



## PROPERTY OF FLUORESCENT HOST MATERIAL ALQ3 ORGANIC LIGHT EMITTING DIODE DEVICE

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### Abstract

We report our simulation study for different physical parameters of Organic Light Emitting Diode (OLED). The energy level of organic material consisting of highest occupied molecular orbital (HOMO) and Lowest occupied molecular orbital (LUMO) study with respect to vacuum level under different stack layer contact. Thus, significant improvement in external quantum efficiency (EQE) 76%&58% is observed in bi layer OLED device for emission layer thickness 120 nm and 160 nm thicknesses. We also addressed the maximum power conversion efficiency 20% for bias voltage 12V. CIE curve of absorbance were studied at a different angle and different Emission layer thickness and observed maximum emission for 120nm EML. We obtained the maximum Emission for OLED in the wavelength region of 300-480nm.

### 1. Introduction

The last decades, Organic Light emitting diode (OLED) have focused much attention toward because of their low operating voltage, high Resist, fast response time, crystal clear picture with wide viewing angle [1]. The invention of OLED leads to the study of variation in different physical parameters phenomenon [2]. For mobile, lighting and display, the power conversion efficiency, EQE, *etc.* become an important parameter for further optimization to enhance the efficiency of the device [3]. The key issue associated with the power efficiency of OLED device was coupling efficiency in which internally light generated were coupled out of the device that also depends upon the type of substrate and the typical external coupling

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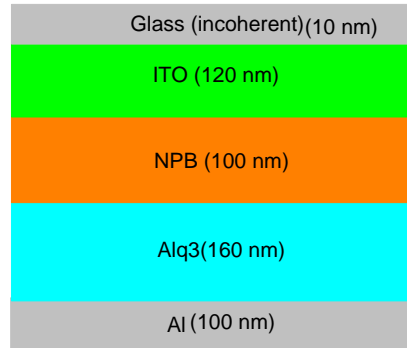
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efficiency is nearly 17%[4]. The coupling efficiency of external, substrate and ITO/organic modes from classical ray theory of optics are 18.9%, 34.2%, and 46.9% and variation in emission layer thickness around 24-52% [5]. It follows that Modeling of the device is important for the study of OLED before the fabrication so that device can be optimized for a better result, thus a lot of research carried out for a better result in OLED [6-12]. In this paper, the typical organic Electro-Luminescent layer of OLED is sandwiched between two metal cathodes. We defined an OLED structure in which we used NPB (*N*, *N'*-b is (naphthalen-1-yl)-*N*, *N'*-b is (phenyl)-benzidine) as an HTL (hole transport layer) and Alq3 (Tr is (8-hydroxy-quinolino) aluminium) as an EML (emission layer). In this paper, we study optical and electrical property, some of the parameter like EQE and power conversion efficiency, etc. As for how the physical parameters of the OLED device will get affected by varying the thickness of the emission layer or by varying the applied bias voltage. In this paper, the electrical and optical property of OLED Performed into the following section. Section 1.1 contains a brief description of the device structure. Section 1.2 contains mathematical modeling, section 1.3 contains result & discussion.

**1.1. Device Structure:** We employ the basic bi layer structure as shown in figure 1.1-Glass (incoherent) 10 nm as a substrate /ITO (indium tin oxide) 120 nm, anode /NPB (*N*, *N'*-b is (naphthalen-1-yl)-*N*, *N'*-b is (phenyl)-benzidine) is an HTL (hole transport layer) of thickness 100 nm/ Alq3(Tris (8-hydroxy-quinolino) Aluminium) is an emissive layer of thickness 160 nm /Al (Aluminium) 100 nm act as a cathode. The basic bi layer OLED is called device. In which organic layer have a different energy level of HOMO and LUMO. Thus, due to the difference in energy level barrier is formed. Under the action of applied bias voltage, hole from anode and electron from cathode face an energy barrier and due to which hole gather at one side of interface and electron gather another side of interface and recombination between electron and hole takes place at EML (electron emission layer) where singlet or triplet exciton (an exciton which is a coulombically bound form of electron-hole pair) which emit light during decay. The energy difference between HOMO and LUMO define the associated color of light [13]. In this paper, we present basic bilayer OLED structure and we sweep the voltage to study the

variation in electron and hole current and also, we sweep the angle and thickness of emission layer to obtain the CIE curve in absorbance.



**Figure 1.** Represents the schematic diagram OLED device.

**1.2. Mathematical Modelling:** The physical parameters of a device depend upon the property of each layer including their energy level, cathode and anode work function, etc. To study the effect of physical parameters we used commercially available software. This used the finite element method and Scharfetter-Gummel technique to solve electrical property and dipole antenna model to solve the optical property of the device, charge transport and recombination following equation was used [14, 15].

$$J_e(x) = e\mu_e(x, E)n(x)E(x) + D(\mu)\frac{dn(x)}{dx} \quad (1)$$

$$\frac{dE(x)}{dx} = \frac{\varepsilon}{\varepsilon\varepsilon_0} [p(x) - n(x)], \quad (2)$$

where in equation (1)  $J_e$  describes the net current of electrons and holes,  $n$  is the density of electrons,  $p$  the density of holes,  $E$  is an electric field and equation is a combination part of drift and diffusion term that satisfies the poisson equation,  $D$  is a Ficki an diffusion constant connate to the charge mobility by the Einstein relation  $eD - \mu kT$ . For optical property we used following a set of the equation: To calculate the layer absorbance and external quantum efficiency, we used the ollowing set of an equation

$$F = \int_0^\infty f(u)du, \quad (3)$$

where  $f(u)$  represents the optical feedback and radiation at any given position and for external quantum efficiency

$$EQE = \eta_{cb}\eta_{st}\eta_{rad}\eta_{out}, \quad (4)$$

where  $\eta_{cb}$  is a charge balance and depend upon injection of charge carrier from an electrode to the organic layer,  $\eta_{st}$  gives a fraction of exciton 0.25 for singlet and 0.75 for the triplet,  $\eta_{rad}$  radiative efficiency and  $\eta_{out}$  is an out-coupling efficiency. To calculate Commission Internationale de  $L$  'Eclairage (CIE) in 1931, which is used to standardize the color perception and from this obtain weighting function  $(x, y, z)$ . Their color matching function.

$$X = \int_0^\infty S(\lambda)x'(\lambda)d\lambda \quad (5)$$

$$Y = \int_0^\infty S(\lambda)y'(\lambda)d\lambda \quad (6)$$

$$Z = \int_0^\infty S(\lambda)z'(\lambda)d\lambda, \quad (7)$$

where  $S(\lambda)$  spectral power distribution and chromaticity values  $[x, y]$  which are calculated from the tristimulus values as:

$$x = \frac{x}{X + Y + Z} \quad (8)$$

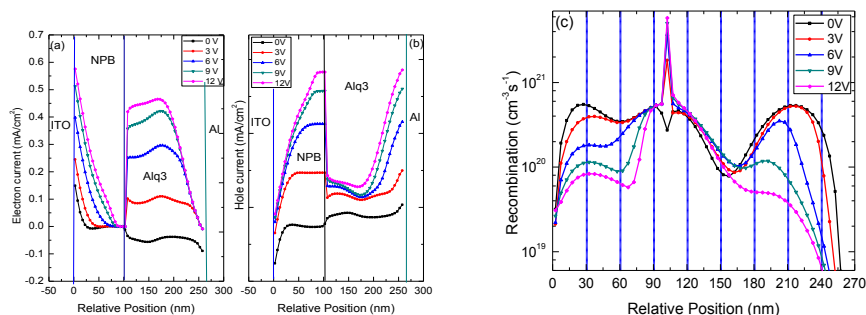
$$y = \frac{y}{X + Y + Z} \quad (9)$$

and  $z = 1 - x - y$ , third chromaticity.

### 1.3. Result and Discussion:

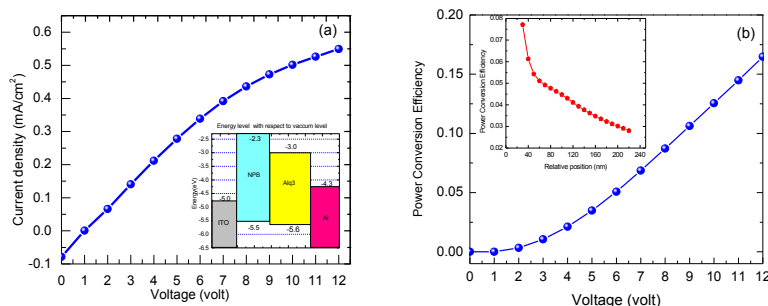
The electrical property of a device derived from equation 1-2. We did the simulation & obtained the electron and hole current under vary distance from the electrode to the organic layer at the different applied voltage as shown in figure 2(a, b). A sharp fall from 0-100nm in electron current is observed in figure 2(a) and increase in hole current in figure 2(b) from 100-260 nm a broad but fluctuating increase of electron current observed to 200 nm under different applied bias voltage, afterward, it falls sharply as shown in figure

2(a). Similarly, in figure 2(b) a constant but fluctuating observed hole current to 180nm afterward start increasing rapidly. As the mobility of HTL is greater than EML hence slow movement of an electronic affected because of lower mobility. Accumulation of electron from cathode/EML gradually move toward EML/HTL interface and from relative position of Alq3 within below 170 nm and above 110 nm a better recombination takes place in EML, as we see, we take 120 nm thickness of emission layer and observed maximum efficiency 76% in figure 4 as shown below.

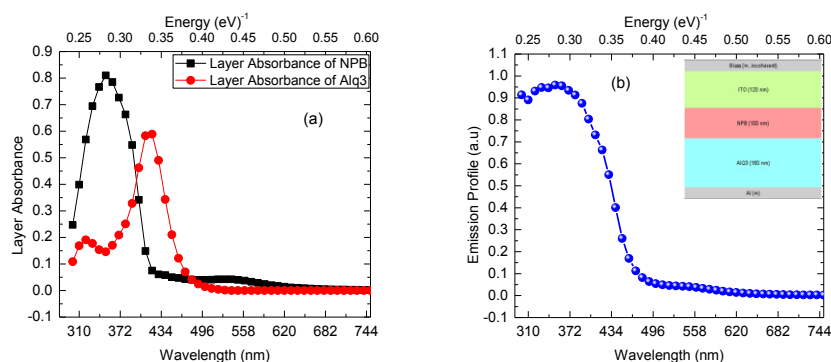


**Figure 2.** Variation of (a) Electron current (b) Hole current (c) Recombination profile for different bias voltage under varying distance from anode to the cathode electrode.

The variation in mean current density observed for different value of applied bias voltage as shown in figure 3(a). It showed a low value of driving voltage because of good transport between NPB/Alq3 organic layer and shows the linear relationship to 5V & after 5V it bends away from the linear relationship. This affects the recombination profile as shown in figure 2(c). The energy level of organic material consisting of highest occupied molecular orbital (HOMO) and Lowest occupied molecular orbital (LUMO)) study with respect to vacuum level under different stack layer contact in figure 3(a). We also addressed the maximum power conversion efficiency 20% for bias voltage 12 V shown in figure 3(b). This increase with the increased of applied voltage but it decreases with an increase of emission layer thickness that also affects the EQE.



**Figure 3.** Variation of (a) mean current density (b) Power conversion efficiency of OLED device for different value of applied bias voltage.

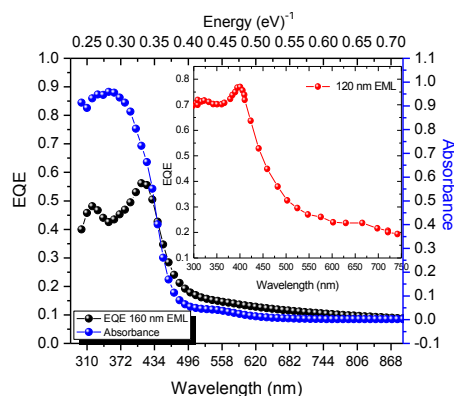


**Figure 4.** (a) Layer absorbance (b) emission profile variation for different value of wavelength.

The layer absorbance of hole transport layer NPB and Alq3 (which act as both missions as well as an electron injecting layer) observed for different value of wavelength shown in figure 4(a). In the wavelength region 300-420 nm, NPB layer absorbance increase to 360 nm wavelength than after it starts decreasing to wavelength 420 nm. For wavelength region 420 nm-750 nm a low absorbance observed for layer NPB. Organic layer Alq3 absorbance start increasing from wavelength 300 nm-320 nm and then decreasing, after 340 nm start again increasing and then observed fall in absorbance to wavelength 490 nm after very low absorbance observed. Figure 4(b) shows the emission profile of the total stack of OLED layer, 90% emission observed in wavelength

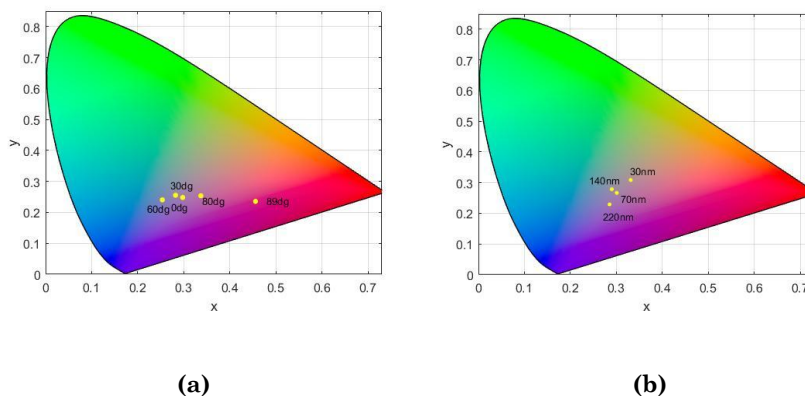
300-390nm after 440 nm onward a low emission observed in OLED stack. As absorbance or emission depend upon reflectance and transmittance which further depend upon refractive index profile of the organic layer.

The external quantum efficiency 40%-58% in the wavelength region 300-440nm for emission layer Alq3 have thickness 160nm and maximum EQE nearly 76% at EML thickness of 120 nm shown in figure 5 comparing with [6] HTL as PVK/Alq3 as EML has an EQE 24-52%. Total absorbance 80%-90% in same above wavelength region, as from thermodynamic principal a good absorber is a good emission of light.



**Figure 5.** Comparison of external quantum efficiency for different wavelength under fixed applied voltage 5V & total absorbance profile.

The  $x$ ,  $y$  coordinate of chromaticity observed at different viewing angle & thickness variation of Alq3 emission layer. This coordinate was represented in a slanted horseshoe, as all the color lies in the slanted horseshoe-shaped region. For Absorbance CIE ( $x$ ,  $y$ ) value represented with specified as string number and we concluded color observation that further depend upon the absorption characteristic of the active layer.



**Figure 6.** CIE curve plotted at (a) different viewing angle in degree (dg) (b) different emission layer thickness indicates the expected color under Absorbance.

**1.4 Conclusion:** The simulation of OLED device studied under various physical parameter conditions for better device performance and obtained maximum EQE 76% & 58% 120nm and 160nm thickness of EML. We also addressed the maximum power conversion efficiency 20% for bias voltage 12V. The maximum layer absorbance and emission profile in wavelength region 300-480nm. CIE graph shows the emitting region of light studied for absorbance at a different angle and different emission layer thickness show the maximum absorption for 120nm thick EML that further depend upon the absorption property of the active layer and refractive index.

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