

Electronic supplementary information

Mn²⁺-Based Narrow-Band Green-Emitting Cs₃MnBr₅ Phosphor and the Performance Optimization by Zn²⁺ Alloying

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Table 1. Main parameters of processing and refinement of the Cs_3MnBr_5 sample

Compound	Cs_3MnBr_5
Sp.Gr.	$14/\text{mcm}$
$a, \text{\AA}$	9.60672 (13)
$c, \text{\AA}$	15.5716 (2)
$V, \text{\AA}^3$	1437.08 (4)
Z	2
2 θ -interval, °	10-105
$R_{wp}, \%$	5.13
$R_p, \%$	3.84
$R_{exp}, \%$	2.31
χ^2	2.21
$R_B, \%$	3.08

Table S2. Fractional atomic coordinates and isotropic displacement parameters (\AA^2) of Cs_3MnBr_5

	x	y	z	B_{iso}
Cs1	0.16040 (14)	0.66040 (14)	0.5	2.5 (2)
Cs2	0	0	0.25	3.0 (2)
Mn1	0	0.5	0.25	1.3 (3)
Br1	0.14742 (16)	0.64742 (16)	0.15389 (11)	3.0 (2)
Br2	0	0	0	2.3 (2)

Table S3. Main bond lengths (\AA) of Cs_3MnBr_5

Cs1—Br1 ⁱ	3.8082 (19)	Cs2—Br1 ^{iv}	3.9646 (16)
Cs1—Br1 ⁱⁱ	3.5439 (19)	Cs2—Br2	3.8929 (1)
Cs1—Br2 ⁱⁱⁱ	3.6080 (13)	Mn1—Br1	2.5002 (16)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $-y+1, -x+1, -z+1/2$; (iii) $-x, y+1, -z+1/2$; (iv) $x, y-1, z$; (v) $-x, y, z+1/2$.

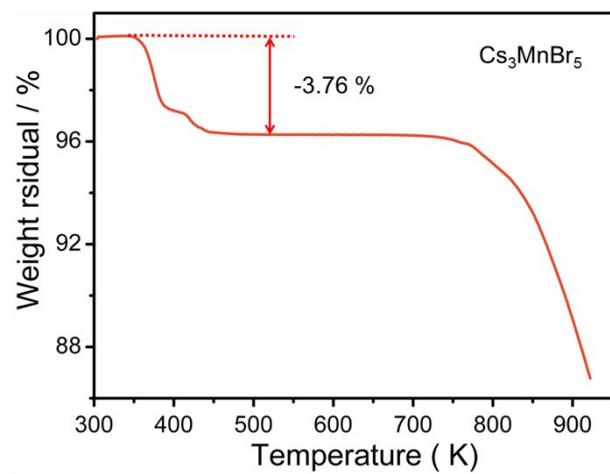


Fig. S1 The TG curve of Cs_3MnBr_5 sample.