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Convergence and Device Innovation: From Low-Dimensional/Lead-Free Perovskite Photovoltaics to Micro/Nano Light-Emitting Displays

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Abstract

Current optoelectronic technologies still face several limitations, including the efficiency ceiling of crystalline silicon, the instability of conventional perovskites, and transfer-related challenges in Micro-LED fabrication. This study centers on the cross-boundary integration of lead-free, low-dimensional perovskite photovoltaics and micro/nano light-emitting displays. Efficient control of carrier dynamics is critical for improving both photovoltaic conversion and light-emitting performance. Through lead-free substitution and dimensional reduction (i.e., the construction of low-dimensional superstructures), an intrinsic water-oxygen barrier is established to significantly enhance the chemical stability of the materials. In addition, quantum confinement modifies the density of states (DOS) distribution, thereby substantially boosting the radiative recombination efficiency. By leveraging fundamental physical strategies such as band engineering, this research may support the development of high-performance optoelectronic devices with improved stability and efficiency.

Keywords

lead-free low-dimensional perovskites, micro/nano light-emitting displays, dimensionality modulation, optoelectronic integration

1. Introduction

High-efficiency clean energy technologies and ultra-high-resolution, low-power-consumption display terminals have attracted increasing attention in recent years [1]. Traditional crystalline silicon photovoltaics are approaching their theoretical efficiency limits, while micro-nano display technologies face significant industrial bottlenecks.

Crystalline silicon solar modules, which currently dominate the photovoltaic market, have efficiencies nearing their physical limits. Meanwhile, third-generation perovskite materials, despite their great potential, urgently need to overcome lead toxicity and the intrinsic instability of three-dimensional perovskite lattices in humid and oxygenated environments. In the field of micro-nano light-emitting displays, both organic light-emitting diodes (OLEDs), which suffer from material aging, and micro light-emitting diodes (Micro-LEDs)—regarded as a promising display technology—encounter formidable industrialization barriers,

including extremely low yields in mass transfer processes and challenging interface defect control between Micro-LEDs and oxide-based driving backplanes. These common challenges highlight a fundamental insight: electroluminescence (electricity-to-light) and photovoltaic conversion (light-to-electricity) are complementary processes. These challenges are closely related to carrier injection, transport, and recombination processes in semiconductors [2].

This study systematically investigates the fundamental mechanisms of light-to-electricity and electricity-to-light conversion, with a particular focus on low-dimensional, lead-free hybrid perovskite photovoltaic materials [3] and the regulatory effects of bandgap engineering and dimensional reduction on the optoelectronic properties of materials. By integrating concepts from photovoltaic and display technologies, this work aims to overcome critical bottlenecks in device efficiency and stability, providing insights into the design of high-performance optoelectronic materials.

2. Core Research Objects and Physical Mechanisms

This research centers on two representative classes of semiconductor optoelectronic systems: electroluminescent display devices and photovoltaic conversion devices. Although these systems belong to distinct application domains—interactive displays and clean energy—they share common underlying principles governed by semiconductor band theory and carrier dynamics. Optimization of device performance in both cases ultimately revolves around the regulation of carrier dynamics.

2.1 Carrier Recombination Mechanism in Electroluminescent Devices

The fundamental operating principle of electroluminescent display devices is the radiative recombination of carriers within the emissive layer, resulting in photon emission. The electroluminescent display systems investigated in this study primarily center on micro-light-emitting diodes (μLEDs), organic light-emitting diodes (OLEDs), and their supporting oxide thin-film transistor (TFT) backplanes—both of which represent mainstream next-generation display materials. The core physical process in these devices relies on stimulated radiative recombination. Under an applied electric field E, electrons and holes are injected from the cathode and anode, respectively, across energy barriers into the multiple-quantum-well emissive layer of μLEDs or the emissive layer (EML) of OLEDs. The injected carriers first form excitons, which subsequently undergo radiative transitions to release photons, thereby realizing electro-optical conversion.

The ultimate efficiency of this process is determined by the quantum yield. The primary bottlenecks include:

(1) Bandgap (Eg) engineering: The bandgap width directly dictates the energy and wavelength of emitted photons, which must precisely match the human visual response curve or specific display color gamut standards. (2) Defect suppression: Deep-level defect states within the material or at interfaces induce non-radiative recombination, causing energy loss in the form of thermal phonons and directly reducing the external quantum efficiency (EQE). (3) Carrier injection dynamics: The energy level alignment between the oxide backplane and the emissive layer governs the injection barriers and transport rates of carriers, thereby influencing device brightness and response speed.

2.2 Photogenerated Carrier Separation Mechanism in Photovoltaic Conversion

The essence of the photovoltaic effect is the directional migration and collection of photogenerated carriers, which determines the conversion efficiency from light to electrical energy. This study selects low-dimensional, lead-free hybrid perovskites as the core photovoltaic material. Distinct from conventional lead-based perovskites, these materials offer environmental friendliness combined with highly tunable optoelectronic properties. In such photovoltaic systems, incident photons excite the semiconductor lattice to generate electron–hole pairs. These carriers are then separated under the influence of the built-in electric field and transported directionally toward their respective electrodes, enabling the collection and extraction of photogenerated charges.

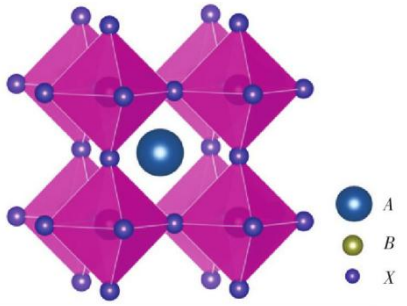
The key factors determining power conversion efficiency (PCE) are as follows: (1) Broad-spectrum light absorption and efficient carrier generation; (2) Passivation of grain boundaries and surface trap states to suppress recombination and enhance open-circuit voltage (Voc); (3) Interfacial charge dynamics: The energy

level alignment at the electron transport layer (ETL)/perovskite and perovskite/hole transport layer (HTL) interfaces critically influences charge extraction efficiency and the probability of back recombination.

3. Structural Design and Optoelectronic Performance Regulation of Low-Dimensional Lead-Free Perovskites

This study centers on novel optoelectronic functional materials based on the ABX_3-type hybrid perovskite system, whose chemical structure is illustrated in Figure 1. The A-site cation primarily serves to balance the lattice charge and support the framework structure, while the B-site metal cation and X-site halide anions together form the $[BX_6]^{4-}$ octahedron, which directly determines the material's band structure and carrier transport properties [4]. To address the toxicity and stability issues of lead-based perovskites, lead-free systems have emerged as an important development direction. Substituting the B-site with Sn^{2+}, Ge^{2+}, or similar ions can effectively tune the bandgap and achieve narrower bandgaps, meeting the requirements for efficient photovoltaic light absorption. Further adjustment of the X-site halide species and their ratios enables continuous bandgap tuning, allowing the material to transition from the optimal bandgap for photovoltaics to wider bandgaps suitable for light emission in display applications. Additionally, double perovskites, designed with multi-component B-site cations, can realize unique emission spectra and enhanced stability.

Figure 1: Schematic illustration of the cubic perovskite crystal structure [5]



Dimensional regulation of the materials also relies on precise compositional design. Introducing large organic cations such as PEA^+ or BA^+ into the ABX_3 precursors disrupts the three-dimensional continuous lattice, driving the system toward two-dimensional (2D) or quasi-two-dimensional (quasi-2D) structures and forming typical Ruddlesden–Popper (RP) or Dion–Jacobson (DJ) phases [6]. These low-dimensional perovskite structures exhibit distinct advantages and inherent limitations.

First, structural and performance advantages. The hydrophobic organic interlayers in layered low-dimensional perovskites effectively block moisture and oxygen ingress, suppress ion migration, and significantly enhance environmental stability. The layered configuration also improves crystallization quality, reduces defect density, and lowers non-radiative recombination losses. In addition, the bandgap can be precisely tuned by controlling the inorganic layer n value and the type of organic cations, making these materials suitable for various devices including photovoltaics, LEDs, and photodetectors. The approach further improves film morphology and enhances the reproducibility of device fabrication.

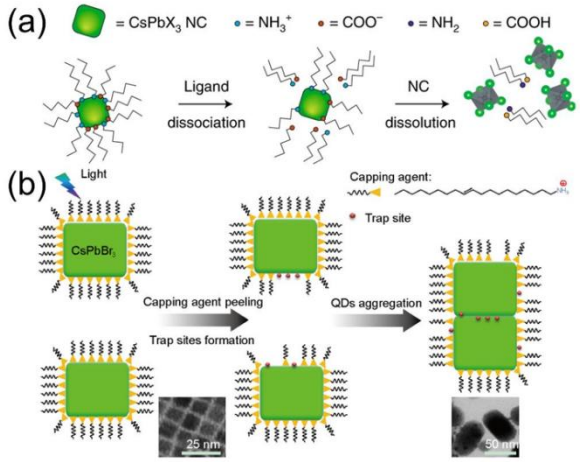
Second, functional and strategic value. By harnessing the intrinsic quantum confinement of low-dimensional architectures, these systems facilitate robust carrier localization and substantially amplify radiative recombination efficiency, thereby providing an inherent structural template for high-performance perovskite LEDs (PeLEDs). Consequently, compositional engineering and dimensionality control serve as the fundamental scientific cornerstones for the rational design of efficient, stable, and environmentally benign multifunctional PV-LED devices.

Even so, these materials also possess intrinsic structural drawbacks. The organic insulating layers create charge transport barriers that severely hinder vertical carrier transport, resulting in lower electrical conductivity and fill factors compared with 3D perovskites. The performance of low-dimensional perovskites is highly dependent on crystal orientation, yet the controllable synthesis of vertically oriented films remains challenging. During solution processing, the formation of mixed n-value phases is common, leading to energy level disorder, aggravated carrier recombination, and compromised overall device performance [7].

This section summarizes the physical foundations of optoelectronic functional materials from three aspects: (1) based on band theory, illustrating that a suitable and tunable bandgap is central to efficient photoelectric conversion; (2) analyzing dielectric polarization mechanisms and the fundamental principles of optical modulation in polar media under electric fields; and (3) discussing electrical behavior under extreme conditions, including the application of ferroelectric polarization switching and superconducting zero-loss transport in devices [8].

When the dimensionality of semiconductor materials is reduced to the nanoscale, the classical continuous band structure becomes discretized due to spatial localization of carriers, giving rise to pronounced quantum confinement effects. In this regime, the material's bandgap and density of states can be artificially modulated by controlling its geometric dimensions (e.g., film thickness) [9].

Figure 2: Schematic of ligand dissociation, dissolution, and photo-induced ligand desorption, trap state formation, and aggregation processes in perovskite quantum dots [10]



As shown in Figure 2, perovskite nanocrystals undergo ligand dissociation and dissolution, while under illumination, ligand shedding, trap state formation, and aggregation occur. Superlattices represent a typical atomic-scale design strategy that exploits size effects, consisting of periodically alternating semiconductor thin layers with different bandgaps. This architecture causes the energy bands to split into discrete minibands and minigaps [11]. By precisely controlling layer thickness and composition, carrier transport and optoelectronic response characteristics can be directionally engineered.

Overall, compared with conventional 3D perovskites, quasi-2D perovskites offer significant competitive advantages in both structure and device applications. Studies have demonstrated that quasi-2D perovskites, constructed with long-chain organic cations forming layered hydrophobic frameworks, can physically isolate external moisture and oxygen, effectively suppress ion migration and lattice thermal distortion within the perovskite system, and substantially mitigate photo-aging and thermal degradation. Consequently, their comprehensive environmental stability and long-term operational performance far exceed those of 3D perovskites.

In terms of film quality and carrier dynamics, the layered crystal configuration optimizes crystallization behavior, reduces intrinsic defects such as vacancies and dislocations, and yields denser, higher-quality films. The well-ordered microstructure lowers non-radiative recombination losses and prolongs photogenerated carrier lifetimes, thereby enhancing the operational stability of photovoltaic devices. Furthermore, through the combination of diverse layered phases (RP, DJ, etc.), inorganic layer n-value modulation, and organic cation engineering, precise customization of bandgap and energy level structures can be achieved to meet the spectral requirements of different photovoltaic devices. In addition, the relatively slow and controllable crystallization rate of quasi-2D perovskites results in superior film uniformity, effectively addressing inhomogeneity issues in large-area fabrication and improving process reproducibility [11].

Nevertheless, quasi-2D perovskites also exhibit inherent limitations and technical bottlenecks: the van der Waals interactions between layers create natural charge transport barriers, leading to a significant decline in vertical carrier migration efficiency—this being the primary factor constraining device performance. At the

fabrication level, preferential film orientation is highly sensitive to parameters such as annealing temperature and solvent composition, resulting in a narrow processing window and high regulatory difficulty. From an industrialization perspective, due to these charge transport limitations, the power conversion efficiencies of current quasi-2D perovskite photovoltaic devices remain significantly lower than those of high-performance 3D perovskite benchmark devices. During solution processing, the system readily forms mixed n-value phases. The disordered distribution of multiple n-phases causes energy level misalignment and band disorder, exacerbating interfacial charge recombination and ultimately leading to fluctuations in device optoelectronic parameters and poor batch-to-batch consistency [12], which is shown in Table 1.

Table 1: Comparison of perovskite structures

Structure Type	Core Advantages	Main Bottlenecks	Suitable Applications
3D Lead-Free Perovskite	Good conductivity, mature processing, high carrier mobility	Poor moisture/oxygen stability, high defect density	Photovoltaic devices
Low-Dimensional (2D/Quasi-2D) Perovskite	Excellent stability, effective defect passivation, tunable bandgap	Limited vertical transport, low charge mobility	Light-emitting diodes (PeLEDs)
Perovskite Superlattice	Combined transport and regulation advantages, good film uniformity	Complex fabrication, high cost	Tandem photovoltaics / Multifunctional devices

4. Novel Luminescent Materials and Micro-Nano Devices

Cathode ray tubes (CRT), plasma display panels (PDP), electroluminescent displays (EL), liquid crystal displays (LCD), and light-emitting diodes (LED) each have their respective application scenarios and performance limitations. Collectively, they reflect an iterative progression in brightness, lifetime, power consumption, and resolution, as summarized in Table 2.

Table 2: Comparison of display technologies

Display Technology	Operating Principle / Emission Mechanism	Current Advantages	Current Disadvantages
LCD	Electric field-induced alignment of liquid crystal molecules to modulate backlight transmission	Mature technology, low cost	Requires backlight, limited contrast, poor flexibility
OLED	Carrier injection and recombination in organic layers	Self-emissive, ultra-thin and flexible, high contrast	Short blue emitter lifetime, prone to burn-in
Mini LED	Refined backlight or direct-view arrays with grain size >100 μm	High brightness, high contrast (local dimming)	Relatively high cost, thermal management challenges
Micro LED	Miniaturized and matrixed self-emissive arrays with grain size <100 μm	Ultra-high brightness, lifetime, and response speed	Extremely low mass transfer yield

Micro-LED is widely regarded as the next-generation mainstream display technology. Yet it faces significant hurdles in industrialization. The technology currently encounters four core challenges: (1) The extremely high difficulty of mass transfer. Achieving high-precision placement of micrometer-scale chips while maintaining efficiency, accuracy, and yield remains a major obstacle, resulting in persistently high production costs. (2) Device performance deteriorates markedly upon miniaturization; surface defects in small-sized chips exacerbate edge effects and non-radiative recombination, causing a rapid decline in internal quantum efficiency. In particular, the efficiency drop in red Micro-LEDs has become the primary barrier to full-color realization. (3) The lack of efficient chip inspection and repair methods makes it difficult to improve overall yield [13]. (4) Stringent requirements for driving technology arise, as high pixel density introduces significant parasitic resistance and capacitance effects, demanding exceptionally high carrier mobility in the backplane and precise current control from the driving ICs. Overall, although Micro-LED offers outstanding performance advantages, its low process maturity and high cost at the present stage limit practical deployment.

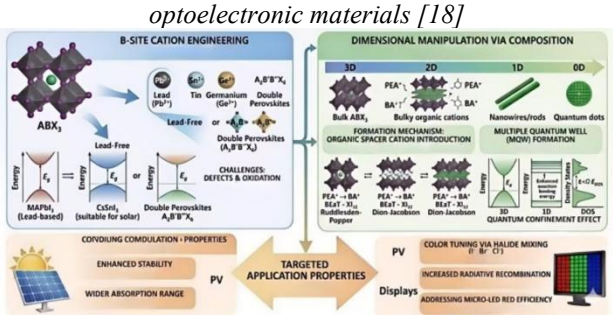
Hybrid perovskites represent a promising class of novel photovoltaic materials with strong industrialization potential, owing to their excellent optoelectronic properties, solution processability, and superior cost-effectiveness compared with conventional crystalline silicon. Even so, their efficiency and stability are highly dependent on the quality of the perovskite layer, film morphology, and interface engineering. Performance is therefore strongly influenced by fabrication processes. Precise regulation of A-site cations, B-site metal cations, and X-site halide anions enables performance optimization. In terms of fabrication methods, the one-step solution process relies on antisolvent quenching to induce uniform nucleation; the two-step method facilitates morphological control and larger grain sizes; while vacuum evaporation is compatible with large-area industrial production and offers precise thickness control. Each approach has distinct advantages and is suited to different needs—laboratory-scale high-efficiency devices, morphology control, or large-area mass production, respectively. Additionally, interface engineering, surface passivation, and interfacial modification are critical strategies for defect passivation and suppression of non-radiative recombination, serving as key means to enhance efficiency and long-term operational stability [14].

To address the toxicity and instability of lead-based perovskites, lead-free compositions and dimensional engineering have become major research directions, each with their own advantages and trade-offs. Figure 3 presents a schematic of lead-free modification and dimensional regulation strategies for perovskite materials. Lead-free systems reduce environmental hazards and are more suitable for flexible and wearable applications. But their three-dimensional (3D) lattices are more susceptible to moisture- and oxygen-induced degradation, and they suffer from severe intrinsic defects and oxidation issues, resulting in suboptimal efficiency and lifetime [15].

In contrast, the introduction of long-chain organic cations (such as PEA^+ and BA^+) to form two-dimensional (2D) layered or quasi-two-dimensional (2D/3D) structures enables molecular-level reconstruction of the crystal superstructure. This approach substantially enhances intrinsic chemical stability, effectively regulates exciton binding energy and carrier transport pathways, suppresses Sn^{2+} oxidation and ion migration, and extends device lifetime while maintaining efficient photoelectric conversion. Yet, these low-dimensional structures impose charge transport limitations, which can reduce optoelectronic efficiency to some extent, and their fabrication processes are more complex, posing greater challenges for large-area processing. In summary, dimensional engineering offers pronounced advantages in stability but still faces shortcomings in efficiency and scalable manufacturing. Future efforts must strike a better balance between performance metrics and practical applicability to achieve both high efficiency and long-term stability [16].

From the perspective of display technology development, the primary advantage lies in the continuous performance improvement of Micro-LED; its disadvantages are the difficulties in industrialization, high cost, and challenges in mass production. From the perspective of perovskite material applications, the advantages include excellent optoelectronic properties, low cost, and ease of processing, with improved environmental friendliness and stability after modification. The disadvantages are efficiency losses in modified materials and increased fabrication complexity due to process limitations [17].

Figure 3: Schematic illustration of lead-free modification and dimensional regulation strategies for perovskite optoelectronic materials [18]



5. Conclusion

This study focuses on two emerging classes of semiconductor materials: lead-free low-dimensional perovskite photovoltaic materials and micro-nano light-emitting display systems centered on Micro-LED and OLED technologies. Motivated by growing demands for sustainable energy and advanced display

technologies, this work targets multiple critical technical bottlenecks in the current optoelectronics field. These include the difficulty of further improving crystalline silicon solar cells that are already approaching their theoretical efficiency limits, the heavy-metal toxicity of lead-based perovskites, and the industrialization challenges of Micro-LED displays due to mass transfer limitations. The results suggest that carrier dynamics play an important role in both photovoltaic and light-emitting processes. By conducting refined compositional design to realize lead-free, non-toxic substitution of perovskites, and integrating bandgap engineering with dimensional reduction strategies, this research improves environmental stability by suppressing moisture and oxygen penetration and significantly enhances radiative recombination efficiency of carriers. These findings may provide useful insights into the design of stable and efficient optoelectronic devices. In summary, lead-free low-dimensional perovskites show potential for applications in both photovoltaic and display technologies. Future studies should further improve defect control and device integration. Subsequent research may explore the use of artificial intelligence methods for process optimization and device design, overcome large-scale production bottlenecks, and promote practical applications in AR/VR, Internet of Things, and other emerging scenarios. These advances may facilitate broader applications of optoelectronic devices in energy and display technologies.

References

[1] Zhou, C. (2024). Research on the photoelectric properties of lead-free perovskite materials (Master's thesis, Guangzhou University). https://doi.org/10.27040/d.cnki.ggzdu.2024.000397.

[2] Wu, S. Y., Ma, S. L., Zhao, C. Y., Li, S. X., Ye, M. Y., Qi, M. Y., ... & Cui, T. (2025). Regulation of photoelectric properties of lead-free double perovskite Cs2TeCl6 under high pressure. *Acta Physica Sinica*, 74(17), 68-75.

[3] Di, J. Y., Cui, Y., Wu, R. X., & Lu, B. (2025). High-performance zero-dimensional lead-free perovskite thin film photodetectors. *Chinese Optics*, 18(04), 748-755.

[4] Zhang, Y. J. (2024). First-principles study based on ABX_3-type inorganic lead-free perovskites (Master's thesis, Hebei University). https://doi.org/10.27103/d.cnki.ghebu.2024.002015.

[5] Yang, J., Pi, M. Y., Zhang, D. K., Tang, X. S., & Du, J. (2021). Research progress of low-dimensional perovskite photodetectors. *Chinese Journal of Luminescence*, 42(06), 755-773.

[6] Peng, X. F. (2023). Defect passivation and mechanism study of quasi-two-dimensional perovskite light-emitting devices (Doctoral dissertation, University of Electronic Science and Technology of China). https://doi.org/10.27005/d.cnki.gdzku.2023.000030.

[7] Liu, R., Hu, X., Xu, M., Ren, H., & Yu, H. (2023). Layered low dimensional Ruddlesden-Popper and Dion-Jacobson perovskites: From material properties to photovoltaic device progress. *ChemSusChem*, 16(19), e202300736. https://doi.org/10.1002/cssc.202300736.

[8] Liu, Z., Liu, S., Zhang, X., Hao, H., Chang, X., Shen, Z., ... & Li, L. (2025). Insights into A-site ion engineering for boosting luminescence efficiency in lead-free perovskites. *Journal of Physical Chemistry Letters*, 7443-7450. https://doi.org/10.1021/acs.jpclett.5c01417.

[9] Yuan, J., Diao, J., Zheng, Y., Hao, J., Sun, B., Zhao, G., ... & Jiang, X. (2025). Hierarchical microfluidic epitaxy of Sn4+-stabilized core–shell perovskites with lead-free double perovskite shells for highly efficient and ultra-stable emission. *Advanced Functional Materials*, 36(10), e13146. https://doi.org/10.1002/adfm.202513146.

[10] Liu, D., Nie, X., Li, X. G., Li, D. L., Chen, Z., Liao, S., ... & Su, S. J. (2025). Highly efficient perovskite/organic hybrid white electroluminescent devices with extended operational lifetime and wide color gamut. *Advanced Materials*, 37(38), e2507820. https://doi.org/10.1002/adma.202507820.

[11] Zhang, L., Liu, B., Lv, X., Zhang, G., Li, C., Zhang, W., ... & Liu, C. (2026). Photovoltage-driven two-transistor-one-diode perovskite pixels for in-cell optical sensing displays. *Advanced Materials*, 38(17), e22776. https://doi.org/10.1002/adma.202522776.

[12] Lee, H., Moon, T., Lee, Y., & Kim, J. (2025). Structural mechanisms of quasi-2D perovskites for next-generation photovoltaics. *Nano-Micro Letters*, 17(1), 139. https://doi.org/10.1007/s40820-024-01609-9.

[13] Zhang, Z., Zhu, R., Li, G., et al. (2026). Photoswitchable isomers to improve grain boundary resilience and perovskite solar cells stability under light cycling. *Nature Energy*, 11, 623–632. https://doi.org/10.1038/s41560-026-01993-z.

[14] Shen, X., Hui, W. T., Hu, S., et al. (2026). Crystal-facet-directed all-vacuum-deposited perovskite solar cells. Nature Materials. Advance online publication. https://doi.org/10.1038/s41563-026-02494-w.

[15] Lian, Y., Wang, Y., Yuan, Y., Ren, Z., Tang, W., Liu, Z., ... & Di, D. (2025). Downscaling micro- and nano-perovskite LEDs. *Nature,* 640(8057), 1-7. https://doi.org/10.1038/s41586-025-08685-w.

[16] Peng, J., Xue, X., Liu, S., Yang, Y., Yang, T., Zhu, B., ... & Ji, W. (2026). Maximizing perovskite electroluminescence with ordered 3D/2D heterojunction. *Nature*, 651(8104), 1-7. https://doi.org/10.1038/s41586-026-10134-1.

[17] Pandey, A., Reddeppa, M., & Mi, Z. (2024). Recent progress on micro-LEDs. *Light: Advanced Manufacturing*, 4(4), 519-542. https://doi.org/10.37188/lam.2023.031.

[18] Xiao, Z. W. (2020). Improving the efficiency of perovskite light-emitting devices by using different defect passivation methods (Master's thesis, Southwest University). https://doi.org/10.27684/d.cnki.gxndx.2020.002385.

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Conflicts of Interest

The authors declare no conflict of interest.

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