Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Suppressing Defect States in $CsPbBr_3$ Perovskite *via* Magnesium Substitution for Efficient All-Inorganic Light-Emitting Diodes

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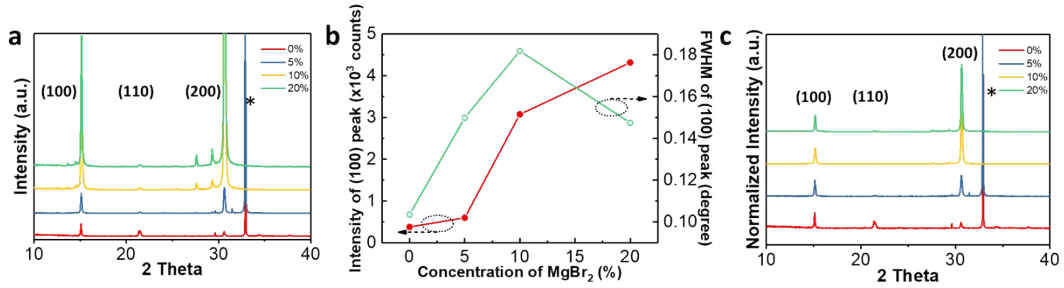

Figure S1. (a) *θ-2θ* XRD patterns, (b) XRD Intensity and FWHM variations of (100) peak, (c) Normalized XRD spectra (set the diffraction peak intensity of (100) plane as 1) of the perovskite films with different $MgBr_2$ concentration ("*" represents the diffraction peak of silicon).

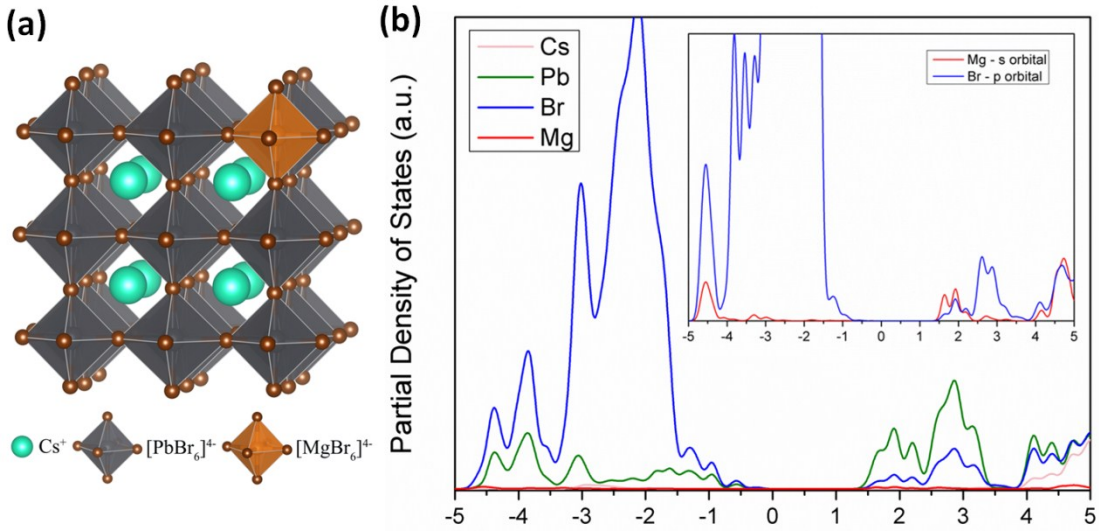

Figure S2. (a) Optimized structure and (b) Partial density of states (PDOS) for Mg-$CsPbBr_3$. Inset figure clearly shows the electrons coupling between *s* orbital of Mg and *p* orbital of Br.

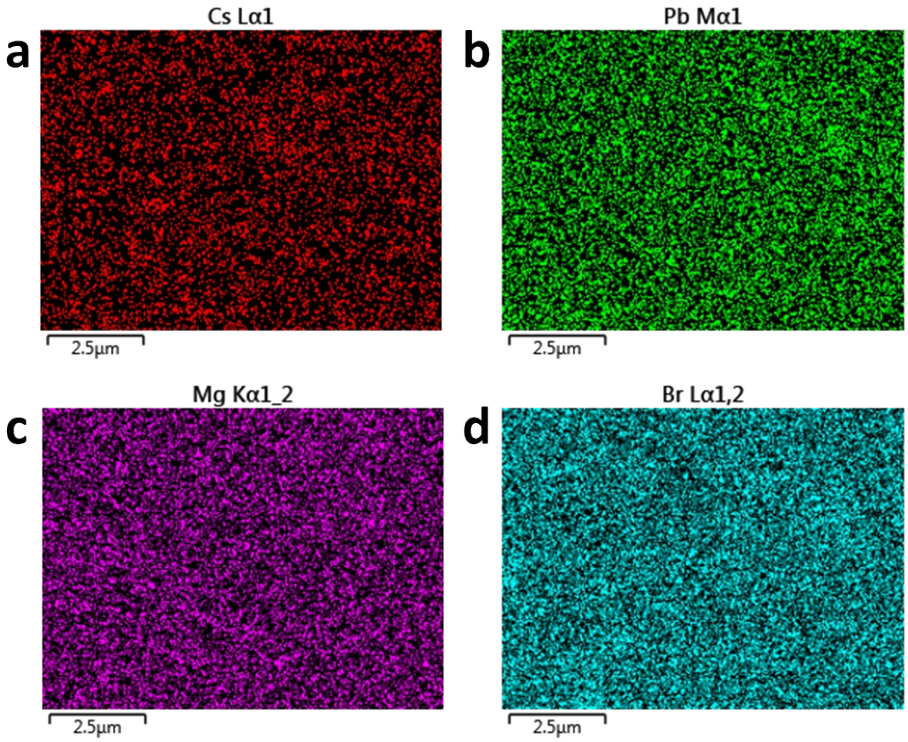

Figure S3. EDX element mapping images of perovskite film with incorporation of 10% $MgBr_2$. (a) Cs, (b) Pb, (c) Mg and (d) Br element mapping.

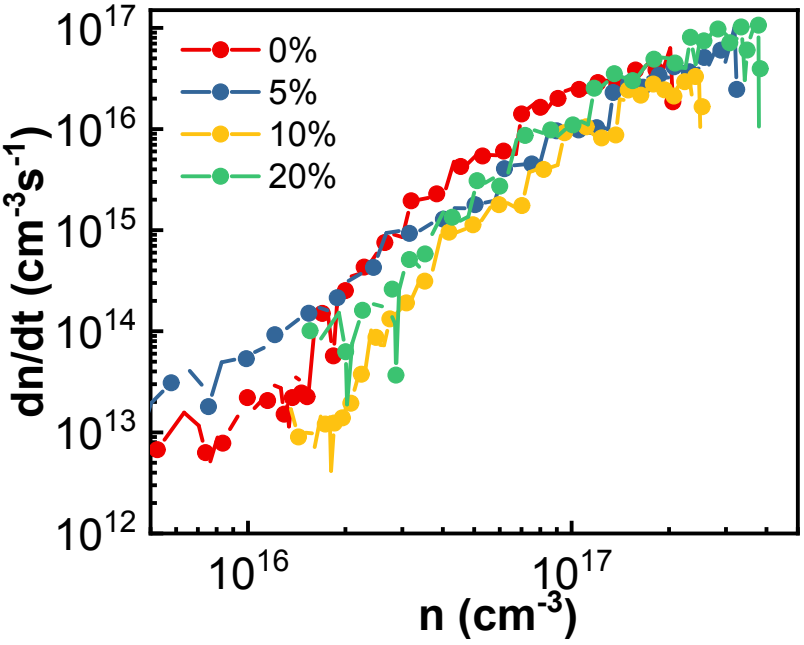

Figure S4. Radiative rate (*dn/dt*) as a function of carrier density for the perovskite films with different Mg^{2+} substitution.

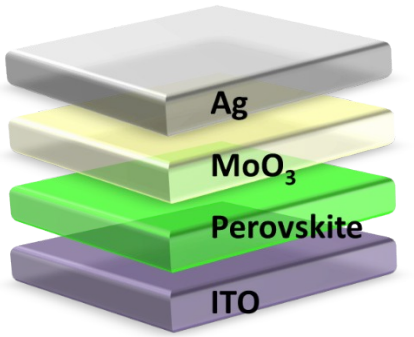

Figure S5. Schematic of hole-only device.

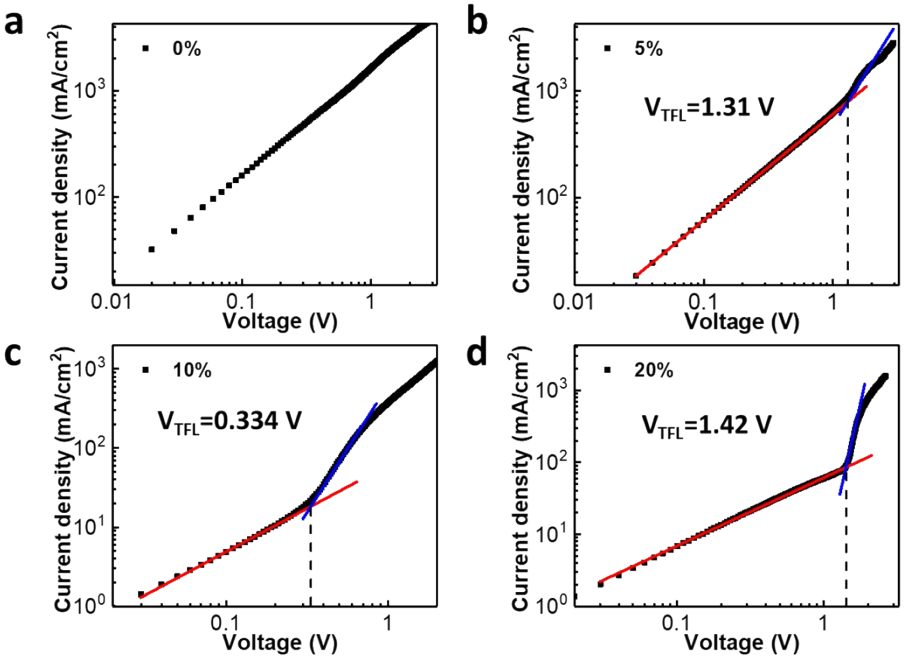

Figure S6. *J-V* characteristic curves of hole-only device based on the perovskite films incorporated with (a) 0%, (b) 5%, (c) 10%, and (d) 20% $MgBr_2$.

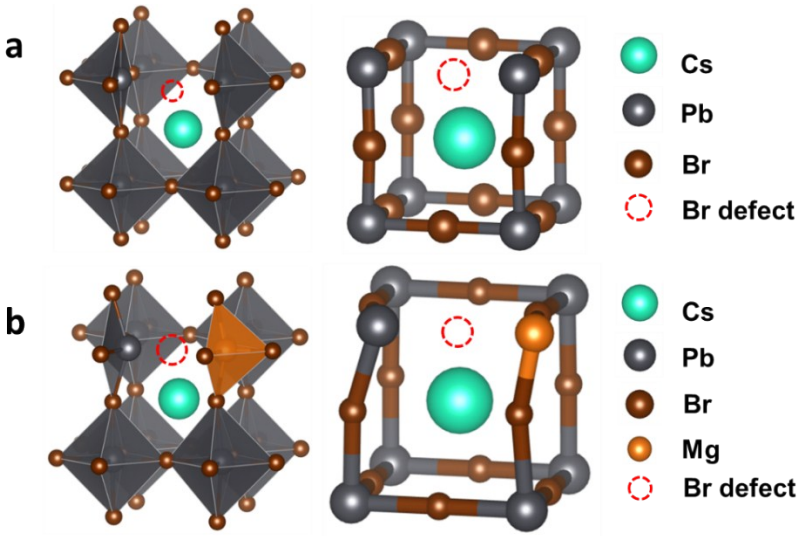

Figure S7. Simulated cubic structures with Br-defect in (a) $CsPbBr_3$ and (b) Mg-incorporated $CsPb_{0.875}Mg_{0.125}Br_3$.

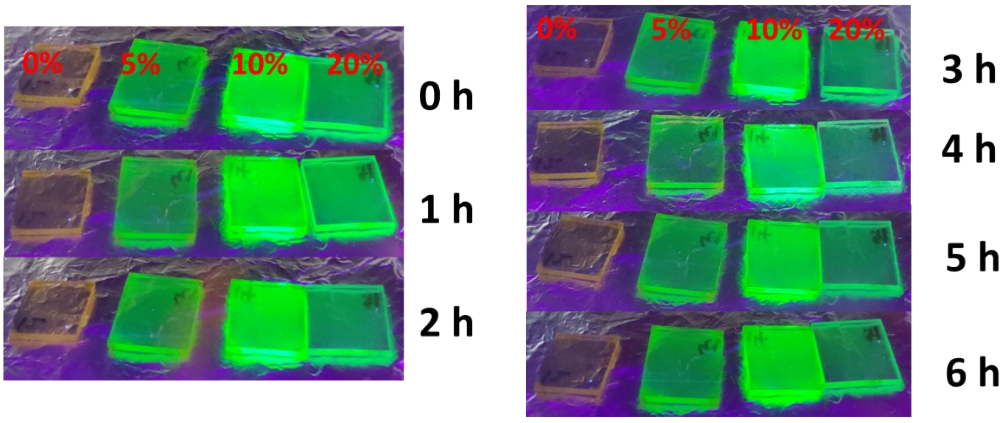

Figure S8. Photographs of $CsPb_{1-x}Mg_xBr_3$ perovskite films with different $MgBr_2$ concentration under 365 nm light illumination for 6 hours.

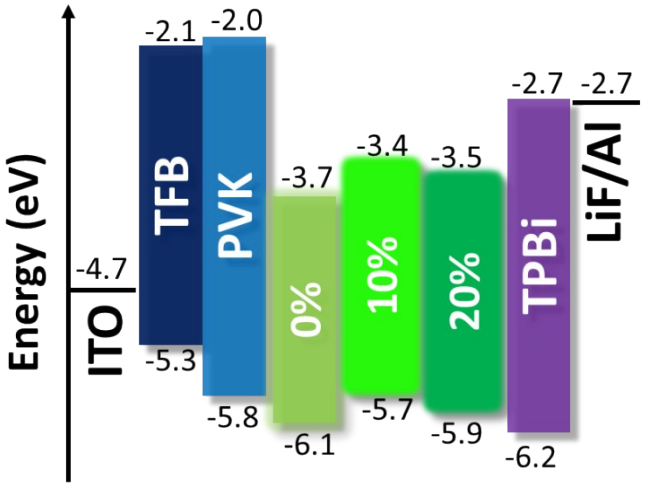

Figure S9. Energy level diagram of different functional layers in PeLEDs.

Table S1. Positions, intensity, and FWHM of (100) diffraction peak and the calculated crystal size of $CsPb_{1-x}Mg_xBr_3$ perovskite films with different $MgBr_2$ concentration.

Sample	2θ (degree)	Intensity ($\times 10^3$ counts)	FWHM (degree)	Crystal size (nm)
0%	15.105	0.382	0.104	76.521
5%	15.134	0.601	0.150	52.871
10%	15.163	3.076	0.182	43.588
20%	15.158	4.315	0.147	53.751

Table S2. PL lifetime value extracted from Figure 3e.

Sample	τ_1 (ns)	τ_2 (ns)	τ_3 (ns)	Average (ns)
0%	17.1	3.12	0.42	0.79
5%	4.59	35.72	3.34	3.80
10%	21.81	90.30	5.42	11.10
20%	19.94	97.41	3.54	6.12

Table S3. Electrical output characteristics of the PeLEDs with different Mg^{2+} concentration.

Sample	V_t (V)	L_{max} (cd m^{-2})	EL (nm)	η_A (cd A^{-1})	EQE (%)
0%	3.5	935	522	0.13	0.036
5%	3.0	10370	520	1.93	0.511
10%	3.0	25450	520	13.13	3.597
20%	3.0	12180	520	3.73	1.027