPEA_2PbBr_4	33.96	32.15	8
R-4MeOPEA_2PbBr_4	34.67	31.66	8

Table S4 Comparison of other low-dimensional lead halide perovskites under pressure

Compound	Magnitude of PL enhancement	White light emission
BA_2PbBr_4	2	**Yes**
$(GA)(MA)_2Pb_2I$	2.5	No
ETA_2PbI_4	4	No
$(PEA)_2PbCl_4$	5	**Yes**
$EAPbI_3$	5	No
$(MA)(BA)_2Pb_2I_7$	5	No
$C_4N_2H_{14}PbBr_4$ NCs	9	**Yes**
$(HA)_2(GA)Pb_2I_7$	12	No
This work	**20**	**YES**

Table S5. The lattice parameters under different pressure conditions

Pressure (GPa)	V (Å^3)	a (Å)	b (Å)	c (Å)
0.0001	2022.57	28.03	8.55	8.44
0.2	1992.89	27.79	8.54	8.40
0.4	1947.07	27.42	8.51	8.34
0.9	1885.26	26.94	8.46	8.27
1.2	1849.55	26.68	8.42	8.23
1.6	1830.18	26.56	8.41	8.20
2.0	1799.67	26.38	8.38	8.14
2.5	1770.24	26.21	8.34	8.10
3.0	1750.23	26.10	8.30	8.08
3.6	1723.70	25.95	8.26	8.04
4.0	1709.95	25.87	8.24	8.02
5.1	1676.89	25.67	8.19	7.97
7.1	1629.68	25.39	8.12	7.91
9.2	1600.69	25.30	8.07	7.84
10.8	1592.97	25.27	8.07	7.82

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