Different Passivation Strategies in Metal-Halide Perovskite Light-Emitting Diodes

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ABSTRACT

Halide perovskite has emerged as one of the most attractive classes of materials for future optoelectronic devices due to its highly tunable band gap, high photoluminescence quantum yield (PLQY), high charge-carrier mobility, and long carrier diffusion length. PeLEDs based on lead halide perovskites have been reported with external quantum efficiency (EQE) exceeding 30% and device lifetimes reaching as high as 180000 hours for green and red emissions. The high darkness, poor stability, and performance of pure-blue PeLEDs (460 to 470 nm) remain a challenge due to the deep trap states, halide ion migration, and unregulated crystallizing phase. These factors lead to non-radiative recombination losses and device instability. Therefore, in this review, we focus on the novel molecular passivation strategies involving fluorinated phosphonic acid, phosphorus oxychloride, choline chloride, malonamide, and tridecylamine in different perovskite systems. Despite their difference in chemical composition, these passivators have improved device performance by passivating undercoordinated Pb^{2+} ions and/or through the stabilization of the halide framework via ionic/hydrogen bonding, with concomitant improvements in PLQY, EQE, and operational stability. Nevertheless, pure blue PeLEDs still lag behind their green and red counterparts, indicating the need for optimized ligand engineering, defect passivation, and device architecture.

Index Terms- halide perovskite, optoelectronics, passivating perovskite, perovskite light-emitting diode

INTRODUCTION

Halide-based perovskites have grown in popularity in recent years and attracted attention among researchers due to their exceptional optoelectronic properties, such as high charge-carrier mobility, tunable band gap, high photoluminescence quantum yield (PLQY), and long free-carrier diffusion length [1], [2], [3]. The general formula of metal halide perovskite is ABX_3, where A^+ is an inorganic or monovalent organic cation; B^{2+} is a divalent metal cation and X^- is a halide anion. Examples of A^+ are $CH_3NH_3^+$, $CH(NH_2)_2^+$, Cs^+. Pb^{2+}, Sn^{2+}, Zn^{2+} are some examples of B^{2+}, examples of X^- are Cl^-, Br^-, I^-, and SCN^- [4]. Metal halide perovskites provide exceptional structural and compositional tunability [5]. Low exciton binding energy and long exciton diffusion length of bulk perovskites negatively affect radiative recombination; hence, the perovskite material is taken to the nanoscale to overcome these issues [6]. Perovskite can conduct both electronic charge carriers and mobile ions. Inside the device, ionic defects can migrate and diffuse under an electric field, which can induce transient efficiency fluctuations and degrade long-term stability [7].In this review, we will extensively focus on lead halide-based perovskite LEDs (PeLEDs). PeLEDs are known for tunable emission wavelength, high color purity, compatibility with low-temperature processing, and an economical solution-processing method [8], [9]. In recent years, PeLEDs have achieved external quantum efficiencies (EQEs) surpassing 30%, and at an initial luminance of 100 cd m^{-2}, the operational half-lifetimes (T_{50}) have reached 180,000 hours [10], [11], [12], [13]. Lead halide perovskite contains water-soluble lead components, which pose a threat to the environment and health.

Review Study

Maimaitizi et al. (2026) have studied the performance of ligand-engineered $CsPb(Br/Cl)_3$ PeLEDs [14]. In recent years, the EQEs of green and red PeLEDs have surpassed 25% [15]. On the other hand, pure blue

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PeLEDs mainly in the 460-470 nm emitting range are lagging [11], [16]. The band gap of mixed halide perovskite nanocrystals (PeNCs) can be precisely tuned by varying the chlorine-to-bromine ratio. This makes the mixed halide PeNCs a promising contender for pure blue LEDs [17], [18]. However, the addition of chlorine in the $CsPb(BrCl)_3$ NCs induces deep-trap states, which leads to suppression of radiative recombination [19].

The halide anions present in the perovskite lattice have low activation energies, which makes them highly susceptible to migration under applied bias voltage and Joule heating [20], [21], [22], [23], [24], [25]. Ion migration of halides degrades the device stability.

Maimaitizi et al. (2026) have introduced a multifunctional fluorinated phosphonic acid (HFPA) molecule to passivate the deep trap states and ion migration in the PeNCs. HFPA stands for (1H,1H,2H,2H-heptadecafluorodec-1-yl) phosphonic acid. The HFPA molecule contains the phosphonyl (-P=O) group, which anchors on the PeNCs and passivates the undercoordinated Pb^{2+} ions [14]. The hydroxyl (-OH) group of HFPA stabilizes the halogen ions and prevents ion migration by forming hydrogen bonds with the halide ions of the PeNCs. Additionally, the terminal fluorine atoms in the HFPA molecule form ionic bonds with the halide octahedra and stabilizes the octahedral structure [14].

The device architecture is as follows: ITO/ PEDOT:PSS /TFB&TCTa/PFI/PeNCs/B_3PyPPM/PO-T2T/LiF/Al [14]. The photoluminescence quantum yield PLQY of the pristine and HFPA-modified devices is 24.7% and 82.1%, respectively [14]. The exciton binding energy of the HFPA-modified device (51.07 meV) is higher than that of the pristine device (43.53 meV) [14]. Lattices of HFPA-based devices are more thermally stable than those of pristine devices. The radiative recombination rate of the HFPA-based device (9.79×10^7 s^{-1}) is also much higher than that of the pristine devices (3.60×10^7 s^{-1}) [14].

The HFPA-treated $CsPb(Br/Cl)_3$ PeLEDs achieved 14.8% EQE, which is 9 times that of the untreated device [14]. The target device reached a maximum luminance of 1052 cd m^{-2}, which is 10-fold of the pristine device. The operational half-lifetime of HFPA-based PeLEDs is about 341.6 seconds, whereas the pristine device has about 27.2 seconds [14].

The HFPA-based PeLEDs showed that the ligand successfully restricted ion migration by maintaining a steady, pure-blue emission peak at precisely 467 nm with minimal spectral shifting [14].

Lead halide perovskite nanocrystals (LHP NCs) exhibit exceptional optoelectronic properties despite high defect density [26], [27], [28], [29]. Chlorine-based LHP NCs suffer from deep trap states as compared to iodide and bromide-based LHP NCs [30], [31], [32]. It is a challenge for $CsPbI_3$ NCs to achieve high PLQY and prolonged stability in the development of violet and blue LEDs [33]. To overcome this issue in $CsPbI_3$ NCs, Fiuza-Maneiro et al. (2026) have synthesized a passivating molecule that contains both phosphorus and chloride to enhance the performance of the NCs [34].

Fiuza-Maneiro et al. (2026) synthesized the phosphorus oxychloride ($POCl_3$) as the passivating molecule. $POCl_3$ is highly reactive and possesses high Lewis acidity [34]. They carried out two different strategies for passivating the PeNCs. In the first method, $POCl_3$ is directly incorporated into the solution during synthesis before the addition of the Cs precursor. In the second method, $POCl_3$ is added after the solution is prepared. It is a post-synthetic process [34]. In the in-situ approach, due to the chemical reactivity of $POCl_3$, it slowly decays into HCl and phosphoric acid. This gradual decomposition has two benefits: (1) It slowly fills the halide vacancies with chloride ions. (2) The deprotonated phosphoric acids coordinate with the undercoordinated Pb^{2+} ions [34].

As time progressed, the PLQY increased for the $POCl_3$-treated PeNCs. The maximum PLQY is achieved after approximately 15 days of synthesis [34]. The data from transient absorption (TA) spectroscopy revealed that the exciton-exciton annihilation rate is 2.09 ± 0.06 cm^2 s^{-1} for $POCl_3$-based NCs, whereas the pristine sample showed 3.54 ± 0.13 cm^2 s^{-1}. This proves that non-radiative recombination is less in $POCl_3$-based NCs as compared to pristine NCs. The PL lifetime for $POCl_3$ NCs is 14.28 ns, whereas for untreated NCs it is 2.27 ns [34].

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The device structure is as follows: ITO/PEDOT: PSS/PVK/PNCs/TPBi/LiF/Al [34]. PVK refers to Poly(9-vinylcarbazole), TPBi is 1,3,5-tris(1-phenyl-1H-benzimidazol-2-yl) benzene, and LiF is lithium fluoride. The turn-on voltage of the $POCl_3$-based PeLEDs is 3.9 V. It showed a maximum EQE of 0.11% and yielded a maximum luminance of 409 cd m^{-2}, which is to date the highest reported for $CsPbI_3$ LEDs. The reported T_{50} lifetime of the device is approximately 40 seconds. It was tested under an electrical bias of 5.7 V and 100 cd m^{-2} initial luminance [34].

In this study, Loganathan et al. (2026) focused on reducing trap states and ion migration on $CH_3NH_3PbBr_3$-based PeLEDs [35]. They employed choline chloride, Ch.Cl as the passivating agent. The device architecture is as follows: ITO/NiOx/ $CH_3NH_3PbBr_3$/LiF/Al.

Loganathan et al. (2026) have studied the time-resolved EL (electro-luminescent) response of PeLEDs under a constant current of 2 mA. The results helped to analyze the influence of trap states in EL dynamics [35]. The EL response is delayed at the beginning for the untreated device. This delay is ascribed to trap-induced carrier accumulation. It initially suppresses radiative recombination. This happens at filled trap sites where it temporarily accumulates injected carriers before radiative recombination [36], [37].

The 3% Ch.Cl-passivated device showed instant EL response. This indicated successful passivation. Initially, the 1% Ch.Cl-passivated device showed a decent EL response, but there was still some delay. The EL response was fast onset for the 5% Ch.Cl-passivated device, but the intensity declined over time, which suggested that injecting excessive Ch.Cl could degrade the film quality or cause charge imbalance [35]. Loganathan et al. (2026) found that the 3% Ch.Cl-passivated devices exhibited the least trap states. The T_{50} lifetime of the 3% Ch.Cl-passivated device is longer than the pristine device. Ion migration is attenuated, and defect-related degradation is less in the 3% Ch.Cl-passivated devices [35].

Guo et al. (2026) observed that defect states and undesired small-n phases (i.e. n=1 phase) cause non-radiative recombination loss in quasi-2D perovskites [38]. They used amide additives to slow down the crystal formation process, prevent the formation of the n=1 phase, and assist in the formation of quasi-2D films. Slower crystal kinetics promote a defect-free film. In the n=1 phase, the defect density is very high, and the non-radiative recombination loss is excessive [39], [40].

The incorporated malonamide additive was effective at suppressing the n=1 phase. The malonamide additive contains C=O and $-NH_2$ groups. The C=O group interacted with the undercoordinated Pb^{2+} ions in the perovskite, while the $-NH_2$ group formed hydrogen bonds with Br/Cl [38]. These interactions assisted in controlling the small-n phases and passivating defects.

The in-situ PL studies show that the quasi-2D perovskite films undergo PL quenching. The quenching is attributed to a fast crystallization process, which induces uneven arrangements of nanoparticles, causing defect sites to form [41], [42]. The malonamide-added perovskite displayed a gradual increment of the fluorescent signal and the PL drop is diminished. This slows down the crystallization process and restrains the phenomenon of luminescence quenching [43]. The DFT calculations reveal the negative and positive electrostatic potential of C=O and $-NH_2$ groups, respectively. This indicates that the amide can act as both Lewis acid and base [44]. The electronegative C=O groups help in passivating undercoordinated Pb2+ ions in the perovskite through Lewis acid-base interactions [38]. The electropositive $-NH_2$ groups form hydrogen bonds with the $Pb(Br/Cl)_6$ octahedra in the perovskite crystals [45].

The absorption peaks at 387, 414, and 440 nm of the perovskite films correspond to n=1, 2, and 3 phases in the quasi-2D perovskite, respectively. Addition of additives could minimize the n=1 phase. The control perovskite films yielded PLQY of 29.57%, and malonamide-based films yielded 68.82% PLQY [38]. The average lifetime of control films is 11.55 ns, while for malonamide-based films it is 14.72 ns [38].

The device configuration is as follows: ITO/PEDOT:PSS/perovskite/TPBi/LiF/Al. The pristine perovskite film is composed of PEABr, BABr, CsCl, FABr and PbBr2 in the ratio 0.6 : 0.4 : 1.1 : 0.075 : 1.0. The fabricated malonamide-based pure-blue PeLED achieved EQE of 9.7% at 470 nm [38].

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Zhu et al. (2026) have studied the stability and performance of $CsPbBr_3$ quantum dots (QDs) assisted with passivating short-chain ligands [46]. Long-chain ligands negatively impact carrier transport in optoelectronic devices [47]. Due to limited surface space, the long-chain ligands are not effective for sky-blue $CsPbBr_3$ QDs.

The difficulty with QDs is that the surface-to-volume ratio is very high, which causes the luminescence intensity to drop and reduces the stability of the device [48]. The main advantage of QDs is the band gap tunability. Quantum confinement allows the band gap to be altered [49].

Typically, the wavelength of $CsPbBr_3$ QDs can be tuned within the range 478-525 nm [46]. The short-chain ligand tridecylamine (TDA) assisted QDs showed enhancement in device stability. The TDA ligand and the QDs exhibited stronger affinity as compared to other ligands [46]. The TDA-capped QDs yielded PLQY of 80.2%. A high PL intensity is maintained by the TDA-capped QDs for 90 days.

The device architecture is as follows: ITO/PEDOT/PSS/PVK/TDA-QDs/TPBi/LiF/Al. The TDA-capped $CsPbBr_3$ QD-based LEDs achieved a maximum EQE of 13.6% with pure and stable EL at 492 nm [46]. The target device achieved maximum luminance of 1268 cd m^{-2}.

The QDs were prepared at relatively high temperatures ranging from 90-130℃. The high-temperature-processed QDs exhibited stable PL, indicating passivation of surface defects. At low-temperature processing, QDs suffered from high surface defects, resulting in an unstable lattice structure[46]. The controlled temperature successfully governed the QD edge length between 4.3 and 12.2 nm. Decreasing the QD edge length resulted in a blue shift of the emission wavelength from 525 to 478 nm [46].

CONCLUSION

All these studies reviewed here demonstrate that the persistent efficiency and stability barriers of pure-blue PeLEDs and their green/red counterparts stem from a common set of defect-related limitations, such as the presence of deep-trap states at undercoordinated sites of Pb2+, halide-vacancy-mediated ion migration, and uncontrolled formation of small-n (n=1) phases in halides and quasi-2D materials. Molecular passivation appears as the common approach for defect passivation across the material platforms studied: $CsPb(Br/Cl)_3$ nanocrystals [14], $CsPbI_3$ nanocrystals [34] and $CH_3NH_3PbBr_3$ thin films [35], quasi-2D perovskites [38] and $CsPbBr_3$ quantum dots [46]. Despite these differences in structure, the multifunctional ligands act on similar chemical principles: electron-donating functional groups (P=O, C=O, OH, NH_2, or Cl) coordinate with the undercoordinated Pb^{2+}, the former occupying halide vacancies, and the latter hydrogen-bonding or ionically interacting with halide ions, which occupy the spaces and so limit their migration under an applied bias.

The improvements in the PLQY achieved by these systems, from below 30% to above 80%, are impressive, as are the several-fold enhancements of EQE, and even the measurable but still modest advances in operational lifetime, that are consistently recorded in the literature following this approach. However, the absolute performance of the pure-blue PeLEDs is still significantly lower than that of their green and red counterparts: reported T_{50} lifetimes are still in the few seconds to minutes range, instead of hours, and the EQE of the bluest emitters (less than 470 nm) are still in the low double digits at best. This gap indicates that surface and lattice passivation are important, but not yet sufficient; it may be necessary to develop a combination of passivation strategies, improve charge-transport layers and device architectures, and gain a better understanding of the interactions between ligand chemistry, crystal-growth kinetics and ion dynamics during device operation.

In the future, the development of multifunctional passivating molecules that can simultaneously suppress trap states, capture halide migration and control nanocrystal growth or phase changes will be crucial to achieve the performance gap for pure-blue PeLEDs. Since these materials contain water-soluble lead-based components, parallel attention will also need to be given to water and toxicological issues, in addition to the lead-free/lead-reduced compositions as this technology proceeds toward practical, large-scale applications in next-generation display and lighting technologies.

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