

Supplementary material

Multicolor emission from hybrid 0D-doped halide (C₈H₁₄N₂)₂CdBr₆ single crystal

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Table S1 Crystal data for C₁₆H₂₈N₄CdBr₆

Compound	MXDA ₂ CdBr ₆
Chemical formula	C ₁₆ H ₂₈ N ₄ CdBr ₆
Fw	868.28
Space group	P1
a/Å	7.961(5)
b/Å	8.835(5)
c/Å	10.498(6)
α/°	100.288(18)
β/°	101.344(18)
γ/°	112.861(17)
Volume	640.0(6)

Table S2 Rietveld refinement of the (MXDA)₂CdBr₆:Mⁿ⁺ samples

Doped ion (M ⁿ⁺)	Space group	A (Å)	B (Å)	C (Å)	Cell volume (Å ³)	R _{wp}	R _p
M=Cu ⁺	P 1	7.940	8.835	10.48 3	638.0	12.01 %	9.05 %
M=Mn ²⁺	P 1	7.959	8.835	10.49 6	639.4	11.23 %	8.03
M=Sb ³⁺	P 1	7.950	8.835	10.49 5	639.8	12.53 %	9.43 %

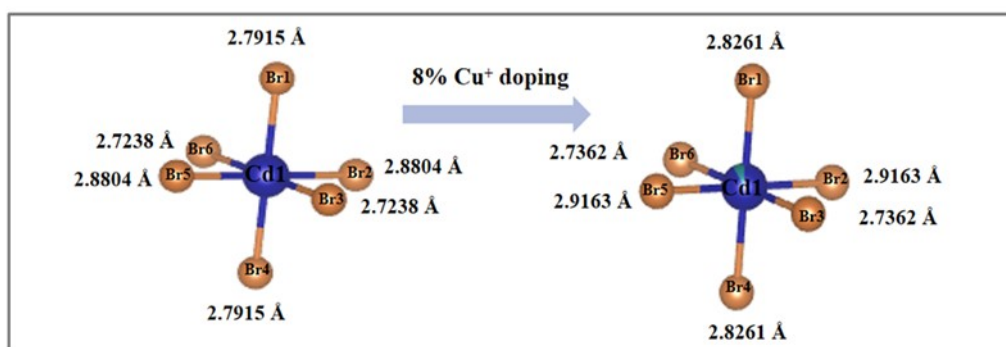


Figure S1 Variation of Cd-Br bond lengths in $[\text{CdBr}_6]^{4-}$ octahedra in $(\text{MXDA})_2\text{CdBr}_6$ before and after 8%Cu⁺ doping

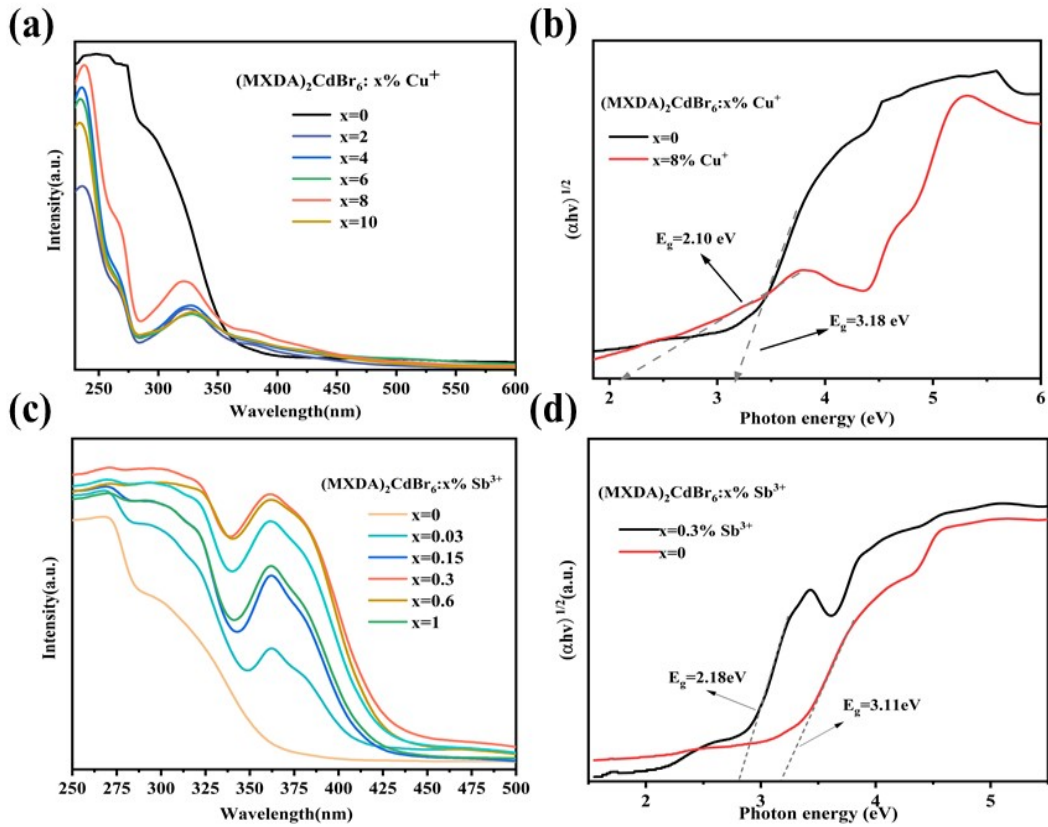


Figure S2 (a) UV-vis absorption spectra of (MXDA)₂CdBr₆:x%Cu⁺ sample, (b) Tauc plots of (MXDA)₂CdBr₆ and (MXDA)₂CdBr₆:x%Cu⁺ samples, (c) UV-Vis absorption spectra of (MXDA)₂CdBr₆:x%Sb³⁺ (x=0-1) sample, and (d) Tauc plots of (MXDA)₂CdBr₆ and (MXDA)₂CdBr₆:x%Sb³⁺ samples

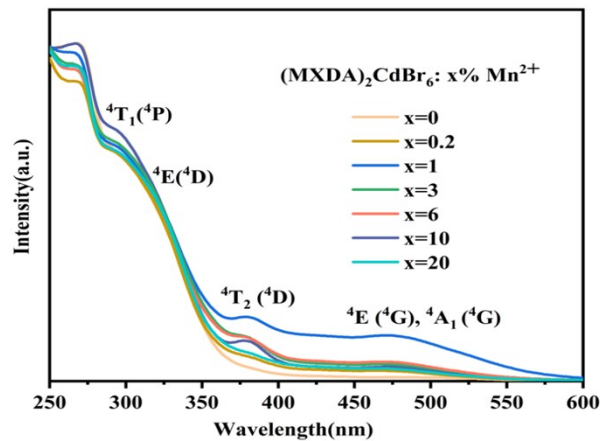


Figure S3 UV-Vis absorption spectra of (MXDA)₂CdBr₆:x%Mn²⁺ samples

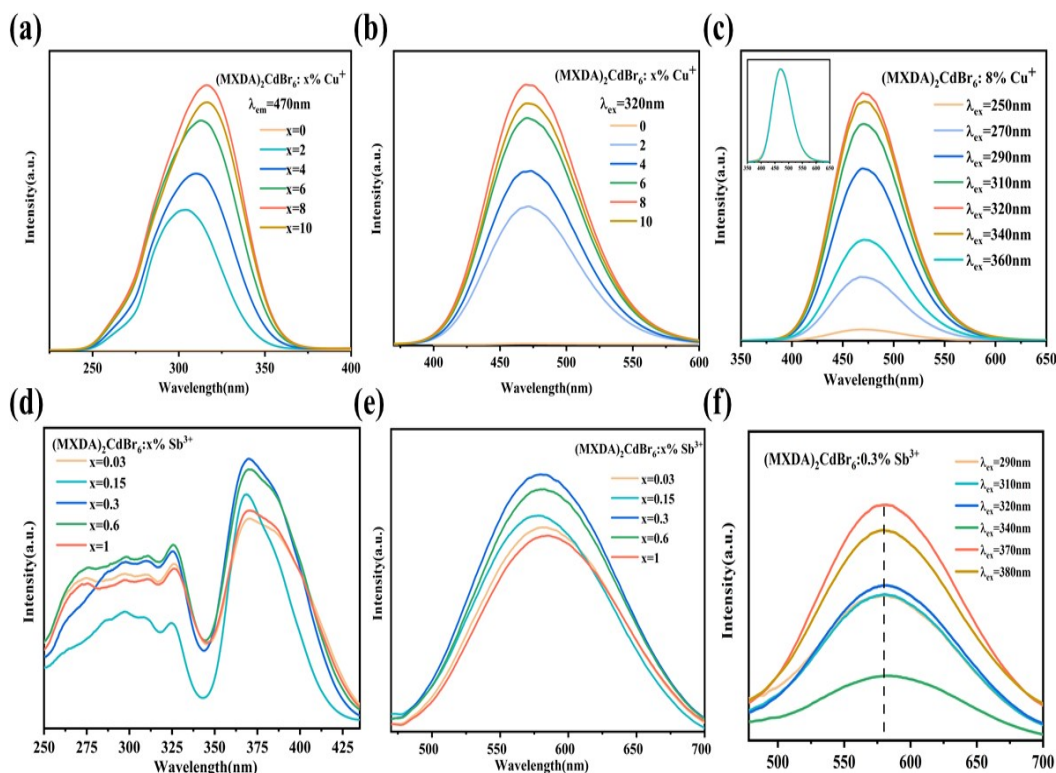


Figure S4 (a) PLE spectra ($\lambda_{em}=470$ nm) of $(MXDA)_2CdBr_6:x\%Cu^+$ samples, (b) PL spectra of $(MXDA)_2CdBr_6:x\%Cu^+$ samples ($\lambda_{ex}=370$ nm), (c) variable excitation spectrum of $(MXDA)_2CdBr_6:8\%Cu^+$ ($\lambda_{em} = 250-360$ nm), (d) PLE spectrum of $(MXDA)_2CdBr_6:x\%Sb^{3+}$ sample ($\lambda_{em}=580$ nm), (e) PL spectrum of $(MXDA)_2CdBr_6:x\%Sb^{3+}$ sample ($\lambda_{ex}=370$ nm), and (f) variable excitation spectrum of $(MXDA)_2CdBr_6:0.3\%Sb^{3+}$ ($\lambda_{em} = 290-380$ nm)

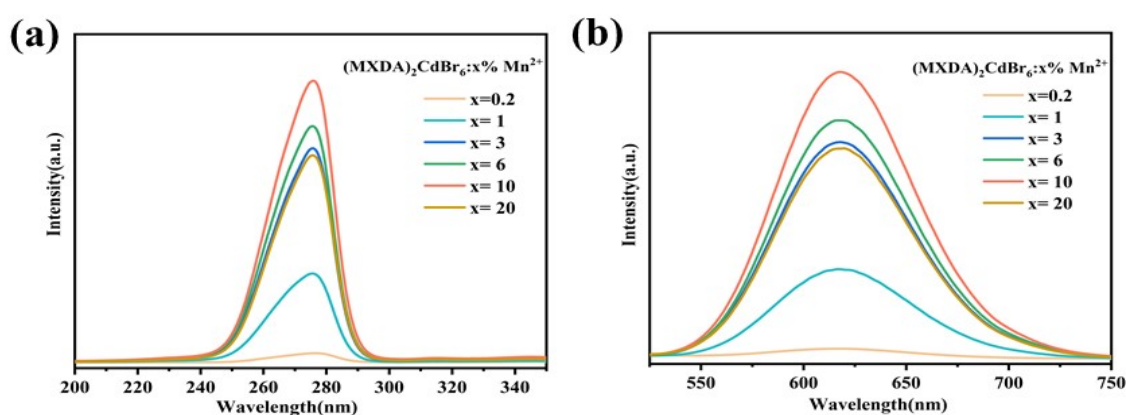


Figure S5 (a) PLE spectra ($\lambda_{em}=618$ nm) of $(MXDA)_2CdBr_6:x\%Mn^{2+}$ samples, and (b) PL spectra of $(MXDA)_2CdBr_6:x\%Mn^{2+}$ samples ($\lambda_{ex}=275$ nm),

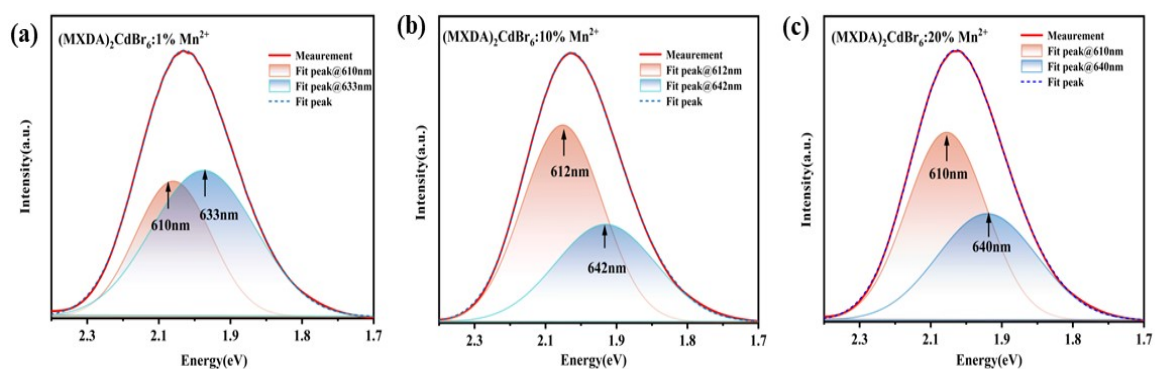


Figure S6 Multi-peak fitting results of PL spectra of $(\text{MXDA})_2\text{CdBr}_6:x\%\text{Mn}^{2+}$ ($x=1, 10, 20$)

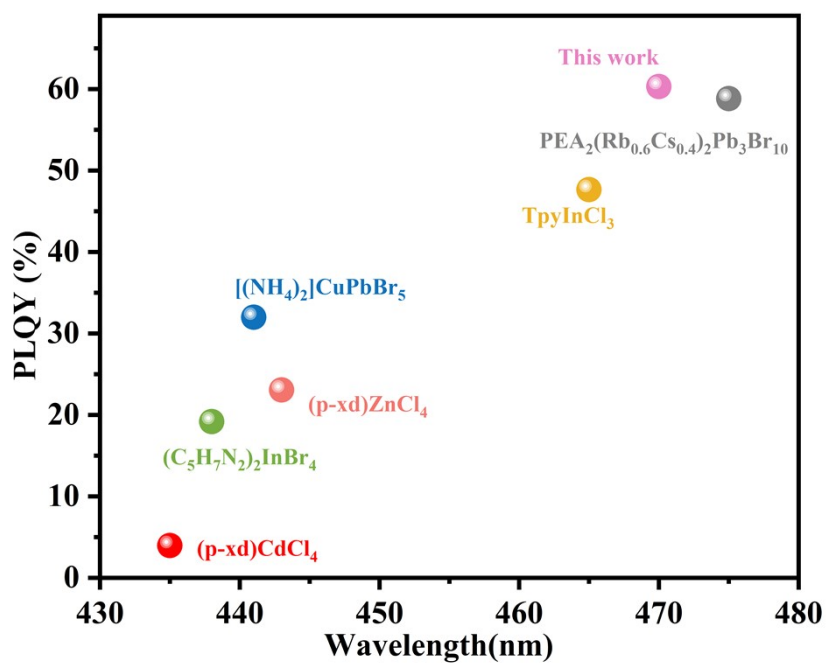


Figure S7 PLQY variation of blue light emission from the organic-inorganic hybrid perovskites in previous studies¹⁻⁵

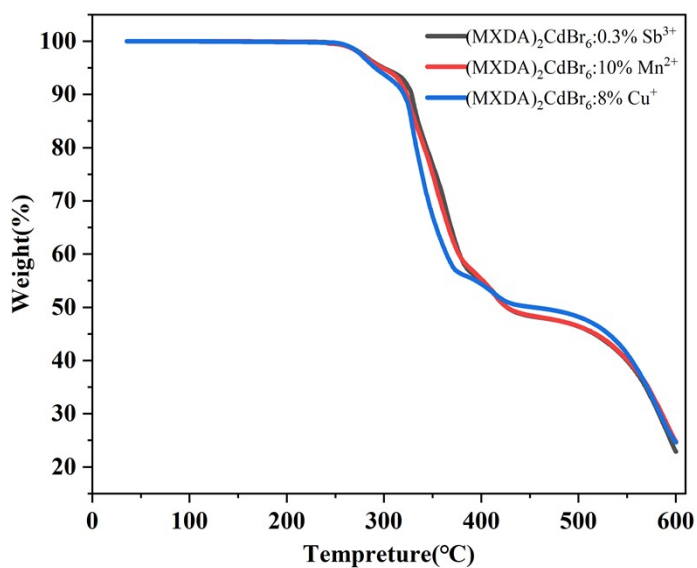


Figure S8 TGA profiles of (MXDA)₂CdBr₆:Mⁿ⁺ (Mⁿ⁺=Cu⁺, Sb³⁺, Mn²⁺)

Reference:

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