# بهبود خروجی دیودنورگسیل پروسکایتی بر پایه شبیه سازی

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**چکیده – در این کار، با استفاده از نرم افزار شبیه ساز دو بعدی، دیود نورگسیل پروسکایتی مورد بررسی قرار گرفته‌است و خروجی نوری آن بهینه شده‌است. بهبود کارآیی این افزاره به عنوان تابعی از ضخامت ناحیه فعال واکاوی شد. نتایج نشان می دهد که بیشترین لومینسانس خروجی با لایه پروسکایتی با ضخامت در محدوده 5-20 نانو متر قابل دستیابی است. همچنین، چگالی حالات تله ها که بیانگر کیفیت لایه فعال است، یکی ازفاکتورهای بسیار مهم در بازدهی دیود نورگسیل پروسکایتی به شمار می‌رود. نشان داده شده است با تغییر طول عمر حامل ها از 5 تا 500 نانو ثانیه که نتیجه تغییر چگالی حالات تله ها از $10^{-12}$ برای پلی کریستال به $10^{-16}$ بر سانتی متر مکعب برای تک کریستال است، لومینسانس نور خروجی از 2.75 به 3.26 وات بر متر مربع افزایش یافته است یعنی افزایش 18.5 در صد برای لومینسانس خروجی نور.**

**کلمات کلیدی: دیود نور گسیل پروسکایتی، شبیه ساز یک بعدی، چگالی حالت تله، بازترکیب SRH.**

# Simulation Based Optimization of Optical Output for Perovskite Light Emitting Diode

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*Abstract- In this work, perovskite light emitting diode (PeLED) has been analyzed using two-dimensional simulation and its optical output is optimized. The device performance is investigated as a function of the perovskite thickness, as the active layer. The result reveals that the highest luminescence can be achieved by a perovskite layer with a thickness in the range of 5-20 nm. Furthermore, the density of trap states which indicates the quality of the active layer, is considered as one of the most substantial parameters to improve the efficiency of PeLEDs. It is shown that by increasing the lifetime of the carriers from 5 ns to 500 ns as a result of density of trap states reduction from $10^{-12}$ $cm^{-3}$ for polycrystalline to $10^{-16}$ $cm^{-3}$ for single crystal perovskite, the maximum luminous power enhances from 2.75 $W/m^2$ to 3.26 $W/m^2$ i.e. 18.5% increment in luminous power.*

*Keywords: Perovskite light emitting diodes, two-dimensional simulation, Trap density of state, SRH recombination*



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## 1 Introduction

Organometal halide perovskites have been regarded as promising materials for optoelectronic applications with high efficiency such as solar cells[1], photodetectors [2] , optical amplifiers, light emitting diodes (LEDs), and laser diodes [3]. In 2014, the first high-brightness infrared and visible electroluminescence (EL) from solution-processed perovskite materials was demonstrated at room temperature [4].This extraordinary feature, along with other unique electrical and optical properties represent perovskite materials as appropriate candidates for high-performance, large area and low cost LEDs [4, 5]. The high colour purity of perovskite with full width at half maximum (FWHM) less than 20 nm distinguish the PeLEDs from conventional LEDs and introduce them as promising candidates for future LEDs [5] .

In spite of rapid progress in the efficiency of PeLED, the operation mechanism and factors affecting PeLEDs performance still have not been fully understood. PeLED can be considered as a device with thin-film structure similar to thin-film compound semiconductor LEDs, such as GaAs that consist of flat layer stacks.

The basic difference between organic and inorganic materials, which used for LEDs as emission layer is exciton type. In typical organic light emitter, the exciton is Frenkel-type. However, perovskite materials have Wannier-type excitons with low exciton binding energy such as $E_b$ ~ 76 or 150 meV for $CH_3NH_3PbBr_3$[5] . In this work, the PeLED is simulated and analyzed. The effect of the active layer thickness and the density of trap states on the device performance is investigated and the optimum conditions are determined.

## 2 Device structure and parameters

Figure 1 shows the schematic structure of the simulated device. As observed, the device has a multilayer structure that consists of ITO/ PEDOT:PSS / $CH_3NH_3PbBr_3$ /ZnO / Ag . The material parameters for PeLED used in simulation has been selected from reported experimental works and shown in Table 1.

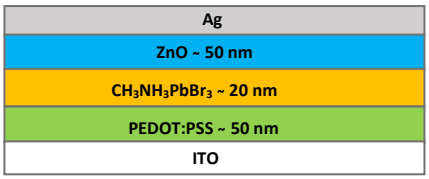



Figure 1. The device architecture of PeLED used in simulation with $CH_3NH_3PbBr_3$ as an active layer.

## 3 Optical and electrical models and parameters

The carrier concentration dependent total recombination rate leading to spontaneous emission can be quantitatively described by the following equation [6, 7] :

$$\frac{dn(t)}{dt} = -k_1\, n(t) - k_2\, n^2(t) - k_3\, n^3(t) \quad (1)$$

Where n (t) is the charge carrier density and $k_1$, $k_2$ and $k_3$ denote the monomolecular, bimolecular and trimolecular recombination rate constants.

Table 1. Material parameters for PeLED used in simulation [7-10].

| Parameter | PEDOT:PSS | $CH_3NH_3PbBr_3$ | ZnO |
|---|---|---|---|
| Thickness (nm) | 50 nm | 10-500 nm | 50 nm |
| $N_A$ ($cm^{-3}$) | $1.0 \times 10^{18}$ | $2.0 \times 10^{15}$ | - |
| $N_D$ ($cm^{-3}$) | - | - | $1.0 \times 10^{18}$ |
| $\varepsilon_r$ | 3 | 18 | 9 |
| $\chi$ (eV) | 2.45 | 3.6 | 4 |
| $E_g$ (eV) | 2.8 | 2.3 | 3.3 |
| $\mu_n$ ($cm^2$ / Vs) | $2 \times 10^{-4}$ | 30 | 100 |
| $\mu_p$ ($cm^2$ / Vs) | $2 \times 10^{-4}$ | 30 | 25 |

### 3.1 Radiative recombination

The simplest carrier decay process is spontaneous band-to-band recombination. Radiative recombination rate without momentum conservation can be written as [11]:

$$R_{np}^{OPT} = B_r\, np \quad (2)$$

$B_r$ is related to transition probability and defined as the coefficient for band-to-band recombination. n and p are the electron and hole concentrations. The total band-to-band recombination is:



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$$R_{np}^{ex} = B_r\,(np - n_i^2) \qquad (3)$$

The $n_i$ is the intrinsic carrier concentration and its value for perovskite is $1.97\times10^7$ $cm^{-3}$.

### 3.2 Auger recombination

Auger recombination has been modelled using the following expression:

$$R_{Auger} = C_n\,(pn^2 - n_0 n_i^2) + C_p(np^2 - p_0 n_i^2) \qquad (4)$$

where $C_n$ and $C_p$ are the Auger coefficients.

### 3.3 Shockley-Read-Hall (SRH) recombination

The basic SRH recombination as a result of trap states in band gap is modelled as follows:

$$R_{SRH} = \frac{pn - n_i^2}{\tau_{n0}\left[p + n_i exp\left(\frac{E_i - E_t}{k_b T}\right)\right] + \tau_{p0}\left[n + n_i exp\left(\frac{E_t - E_i}{k_b T}\right)\right]} \qquad (5)$$

$k_b$ is Boltzmann's constant and $E_i$ and $E_t$ are the intrinsic Fermi level and trap energy level, respectively. $\tau_{n0}$ and $\tau_{p0}$ are the electron and hole lifetimes, respectively.

By solving Poisson equation along with electron and hole continuity equations, the current density- voltage curves are obtained.

The Auger, SRH and radiative recombination rate are included in the recombination term in the carrier continuity equations. According to equation 1 the values of the radiative and nonradiative constants for perovskite film has been obtained from experimental data [6, 7] and shown in Table 2.

Table 2. The values of the radiative and nonradiative constants for perovskite film[6].

| | $k_1$ ($\mu s^{-1}$) | $k_2$ ($cm^3\ s^{-1}$) | $k_3$ ($cm^6\ s^{-1}$) |
|---|---|---|---|
| $CH_3NH_3PbBr_3$ | 27.2 | $4.9\times10^{-10}$ | $13.5\times10^{-28}$ |

## 4 Results and discussion

The thickness of the emission layer is one of the most important parameters to determine the performance of PeLEDs. Here, the impact of $CH_3NH_3PbBr_3$ thickness on the optical output of the device is investigated. The I-V (Current-Voltage) curves are shown in Figure 2 and the luminous-Current curves are presented in Figure 3. From these results we can find that the optical output of PeLED increases with decreasing the thickness of perovskite layer. In Figure 2 we can see that for 5 nm perovskite thickness the maximum current passing through active layer at 7 V is greater than other. The thinner perovskite layer leads to lower resistance and thus higher current. A large current means that the number of carriers that reaches to active layer is high. The luminous power of PeLED with 5 nm perovskite thickness is greater than other as a result of higher current, which show in Figure 3. The maximum current efficiency of PeLED for different perovskite thickness 3, 5, 20, 50, and 100 nm calculated 0.66, 0.74, 0.71, 0.68, and 0.61 cd/A, respectively. These results show that the optimum thickness for PeLEDs is 5 nm. Considering device manufacturing constraints, we introduce the optimum 20 nm thickness for perovskite layer which is consistent with the experimental data [4] . It should be noted that the maximum luminous power of 3.3 $W/m^2$ is equivalent to 2186 $cd/m^2$ that in line with experimental data[12].

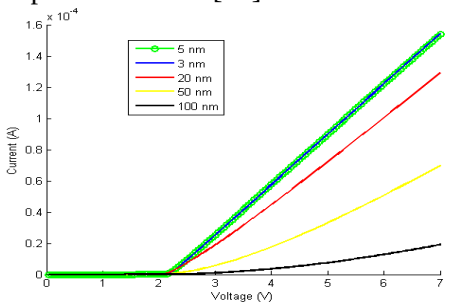



Figure 2. The I-V curves for different perovskite thicknesses.

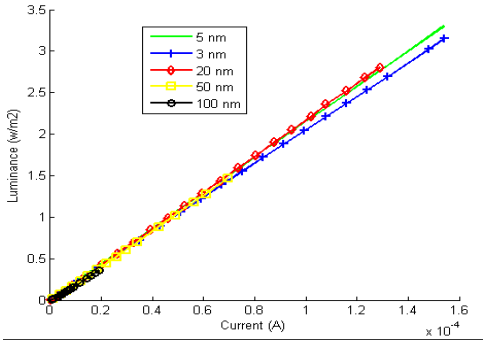



Figure 3. The luminous-current curves for different perovskite thicknesses.

In addition to thickness, the quality of active layer is regarded as one of the most substantial parameters to improve the efficiency of PeLEDs. Model that obtains the impact of emission layer quality on the efficiency of PeLEDs is SRH recombination. According to equation 5, by

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changing the carrier lifetime which is proportional to the defect density, the impact of active layer quality on the device performance can be obtained. It is revealed that in the perovskite layer with lower density of trap states and higher carrier lifetime, SRH recombination reduces and subsequently leads to the device performance enhancement. Figure 4 shows that by increasing the lifetime of the carriers from 5 ns to 500 ns as a result of density of trap states reduction from $10^{-12}$ for polycrystalline to $10^{-16}$ for single crystal perovskite, the maximum luminous power enhanced from 2.75 W/m$^2$ to 3.26 W/m$^2$ i.e. 18.5% increasing in luminous power. In addition, the maximum current efficiency enhanced from 0.71 cd/A to 0.76 cd/A.

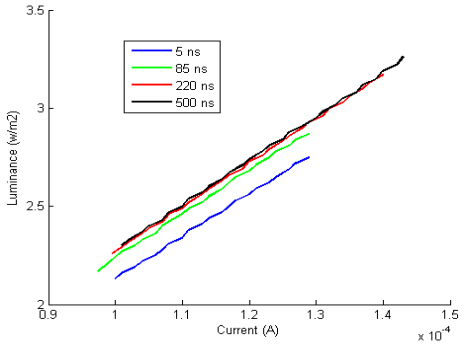



Figure 4. The luminous -current curves for different carrier lifetimes.

## 5 Conclusion

In summary, perovskite LED was electrically and optically simulated and analysed. The effect of active layer thickness on the performance was investigated and the optimum value for achieving the highest efficiency was determined to be in the range of 5-20nm. Further, the performance of the device was investigated as a function of the density of trap stats in perovskite layer. It was revealed that by reducing the defect density and enhancing charge lifetime, the SRH recombination decreases and the device efficiency improved.

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