

## Supporting Information

### Enhancing Carrier Transport Properties of Melt-grown CsPbBr<sub>3</sub> Single Crystals by Eliminating Inclusions

Peng Zhang,<sup>†</sup> Qihao Sun,<sup>‡</sup> Yadong Xu,<sup>‡</sup> Xiang Li,<sup>†</sup> Lin Liu,<sup>†</sup> Guodong Zhang,<sup>\*,†</sup> and Xutang Tao<sup>\*,†</sup>

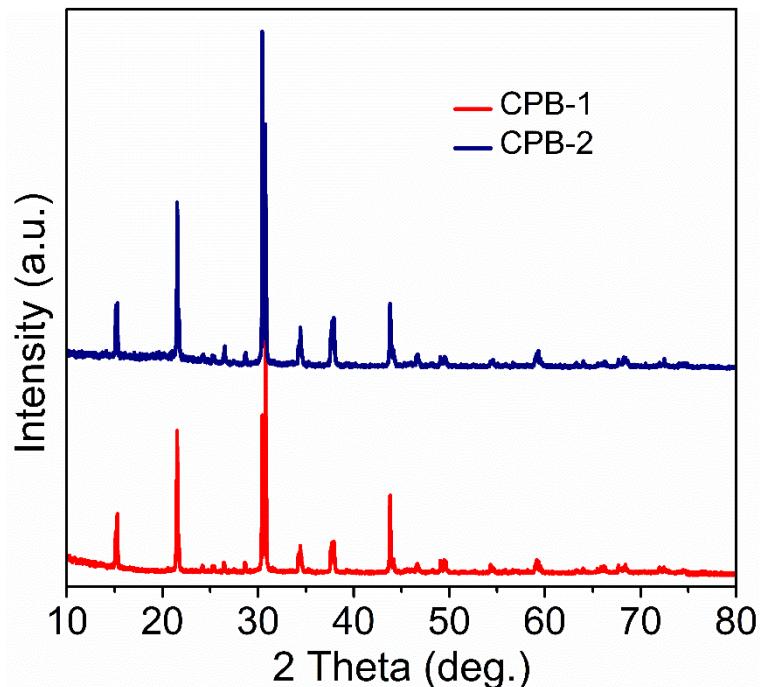
<sup>†</sup>State Key Laboratory of Crystal Materials, Institute of Crystal Materials, Shandong University, Jinan 250100, PR China.

<sup>‡</sup>State Key Laboratory of Solidification Processing, School of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an 710072, China.

#### Corresponding Author

\* E-mail: txt@sdu.edu.cn; Phone: 86-531-88364963

\* E-mail: zgd@sdu.edu.cn; Phone: 86-531-88369099



**Figure S1.** PXRD of the CPB-1 and CPB-2.

**Table S1.** GDMS of the CPB-1.

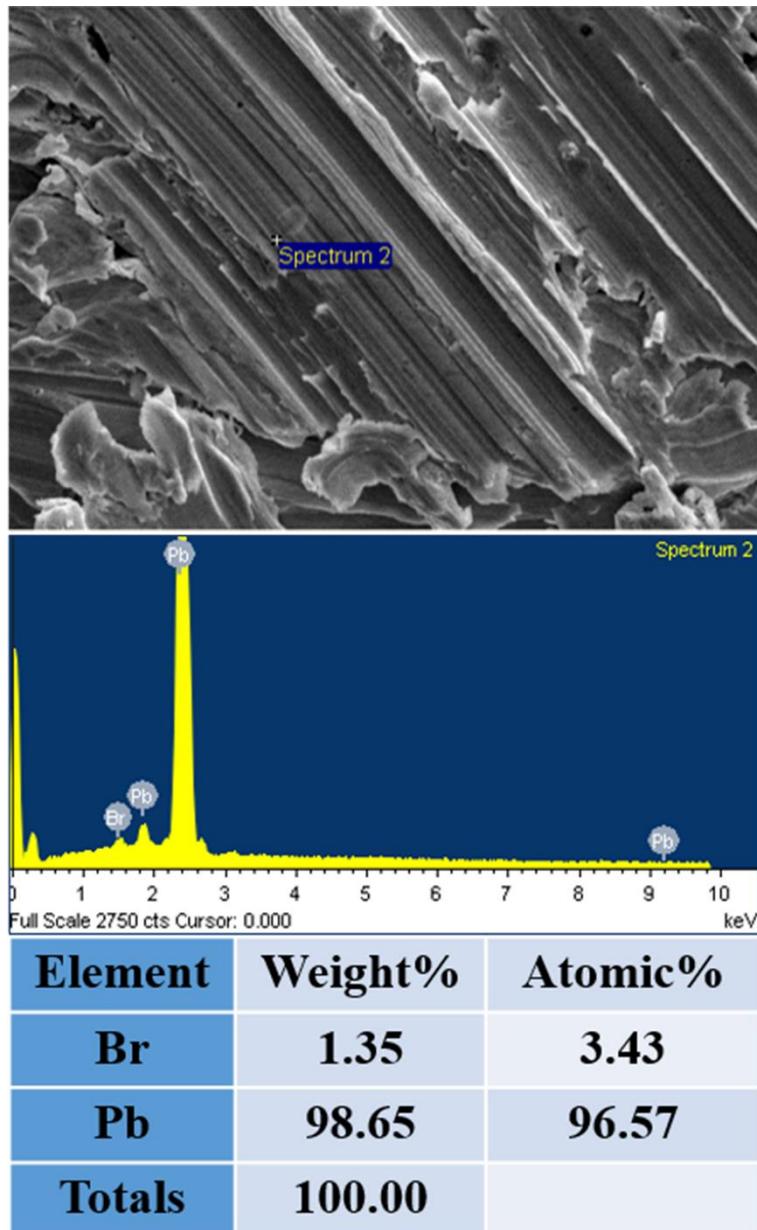
Elements	Concentration (ppm)	Elements	Concentration (ppm)	Elements	Concentration (ppm)
Li	<0.005	Cr	0.92	Sr	<0.005
B	0.019	Mn	0.007	Cd	0.013
C	16	Fe	4.6	Ag	0.012
F	<0.005	Ni	0.18	Sn	1.8
Na	0.032	Co	0.017	Sb	0.51
Mg	0.05	Cu	0.011	Te	0.023
Al	3.7	Zn	0.28	I	0.26
Si	0.056	Ga	0.009	Ba	0.031
S	0.078	Ge	0.013	Au	<0.005
Cl	1.6	As	<0.005	Hg	<0.005
K	<0.5	Se	<0.005	Tl	<0.005
Ca	2.6	Rb	<0.005	Bi	<0.005
<b>Cs</b>	<b>Matrix</b>	<b>Pb</b>	<b>Matrix</b>	<b>Br</b>	<b>Matrix</b>

**Table S2.** GDMS of the CPB-2.

Elements	Concentration (ppm)	Elements	Concentration (ppm)	Elements	Concentration (ppm)
Li	<0.005	Cr	0.074	Sr	<0.005
B	<0.005	Mn	0.011	Cd	0.009
C	4.9	Fe	7.9	Ag	0.013
F	0.034	Ni	0.041	Sn	0.51
Na	0.075	Co	<0.005	Sb	<0.05
Mg	0.037	Cu	0.006	Te	<0.005
Al	0.28	Zn	0.15	I	0.26
Si	0.057	Ga	<0.005	Ba	0.031
S	0.67	Ge	0.012	Au	<0.005
Cl	2.8	As	<0.005	Hg	0.22
K	<0.5	Se	<0.005	Tl	<0.005
Ca	1.7	Rb	0.021	Bi	<0.005
<b>Cs</b>	<b>Matrix</b>	<b>Pb</b>	<b>Matrix</b>	<b>Br</b>	<b>Matrix</b>



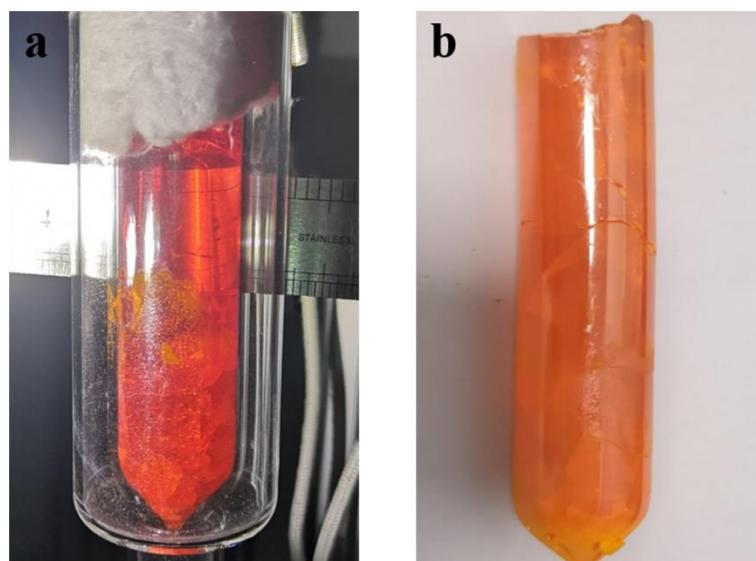
**Figure S2.** Pb particle with silver color in size about 0.5 mm in the cusp of CsPbBr<sub>3</sub> crystal.



**Figure S3.** EDS of the particle with silver color in the cusp of  $\text{CsPbBr}_3$  crystal.

**Table S3.** CsPbBr<sub>3</sub> single crystals grown by modified VB method with different crystal growth parameters.

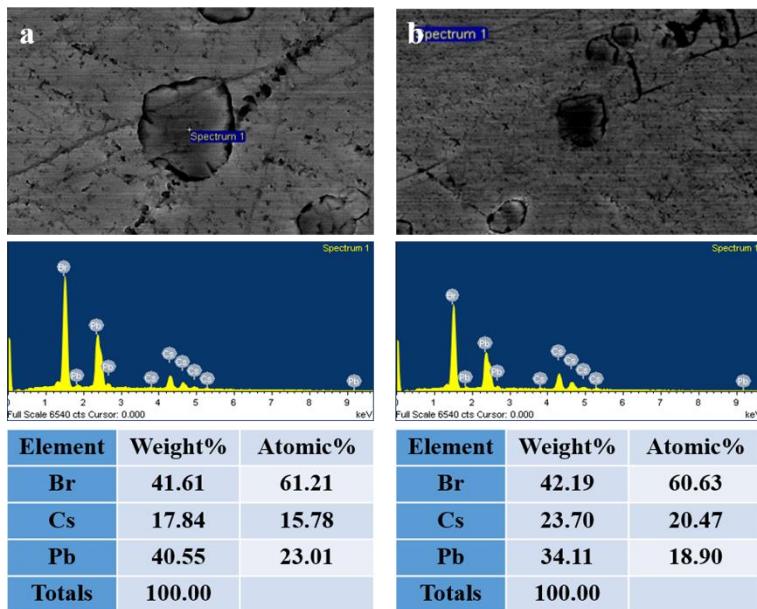
Crystal Photos	Temperature Gradient	Growth Rate	Cooling Rate
	30 ° C/cm	1 mm/h	10 ° C/h
	30 ° C/cm	0.5 mm/h	10 ° C/h
	30 ° C/cm	0.5 mm/h	15 ° C/h
	30 ° C/cm	0.2 mm/h	5 ° C/h



**Figure S4.** (a) Photograph of the as-grown CsPbBr<sub>3</sub> crystal which putted forward at 180 °C. (b) The picture of the CsPbBr<sub>3</sub> crystal after cooling down to room temperature in air.

**Table S4.** Thermal expansion coefficient of CsPbBr<sub>3</sub> crystal.

Thermal expansion coefficient (K <sup>-1</sup> )	25 °C~90 °C	91 °C~131 °C	132 °C~450 °C
<i>a</i> axis	4.09×10 <sup>-5</sup>		
<i>b</i> axis	3.05×10 <sup>-5</sup>		2.92×10 <sup>-5</sup>
<i>c</i> axis	4.26×10 <sup>-5</sup>	1.95×10 <sup>-5</sup>	



**Figure S5.** EDS of the inclusion in CPB-1.