

Synergistic phase regulation and defect passivation for efficient deep-blue quasi-2D perovskite light-emitting diodes

Yuyu Zhang¹, Jintao Wang² (✉), Yingjie Shen¹, Rui Han¹, Jinwen Liu¹, Haochen Yi¹, Xiaoke Li¹, Dejian Gao¹, Ren Sheng¹ (✉), Ping Chen¹ (✉)

¹ Institute of Physics and Electronic Information, Yantai University, Yantai 264005, China

² School of Information Engineering, Yantai Institute of Technology, Yantai 264005, China

Nano Res., **Just Accepted Manuscript** • <https://doi.org/10.26599/NR.2026.94909114>

<https://www.sciopen.com/journal/1998-0124> on Aug. 13, 2026

© The Authors(s)

Just Accepted

This is a “Just Accepted” manuscript, which has been examined by the peer-review process and has been accepted for publication. A “Just Accepted” manuscript is published online shortly after its acceptance, which is prior to technical editing and formatting and author proofing. Tsinghua University Press (TUP) provides “Just Accepted” as an optional and free service which allows authors to make their results available to the research community as soon as possible after acceptance. After a manuscript has been technically edited and formatted, and the page proofs have been corrected, it will be removed from the “Just Accepted” web site and published officially with volume and article number (e.g., *Nano Research*, **2025**, *18*, 94906990). Please note that technical editing may introduce minor changes to the manuscript text and/or graphics which may affect the content, and all legal disclaimers that apply to the journal pertain. In no event shall TUP be held responsible for errors or consequences arising from the use of any information contained in these “Just Accepted” manuscripts. To cite this manuscript please use its Digital Object Identifier (DOI®), which is identical for all formats of publication.

Synergistic phase regulation and defect passivation for efficient deep-blue quasi-2D perovskite light-emitting diodes

Yuyu Zhang¹, Jintao Wang² , Yingjie Shen¹, Rui Han¹, Jinwen Liu¹, Haochen Yi¹, Xiaoke Li¹, Dejian Gao¹, Ren Sheng¹ , and Ping Chen¹ 

¹ Institute of Physics and Electronic Information, Yantai University, Yantai 264005, China

² School of Information Engineering, Yantai Institute of Technology, Yantai 264005, China

Received: 25 June 2026; Revised: 3 August 2026; Accepted: 13 August 2026

 Address correspondence to Jintao Wang, wangjintao@yitsd.edu.cn; Ren Sheng, rensheng@ytu.edu.cn; Ping Chen, chenping@ytu.edu.cn

 Cite this article: Nano Research, 2026, 19, 94909114 <https://doi.org/10.26599/NR.2026.94909114>

ABSTRACT: Quasi-two-dimensional (quasi-2D) metal-halide perovskite light-emitting diodes (PeLEDs) have attracted extensive attention for next-generation display and lighting applications, while achieving efficient and stable deep-blue emission below 460 nm remains challenging, primarily attributed to the unfavorable phase distribution severe, trap-assisted nonradiative recombination and ion migration. Herein, the multifunctional defect-passivation strategy by using 3-(N-morpholino)-2-hydroxypropanesulfonic acid (MOPSO) as an additive is investigated. The sulfonate ($-\text{SO}_3^-$) and hydroxyl ($-\text{OH}$) groups in MOPSO enable dual interactions with the perovskite lattice. Specifically, the electron-rich sulfonate group chelates with undercoordinated Pb^{2+} ions, while the hydroxyl group forms hydrogen bonds with halide ions. The synergistic interactions regulate the crystallization process to tailor phase distribution, suppress trap-assisted nonradiative recombination and inhibit ion migration. As a result, the optimized deep-blue PeLEDs exhibit a peak external quantum efficiency of 4.13% and a maximum luminance of 1055 cd/m^2 , with a well-defined electroluminescence peak at 456 nm. Moreover, negligible spectral shift is observed over a wide driving-voltage range, indicating improved operational stability. This work demonstrates a simple molecular engineering strategy for advancing efficient and stable deep-blue quasi-2D PeLEDs.

KEYWORDS: deep-blue perovskite light-emitting diodes; quasi-2D perovskite; phase regulation; crystallization kinetics; defect passivation.

1 Introduction

Metal halide perovskite light-emitting diodes (PeLEDs) have attracted considerable attention for next-generation display and lighting applications, owing to their tunable bandgaps, high color purity and solution processability [1-3]. In recent years, the performance of PeLEDs has been significantly improved, with the external quantum efficiency (EQE) approaching 30% for green and red devices [4, 5]. However, as a crucial part of solid-state lighting and full-color displays, the development of deep blue PeLEDs below 460 nm remains particularly unsatisfactory [6, 7].

Quasi-two-dimensional (quasi-2D) perovskites offer a promising approach for realizing deep-blue emission by incorporating bulky organic spacer cations to reduce structural dimensionality, and the resulting dimensional confinement widens the bandgap [8, 9]. Nevertheless, the optoelectronic performance of quasi-2D perovskites is highly sensitive to phase distribution and defect states, which would induce inefficient energy transfer, poor carrier utilization, and severe nonradiative recombination losses [10, 11]. Therefore, rational regulation of phase arrangement and effective suppression of defect formation are essential for further improving the performance of deep-blue quasi-2D PeLEDs [12]. Diverse strategies, including

compositional engineering, interfacial modulation, and additive engineering, have been explored [13]. Among them, additive engineering has emerged as a particularly effective approach to simultaneously regulate crystallization dynamics, tailor phase evolution, and passivate defect states [14, 15]. Typically, Lewis base-containing molecules can chelate with undercoordinated Pb^{2+} ions, thereby tailoring crystallization process and suppressing trap-assisted nonradiative recombination [16]. On this basis, various multifunctional additives have been developed [17, 18]. For instance, Lee and co-workers introduced thiourea with thiocarbonyl and amino groups to regulate phase distribution and passivate defects in quasi-2D perovskite films, leading to improved recombination balance and reduced nonradiative losses, and thereby enabling stable pure-blue emission centered at 466 nm [19]. Similarly, Kong et al. employed methanesulfonate (MeS) to reconstruct quasi-2D perovskite structures through strong hydrogen-bonding interactions with spacer cations to achieve smooth energy-transfer pathway by increasing the proportion of high-n phases, and reduce uncoordinated Pb^{2+} -related defects, resulting in efficient light-emitting devices with emission peaks at around 512 nm [20]. Therefore, effective phase regulation and defect suppression represent key strategies for realizing high-efficiency deep-blue perovskite

light-emitting diodes.

Herein, 3-(N-morpholino)-2-hydroxypropanesulfonic acid (MOPSO), which contains both sulfonate ($-\text{SO}_3^-$) and hydroxyl ($-\text{OH}$) functional groups, is introduced as a multifunctional additive to enable multiple interactions with perovskite components. Specifically, the electron-rich oxygen atoms in the $-\text{SO}_3^-$ group can coordinate with undercoordinated Pb^{2+} ions, while the $-\text{OH}$ group can form hydrogen bonds with halide ions. The synergistic interactions enable MOPSO to regulate crystallization process, suppress defect formation and ion migration, and ultimately improve the optoelectronic performance of deep-blue quasi-2D PeLEDs. Consequently, the optimized devices deliver a peak external quantum efficiency of 4.13% and a maximum luminance of 1055 cd/m^2 , accompanied by a well-defined electroluminescence emission at 456 nm. Notably, the devices exhibit negligible spectral shift over a wide driving-voltage range. This strategy provides insight into deep-blue PeLEDs fabrication and highlights the role of defect passivation and phase regulation in improving device performance and stability.

2 Results and discussion

MOPSO, which contains sulfonate and hydroxyl group, is incorporated into precursor to achieve multifunctional effects through strong interactions with perovskite components. As illustrated in Figure 1a and Figure S1 in the ESM, the electrostatic potential (ESP) distribution reveals the distinct electronic characteristics of these functional groups. The ESP distribution demonstrates a pronounced negative electrostatic potential localized around the $-\text{SO}_3^-$ group, suggesting the possible interaction of electron-rich

SO_3^- group with undercoordinated Pb^{2+} defects through Lewis acid-base interactions [21]. Meanwhile, the hydroxyl group in MOPSO may form hydrogen bonds with halide ions [22].

To further elucidate the chemical interactions between MOPSO and the perovskite components, Fourier-transform infrared spectroscopy (FTIR), ^1H nuclear magnetic resonance (NMR), and X-ray photoelectron spectroscopy (XPS) were employed. As shown in the FTIR spectra (Figure 1b), the characteristic stretching vibration of the $-\text{SO}_3^-$ group shifts to a lower wavenumber in the MOPSO + PbBr_2 sample, suggesting a coordination interaction between the sulfonate group and Pb^{2+} [23, 24]. The O-H stretching vibration also undergoes a red shift (Figure 1c), suggesting the formation of hydrogen-bonding interactions between the hydroxyl group and halide ions [25]. This hydrogen bond interaction is further confirmed by the ^1H NMR spectra (Figure S2 in the ESM), where the hydroxyl proton signals become broadened and undergo noticeable chemical-shift changes after PbBr_2 addition, reflecting the formation of hydrogen-bonding interactions [26]. Meanwhile, the XPS spectrum of Pb 4f peaks shown in Figure 1d shift toward lower binding energies in the MOPSO-incorporated perovskite film (denoted as target film), indicating increased electron density around Pb^{2+} . In contrast, the S 2p peaks shift toward higher binding energies (Figure 1e), implying electron depletion around the $-\text{SO}_3^-$ group attributed to the coordination interaction with Pb^{2+} [27]. In addition, the Cl 2p and Br 3d spectra shown in Figure S3 in the ESM exhibit shifts toward lower binding energies, which may arise from the synergistic effects of Pb-O coordination and hydrogen-bonding interactions [28, 29].

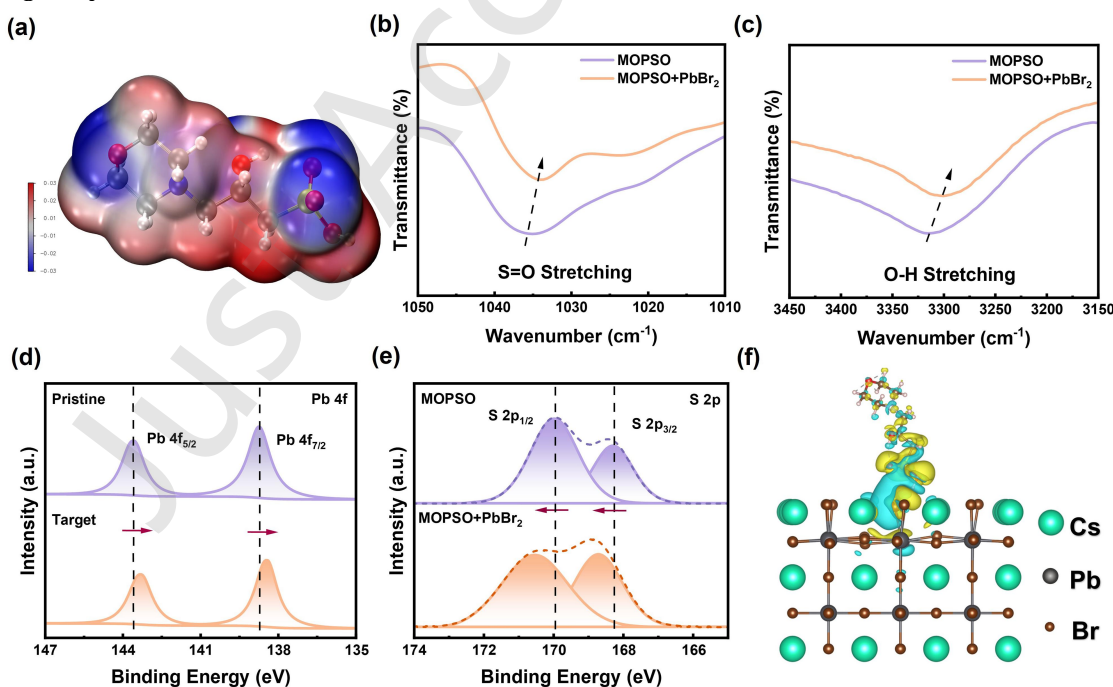


Figure 1 (a) Molecular structure and electrostatic potential simulation of MOPSO. (b) FTIR spectra of S=O modes of MOPSO and MOPSO incorporated PbBr_2 . (c) FTIR spectra of O-H modes of MOPSO and MOPSO incorporated PbBr_2 . (d) The XPS analysis of the Pb 4f for the pristine and target perovskite films. (e) The XPS analysis of the S 2p for the MOPSO and a mixture of samples with PbBr_2 . The XPS spectra are calibrated to the adventitious C 1s peak at 284.8 eV. (f) The differential charge density plot of the quasi-2D perovskites with MOPSO.

To evaluate the interaction between MOPSO and undercoordinated Pb^{2+} sites, the adsorption energy was calculated to be -0.28 eV , indicating a thermodynamically favorable interaction. The differential charge density plot further reveals pronounced charge redistribution around Pb^{2+} , supporting electron donation from the $-\text{SO}_3^-$ group to

undercoordinated Pb^{2+} sites and the formation of Pb-O coordination (Figure 1f) [30]. These results confirm that MOPSO interacts with the perovskite lattice through a dual mechanism, involving sulfonate- Pb^{2+} coordination and hydroxyl-mediated hydrogen bonding. These synergistic interactions may effectively tailor crystallization process to

regulate phase distribution, passivate undercoordinated Pb^{2+} sites, while stabilizing the perovskite lattice and potentially suppressing halide-ion migration.

Since the interaction between MOPSO and perovskite components has been confirmed, we further elucidate the evolution of defects with MOPSO incorporation. Steady-state photoluminescence (PL) measurement was conducted to evaluate the radiative recombination behavior (Figure S4 in the ESM). Compared with the pristine film, the target film exhibits markedly enhanced PL emission. The PL mapping further confirms that MOPSO modification improves the spatial homogeneity of PL emission compared with the pristine counterpart (Figure S5 in the ESM). To further elucidate the defect passivation mechanism, we conducted temperature-dependent PL measurements. As shown in Figure 2a and b, the target perovskite film maintains a high PL intensity across varying temperatures. In contrast, the pristine film exhibits significant PL quenching with increasing temperature, which arises from the activation of defects states. This phenomenon can be attributed to the suppression of defect formation and defect-assisted carrier trapping by MOPSO incorporation, which mitigates nonradiative recombination in the perovskite film [31]. The exciton binding energy (E_b) was extracted by fitting the temperature-dependent PL intensity, as shown in Figure S6 in the ESM. The E_b values of the pristine and target films are estimated to be 34.2 meV and 49.8 meV, respectively. The increased E_b upon MOPSO incorporation may be attributed to its defect passivation effect, which alleviates defect-

induced exciton dissociation. Consequently, the higher E_b of the target film indicates stronger exciton confinement and a lower probability of exciton dissociation into free carriers, thereby promoting radiative recombination [32]. Furthermore, the temperature-dependent full width at half maximum (FWHM) of the PL spectra was analyzed to evaluate the exciton-phonon interaction, as shown in Figure S7 in the ESM. The fitted optical phonon energy ($\hbar\omega_{\text{op}}$) value increases from 25.62 meV for the pristine film to 40.5 meV for the target film, suggesting suppressed defect-assisted exciton-phonon interactions. The increased $\hbar\omega_{\text{op}}$ value indicates that MOPSO effectively passivates trap states and suppresses phonon-mediated nonradiative relaxation pathways, thereby reducing energy loss and improving exciton stability [33, 34]. To further verify the influence of defect passivation on carrier recombination behavior, time-resolved photoluminescence (TRPL) measurements were subsequently conducted. As shown in Figure 2c, the decay curves were fitted with a biexponential function, and the corresponding fitting parameters are summarized in Table S1 in the ESM. The target film exhibits a significantly prolonged average lifetime ($\tau_{\text{avg}} = 25.62$ ns) compared with the pristine film ($\tau_{\text{avg}} = 16.28$ ns). The radiative (k_r) and nonradiative (k_{nr}) recombination rates shown in Table S2 are calculated from the PLQY and TRPL in the ESM. The k_{nr} value decreases from $5.04 \times 10^7 \text{ s}^{-1}$ for the pristine film to $2.54 \times 10^7 \text{ s}^{-1}$ for the target film, indicating that MOPSO effectively suppresses trap-assisted nonradiative recombination, thereby prolonging the carrier lifetime [35].

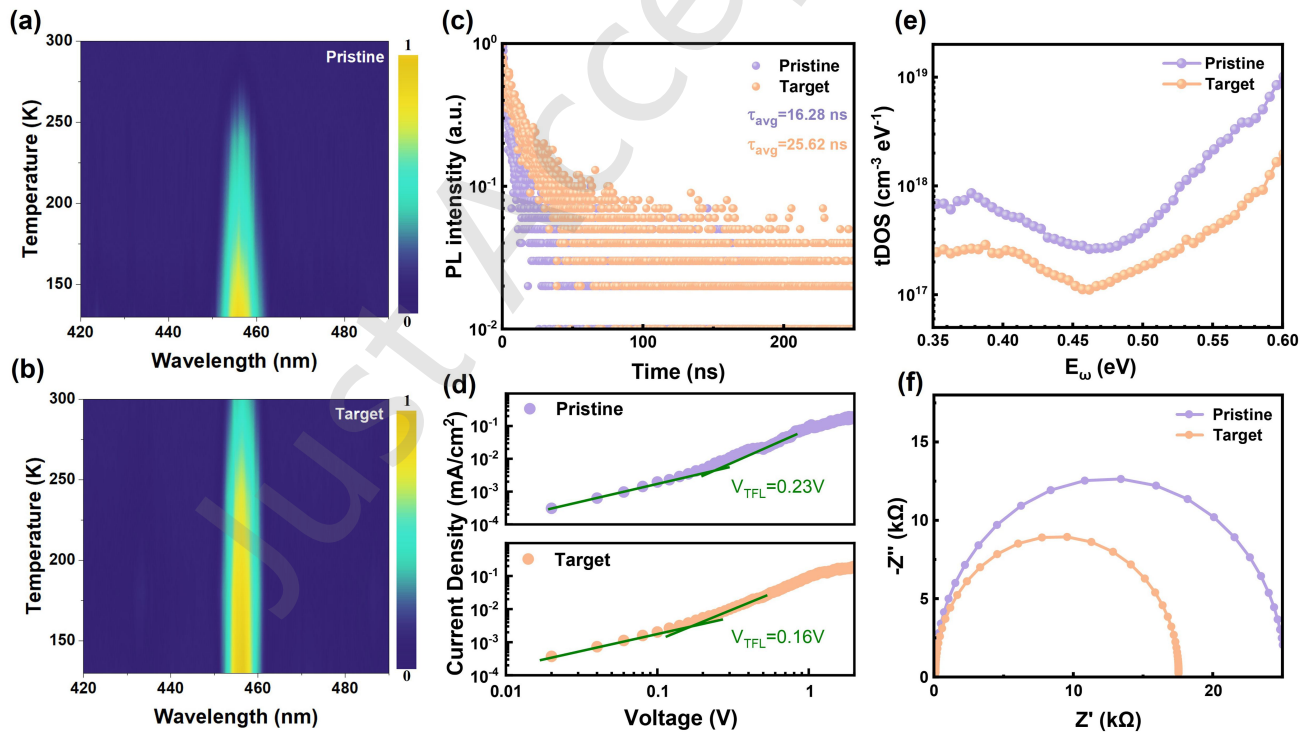


Figure 2. Temperature-dependent PL spectra for (a) pristine perovskite film and (b) target films. (c) TRPL decay of the pristine and target perovskite films. (d) SCLC measurement for the pristine and target perovskite films. (e) $t\text{DOS}$ of the pristine and target perovskite films. (f) EIS results of pristine and target devices.

To further investigate the beneficial effect of MOPSO incorporation on suppressing trap states, space-charge-limited current (SCLC) measurements were performed using hole-only devices with the structure of ITO/poly(9-vinylcarbazole) (PVK)/perovskite/TAPC/Al. As shown in Figure 2d, the trap-filled limit voltage (V_{TFL}) decreases from 0.23 V for the pristine device to 0.16 V after MOPSO incorporation. Accordingly, the calculated trap density is reduced from 9.0×10^{17} to $6.3 \times 10^{17} \text{ cm}^{-3}$, indicating a reduced trap density in the perovskite film [36].

Capacitance-frequency measurements were performed to extract the trap density of states ($t\text{DOS}$). As shown in Figure 2e and Figure S8 in the ESM, the target perovskite exhibits a significantly reduced $t\text{DOS}$ compared with the pristine film across the measured energy range, which can be attributed to the coordination interaction between the $-\text{SO}_3^-$ group and undercoordinated Pb^{2+} sites, together with the hydrogen bonding between hydroxyl group and halide ions. The decreased defect density is consistent with the SCLC results, confirming the effective suppression of defect states by

MOPSO [37-39]. Meanwhile, the charge transport behavior was examined by EIS analysis. As shown in Figure 2f, the target device displays a smaller semicircle in the Nyquist plot, indicating reduced charge-transfer resistance and enhanced charge transport efficiency [40]. The results collectively demonstrate that MOPSO effectively suppresses defect-assisted nonradiative recombination and improves charge-transport dynamics in perovskite films.

The effect of the interaction between MOPSO and perovskite components on modulating film formation, phase evolution, and surface morphology was further investigated. To directly monitor the effect of MOPSO on the crystallization dynamics of quasi-2D perovskites, in situ PL measurements were performed during the annealing process under 365 nm excitation, where the temporal evolution of PL intensity was recorded. It could be concluded that the time required for the PL intensity to reach its maximum is significantly prolonged after MOPSO incorporation (Figure 3a and b), suggesting that the interaction between MOPSO and perovskite components retard the crystallization process [41]. To verify the final phase distribution, UV-vis absorption spectroscopy was

subsequently conducted. As shown in Figure 3c, both the pristine and target films display four distinct excitonic absorption peaks at 380, 403, 426, and 453 nm, corresponding to quasi-2D perovskite phases with $n = 1, 2, 3$, and $n \geq 4$, respectively. Compared with the pristine film, the target film demonstrates an enhanced absorption contribution of the $n \geq 4$ phase and weakened features for the $n = 1-3$ phases, suggesting that MOPSO incorporation shifts the phase distribution toward higher- n domains. Such phase redistribution is expected to facilitate cascade energy transfer from low- n phases to the desired high- n emissive domains [42]. Grazing-incidence X-ray diffraction (GIXRD) measurements further support this phase redistribution. As plotted in Figure 3d, the diffraction signal assigned to the $n = 2$ phase is weakened in the target film, indicating suppressed formation of low- n phases after MOPSO incorporation, consistent with the UV-vis absorption results. This phase-distribution modulation can be attributed to the strong interactions between MOPSO and perovskite components, which regulate the crystallization process and promote phase redistribution toward higher- n domains.

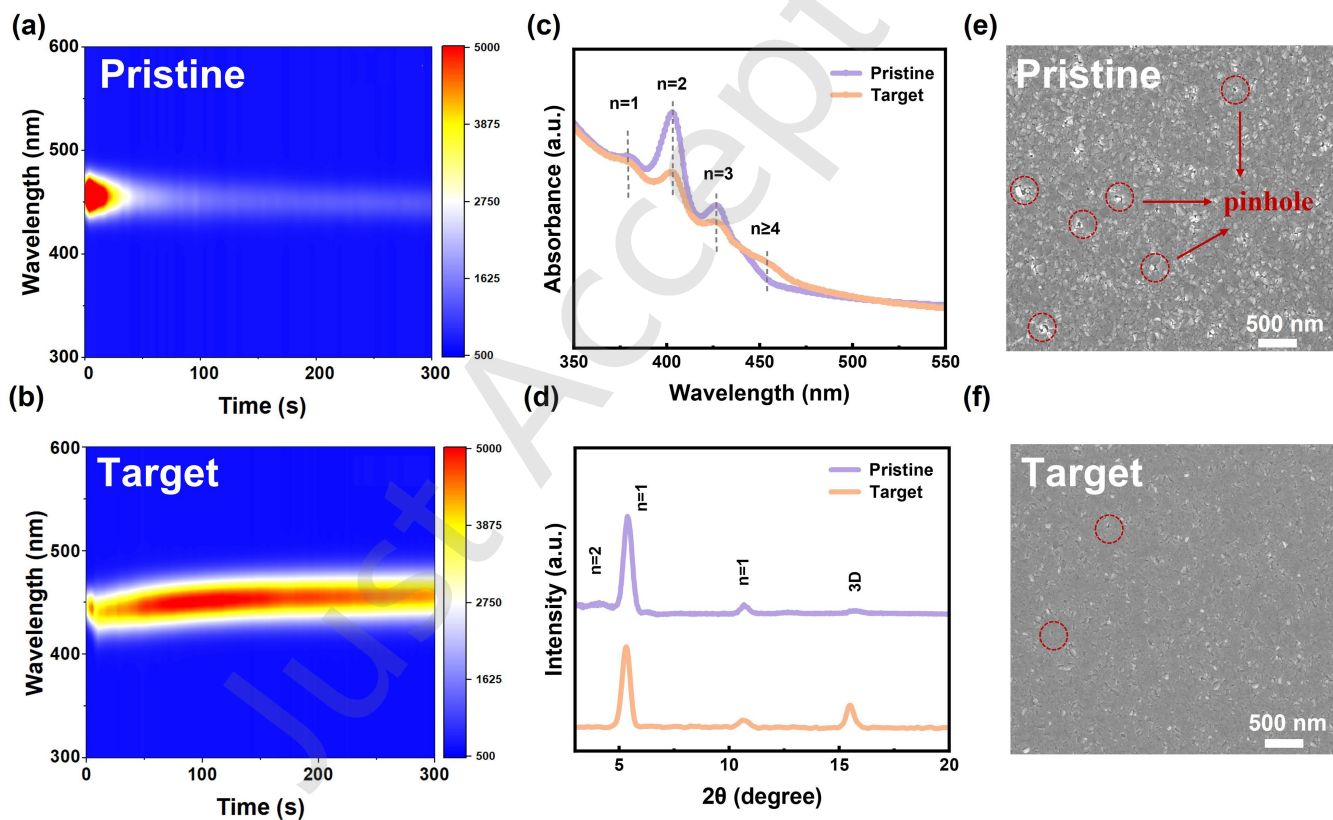


Figure 3. In situ PL spectra of the pristine (a) and target (b) films during the annealing process. (c) UV-vis absorption of the pristine and target perovskite films. (d) GIXRD patterns of the pristine and target perovskite films. SEM images of (e) pristine and (f) target perovskite films.

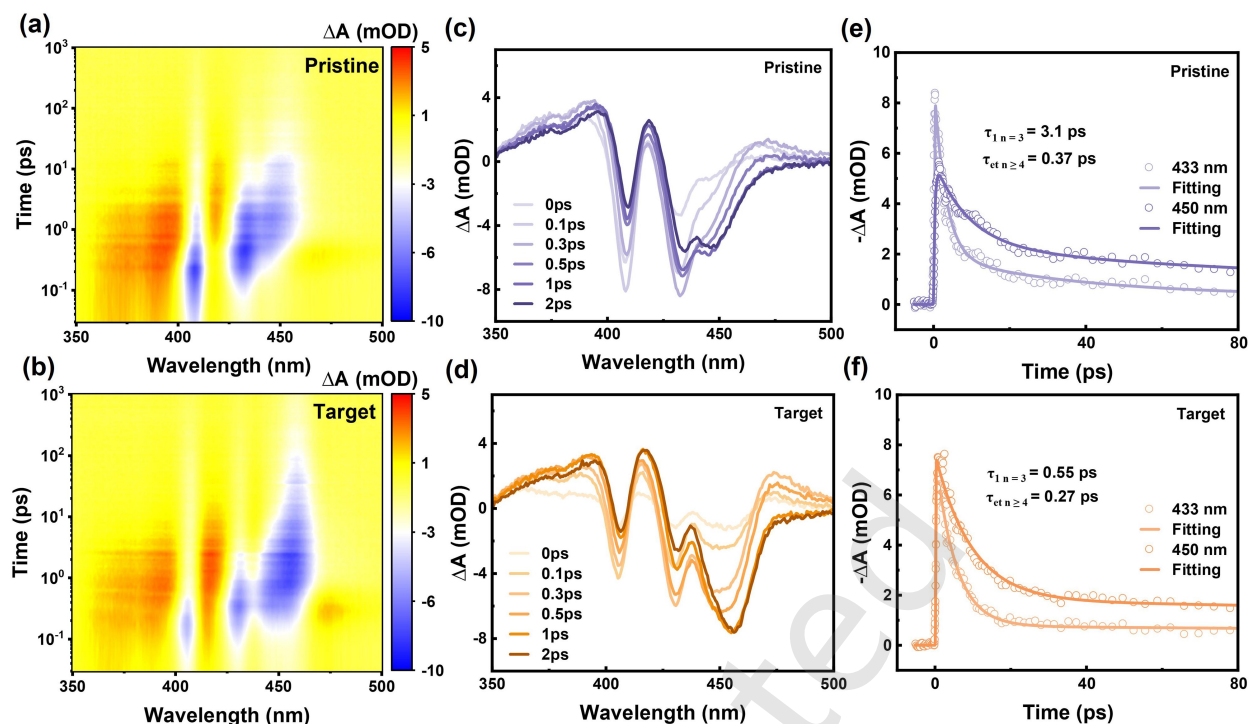


Figure 4. TA time spectrograms of (a) pristine and (b) target perovskite films. TA spectra at different probe delay times and TA kinetics probed at selected wavelengths for pristine (c, e) and target (d, f) perovskite films, respectively.

After confirming the evolution of crystallization dynamics after MOPSO incorporation, the film morphology variation was investigated by scanning electron microscopy (SEM) and atomic force microscopy (AFM) measurements. As shown in Figure 3e and f, the pristine film exhibits noticeable pinholes and uneven surface morphology, while the target sample features a more compact and continuous surface morphology with fewer pinholes after MOPSO incorporation. The AFM images shown in Figure S9 in the ESM demonstrate that the root-mean-square (RMS) roughness decreased from 2.92 nm to 1.22 nm after MOPSO incorporation, indicating a significantly smoother perovskite surface. This trend is also supported by the 3D topography images and corresponding height profiles. Kelvin probe force microscopy (KPFM) measurements show fewer localized surface-potential fluctuations in the target film compared with the pristine film (Figure S10 in the ESM), indicating reduced electrical inhomogeneity after MOPSO incorporation. This is likely associated with the smoother and more uniform surface morphology of the target film [43].

Given the fact that phase distribution critically influences cascade energy transfer in quasi-2D perovskites, transient absorption (TA) measurements were performed to gain deeper insight into the energy transfer dynamics of the pristine and target perovskite films. As shown in Figure 4a and b, both films exhibit distinct ground-state bleach (GSB) signals at 408, 430, and 450 nm, corresponding to the $n = 2$, $n = 3$, and $n \geq 4$ phases, which are consistent with the steady-state absorption spectra. The TA spectra at different delay times (Figures 4c and d) reveal the fact that compared with the pristine film, the target film exhibits suppressed GSB intensities for the $n = 2$ and $n = 3$ phases and an enhanced GSB signal for the $n \geq 4$ phase, indicating that the target perovskite film formed the favorable phase distribution for luminescence. The evolution of GSB signals of $n = 3$ and $n \geq 4$ phases was extracted to analyze the energy transfer process. As shown in Figure 4e and f and Table S3 in the ESM, the fast decay time constant τ_1 for the $n = 3$ phase decreased from

3.1 to 0.55 ps with the introduction of MOPSO, indicating faster energy transfer dynamics, which would be beneficial to reduce the exciton accumulation in low- n phases, thus decreasing exciton annihilation [44]. Meanwhile, the formation time constant τ_{et} also decreased from 0.37 ps for the pristine film to 0.27 ps for the target film. The reduced τ_{et} could play an important role in inhibiting energy loss and promoting radiative recombination, thereby enhancing the performance of the deep-blue PeLEDs [20].

To evaluate the device-level impact of MOPSO, deep-blue PeLEDs were fabricated and systematically characterized. PeLEDs were fabricated with a device architecture of ITO/PVK/perovskite/PO-T2T/Liq/Al, as schematically illustrated in Figure 5a. Photoluminescence quantum yield (PLQY) measurements were conducted as a function of MOPSO concentration to determine the optimal additive loading (Figure S11 in the ESM). The PLQY increases from 18% for the pristine film to a maximum value of 35% at 2 mol% MOPSO, followed by a gradual decrease at higher concentrations. The corresponding device performance comparisons under various MOPSO concentrations are summarized in Figure S12 in the ESM. Therefore, 2 mol% MOPSO was identified as the optimal concentration. The current density-luminance-voltage (J-V-L) characteristics and EQE-luminance curves of the champion devices are shown in Figure 5b and c. The target device achieves a peak EQE of 4.13%, which is approximately 2.1 times that of the pristine device. This improvement is further supported by the statistical distribution of 20 devices, where the target devices exhibit an average EQE of 3.8%, indicating good reproducibility (Figure S13 in the ESM). The normalized EL spectra indicate that both devices exhibit similar deep-blue emission centered at around 456 nm with the CIE coordinates of (0.153, 0.068) for the optimized device (Figure S14 in the ESM). The operational and spectral stability of the devices were further evaluated. All device stability measurements were performed on unencapsulated devices in a nitrogen-filled glovebox. As shown in Figure 5d

and e, the pristine device shows a pronounced redshift of the electroluminescence (EL) peak from 456 to 490 nm as the bias voltage increases from 4.0 to 6.5 V. In contrast, the target device exhibits only a slight spectral shift, with the EL peak remaining close to 456 nm, indicating significantly improved color stability. Meanwhile, the PL peak of the perovskite film with MOPSO incorporation demonstrates a slight shift under 65°C thermal annealing for 30 min (Figure S15 in the ESM), implying inhibited ion migration. Under continuous operation at 4.0 V, the EL wavelength of the target device also remains nearly unchanged over 30 min,

with negligible spectral deviation observed (Figure S16 in the ESM). In addition, the T_{50} lifetime, defined as the time required for the luminance to decay to 50% of its initial value, is extended to 10 min for the target device under a constant current density of 10 mA/cm², representing a twofold improvement in operational stability compared with the pristine device. Overall, the improved efficiency and excellent spectral stability are attributed to the multifunctional passivation effect of MOPSO, which reduces defect density, stabilizes the perovskite lattice, and suppresses halide ion migration, as illustrated by the proposed mechanism in Figure S17 in the ESM.

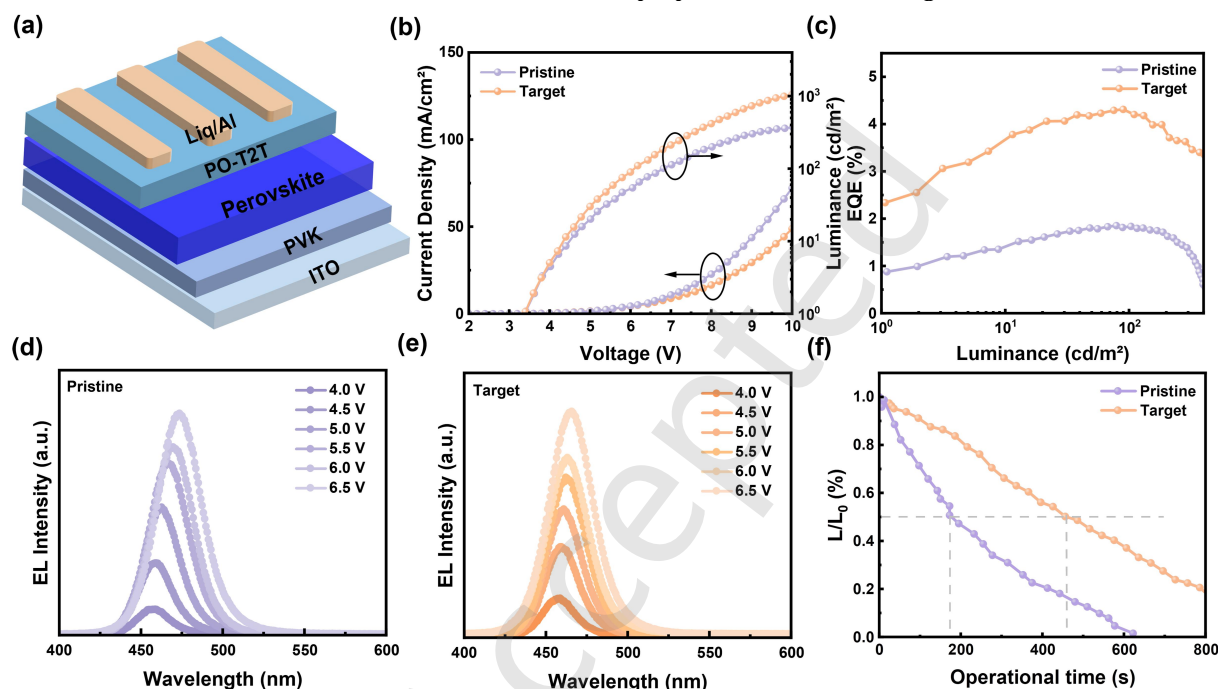


Figure 5. (a) Device architecture. (b) J-V-L and (c) EQE-L curves of the pristine device and target device. The EL spectra of the (d) pristine and (e) target devices under different voltages from 4.0 to 6.5 V. (f) Operational lifetime measurement for the pristine and target devices measured under a constant current density of 10 mA/cm².

3 Conclusions

In summary, MOPSO was introduced as a multifunctional additive to regulate the crystallization behavior and defect states of deep-blue quasi-2D perovskites. The sulfonate group in MOPSO coordinates with undercoordinated Pb²⁺ sites through Pb-O interactions, while the hydroxyl group forms hydrogen bonds with halide ions. These synergistic interactions lead to a more favorable phase distribution, suppressed ion migration, and effective defect passivation within the perovskite films. As a result, the suppressed nonradiative recombination and improved film quality are achieved. Benefiting from these effects, the target PeLEDs exhibit improved electroluminescence efficiency and operational stability. This work demonstrates that multifunctional molecular additives provide an effective strategy for simultaneously regulating phase evolution and defect states in deep-blue quasi-2D PeLEDs.

Electronic Supplementary Material: Supplementary material (Figures S1-S17 and Tables S1-S3) is available in the online version of this article at <https://doi.org/10.26599/NR.2026.94909114>.

Data availability

All data needed to support the conclusions in the paper are presented in the manuscript and/or the Electronic SupplementaryMaterial. Additional data related to this paper

may be requested from the corresponding author upon request.

Acknowledgements

This work was supported by the Natural Science Foundation of Shandong Province (ZR2026QC0805), the National Natural Science Foundation of China (62474154, 62205281).

Declaration of competing interest

All the contributing authors report no conflict of interests in this work.

Author contribution statement

Y.Y.Z.: Validation, writing manuscript. J.T.W.: Experimental design, revised manuscript. Y.J.S. and R.H.: methodology and visualization. J.W.L. and H.C.Y.: data curation and investigation. X.K.L. and D.J.G.: data curation and methodology. R.S.: Funding acquisition. P.C.: Project administration, funding acquisition. All authors contributed to manuscript preparation and discussions.

Use of AI statement

None.

References

- [1] Kim, J. S.; Heo, J.-M.; Park, G.-S.; Woo, S.-J.; Cho, C.; Yun, H. J.;

- Kim, D.-H.; Park, J.; Lee, S.-C.; Park, S.-H.; Yoon, E.; Greenham, N. C.; Lee, T.-W., Ultra-bright, efficient and stable perovskite light-emitting diodes. *Nature* 2022, 611, 688-694.
- [2] Zhang, L.; Sun, C.; He, T.; Jiang, Y.; Wei, J.; Huang, Y.; Yuan, M., High-performance quasi-2D perovskite light-emitting diodes: from materials to devices. *Light: Science & Applications* 2021, 10, 61.
- [3] Wang, J.; Shang, J.; Chen, S.; Jiang, X.; Zhao, F.; Ma, X.; Sheng, R.; Chen, P., White light-emitting diode enabled by perovskite/excimer hybrids with excellent performance. *J. Lumin.* 2026, 121830.
- [4] Bai, W.; Xuan, T.; Zhao, H.; Dong, H.; Cheng, X.; Wang, L.; Xie, R. J., Perovskite light-emitting diodes with an external quantum efficiency exceeding 30%. *Adv. Mater.* 2023, 35, 2302283.
- [5] Kong, L.; Sun, Y.; Zhao, B.; Ji, K.; Feng, J.; Dong, J.; Wang, Y.; Liu, Z.; Maqbool, S.; Li, Y., Fabrication of red-emitting perovskite LEDs by stabilizing their octahedral structure. *Nature* 2024, 631, 73-79.
- [6] Yang, X.; Ma, L.; Yu, M.; Chen, H.-H.; Ji, Y.; Hu, A.; Zhong, Q.; Jia, X.; Wang, Y.; Zhang, Y., Focus on perovskite emitters in blue light-emitting diodes. *Light: Science & Applications* 2023, 12, 177.
- [7] Luo, X.; Xu, W.; Zheng, G.; Tammireddy, S.; Wei, Q.; Karlsson, M.; Zhang, Z.; Ji, K.; Kahmann, S.; Yin, C., Effects of local compositional heterogeneity in mixed halide perovskites on blue electroluminescence. *Matter* 2024, 7, 1054-1070.
- [8] Shang, J.; Wang, J.; Chen, C.; Zhang, Y.; Liu, J.; Sheng, R.; Chen, P., Recent Progress in High-Efficiency Blue Perovskite Light-Emitting Diodes. *Advanced Optical Materials* 2025, 13, e01924.
- [9] Yuan, S.; Dai, L.; Sun, Y.; Auras, F.; Zhou, Y.-H.; An, R.-Z.; Liu, Y.; Ding, C.; Cassidy, C.; Tang, X., Efficient blue electroluminescence from reduced-dimensional perovskites. *Nat. Photonics* 2024, 18, 425-431.
- [10] Ma, D.; Lin, K.; Dong, Y.; Choubisa, H.; Proppe, A. H.; Wu, D.; Wang, Y.-K.; Chen, B.; Li, P.; Fan, J. Z., Distribution control enables efficient reduced-dimensional perovskite LEDs. *Nature* 2021, 599, 594-598.
- [11] Jin, G.; Liu, T.; Li, Y.; Zhou, J.; Zhang, D.; Pang, P.; Ye, Z.; Xing, Z.; Xing, G.; Chen, J., Low-dimensional phase suppression and defect passivation of quasi-2D perovskites for efficient electroluminescence and low-threshold amplified spontaneous emission. *Nanoscale* 2022, 14, 919-929.
- [12] Yu, M.; Qin, T.; Gao, G.; Zu, K.; Zhang, D.; Chen, N.; Wang, D.; Hua, Y.; Zhang, H.; Zhao, Y.-B., Multiple defects renovation and phase reconstruction of reduced-dimensional perovskites via in situ chlorination for efficient deep-blue (454 nm) light-emitting diodes. *Light: Science & Applications* 2025, 14, 102.
- [13] Fakharuddin, A.; Gangishetty, M. K.; Abdi-Jalebi, M.; Chin, S.-H.; bin Mohd Yusoff, A. R.; Congreve, D. N.; Tress, W.; Deschler, F.; Vasilopoulou, M.; Bolink, H. J., Perovskite light-emitting diodes. *Nature Electronics* 2022, 5, 203-216.
- [14] Wang, S.; Sun, X.; Shi, J.; Zhao, R.; Zhang, B.; Lu, S.; Li, P.; Li, F.; Manna, L.; Zhang, Y., Additive-Driven Enhancement of Crystallization: Strategies and Prospects for Boosting Photoluminescence Quantum Yields in Halide Perovskite Films for Light-Emitting Diodes. *Adv. Mater.* 2024, 36, 2413673.
- [15] Guo, Z.; Zhang, Y.; Wang, B.; Wang, L.; Zhou, N.; Qiu, Z.; Li, N.; Chen, Y.; Zhu, C.; Xie, H., Promoting energy transfer via manipulation of crystallization kinetics of quasi-2D perovskites for efficient green light-emitting diodes. *Adv. Mater.* 2021, 33, 2102246.
- [16] Wang, J.; Shang, J.; Zhang, B.; Chen, S.; Yi, H.; Zhang, Y.; Liu, J.; Sheng, R.; Chen, P., High-Performance Perovskite Solar Cells Enabled by the Guanidine Derivative. *ACS Appl. Mater. Interfaces* 2026.
- [17] Li, M.; Zhao, Y.; Guo, J.; Qin, X.; Zhang, Q.; Tian, C.; Xu, P.; Li, Y.; Tian, W.; Zheng, X., Phase regulation and defect passivation enabled by phosphoryl chloride molecules for efficient quasi-2D perovskite light-emitting diodes. *Nano-Micro Letters* 2023, 15, 119.
- [18] Dong, J.; Zhao, B.; Ji, H.; Zang, Z.; Kong, L.; Chu, C.; Han, D.; Wang, J.; Fu, Y.; Zhang, Z.-H., Multivalent-effect immobilization of reduced-dimensional perovskites for efficient and spectrally stable deep-blue light-emitting diodes. *Nat. Nanotechnol.* 2025, 20, 507-514.
- [19] Lee, H. J.; Jung, J. W., Multivalent Engineering of Quasi-2D Perovskite Emitter Films for Phase-Pure Blue Perovskite Light-Emitting Diodes. *ACS Energy Letters* 2025, 10, 5405-5413.
- [20] Kong, L.; Zhang, X.; Li, Y.; Wang, H.; Jiang, Y.; Wang, S.; You, M.; Zhang, C.; Zhang, T.; Kershaw, S. V., Smoothing the energy transfer pathway in quasi-2D perovskite films using methanesulfonate leads to highly efficient light-emitting devices. *Nat. Commun.* 2021, 12, 1246.
- [21] Shen, C.; Wang, H.; Liang, X.; Chen, H.; Cai, B.; Wei, Y.; Hu, S.; Luo, Y.; Zhang, F.; Xu, Q., Simultaneous Interfacial Modification and Crystallization Regulation for High-Performance Pure-Blue Quasi-2D Perovskite Light-Emitting Diodes. *ACS Energy Letters* 2025, 10, 3638-3646.
- [22] Zou, G.; Li, Z.; Chen, Z.; Chu, L.; Yip, H. L.; Cao, Y., Color-stable deep-blue perovskite light-emitting diodes based on Organotrichlorosilane post-treatment. *Adv. Funct. Mater.* 2021, 31, 2103219.
- [23] Yu, Y.; Wang, B. F.; Shen, Y.; Su, Z. H.; Zhang, K.; Ren, H.; Zhang, Y. F.; Gao, X.; Tang, J. X.; Li, Y. Q., Regulating perovskite crystallization through interfacial engineering using a zwitterionic additive potassium sulfamate for efficient pure-blue light-emitting diodes. *Angew. Chem.* 2024, 136, e202319730.
- [24] Yang, H.; Fang, K.; Duan, J.; Dong, J.; Li, Y.; Yang, S.; Liang, J.; Jiang, Y.; Li, M.; Liu, Y., Selective facet shielding induced epitaxial deposition along the Zn (101) plane for highly reversible Zn-Ion batteries. *Energy Storage Materials* 2025, 75, 103995.
- [25] Cohen, B.-E.; Binyamin, T.; Ben-Tzvi, T.; Goldberg, O.; Schlesinger, A.; Balberg, I.; Millo, O.; Gross, E.; Azulay, D.; Etgar, L., Hydroxyl functional groups in two-dimensional Dion-Jacobson perovskite solar cells. *ACS Energy Letters* 2021, 7, 217-225.
- [26] Meng, X.; Lin, J.; Liu, X.; He, X.; Wang, Y.; Noda, T.; Wu, T.; Yang, X.; Han, L., Highly stable and efficient FASnI₃-based perovskite solar cells by introducing hydrogen bonding. *Adv. Mater.* 2019, 31, 1903721.
- [27] Lee, S.; Kim, J.; Kim, H.; Kim, C.; Kim, S.; Kim, C.; Lee, H.; Choi, B.; Muthu, C.; Kim, T., Brightening deep-blue perovskite light-emitting diodes: A path to Rec. 2020. *Science Advances* 2024, 10, eadn8465.
- [28] Chen, Z.; Liu, X. K.; Wang, H.; Liu, X.; Hou, L.; Gao, F., Photoluminescence enhancement for efficient mixed-halide blue perovskite light-emitting diodes. *Advanced Optical Materials* 2023, 11, 2202528.
- [29] Shang, J.; Wang, J.; Yang, L.; Sheng, R.; Zhang, F.; Chen, P., Stable and efficient blue quasi-2D perovskite light-emitting diodes enabled by synergistic passivation engineering. *Nano Research* 2025, 18.
- [30] Chen, H.; Liu, C.; Xu, J.; Maxwell, A.; Zhou, W.; Yang, Y.; Zhou, Q.; Bati, A. S.; Wan, H.; Wang, Z., Improved charge extraction in inverted perovskite solar cells with dual-site-binding ligands. *Science* 2024, 384, 189-193.
- [31] Zhang, D.; Fu, Y.; Zhan, H.; Zhao, C.; Gao, X.; Qin, C.; Wang, L., Suppressing thermal quenching via defect passivation for efficient quasi-2D perovskite light-emitting diodes. *Light: Science & Applications* 2022, 11, 69.
- [32] Maimaitizi, H.; Ågren, H.; Chen, G., Multifunctional ligand engineering enables high-performance CsPb (Br/Cl) 3 nanocrystals toward efficient and stable pure-blue perovskite LEDs. *Light: Science & Applications* 2026, 15, 135.
- [33] Dong, J.; Lu, F.; Han, D.; Wang, J.; Zang, Z.; Kong, L.; Zhang, Y.; Ma, X.; Zhou, J.; Ji, H., Deep-Blue Electroluminescence of Perovskites with Reduced Dimensionality Achieved by Manipulating Adsorption-Energy Differences. *Angew. Chem.* 2022, 134, e202210322.
- [34] Gong, X.; Voznyy, O.; Jain, A.; Liu, W.; Sabatini, R.; Piontkowski, Z.; Walters, G.; Bappi, G.; Nokhrin, S.; Bushuyev, O., Electron-phonon interaction in efficient perovskite blue emitters. *Nat. Mater.* 2018, 17, 550-556.
- [35] Shen, Y.; Li, Y. Q.; Zhang, K.; Zhang, L. J.; Xie, F. M.; Chen, L.; Cai, X. Y.; Lu, Y.; Ren, H.; Gao, X., Multifunctional crystal regulation enables efficient and stable sky-blue perovskite light-emitting diodes. *Adv. Funct. Mater.* 2022, 32, 2206574.
- [36] Duijnste, E. A.; Ball, J. M.; Le Corre, V. M.; Koster, L. J. A.; Snaith, H. J.; Lim, J., Toward understanding space-charge limited current measurements on metal halide perovskites. *ACS Energy Letters* 2020, 5, 376-384.
- [37] Jiang, Y.; Qin, C.; Cui, M.; He, T.; Liu, K.; Huang, Y.; Luo, M.; Zhang, L.; Xu, H.; Li, S., Spectra stable blue perovskite light-emitting diodes. *Nat. Commun.* 2019, 10, 1868.
- [38] Ren, Z.; Yu, J.; Qin, Z.; Wang, J.; Sun, J.; Chan, C. C.; Ding, S.; Wang, K.; Chen, R.; Wong, K. S., High-performance blue perovskite light-emitting diodes enabled by efficient energy transfer between coupled quasi-2D perovskite layers. *Adv. Mater.* 2021, 33, 2005570.
- [39] Xiao, X.; Ye, T.; Sun, J.; Qu, X.; Ren, Z.; Wu, D.; Ding, S.; Sun, X. W.; Choy, W. C.; Wang, K., Capacitance-voltage characteristics of perovskite light-emitting diodes: Modeling and implementing on the analysis of carrier behaviors. *Appl. Phys. Lett.* 2022, 120.
- [40] Li, Z.; Chen, Z.; Shi, Z.; Zou, G.; Chu, L.; Chen, X.-K.; Zhang, C.; So, S. K.; Yip, H.-L., Charge injection engineering at organic/inorganic heterointerfaces for high-efficiency and fast-response perovskite light-emitting diodes. *Nat. Commun.* 2023, 14, 6441.
- [41] Li, Z.; Guo, Y.; Liu, Z.; Wu, J.; Tang, Z.; Fu, Y.; Xie, Z., Defect Passivation and Lattice Stabilization by Dual-Functional Additive Enables High-Efficiency Pure Blue Quasi-2D Perovskite Light-Emitting Diodes. *Advanced Optical Materials* 2026, e71306.
- [42] Wang, K.; Lin, Z.-Y.; Zhang, Z.; Jin, L.; Ma, K.; Coffey, A. H.;

Atapattu, H. R.; Gao, Y.; Park, J. Y.; Wei, Z., Suppressing phase disproportionation in quasi-2D perovskite light-emitting diodes. *Nat. Commun.* 2023, 14, 397.

[43] Pan, Y.; Wang, J.; Sun, Z.; Zhang, J.; Zhou, Z.; Shi, C.; Liu, S.; Ren, F.; Chen, R.; Cai, Y., Surface chemical polishing and passivation minimize non-radiative recombination for all-perovskite tandem solar cells. *Nat. Commun.* 2024, 15, 7335.

[44] Liu, Y.; Wang, S.; Yu, Z.; Chen, G.; Wang, C.; Wang, T.; Ke, W.; Fang, G., A multifunctional additive strategy enables efficient pure-blue perovskite light-emitting diodes. *Adv. Mater.* 2023, 35, 2302161.

Just Accepted

Electronic Supplementary Material

Synergistic phase regulation and defect passivation for efficient deep-blue quasi-2D perovskite light-emitting diodes

Yuyu Zhang¹, Jintao Wang² , Yingjie Shen¹, Rui Han¹, Jinwen Liu¹, Haochen Yi¹, Xiaoke Li¹, Dejian Gao¹, Ren Sheng¹ , and Ping Chen¹ 

¹ Institute of Physics and Electronic Information, Yantai University, Yantai 264005, China

² School of Information Engineering, Yantai Institute of Technology, Yantai 264005, China

 Address correspondence to Jintao Wang, wangjintao@yitsd.edu.cn; Ren Sheng, rensheng@ytu.edu.cn; Ping Chen, chenping@ytu.edu.cn

Supporting information to <https://doi.org/10.26599/NR.2026.94909114>

1 Experimental Section

Materials

P-F-PEABr, CsBr (99.999%), PbCl₂ (99.999%), PbBr₂ (99.999%), poly(9-vinylcarbazole) (PVK, 99.999%), dimethyl sulfoxide (DMSO) (anhydrous, 99.9%), and chlorobenzene were purchased from Liaoning Preferred New Energy Technology Co., LTD. MOPSO (99.99%) was purchased from Shanghai Aladdin Biochemical Technology Co., LTD. 8-Hydroxyquinolitolithium (Liq) and Al were purchased from Xi'an Bath Sunlight Technology Co., LTD. TAPC and ((1,3,5-triazine-2,4,6-triyl) tris(benzene-3,1-diyl)) tris(diphenylphosphine oxide) (PO-T2T) (99.9%) was purchased from Shenzhen Purui Material Technology Co., LTD. All materials were used directly and required no further purification.

Synthesis of precursor solution

Precursor solution preparation: PVK was dissolved in chlorobenzene at a concentration of 6 mg/mL. The perovskite precursor solution was prepared by adding P-F-PEABr, CsBr, PbCl₂ and PbBr₂ to DMSO at specific molar ratios. For the pristine sample, the ratio was 0.8:1:0.7:0.25, and the molar concentration of CsBr was kept at 0.12 M. For the target sample, MOPSO was added to the precursor solution at various molar ratios relative to CsBr. Before use, all solutions were stirred for 2 h.

Device fabrication

The indium tin oxide (ITO) substrate was scrubbed sequentially with acetone and ethanol. Then, the cleaned ITO substrates were dried with N₂ and treated under ultraviolet (UV) ozone for 20 min. The device was fabricated using a multilayer structure of ITO/PVK/perovskite/PO-T2T (25 nm)/Liq (2 nm)/Al (100 nm). Before use, the PVK solution was filtered through a 0.2 μm PTFE film filter. It was spin-coated onto ITO substrate at 5000 rpm for 35 s and then annealed at 120°C for 15 min. The perovskite films were subsequently spin-coated at 6000 rpm for 100 s and then treated at 65°C for 5 min. PO-T2T (25 nm), Liq (2 nm), and Al (100 nm) were evaporated in a thermal evaporation chamber with vacuum pressure < 5 × 10⁻⁴ Pa. PO-T2T was grown at the rate of 0.1–0.2 Å/s, while Liq was deposited at the rate of 0.02–0.08 Å/s, and Al cathode was deposited at the rate of 0.5 Å/s. The effective area of the device was 0.09 cm².

Film and device characterization

Fourier transform infrared (FTIR) spectra were measured using an absorption infrared spectrometer (Thermo Fisher Scientific Nicolet iS20). X-ray photoelectron spectroscopy (XPS) (Thermo Scientific ESCALAB 250Xi) was utilized to analyze the chemical environment of elements. ¹H nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AV-400 nuclear magnetic resonance spectrometer. Photoluminescence quantum yield (PLQY) measurements were taken in an integrating sphere and photoexciting with a 405 nm continuous-wave laser. The absorption spectra of the perovskite films were recorded with a Shimadzu UV2700 spectrometer. PL spectra and time-resolved fluorescence (TRPL) spectra of light excitation at 400 nm were measured using an FLS980 transient fluorescence spectrometer at room temperature. Grazing-incidence X-ray diffraction (GIXRD) spectra were obtained using a Rigaku Smartlab 3 kW with a grazing angle of 0.1°. Scanning electron microscope (SEM) images were acquired using field emission SEM (TESCAN MIRA LMS). Atomic force microscopy (AFM) measurements were performed on a Bruker Dimension Icon. The electrochemical impedance spectroscopy (EIS) measurements were conducted with a PARSTAT 4000A analyzer from 1 kHz to 1 MHz. The Mott-Schottky characterization was carried out by using Solartron ModuLab XM MTS. Electroluminescence information of the devices was simultaneously measured by a PR655 Spectro-scan spectrometer. The current-voltage and luminance-voltage characteristics were recorded by combining the spectrometer with a programmable Keithley 2450 voltage-current source. The EQE of the devices (calculated in the range of 380–900 nm) was obtained by measuring the light intensity in the forward direction.

2 Supplementary Note

Supplementary Note 1. Extraction of exciton binding energy

Based on the temperature-dependent PL spectra, we fitted the exciton binding energy (Eb) values using the following formula[1]:

$$I(T) = \frac{I_0}{1 + Ae^{\frac{-E_b}{k_B T}}} \quad \#(1)$$

Where $I(T)$ is the temperature-dependent integrated PL intensity, T is the temperature, I_0 is the integrated PL intensity extrapolated at 0 K, A is a constant, E_b is the exciton binding energy and k_B is the Boltzmann constant.

Supplementary Note 2. The variation of full width at half maximum

The variation of full width at half maximum (FWHM) with temperature can be described using the independent Boson model[2]:

$$\Gamma_T = \Gamma_0 + \sigma T + \frac{\Gamma_{op}}{e^{\frac{\hbar\omega_{op}}{k_B T}} - 1} \quad \#(2)$$

Where Γ_T refers to the FWHM at a given temperature T , while Γ_0 is the inhomogeneous broadening contribution, $\hbar\omega_{op}$ represents the optical phonon energy, σ and Γ_{op} are the exciton-acoustic phonon interaction and the exciton-optical phonon contribution to the linewidth broadening, respectively.

Supplementary Note 3. TRPL Measurement

The TRPL decay curves can be fitted by a biexponential function[3]:

$$I(t) = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right) \quad \#(3)$$

Where A_1 and A_2 are the amplitudes and τ_1 and τ_2 are time constants for fast and slow decay components, respectively. The average lifetime τ_{avg} was calculated by the relation:

$$\tau_{avg} = \frac{A_1 \tau_1^2 + A_2 \tau_2^2}{A_1 \tau_1 + A_2 \tau_2} \quad \#(4)$$

Supplementary Note 4. Extraction of recombination rate constants

The average PL lifetime is related to the radiative and nonradiative recombination rate constants by:

$$\tau_{avg} = \frac{1}{k_r + k_{nr}} \quad \#(5)$$

The PLQY is expressed as:

$$PLQY = \frac{k_r}{k_r + k_{nr}} \quad \#(6)$$

Accordingly, the radiative and nonradiative recombination rate constants can be calculated as:

$$k_r = \frac{PLQY}{\tau_{avg}} \quad \#(7)$$

$$k_{nr} = \frac{1 - PLQY}{\tau_{avg}} \quad \#(8)$$

Supplementary Note 5. Calculations of the SCLC

The linear response at low bias and the sharp increase in current at high bias are assigned to the ohmic and trap-filled regions, and the trap-filling limit voltage (V_{TFL}) can be represented as[4]:

$$V_{TFL} = \frac{eN_t L^2}{2\epsilon\epsilon_0} \quad \#(9)$$

Where e is the elementary charge, L represents the thickness of the perovskite film, N_t refers to the trap density, ϵ represents the relative dielectric constant, and ϵ_0 corresponds to the dielectric constant of the vacuum[5].

Supplementary Note 6. Calculations of the tDOS (N_T) in energy (E_ω) of pristine and target devices

The tDOS (N_T) in energy (E_ω) was deduced on the basis of the following equation:

$$N_T = -\frac{V_{bi}}{qW} \frac{dC}{d\omega} \frac{\omega}{k_B T} \quad \#(10)$$

$$E_\omega = k_B T \left(\ln \frac{2\pi v_0 T^2}{\omega} \right) \quad \#(11)$$

where V_{bi} is the built-in potential, q is the elementary charge, W is the depletion width, C is the capacitance, ω is the angular frequency, k_B is the Boltzmann constant, v_0 is the attempt-to-escape frequency, and T is the temperature. V_{bi} and W were obtained from the Mott-Schottky analysis[6].

Supplementary Note 7. The kinetics of each GSB

The decay functions of GSB peaks were fitted using the following exponential function:

$$\Delta A(t) = A_1 e^{-t/\tau_1} + A_2 e^{-t/\tau_2} + A_3 e^{-t/\tau_3} - c e^{-t/\tau_{et}} \quad \#(12)$$

where A_1 , A_2 , A_3 and c are amplitudes; τ_1 represents the fast decay time constant associated with energy-cascading processes in quasi-two-dimensional perovskite; τ_2 and τ_3 represent slow decay time constants; and τ_{et} represents the formation time constant.

Supplementary Note 8. The calculation of DFT

We performed the first-principles calculations in the frame of density functional theory (DFT). The exchange-correlation energy is described by the Perdew-Burke-Ernzerhof (PBE) form of generalized-gradient approximation (GGA) exchange-correlation energy functional. The structure optimization of CsPbBr₃ perovskite has been carried out by allowing all atomic positions and lattice parameters to vary and relax until the energy difference of successive atom configurations was less than 10⁻⁶ eV. The force on each atom in the relaxed structures was less than 0.015 eV Å⁻¹. The cutoff energy for the plane-wave basis set was set to 400 eV. The k-point spacing was set to be smaller than 0.03 Å⁻¹ over Brillouin zone (BZ).

Supplementary Note 9. Charge Difference Density between perovskite (001) surface and MOPSO

To intuitively observe the interfacial binding between MOPSO molecule and the (001) surface, their charge density difference (CDD) was calculated according to [7]:

$$\Delta\rho = \rho_{system} - \rho_{CsPbBr_3} - \rho_{MOPSO} \quad (13)$$

Where ρ_{system} is the charge density of the MOPSO-incorporated (001) surface and ρ_{CsPbBr_3} and ρ_{MOPSO} are the charge densities of (001) surface and MOPSO molecule, respectively.

Supplementary Note 10. Adsorption energy

To calculate the adsorption energy of a MOPSO molecule on the perovskite surface containing an undercoordinated Pb²⁺ site, a 3*3*2 supercell was constructed. During structural optimization, the middle two layers were fixed, and a 15 Å vacuum layer was introduced along the z direction. The exchange-correlation functional and convergence criteria were consistent with those used for the bulk calculation, while a 2*2*1 k-point mesh was employed. The adsorption energy was calculated using the following equation:

$$\Delta E = E_{system} - E_{slab} - E_{adsorption} \quad (14)$$

Where E_{system} , E_{slab} and $E_{adsorption}$ represent the total energies of the adsorption system, substrate surface and adsorbate, respectively.

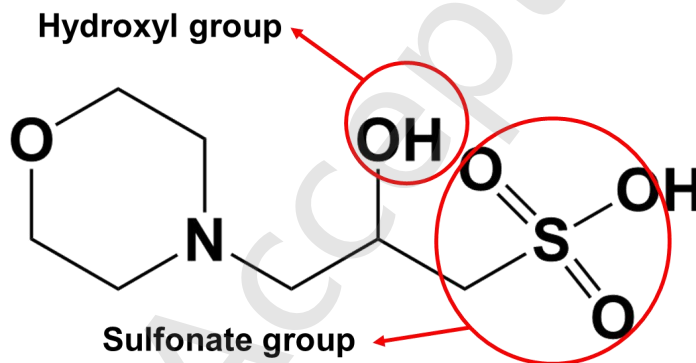
3 Figure S1-17

Figure S1. The molecular structure of MOPSO.

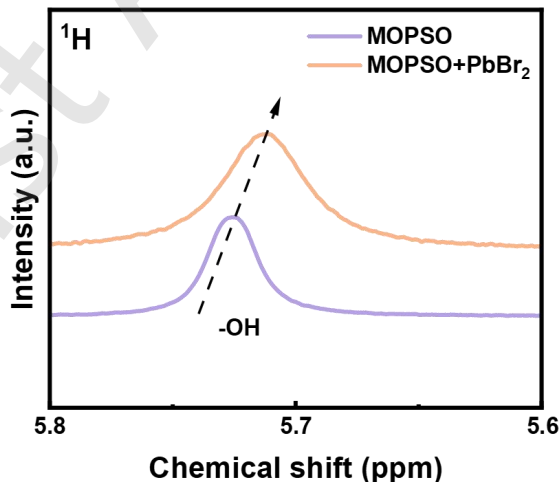


Figure S2. ¹H NMR spectra of MOPSO and a mixture of samples with PbBr₂.

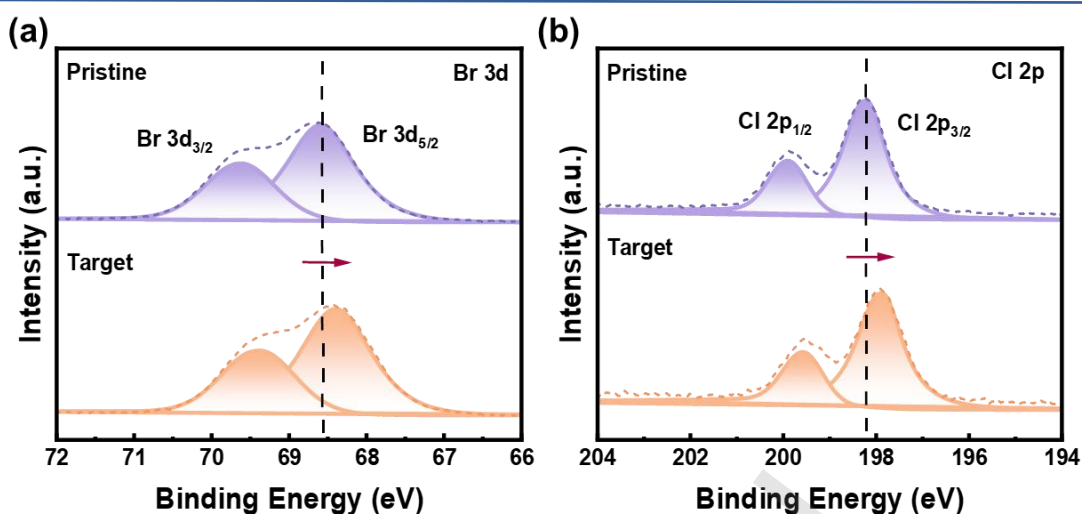


Figure S3. The XPS analysis of the (a) Br 3d and (b) Cl 2p peak for the pristine and target perovskite films.

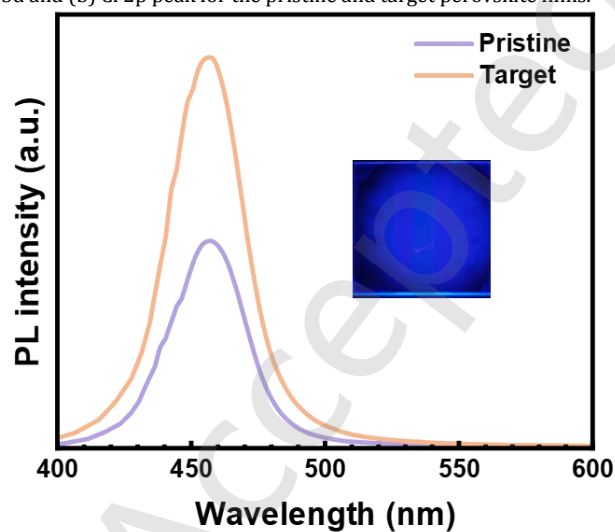


Figure S4. Steady-state PL spectra of the pristine and target perovskite films (inset is a photo image of the target film under UV illumination).

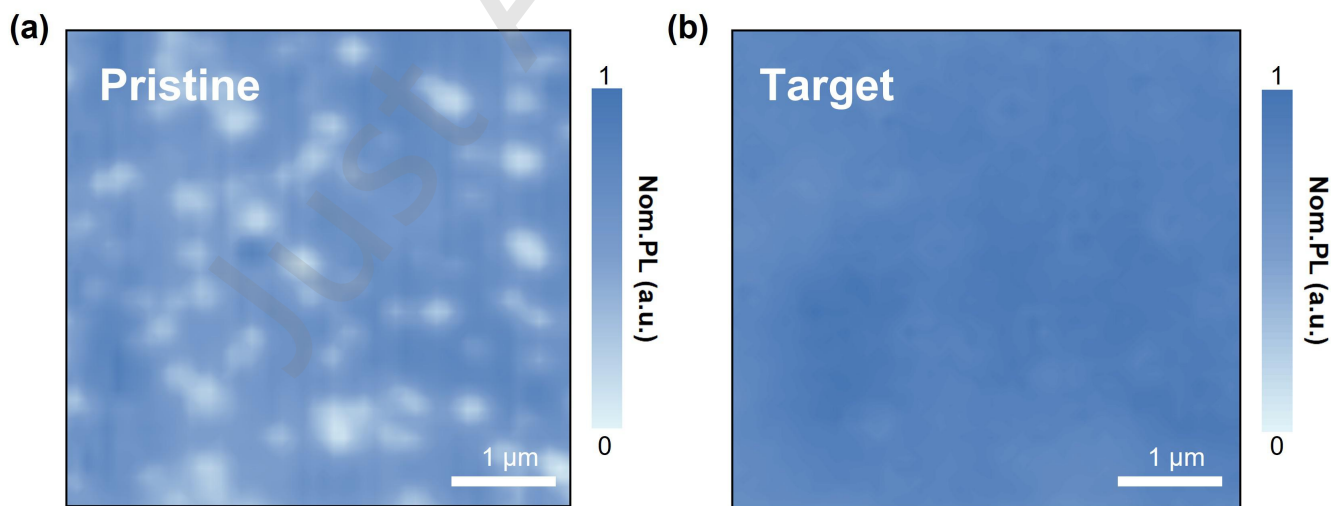


Figure S5. PL mapping of pristine and target perovskite films.

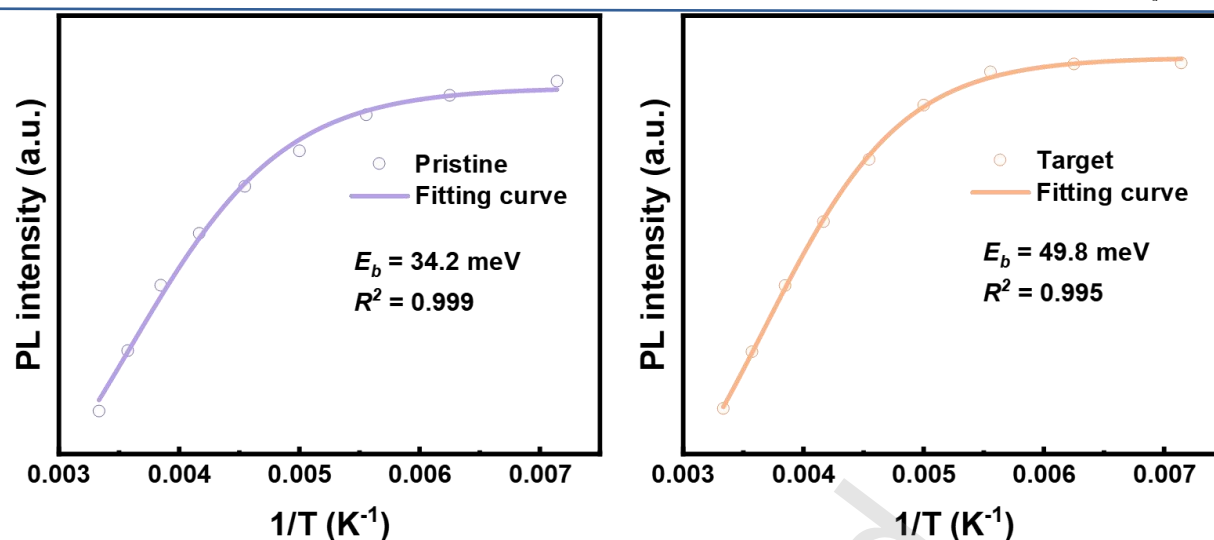


Figure S6. Fitted curves of the integrated photoluminescence (PL) intensity as a function of $1/T$ for the perovskites with and without MOPSO.

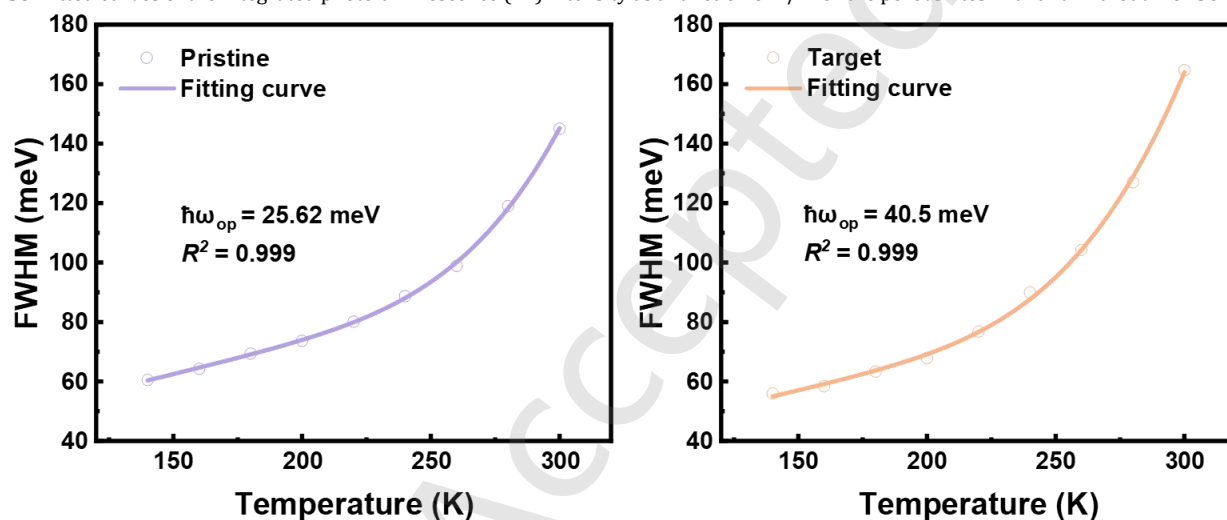


Figure S7. FWHM as a function of temperature for the films without and with MOPSO, which were extracted from temperature-dependent steady-state PL spectra.

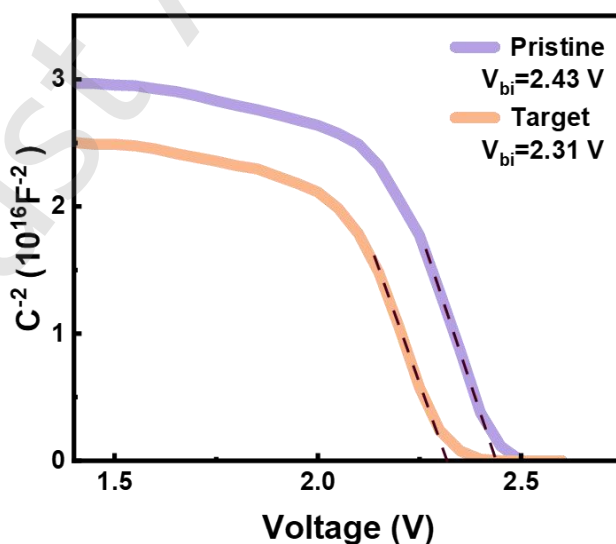


Figure S8. The capacitance behavior and Mott-Schottky curves for the pristine and target devices.

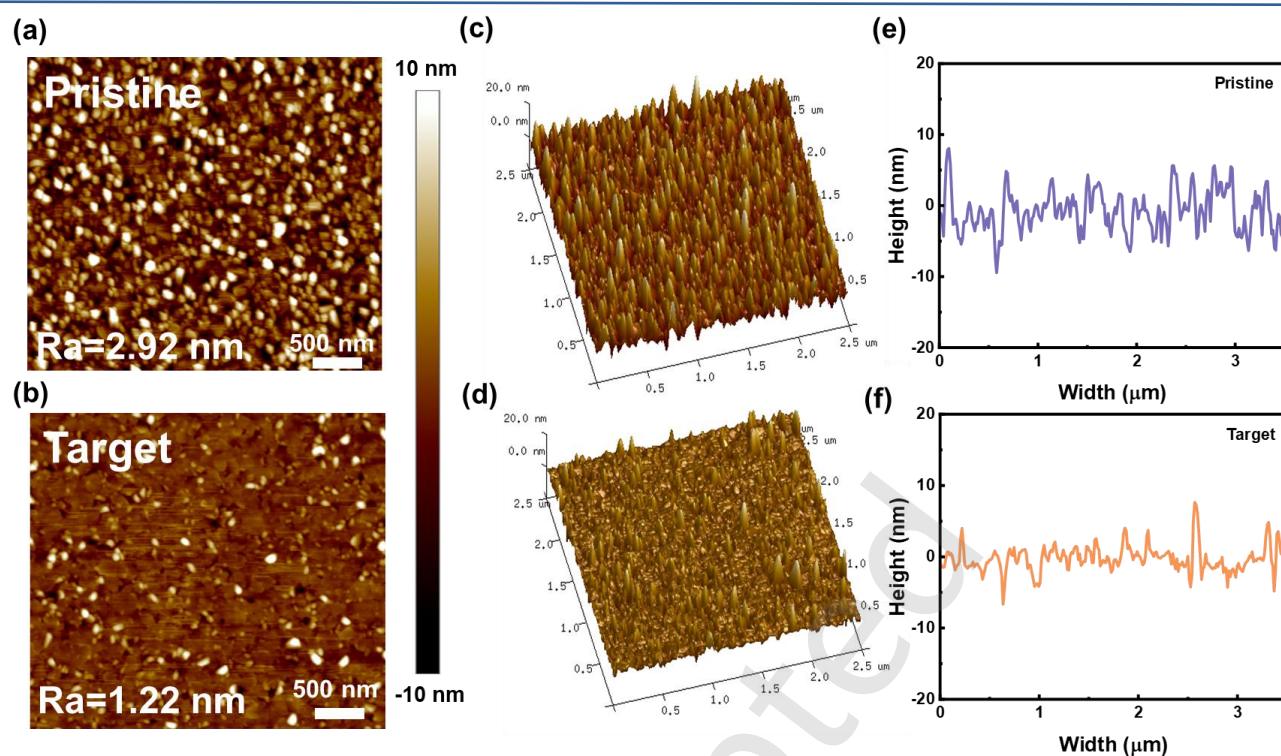


Figure S9. Atomic force microscopy (AFM) 3D images of (a) pristine and (b) target perovskite films, together with the line profiles corresponding to the middle horizontal lines.

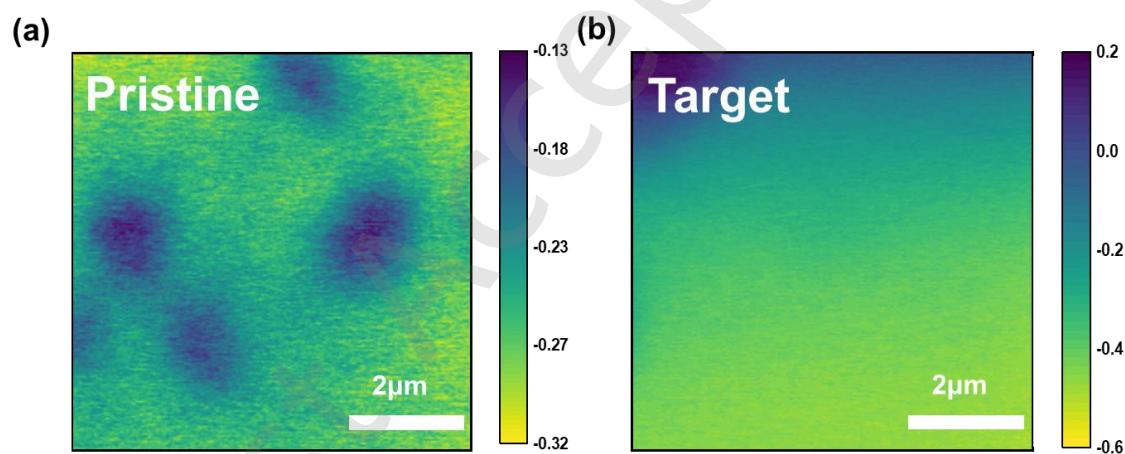


Figure S10. KPFM images of (a) pristine and (b) target perovskite films.

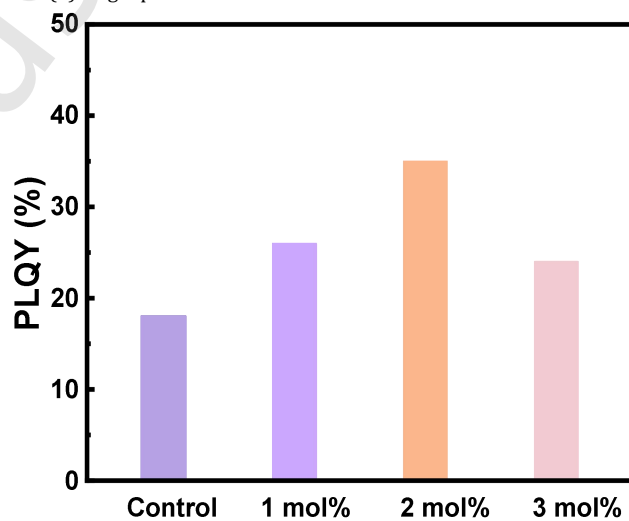


Figure S11. PLQY of perovskite films with varied concentration of MOPSO additive.

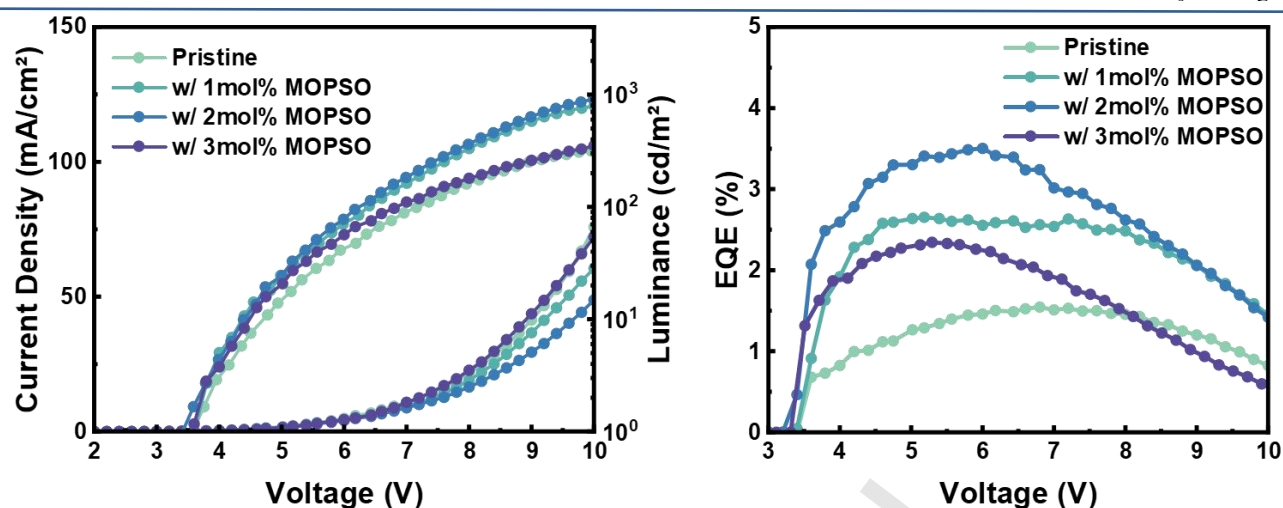


Figure S12. J-V, L-V and EQE-V curves for the pristine device and PeLEDs with varying MOPSO doping contents of 1, 2 and 3 mol%.

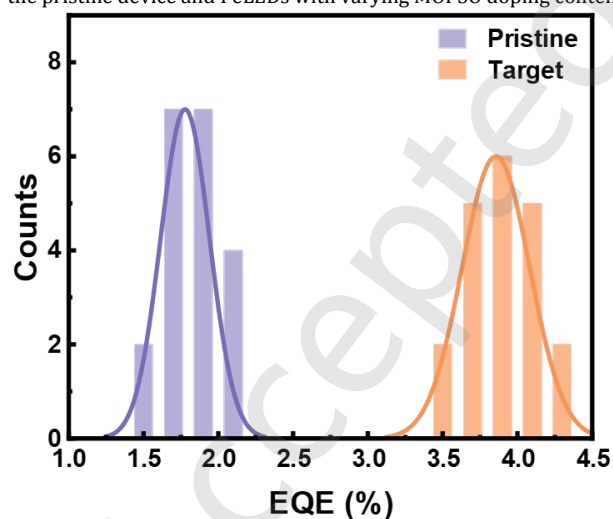


Figure S13. EQE distribution of deep-blue PeLEDs based on over 20 devices.

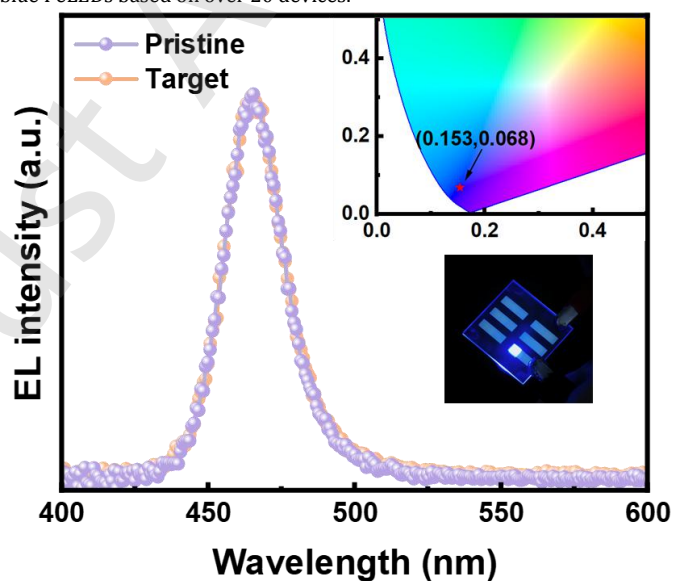


Figure S14. EL emission characteristics of the pristine and target devices.

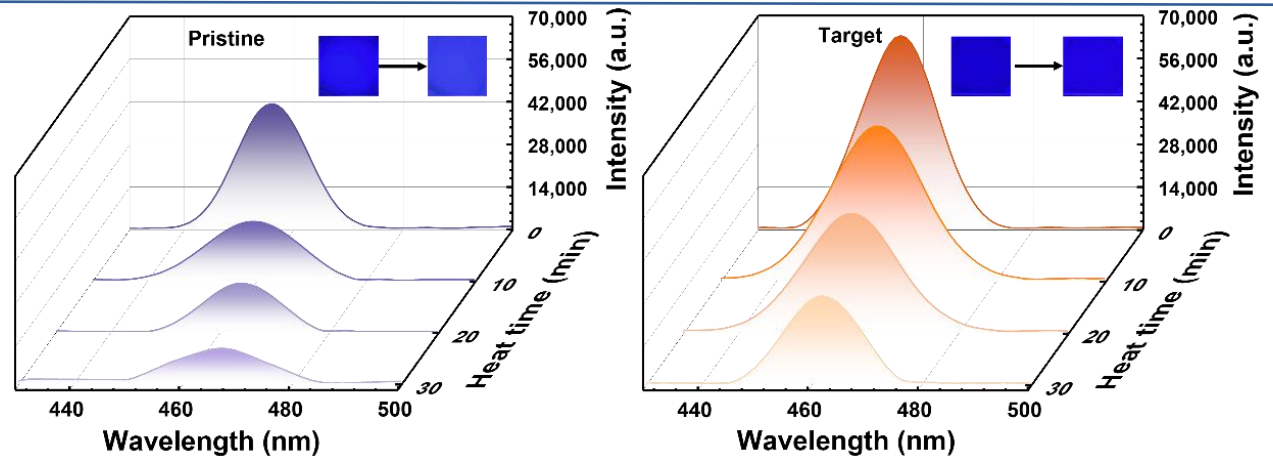


Figure S15. Time evolution of the PL spectra for the pristine and target perovskite films after heating at 65°C for 30 min, and the inset shows a photograph of the corresponding films before and after heating for 30 min.

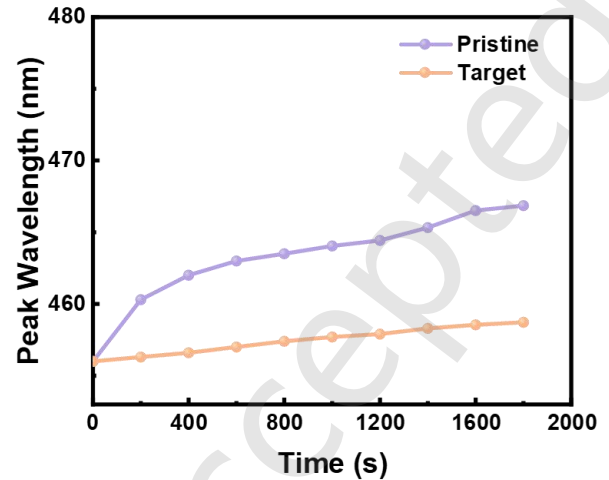


Figure S16. The spectral deviation under continuous bias operation (lasting 30 minutes at 4.0 V).

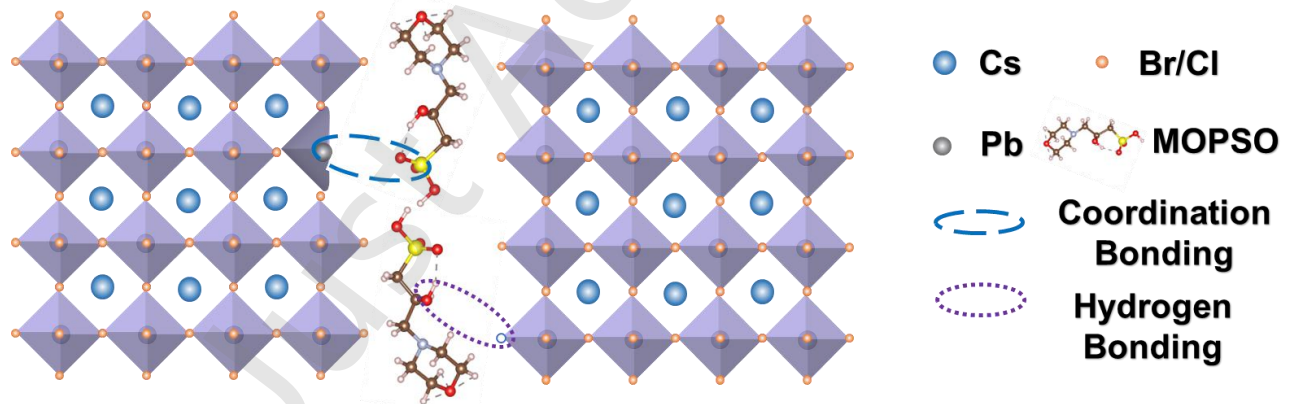


Figure S17. The schematic diagram of MOPSO passivation.

4 Table S1,2,3

Table S1. The fitting parameters of TRPL curves of pristine and target film.

Perovskite film	A ₁	τ ₁ (ns)	A ₂	τ ₂ (ns)	τ _{avg} (ns)
Pristine	0.75	2.72	0.13	24.78	16.28
Target	0.48	7.23	0.22	34.23	25.62

Table S2. PLQY, PL average lifetimes (τ_{avg}), radiative decay rates (k_r), and nonradiative recombination rates (k_{nr}) of pristine and target perovskite films.

	Pristine	Target
PLQY (%)	18	35
τ_{avg} (ns)	16.28	25.62
k_r (10^7 s^{-1})	1.11	1.37
k_{nr} (10^7 s^{-1})	5.04	2.54

Table S3. Extracted TA data of perovskite films.

Sample	n=3				n≥4			
	τ_1 (ps)	τ_2 (ps)	τ_3 (ps)	τ_{et} (ps)	τ_{et} (ps)	τ_1 (ps)	τ_2 (ps)	τ_3 (ps)
Pristine	3.1	43	239.3	146.5	0.37	9.06	87.2	5219
Target	0.55	2.38	4.27	0.82	0.27	10.2	17.35	346.9

References

- [1] Xia, Y.; Song, B.; Zhang, Z.; Wang, K. L.; Li, Y. H.; Li, N.; Chen, C. H.; Chen, J.; Xing, G.; Wang, Z. K., Vertically concentrated quantum wells enabling highly efficient deep-blue perovskite light-emitting diodes. *Angew. Chem.* **2024**, *136*, e202403739.
- [2] Dong, J.; Lu, F.; Han, D.; Wang, J.; Zang, Z.; Kong, L.; Zhang, Y.; Ma, X.; Zhou, J.; Ji, H., Deep-Blue Electroluminescence of Perovskites with Reduced Dimensionality Achieved by Manipulating Adsorption-Energy Differences. *Angew. Chem.* **2022**, *134*, e202210322.
- [3] Wang, Q.; Wang, X.; Yang, Z.; Zhou, N.; Deng, Y.; Zhao, J.; Xiao, X.; Rudd, P.; Moran, A.; Yan, Y., Efficient sky-blue perovskite light-emitting diodes via photoluminescence enhancement. *Nat. Commun.* **2019**, *10*, 5633.
- [4] Maimaitizi, H.; Ågren, H.; Chen, G., Multifunctional ligand engineering enables high-performance CsPb (Br/Cl)₃ nanocrystals toward efficient and stable pure-blue perovskite LEDs. *Light: Science & Applications* **2026**, *15*, 135.
- [5] Shen, Y.; Li, Y. Q.; Zhang, K.; Zhang, L. J.; Xie, F. M.; Chen, L.; Cai, X. Y.; Lu, Y.; Ren, H.; Gao, X., Multifunctional crystal regulation enables efficient and stable sky-blue perovskite light-emitting diodes. *Adv. Funct. Mater.* **2022**, *32*, 2206574.
- [6] Shang, J.; Wang, J.; Yang, L.; Sheng, R.; Zhang, F.; Chen, P., Stable and efficient blue quasi-2D perovskite light-emitting diodes enabled by synergistic passivation engineering. *Nano Research* **2025**, *18*.
- [7] Shen, C.; Wang, H.; Liang, X.; Chen, H.; Cai, B.; Wei, Y.; Hu, S.; Luo, Y.; Zhang, F.; Xu, Q., Simultaneous Interfacial Modification and Crystallization Regulation for High-Performance Pure-Blue Quasi-2D Perovskite Light-Emitting Diodes. *ACS Energy Letters* **2025**, *10*, 3638-3646.