# Modeling of Carrier Transport and Exciton Diffusion in Organic Light Emitting Diodes with Different Doping Effects

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***Abstract*—In this paper, we use Poisson and drift-diffusion solver, effective Gaussian shape density of state model and Poole-Frenkel field dependent mobility model to simulate organic light emitting diode. Furthermore, to describe the model exactly, we also considered the mechanism of exciton diffusion and exciton annihilation. Finally, we study the influences of different doping region to the IV and exciton diffusion mechanism.**

***Keywords*—1D model, Exciton, BImBP, FIrpic, OLED**

## I. Introduction

In recent years, organic materials are getting more and more popular. Due to their applications in display and solid state lighting applications. However, because the organic material is unstable in common, which makes it hard to provide a reliable commercial product. Therefore, new materials for lighting applications especially for blue are very important. The current trend is to use Firpic as dopants as the blue light source and founding a good host material to improve the device performance.

As we know, organic materials are quite different from inorganic semiconductors including the distribution of density of states and the mechanism of mobility. The carrier transport is known as hopping process. In 1993 [1], Bässler et. al. presented Gaussian-like Density of State to describe the state distribution in organic materials. The hopping process can be described with this Gaussian shape density of states models. The shape of Gaussian shape of tail states can be determined by absorption spectrum or molecular simulations. In this paper, the structure of OLED, we use is shown in Fig.1. We do not only model the carrier transport and recombination behavior but also calculate exciton diffusion equations. Finally, we had modeled three different doping area cases to studied the influence of carrier transport and recombination behavior.

## II. Methodology

According to the absorption spectrum of organic materials, there are some Gaussian-like DOS and some tail state near the occupied orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). In this paper, we use Gaussian-like DOS to describe the material properties. (1)

$$N_{tail,dos}(E) = N_t \frac{1}{\sigma\sqrt{2\pi}} exp\left[-\frac{(E-E_t)^2}{2\sigma^2}\right] \quad (1)$$

where $N_t$ is totally Gaussian-like DOS, $\sigma$ is the FWHM of the Gaussian-like DOS, $E_t$ is the depth of DOS.

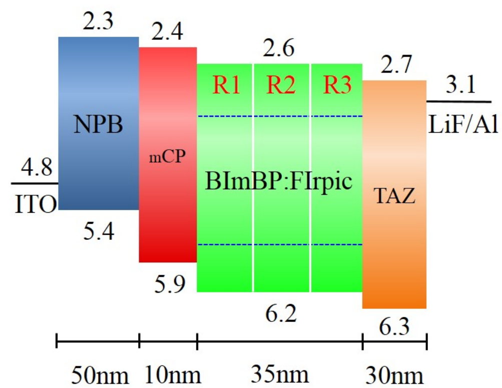



Fig. 1: Structure of OLEDs, where NPB is the hole injection layer (HIL), mCP is the hole transport layer, BImBP:FIrpic is the emitting layer (EML) and TAZ is the electron transport layer (ETL).

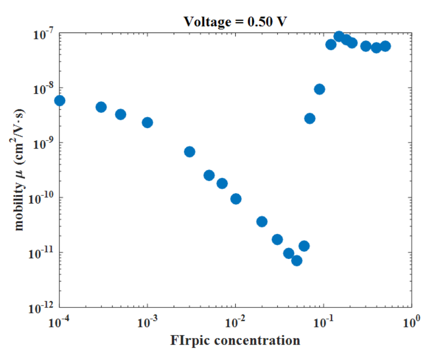



Fig. 2: We have calculated the mobility after doping.

Then, we use the Poole-Frenkel field dependent mobility (2) to describe the behavior of mobility. When the electrical field is increased, the mobility becomes large. [2]

$$\mu = \mu_0 \times exp\left(\beta\sqrt{E}\right) \quad (2)$$

where $\mu$ is the mobility, $\mu_0$ is the mobility when electrical field is equal to zero , $\beta$ is the factor of the field dependence, and $E$ is the electrical field.

TABLE I: Simulation parameters settings for OLED

| Material | $N_{te}\ (cm^{-3})$ | $E_{te}(eV)$ | $\sigma_e(eV)$ | $N_{th}\ (cm^{-3})$ | $E_{th}(eV)$ | $\sigma_h(eV)$ | $\mu_{0e}\left(\frac{cm^2}{Vs}\right)$ | $\beta_e\left(\frac{cm^{0.5}}{V^{0.5}}\right)$ | $\mu_{0h}\left(\frac{cm^2}{Vs}\right)$ | $\beta_h\left(\frac{cm^{0.5}}{V^{0.5}}\right)$ |
|---|---|---|---|---|---|---|---|---|---|---|
| NPB | $1 \times 10^{21}$ | 2.3 | 0.15 | $1 \times 10^{21}$ | 5.4 | 0.13 | $1 \times 10^{-7}$ | 0.005 | $2 \times 10^{-4}$ | 0.0015 |
| mCP | $1 \times 10^{21}$ | 2.4 | 0.15 | $1 \times 10^{21}$ | 5.9 | 0.15 | $4 \times 10^{-5}$ | 0.00426 | $1.2 \times 10^{-4}$ | 0.00254 |
| FIrpic | $8 \times 10^{19}$ | 2.6 | 0.3 | $8 \times 10^{19}$ | 5.8 | 0.3 | $1.1 \times 10^{-9}$ | 0.096 | $1.1 \times 10^{-10}$ | 0.0084 |
| BImBP | $1 \times 10^{17}$ | 2.6 | 0.111 | $1 \times 10^{17}$ | 6.2 | 0.111 | $1.9 \times 10^{-9}$ | 0.0101 | $6.0 \times 10^{-10}$ | 0.0025 |
| TAZ | $1 \times 10^{21}$ | 2.7 | 0.07 | $1 \times 10^{21}$ | 6.3 | 0.08 | $8.57 \times 10^{-6}$ | 0.003 | $1.4 \times 10^{-8}$ | 0.0035 |

Recently studies have shown that the change in mobility is not linear variation with doping concentration.[3][4] Hence, to simulate the doping effect, we use 2D simulation with random dopants that developed by our laboratory. We have calculated the electron mobility after doping (Fig.2). Afterwards, we take this result into the 1D simulation. Finally, we calculate the exciton diffusion equation.(3) Since, the light emitted from OLED is decide by exciton distribution, we consider the exciton diffusion behavior by modeling following equations.

$$\frac{\mathrm{d}n_{ex}}{\mathrm{d}t} = D\nabla^2 n_{ex} - (K_r + K_{nr})n_{ex} - \gamma {n_{ex}}^2 + G_r \quad (3)$$

## III. Results And Discussion

We has demonstrate three cases, case 1, case 2 and case 3. The case 1 means non-doping case. The case 2 means the EML was doped by 12% FIrpic. And case 3 means the EML was partially doped by 12% FIrpic at R1 and R2 (shown in Fig.1). Fig.3 shows the current-voltage curve of experiment and simulation. At doping region, we set electron mobility of doping layer as $10^{-12}$ (cm$^2$/Vs) and hole mobility is $2\times10^{-12}$ (cm$^2$/Vs). And we set $\beta_e$ and $\beta_h$ as 0.0096 (cm$^{0.5}$/V$^{0.5}$) and 0.0092 (cm$^{0.5}$/V$^{0.5}$). The mobility is calculated by 2D random dopants simulation. We compared the J-V curve for all cases. This result proved our simulation tool is correct and credible. Then we use exciton diffusion equation (3) to solve the exciton distribution (shown in Fig. 4(a)).

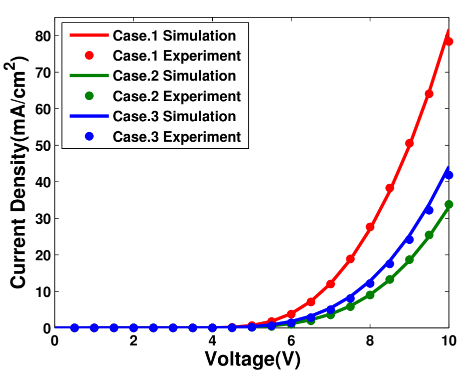
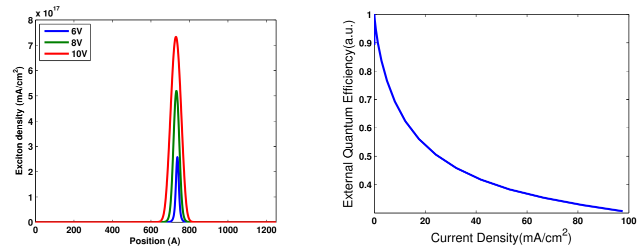



Fig. 3: The current-voltage curve of experiment and simulation. Red line means result of case.1, blue line means result of case.2 and green line means result of case.3. The dot is experiment data, the solid line is simulation result.




(a) The exciton distribution with variable bias voltage.

(b) The quantum efficiency, and we can observe the efficiency droop effect.

Fig. 4: We calculated the exciton distribution including exciton diffusion and exciton annihilation.

## IV. Conclusion

In this paper, we calculated not only the Poisson-drift diffusion equation but also used exciton diffusion equation to solve distribution of excitons. And we use 2D random simulation to calculate mobility of doping layer. We can get correct current-voltage curve with different doping region.

## V. Acknowledgments

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