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Synergistic Effect of $SrCl_2$ and LiBr Additives on the Performance of High-Purity Green Perovskite Light-Emitting Diodes

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Abstract. This study demonstrates a significant performance enhancement in all-inorganic green perovskite light-emitting diodes (PeLEDs) by utilizing a p–i–n architecture (ITO/PEDOT:PSS/$CsPbBr_3$/TPBi/LiF/Al). The research focuses on the synergistic effects of incorporating Strontium Chloride ($SrCl_2$) and Lithium Bromide (LiBr) as dual-additives into the $CsPbBr_3$ emissive layer. The introduction of these additives effectively passivates surface defects and halide vacancies, which reduces non-radiative energy losses and improves charge carrier transport within the device structure. Experimental results show that the optimized devices achieve a peak external quantum efficiency (EQE) of 2.95%, representing a nearly 50% improvement over the 1.9% efficiency of the control samples. Furthermore, the additives ensure a high-purity green emission at 512 nm with improved color saturation. These findings provide a clear and reproducible pathway toward developing high-efficiency, stable, and cost-effective all-inorganic green LEDs for next-generation optoelectronic applications.

Keywords: $CsPbBr_3$, perovskite LED, green emission, p-i-n structure, optoelectronic devices, external quantum efficiency (EQE), electroluminescence (EL), bandgap tuning, device optimization.

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1. Introduction

Light-emitting diodes (LEDs) are fundamental components of modern optoelectronics, valued for their high efficiency, long operational life, and diverse applications in lighting and display technologies [1-3]. Recently, research has intensified to find new semiconducting materials that offer high performance at low fabrication costs [4, 5]. Among these, metal halide perovskites (MHPs) have emerged as revolutionary candidates. They are characterized by exceptional photoluminescence quantum yield (PLQY), high color purity with narrow emission bands, and tunable bandgaps [6-8]. Additionally, their compatibility with low-temperature solution-processing makes them ideal for large-scale production [9, 10]. Despite the rapid progress of perovskite LEDs (PeLEDs), long-term stability remains a major challenge. Organic-inorganic hybrid perovskites easily degrade when exposed to moisture, oxygen, or heat [11, 12]. As a more robust alternative, all-inorganic cesium lead halide perovskites, specifically $CsPbBr_3$, have gained interest due to their superior thermal stability and high-purity green emission [13, 14]. However, $CsPbBr_3$ devices often face limitations such as poor film morphology, high surface defect density, and unbalanced charge injection, leading to non-radiative recombination losses [15-17]. To overcome these issues, additive engineering has become a key strategy for controlling crystallization and passivating electronic traps [18, 19]. This study focuses on the synergistic effects of a dual-additive, Strontium Chloride ($SrCl_2$) and Lithium Bromide (LiBr). Previous research suggests that divalent cations like Sr^{2+} can effectively passivate grain boundaries and reduce defect density within the perovskite lattice [20, 21]. Meanwhile, alkali metal halides like LiBr have been shown to improve charge transport and optimize the interfaces between the layers [22, 23]. In this work, a systematic optimization of green PeLEDs is presented using a p–i–n architecture (ITO/PEDOT:PSS/$CsPbBr_3$/TPBi/LiF/Al). It is shown that the incorporation of $SrCl_2$

and LiBr additives significantly improves the device parameters, leading to enhanced brightness and external quantum efficiency (EQE). The influence of these additives on the optical, and electrical properties is discussed in detail, providing a clear path toward high-performance and stable all-inorganic green LEDs [24, 25].

2. Results and Discussions

The optoelectronic performance of the fabricated $CsPbBr_3$ based PeLEDs was systematically evaluated to understand the impact of $SrCl_2$ and LiBr dual-additives. The comparison between the control devices (WO - without additives) and the optimized devices (WE - with additives) reveals significant improvements in efficiency and brightness. The current-voltage (I-V) curves for both devices are presented in Figure 1. Both samples exhibit typical rectifying diode behavior with a clear turn-on voltage at approximately 3.0 V. The device with $SrCl_2$ and LiBr additives (WE) shows a higher current at the same applied voltage compared to the control device (WO). This increase in current indicates that the dual-additives enhance charge carrier injection and transport within the perovskite layer, likely due to improved film morphology and reduced resistive losses at the interfaces.

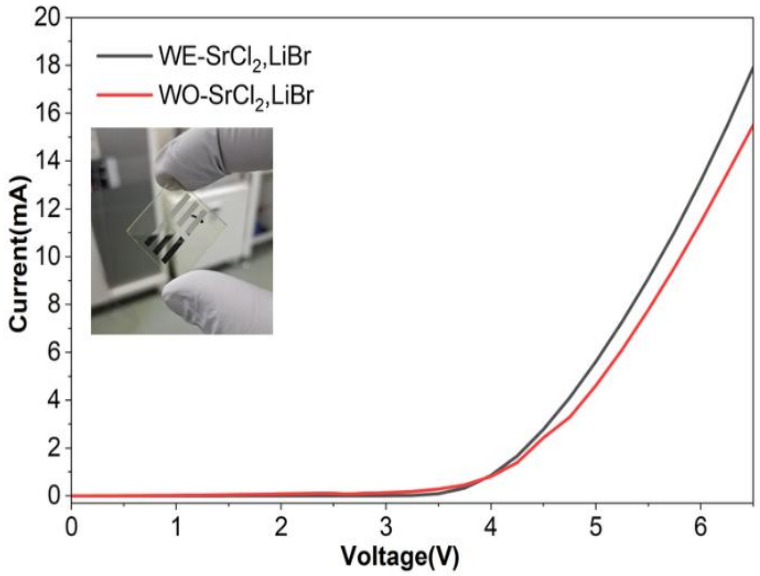

Figure 1. Current-voltage (I-V) characteristics of the PeLED devices fabricated with and without $SrCl_2$ and LiBr additives. The inset shows a photograph of the fabricated perovskite device.

The most striking improvement is observed in the external quantum efficiency (EQE) trends shown in Figure 2. The peak EQE of the optimized device (WE) reaches approximately 2.95% at 4.0 V, which is a significant enhancement compared to the control device's peak of 1.9%. This improvement can be attributed to the passivation of halide vacancies and surface defects by Sr^{2+} and Li^{+} ions, which suppresses non-radiative recombination processes. However, both devices exhibit efficiency roll-off at higher voltages (above 4.5 V), a common phenomenon in PeLEDs often associated with joule heating or auger recombination at high injection levels.

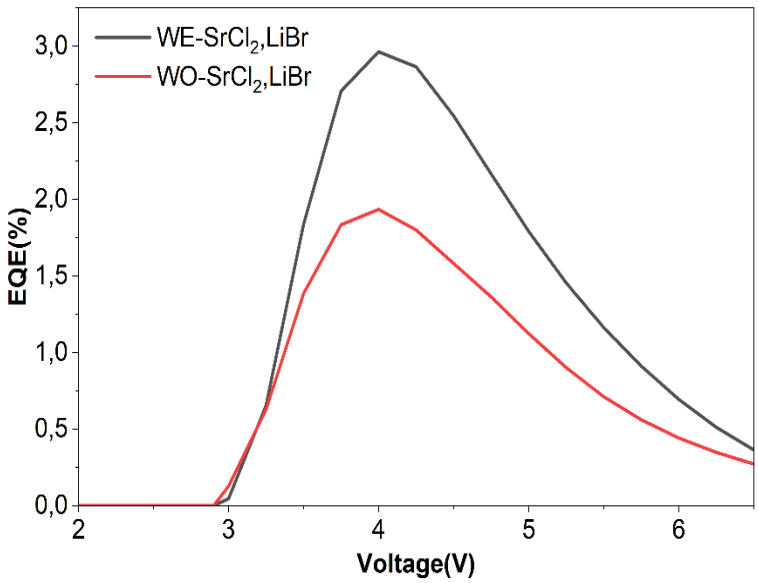

Figure 2. EQE-V characteristics of PeLEDs. The dual-additive device (WE) achieves a peak EQE of ~3.0% at 4 V.

Figure 3 illustrates the electroluminescence (EL) spectra of the devices. Both samples exhibit a sharp green emission peak centered at approximately 512 nm, characteristic of the $CsPbBr_3$ perovskite phase. The peak intensity of the WE device is substantially higher than that of the WO device, confirming the superior radiative recombination efficiency enabled by the additives.

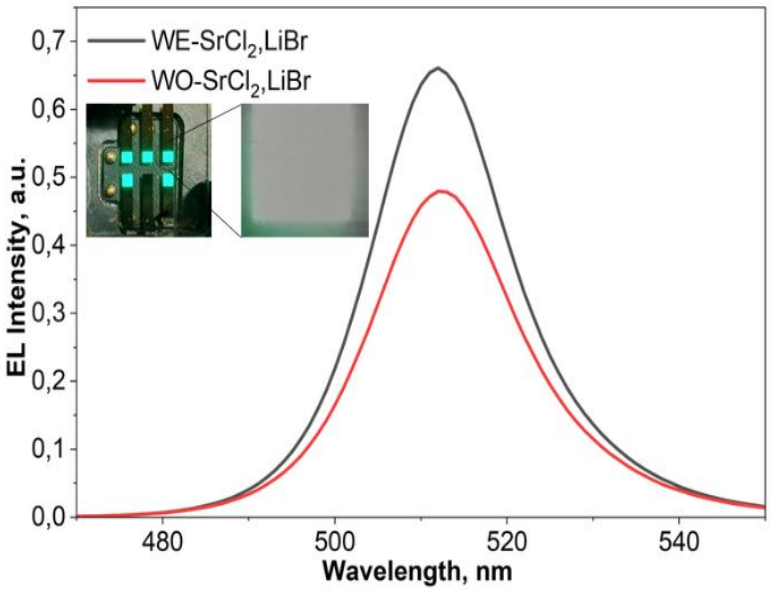

Figure 3. EL spectra of the $SrCl_2$, LiBr modified (WE) and control (WO) devices. The inset displays the working green PeLED pixels.

The narrow full-width at half-maximum (FWHM) remains consistent, suggesting that the incorporation of $SrCl_2$ and LiBr does not introduce deep-level impurity states or alter the crystal structure of the perovskite. The color characteristics were evaluated using the CIE 1931 chromaticity diagram (Figure 4).

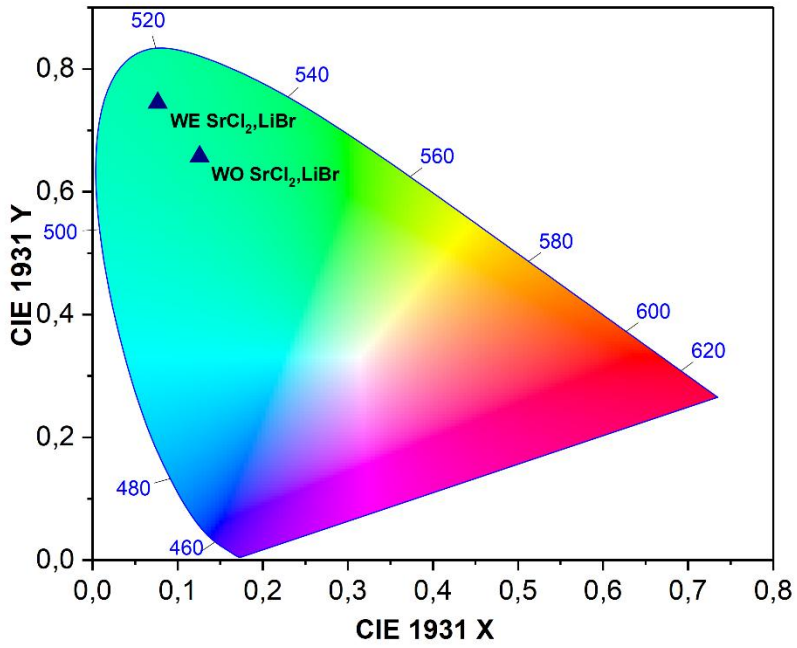

Figure 4. CIE 1931 chromaticity diagram showing the emission coordinates for $SrCl_2$ and LiBr modified (WE) and control (WO) PeLEDs.

It is observed that the emission for both devices is located within the green region of the color gamut. Notably, the introduction of $SrCl_2$ and LiBr additives results in a detectable shift of the chromaticity coordinates toward the saturated green region. This shift indicates that the dual-additive engineering not only enhances the device efficiency but also ensures a higher color purity for the $CsPbBr_3$ LEDs. The optimized sample (WE) demonstrates a more pronounced and stable green emission, which is essential for high-quality display applications requiring precise color saturation.

3. Methods and Materials

3.1 Materials

Indium tin oxide (ITO)-coated glass substrates were used as the bottom electrode. PEDOT:PSS, containing cesium chloride (CsCl) and sodium polystyrene sulfonate (PSS-Na), was used as the hole transport layer (HTL). For perovskite emissive layer was used composed of lead bromide ($PbBr_2$), cesium bromide (CsBr), phenethylammonium bromide (PEABr), strontium chloride ($SrCl_2$), formamidinium bromide (FABr), and lithium bromide (LiBr), with dimethyl sulfoxide (DMSO) as the solvent. TPBi was used as the electron transport layer (ETL), lithium fluoride (LiF) and aluminum (Al) was used as a top electrode.

3.2 Device fabrications

The ITO-coated glass substrates were sequentially cleaned in an ultrasonic bath using DT water, deionized (DI) water, acetone, and isopropanol, with each step performed for 15 minutes, followed by drying under a nitrogen flow. The cleaned substrates were then treated with UV-ozone for 30

minutes to improve surface wettability. For the hole transport layer (HTL) 0.065 g of PSS-Na and 0.030 g of cesium chloride (CsCl**)** were dissolved in 0.75 mL of deionized (DI) water and sonicated for 15 minutes**.** After complete dissolution, 2mL of PEDOT:PSS was added to the solution, and the mixture was sonicated for an additional 15 minutes. The resulting solution was then filtered through a 0.2 μm PES filter. The HTL was deposited by dropping 160 μL of the solution, followed by spin coating at 4000 rpm for 60 s, and annealed at 150 °C for 15 min. The perovskite emissive layer was fabricated in a nitrogen filled glovebox (H_2O, O_2 < 0.1 ppm). The precursor solution was prepared by dissolving $PbBr_2$ (0.0712 g, 97 mM), CsBr (0.0340 g, 80 mM), PEABr (0.0202 g, 50 mM), FABr (0.0087 g, 35 mM), $SrCl_2$ (0.0010 g, 3.15 mM), and LiBr (0.0003 g, 1.7 mM) in 2 mL of anhydrous DMSO. The solution was spin-coated onto the HTL at 4000 rpm for 90 s. The resulting films were annealed at 90 °C for 10 min. TPBi (40 nm), LiF (1 nm), and Al (100 nm) were deposited via thermal evaporation a base pressure of less than 10^{-6} Torr.

3.3 Optoelectronic Characterization

To evaluate device performance, current density-voltage (J–V) and luminance characteristics were recorded using a Keithley 2400 SourceMeter and a TOPCON SR-3AR Spectroradiometer, followed by the analysis of electroluminescence (EL) spectra, external quantum efficiency (EQE), and CIE 1931 chromaticity coordinates to quantify optoelectronic performance and verify color consistency.

4. Conclusion

The experimental results demonstrate that additive engineering is a highly effective strategy for enhancing the optoelectronic properties of green PeLEDs fabricated in a p–i–n architecture. The incorporation of Sr^{2+} and Li^{+} ions led to a significant improvement in charge carrier transport and radiative recombination efficiency. Specifically, the optimized devices (WE) exhibited a substantial increase in current density and a peak external quantum efficiency (EQE) of approximately 2.95%, representing a nearly 50% enhancement compared to the control devices. This improvement is attributed to the effective passivation of surface defects and halide vacancies, which significantly suppressed non-radiative losses. Electroluminescence measurements confirmed high-purity green emission centered at 512 nm, with excellent spectral stability and narrow emission bandwidths. Overall, the findings presented in this study highlight the critical role of chemical additives in modulating the performance of $CsPbBr_3$ based devices. The demonstrated approach provides a clear and reproducible pathway toward developing high-efficiency, stable, and cost-effective all-inorganic green light-emitting diodes, contributing to the advancement of next-generation perovskite-based optoelectronic technologies.

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