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CHARGE TRANSPORT MECHANISMS AND ENERGY LEVEL ALIGNMENT IN $KPbBr_3$ - BASED PEROLED STRUCTURES

M.Rahmonova, N. Mukhamadiev
Samarkand State University named after Sharof Rashidov, Samarkand, Uzbekistan.

M.Rahmonova Samarkand State University named after Sharof Rashidov, Samarkand, Uzbekistan.

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Abstract. This study investigates charge transport mechanisms and energy level alignment in peroLED structures based on inorganic halide perovskite $KPbBr_3$. The device architecture ITO / $KPbBr_3$–PEO / Ga–In was fabricated using a low-temperature solution-based method with polymer-assisted stabilization. Current density–voltage (J–V) characteristics were analyzed to identify different conduction regimes, including ohmic conduction, injection-controlled transport, space-charge-limited current (SCLC), and trap-filled limit behavior. An energy level diagram was constructed to interpret carrier injection processes and internal electric field formation. The results demonstrate that charge transport is governed by the combined influence of energetic alignment, trap states associated with halide vacancies, and field-assisted carrier injection. The study provides insight into transport physics in inorganic perovskite light-emitting structures and highlights the importance of defect engineering for optimizing device performance.

Keywords: charge transport; energy level alignment; $KPbBr_3$ perovskite; peroLED; perovskite light-emitting devices; space-charge-limited current; trap states.

$KPbBr_3$ asosidagi peroled tuzilmalarida zaryad tashish mexanizmlari va energetik sathlarning moslashuvi

Annotatsiya. Mazkur ishda noorganik galogenid perovskit $KPbBr_3$ asosidagi peroLED tuzilmalarida zaryad tashish mexanizmlari va energetik sathlarning moslashuvi o‘rganildi. ITO / $KPbBr_3$–PEO / Ga–In arxitekturali qurilma past haroratli eritma usuli yordamida polimer stabilizatsiyasi bilan tayyorlandi. Tok zichligi–kuchlanish (J–V) xarakteristikalari tahlili orqali o‘tkazuvchanlikning turli rejimlari, jumladan omik o‘tkazuvchanlik, injeksiya bilan boshqariladigan transport, fazoviy zaryad bilan cheklangan tok (SCLC) va tuzoqlar to‘lishi rejimi aniqlangan. Energetik diagramma zaryad tashuvchilar injeksiyasi va ichki elektr maydon hosil bo‘lishini tushuntirish uchun qo‘llanildi. Natijalar zaryad tashish jarayoni energetik moslashuv, tuzoq holatlari va maydon ta’siridagi injeksiya bilan belgilanadi degan xulosani ko‘rsatadi.

Kalit so‘zlar: energetik sathlar moslashuvi; fazoviy zaryad bilan cheklangan tok; $KPbBr_3$ perovskit; peroLED; perovskit asosidagi yorug‘lik chiqaruvchi qurilmalar; tuzoq holatlari; zaryad transporti.

Механизмы переноса заряда и согласование энергетических уровней в peroled-структурах на основе $KPbBr_3$

Аннотация. В работе исследованы механизмы переноса заряда и согласование энергетических уровней в peroLED-структурах на основе неорганического галогенидного

перовскита $KPbBr_3$. Устройство с архитектурой ITO / $KPbBr_3$–PEO / Ga–In было получено методом низкотемпературного растворного синтеза с использованием полимерной стабилизации. Анализ вольт-амперных характеристик (ВАХ) позволил выделить различные режимы проводимости, включая омическую проводимость, инжекционно-ограниченный транспорт, ток, ограниченный пространственным зарядом (SCLC), и режим заполнения ловушек. Энергетическая диаграмма использована для интерпретации процессов инжекции носителей заряда и формирования внутреннего электрического поля. Показано, что перенос заряда определяется энергетическим согласованием, наличием ловушечных состояний и полевым усилением инжекции. Полученные результаты расширяют представления о физике переноса в перовскитных светоизлучающих структурах.

Ключевые слова: ловушечные состояния; перовскит $KPbBr_3$; перенос заряда; перовскитные светоизлучающие устройства; peroLED; ток ограниченный пространственным зарядом; энергетическое согласование.

Introduction. Halide perovskites have emerged as a promising class of materials for optoelectronic applications due to their outstanding electronic and optical properties, including high absorption coefficients, tunable band structures, efficient radiative recombination, and solution-processable fabrication routes. These advantages have enabled rapid progress in devices such as solar cells, photodetectors, and light-emitting diodes. In particular, inorganic halide perovskites have attracted increasing attention as alternatives to hybrid organic–inorganic systems because of their improved thermal stability, reduced sensitivity to moisture, and enhanced structural robustness.

Among various perovskite compositions, bromide-based materials are of special interest for light-emitting applications owing to their favorable bandgap and efficient excitonic emission. While significant research has focused on cesium-based perovskites, potassium lead bromide ($KPbBr_3$) remains comparatively less explored, especially in simplified device architectures designed to investigate fundamental charge transport processes. Understanding the mechanisms governing charge injection, transport, and recombination in such systems is essential for optimizing device performance and improving operational stability.

Charge transport in perovskite-based light-emitting structures is strongly influenced by interfacial energetics and defect-related phenomena. The alignment of energy levels between electrodes and active materials determines carrier injection efficiency and internal electric field distribution, while structural defects such as halide vacancies and grain boundary states introduce trap levels that modify carrier mobility and recombination dynamics. As a result, current–voltage characteristics often exhibit multiple conduction regimes, including ohmic transport, injection-controlled behavior, and space-charge-limited current (SCLC). Detailed analysis of these regimes provides insight into carrier dynamics and device physics.

Recent studies have highlighted the role of polymer-assisted perovskite composites in improving film formation and stabilizing device performance. Incorporating polymer matrices can enhance mechanical stability and partially passivate surface defects, although the resulting energetic disorder may influence charge transport pathways. Investigating how these competing effects impact electrical characteristics is therefore crucial for understanding the operation of simplified perovskite light-emitting structures such as peroLED devices.

The present work aims to analyze charge transport mechanisms and energy level alignment in $KPbBr_3$-based peroLED structures fabricated using a low-temperature solution approach. By combining energy level analysis with experimental current density–voltage measurements, different conduction regimes are identified and interpreted within the framework of injection-controlled transport and trap-mediated dynamics. The obtained results contribute to a deeper understanding of transport physics in inorganic perovskite light-emitting devices and provide insights for improving their performance through defect engineering and interface optimization.

Literature review. All-inorganic halide perovskites have attracted considerable attention due to their unique combination of optical and electronic properties, including tunable bandgap, high absorption coefficients, efficient excitonic emission, and compatibility with low-temperature solution processing. Early studies demonstrated that cesium lead halide perovskites exhibit enhanced thermal stability compared to hybrid organic–inorganic counterparts, which makes them promising candidates for optoelectronic devices operating under practical conditions [1,2]. The ability to tailor bandgap and emission characteristics through compositional engineering and structural modification has enabled significant progress in perovskite-based light-emitting applications [3–5].

Extensive research has been devoted to the synthesis and surface engineering of cesium lead halide nanocrystals, where ligand chemistry and reaction conditions strongly influence optical properties and stability [6–9]. Surface termination, passivation strategies, and defect control play a critical role in determining photoluminescence efficiency and long-term device performance, as defects such as halide vacancies introduce trap states that affect carrier dynamics [10–12]. Various approaches, including ligand-mediated growth, anion exchange reactions, and compositional tuning, have been proposed to optimize nanocrystal morphology and emission properties [13–16].

Recent investigations have emphasized the importance of defect engineering and doping strategies to control optical response and improve luminescent efficiency. Incorporation of transition metal ions or surface passivation layers has been shown to enhance quantum yield and color stability while modifying carrier recombination pathways [17–21]. Additionally, polymer-assisted strategies and surface chemical modifications have been explored to stabilize perovskite nanocrystals and suppress nonradiative recombination processes [22,23].

Despite extensive studies on optical properties, understanding charge transport mechanisms remains essential for improving device performance. Carrier injection and transport in perovskite-based light-emitting structures are strongly influenced by interfacial energetics, trap states, and space-charge effects. Previous works have shown that charge transfer processes and defect-mediated recombination govern electrical characteristics, including nonlinear current–voltage behavior and transitions between conduction regimes [24,25]. Analysis of these regimes provides insight into carrier mobility, trap density, and the role of energetic alignment between electrodes and active layers.

While cesium-based systems have been widely investigated, potassium lead bromide ($KPbBr_3$) remains comparatively less explored, particularly in simplified device architectures aimed at studying fundamental transport processes. Recent studies by Rahmonova et al. demonstrated that $KPbBr_3$ materials exhibit promising optical properties and stability, highlighting their potential for optoelectronic applications [26–30]. However, the mechanisms governing charge injection, energy level alignment, and transport regimes in $KPbBr_3$-based light-emitting structures require further investigation.

Therefore, a detailed analysis of charge transport mechanisms combined with energy level modeling is necessary to better understand the operation principles of $KPbBr_3$-based peroLED devices and to identify pathways for improving their performance.

Materials and methods. Halide perovskite $KPbBr_3$ was synthesized using a low-temperature solution-based ligand-assisted method. Potassium bromide and lead precursor salts were used as starting materials, while dimethyl sulfoxide (DMSO) served as the coordinating solvent to ensure complete dissolution of precursors and controlled crystallization. Oleic acid and oleylamine were employed as stabilizing ligands to regulate nucleation and growth processes and to improve the stability of the perovskite phase. Polyethylene oxide (PEO) was introduced as a polymer matrix to form a composite active layer and to enhance film uniformity and mechanical stability.

The peroLED structure was fabricated on indium tin oxide (ITO)-coated glass substrates, which were used as transparent bottom electrodes. Prior to deposition, the substrates were cleaned using standard solvent treatment procedures to remove organic contaminants and ensure good adhesion of the active layer. The $KPbBr_3$–PEO composite film was formed by solution deposition followed by drying under ambient conditions to remove residual solvent and stabilize the film morphology. A eutectic gallium–indium (Ga–In) alloy was applied as the top contact, resulting in a simple device architecture with the configuration ITO / $KPbBr_3$–PEO / Ga–In.

Electrical characterization was performed by measuring current density–voltage (J–V) characteristics at room temperature using a precision source-measure unit (SMU), such as a Keithley 2400 series instrument or equivalent. Voltage was applied in the range of 0–4.0 V, and the resulting current response was recorded to analyze the charge transport behavior and identify different

conduction regimes. The experimental data were further analyzed through theoretical approximation to determine the dominant transport mechanisms, including ohmic conduction, injection-controlled transport, and space-charge-limited current behavior.

The energy level diagram of the device was constructed using literature values for work functions and electronic energy levels of ITO, $KPbBr_3$, PEO, and Ga–In electrodes. This diagram served as the basis for interpreting carrier injection processes, band alignment effects, and recombination mechanisms responsible for the electrical characteristics observed in the peroLED structure.

Results and discussion. Charge transport in the $KPbBr_3$-based peroLED structure is governed by the combined effects of energy level alignment, defect-mediated trapping, and field-assisted carrier injection. The energy diagram (Fig. 1) illustrates the relative positions of the work functions of ITO and Ga–In electrodes with respect to the conduction and valence band edges of $KPbBr_3$ and the HOMO/LUMO levels of the polymer matrix (PEO). Such energetic alignment enables asymmetric carrier injection and establishes internal electric fields that control charge accumulation and recombination processes within the active layer.

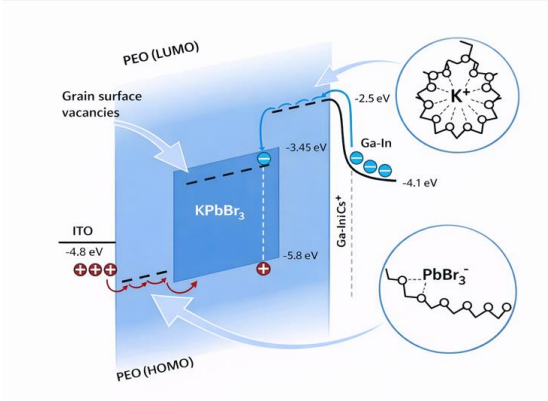


Figure 1. Energy level diagram of the $KPbBr_3$-based peroLED structure.

The evolution of transport regimes with increasing applied voltage reflects a gradual transition from equilibrium carrier transport to injection-dominated conduction. At low voltages, approximately 0–1.2 V, the current density exhibits behavior consistent with ohmic conduction (Fig. 2a), where the injected carrier density remains comparable to the intrinsic carrier concentration. In this regime, transport is primarily governed by drift motion of carriers with limited influence of trap states, indicating relatively efficient initial injection and moderate defect density within the perovskite–polymer composite.

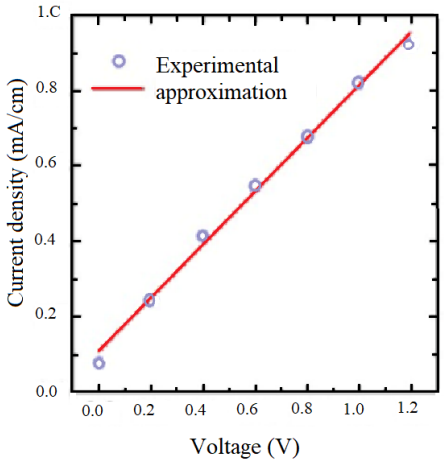


Figure 2. Approximation of experimental J–V characteristics in the ohmic regime.

With increasing applied voltage, in the range of approximately **2.0–3.0 V**, the device exhibits a transition toward diode-like injection behavior, characterized by a nonlinear increase in current density consistent with Shockley-type transport mechanisms. The current density in this regime can be described by the relation:

$$J = J_0(e^{\frac{qV}{nkT}} - 1)$$

where J_0 represents the saturation current density, q is the elementary charge, n is the ideality factor, k is Boltzmann's constant, and T is temperature. The quasi-exponential current growth indicates enhanced carrier injection due to the reduction of interfacial barriers under increasing electric field. The energetic configuration presented in Fig. 1 supports this mechanism, as asymmetric band alignment facilitates carrier injection from both electrodes. However, deviations from ideal diode behavior suggest the involvement of trap-assisted transport and recombination processes.

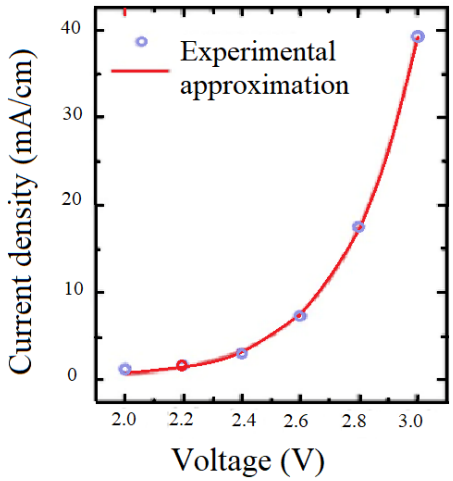


Figure 2b — Space-charge-limited current (SCLC) region

At higher voltages, approximately **2.5–3.5 V**, the transport regime becomes dominated by space-charge effects, as evidenced by the nonlinear current increase shown in Fig. 2b. In this region, injected carrier density exceeds the equilibrium carrier population, leading to charge accumulation and modification of the internal electric field distribution. The current density can be approximated using the Mott–Gurney expression for space-charge-limited current (SCLC):

$$J = \frac{9}{8}\varepsilon\mu\frac{V^2}{L^3}$$

where ε is the dielectric permittivity, μ is carrier mobility, V is applied voltage, and L is the active layer thickness. The observed deviation from ideal quadratic dependence indicates trap-controlled SCLC transport, which is typical for solution-processed perovskite films containing grain-boundary defects and halide vacancies.

Further increase in applied voltage to approximately 3.0–4.0 V leads to the trap-filled limit (TFL), associated with a sharp increase in current density (Fig. 2c). This transition corresponds to the saturation of trap states, after which injected carriers contribute directly to conduction. The filling of traps effectively reduces carrier scattering and increases mobility, enabling more efficient charge transport across the perovskite layer.

According to the energy diagram (Fig. 1), this regime promotes enhanced electron–hole recombination within emissive domains, which is essential for efficient light emission in peroLED structures.

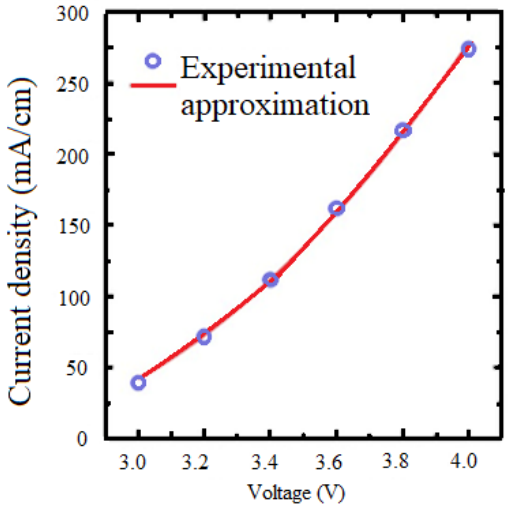


Figure 2c — Trap-filled limit regime at high voltages.

The overall evolution of transport behavior—from ohmic conduction to injection-controlled transport, followed by trap-limited SCLC and finally trap-filled conduction—reflects a complex interplay between energetic alignment and defect physics. Similar transport mechanisms have been reported in halide perovskite optoelectronic devices, where halide vacancies and interfacial energetics strongly influence carrier dynamics. In the $KPbBr_3$–PEO system, the polymer matrix likely provides partial surface passivation while introducing energetic disorder, leading to distributed trap states responsible for the observed transport transitions.

Thus, the combined analysis of the energy diagram and experimentally approximated J–V characteristics reveals that charge transport in the studied peroLED structure is governed by field-assisted injection, trap-mediated carrier dynamics, and space-charge effects. These findings emphasize the importance of controlling defect density and energy level alignment for optimizing the performance of perovskite-based light-emitting devices.

Conclusions.

1. In this work, charge transport mechanisms and energy level alignment in $KPbBr_3$-based peroLED structures were systematically investigated in order to clarify the physical processes governing carrier injection and conduction in inorganic halide perovskite light-emitting devices. The initial motivation of this study was to address the limited understanding of transport behavior in potassium-based perovskite systems compared to more extensively studied cesium analogues, particularly within simplified device architectures designed for fundamental analysis.
2. The combined evaluation of energy level alignment and experimental current density–voltage characteristics revealed a sequential evolution of conduction regimes, including ohmic transport at low applied voltages, injection-controlled behavior described by Shockley-type mechanisms, space-charge-limited current (SCLC), and trap-filled limit conduction at higher electric fields. These transitions demonstrate that charge transport in $KPbBr_3$-based structures is governed by the interplay between energetic band alignment, trap states associated with structural defects, and field-assisted carrier injection processes.
3. The constructed energy level diagram provided a consistent framework for interpreting asymmetric carrier injection and internal electric field formation, explaining the observed nonlinear electrical response. The presence of distributed trap states was identified as a key factor controlling carrier mobility and the transition between transport regimes. Additionally, incorporation of a polymer matrix contributes to structural stabilization while influencing energetic disorder and carrier dynamics within the active layer.
4. Overall, the obtained results provide deeper insight into the transport physics of inorganic $KPbBr_3$ perovskite light-emitting structures and highlight the importance of optimizing energy level alignment and defect engineering to improve device performance. The presented approach demonstrates that simplified peroLED architectures can serve as effective model sys-

tems for investigating fundamental charge transport mechanisms in perovskite optoelectronics and may contribute to the future development of stable and efficient light-emitting devices.

5. Future perspectives include further investigation of interfacial engineering strategies, trap density control, and compositional optimization aimed at enhancing carrier balance and improving electroluminescence efficiency in potassium-based perovskite systems.

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