Supporting Information

Pressure-Induced Fluorescent Enhancement of $FA_\alpha PbBr_{2+\alpha}$ Composite Perovskites

Lan Anh Thi Nguyen,[1,2] Duong Nguyen Minh,[3] Ye Yuan,[5] Sudeshna Samanta,[2,5] Lin Wang,[5] Dongzhou Zhang,[6] Naohisa Hirao[7] Jaeyong Kim[1,2*], Youngjong Kang,[3,4*]

Experimental Details

Sample preparation. $PbBr_2$-98% and hydrobromic acid HBr-48% were purchased from Sigma-Aldrich. Dimethylsulfoxide ≥ 99.5% was purchased from Daejung company, Korea. Formamidine acetate ≥ 98% was supported by TCI company. $PbBr_2$-DMSO and FABr were synthesized following the procedure reported.[27] FABr was re-dissolved by ethanol following by slowly added to toluene in the purpose to get fine powder sample. The final powder was collected for further experiment after dry 12 hours in a vacuum oven.

High pressure generation. High pressure experiments were carried out using a symmetric DAC. Consider that the samples are air-sensitive, the sample loading processes were carefully conducted in a Ag-filled glove box. A T301 stainless steel gasket with a thickness of 50 μm and a 250 μm diameter of hole was used as the sample chamber. An approximately 5 micrometer ruby ball was inserted into the sample compartment for in-situ pressure calibration, by the standard ruby fluorescence technique. Silicone oil was used as pressure transmitting medium for high pressure optical absorption, PL and XRD measurements. All the measurements were performed at room temperature.

Absorbance and PL measurements. Absorbance spectra were measured in the exciton absorption band region using a Deuterium-Halogen light source. PL spectra were collected by using a Horiba LabRAM HR Evolution Raman spectrometer, excited by 473 nm laser. In-situ high pressure Raman spectra were recorded using a silicon CCD detector. A Renishaw Via Raman system was used to collect Raman signal from the sample in the DAC. A 633 nm radiation of a He-Ne laser with 17 mW output power was used to excite the sample.

XRD measurements. High pressure XRD measurements were conducted at the BL10XU beamline of Spring-8, Japan, and GSECARS-13BMC of APS at Argonne National Laboratory, USA, with beam energies of 30, and 28.6 keV, respectively. The diffracted x-rays were collected using the Rigaku

imaging plate area detector at SPring-8 and MAR CCD at APS. CeO_2 (Spring-8) and Lab_6(APS) were used as the standard samples to calibtrate the sample-detector distance and detector tilting. The Dioptas program was used to integrate and analyze the collected 2D images. The XRD patterns were refined by using the crystallography data analysis program of General Structure Analysis System (GSAS) and a 3D simulation software Visualization Electronic and STructural Analysis.

A. Table and Figures

Table S1.

Pressure (GPa)	Peak position (nm)	FWHM (nm)	Intensity (%)
0	542.3	19.2	100
0.1	545.7	18.5	696.1
0.3	554.3	18.8	694.1
0.4	558.9	18.7	664.7
0.5	562.6	20.9	293.7
0.8	570.3	19.9	475.2
1.0	576.2	17.9	548.9
1.2	579.3	18.5	974.9
1.5	584.02	19.5	959.8
1.7	588.5	18.0	1005.8
2.0	589.1	19.3	2146.4
2.4	586.1	21.6	1100.5
3.0	563.0	23.6	147.5
3.5	555.8	25.2	14.13
0 (Release)	534.4	21.5	49.2

Table S2.

		Ambient	**0.8 GPa**	**2.0 GPa**	**Release**
0D structure	Space group	$R\bar{3}c$	$R\bar{3}c$	$R\bar{3}c$	$R\bar{3}c$
	a / Å	13.07	13.79	13.32	13.94
	b / Å	13.07	13.79	13.32	13.94
	c / Å	18.45	17.50	17.88	17.69
3D structure	Space group	$Pm\bar{3}m$	$Im\bar{3}$	*Pnma*	$Pm\bar{3}m$
	a / Å	5.99	11.12	8.18	5.94
	b / Å	5.99	11.12	11.44	5.94
	c / Å	5.99	11.12	8.49	5.94

Table S3.

	Ambient	**Released**
Mismatching (%)	2.61	0.73
3D facet	(100)	(100)
0D facet	(300)	(300)
Mismatching (%)	0.59	0.47
3D facet	(200)	(210)
0D facet	(312)	$(31\bar{4})$

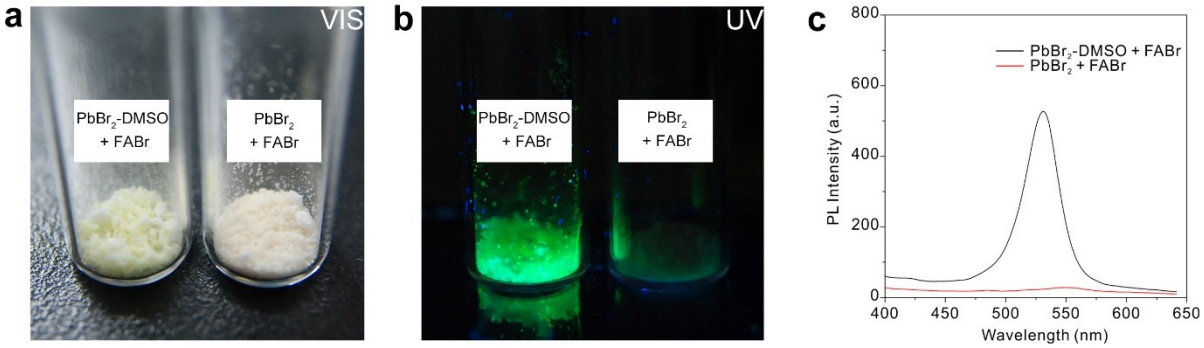

Figure S1. Pictures of the mixture of $PbBr_2$-DMSO and $PbBr_2$ with FABr under (a) visible light, and (b) UV illumination. (c) PL spectra of the mixtures of $PbBr_2$-DMSO/FABr and $PbBr_2$/FABr.

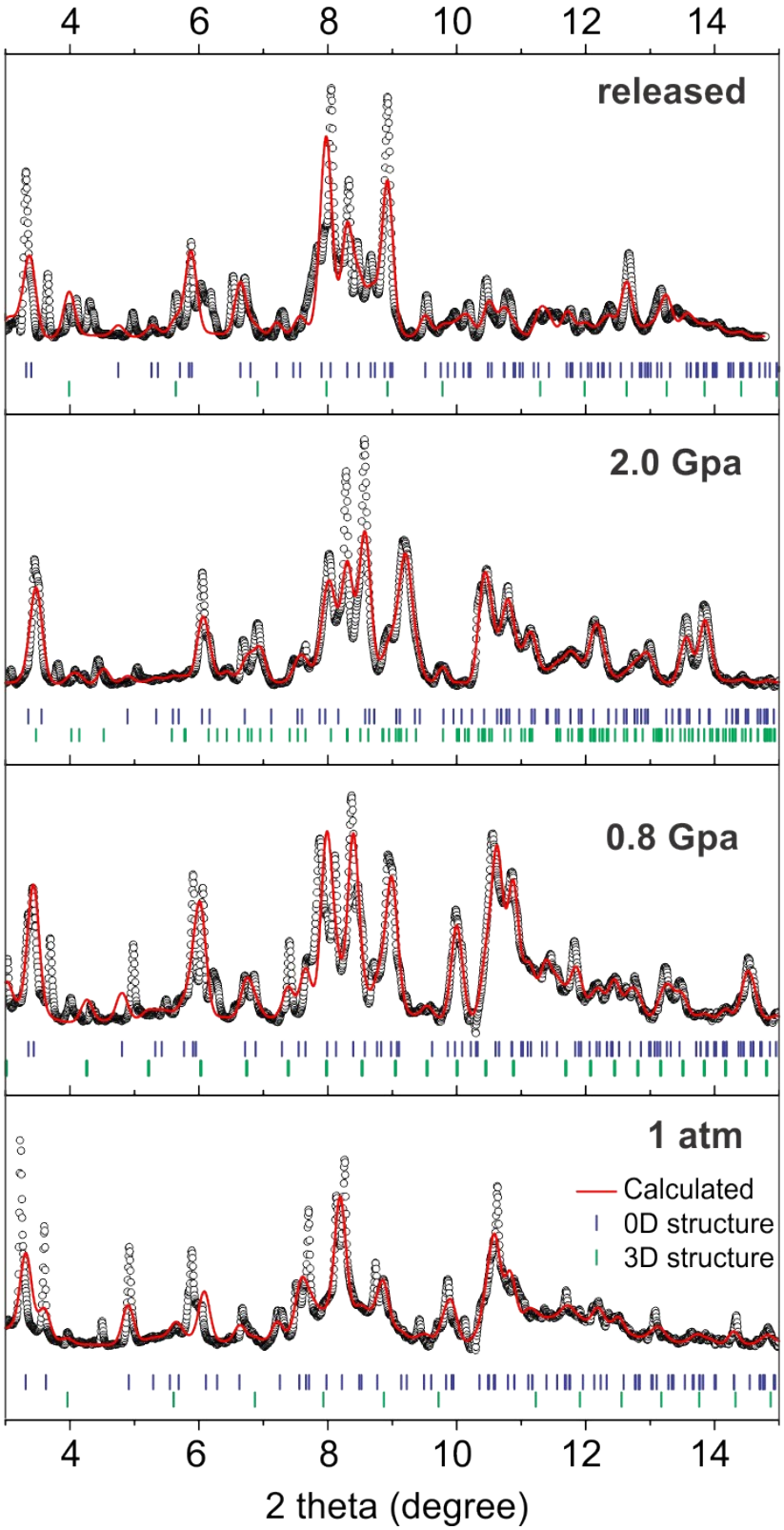

Figure S2. XRD analysis of $FA_{\alpha}PbBr_{2+\alpha}$ composite perovskite at a) ambient, b) 0.8 GPa, c) 2.0 GPa and d) after release. The expected peak positions for 0D and 3D structures from the GSAS calculation are marked and shown at the bottom of each result.

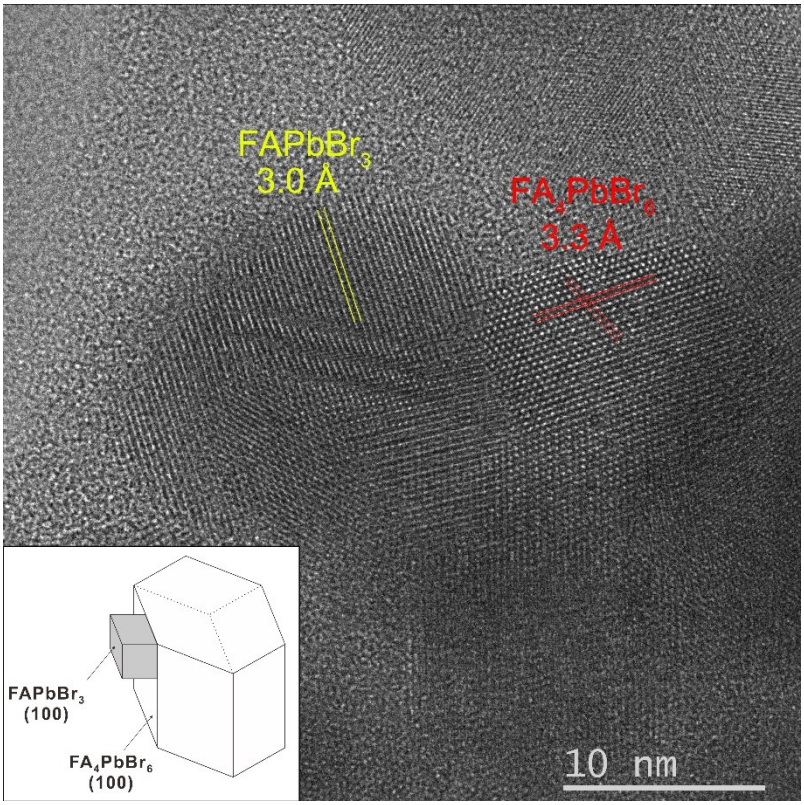

Figure S3. HR-TEM micrograph of $FA_{\alpha}PbBr_{2+\alpha}$ composite perovskite showing interface between FA_4PbBr_6 and $FAPbBr_3$ nanoparticles.

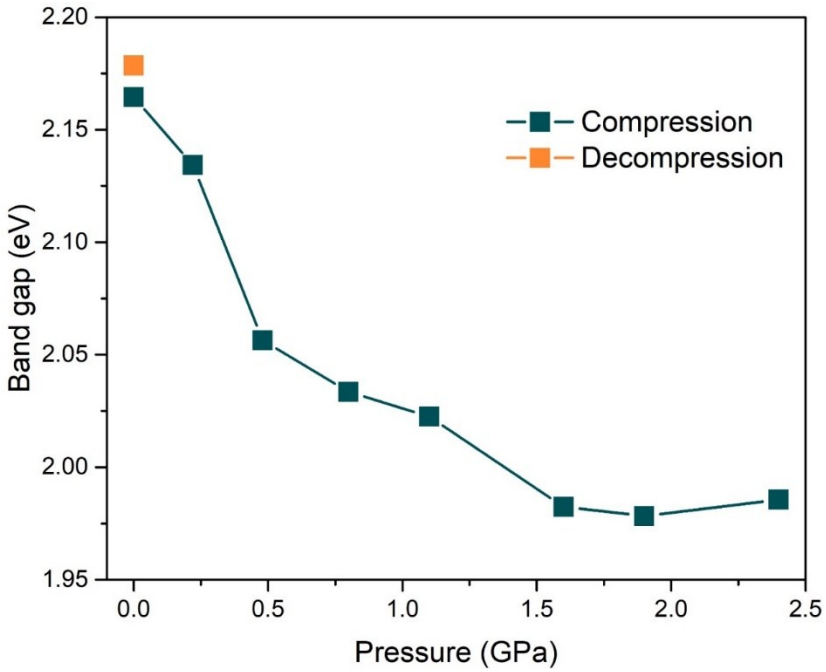

Figure S4. Pressure dependent band gap of $FA_{\alpha}PbBr_{2+\alpha}$ composite perovskite.

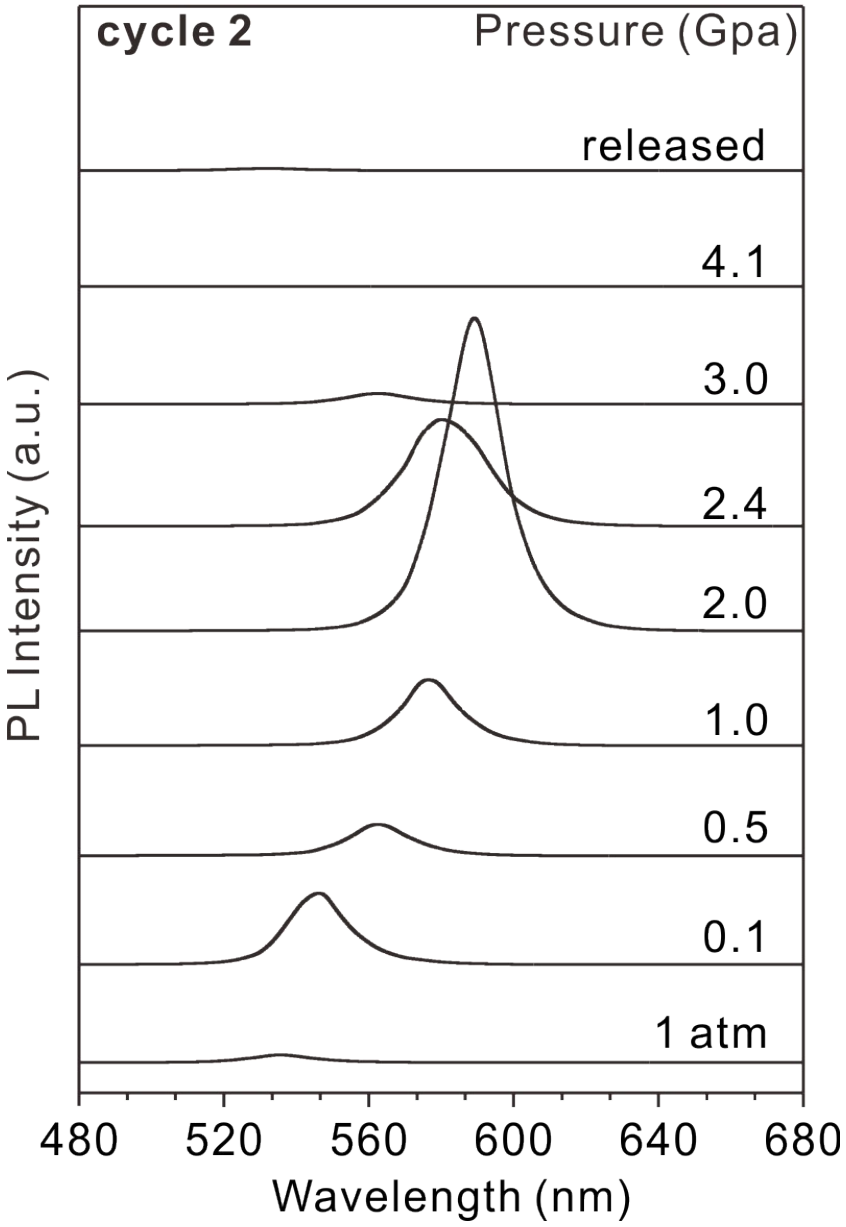

Figure S5. PL spectra of $FA_{\alpha}PbBr_{2+\alpha}$ composite perovskite at the second cycle of compression.