Investigation of Efficient Hole Injection Layer for Enhancement of Opto-Electrical Properties of an Organic Light Emitting Diode

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Abstract. A multilayer Organic Light Emitting Diode (OLED) has been simulated and analysed for the investigation of an efficient Hole Injection Layer (HIL). Study includes the simulation of different devices which comprises of the different materials as HIL. Three devices have been simulated and their characteristics have been extracted to compare the electrical and optical properties of the OLEDs. It has been found that the device with HAT-CN as HIL has achieved the highest value of the current at the mentioned applied voltage and hence the current density. There is drastic enhancement in the current density of the device when an HIL is inserted in comparison to when it is not used in the OLED. Also, there is an approximate enhancement of around 20% in the device performance when HIL is changed from MoO3 to HAT-CN. The device without any HIL included has the highest electric field at the given voltage. Optical characteristics of the device includes Electroluminescence Intensity with respect to the varying wavelength and it has been observed that OLED achieved the maximum light intensity at an approximate wavelength of around 320 nm.

Keywords: Organic Light Emitting Diode, HAT-CN, Hole Injection Layer, Electroluminescence Intensity.

1. Introduction
Organic Light Emitting Diodes (OLEDs) have registered with capable emissions in flat-panel displays, display screens etc substituting displays in LEDs or cathode ray tubes (CRTs). Solid-state lighting applications of OLEDs make it informal to fabricate flexible displays. OLEDs can be stated as thin-film light-emitting devices in which organic semiconductor layer is sandwiched. OLEDs generally comprise of a thin film of organic layer crammed between two electrodes termed as anode and cathode. Light is generated as a result of recombination of holes and electrons injection at the electrodes [1]–[3].

Some of the applications for OLED displays demand highly reliable response and its high readability. This may mainly include some digital devices like television displays, computer screens, small displays like screens of Android phones, portable gaming consoles and some mini-screens. OLEDs also attains some recompenses like it results in less consumption of power and deliver high-quality displays in addition to high efficiency, large colour fidelity and highly stable in its operation. OLEDs exhibit the semiconductors that have wide energy gap in them and they involve singlet and triplet exciton phenomenon of radiation when compared with that of LEDs and LCDs. This phenomena makes OLEDs capable of consuming less power and hence can be considered for use in devices such as android phones, portable gaming consoles, media players, digital cameras etc [4]–[6].

OLED device can consist of a single layer or it can have multiple layers. This can include buffer layers like hole injection layer (HIL), electron injection layer (EIL), transport layers i.e., hole transport layer (HTL), electron transport layer (ETL), electron and hole blocking layers, emitting layer and electrodes. For efficient injection of charge carriers, HTL and ETL should have high hole and electron
mobilities respectively. This property makes it capable of injecting the charge carriers from the electrodes towards EML. In addition to transport layers, buffer layers can be inserted in an OLED structure which will help in reducing the energy barrier which will ease the transport of carriers towards the emitting side [7][8][9]. Intensity of light from the emitting layer depends on the applied electric field. Sometimes blocking layer has to be added in the structure in order to prevent the carriers to move to the opposite electrodes which can reduce the efficiency of the device [10]. In the present work, insertion of an efficient HIL has been investigated in the OLED. Initially the device with and without HIL has been analysed and then the selection of a perfect HIL has been investigated by comparing the results from different HIL materials. Selection of a proper HIL in a device is very important since it affects the efficacy and constancy of the device which results in creating a barrier at the interface between HIL and EML or HTL and EML interface. The examples of some HIL materials can be given as PEDOT: PSS, Molybdenum trioxide (MoO3), HAT-CN, Rhenium Oxide (ReO) etc. Insertion of such layer in the device has the capability of modifying the electronic properties of the device [11][12].

The paper is organized as given. Section 1 includes introduction to the structure and materials included for its simulation. Section 2 explains the simulation model. Section 3 discusses the mathematical model for the structure and physics involved with it. Section 4 discusses the results and discussion related to it.

2. SIMULATION MODEL

A general and simplest structure of an OLED consists of an organic layer amalgamated between two electrodes i.e., anode and cathode. Other layers like HTL, ETL, EIL, HIL etc can be inserted in the structure to improve the efficiency of the device both in terms of electrical as well as optical characteristics. Figure 1 shows the structures that are simulated in this study. Figure 1 (a) shows an OLED which consists of 2, 7-bis [N, N-bis (4-methoxy-phenyl) amino]-9, 9-spirobifluorene (Meo-Spiro TPD) as HTL, 4,4'-N, N dicarbazolylbiphenyl (CBP) with 5% fac-Tris(2-phenylpyridine) iridium (Ir(ppy)3) acts as a host-guest system, Alq3 is the emitting layer, Lithium Fluoride (LiF) is the buffer layer and Indium Tin Oxide (ITO) and Aluminium (Al) are acting as electrodes. HIL is not used in the structure shown in figure 1(a). Figure 1 (b) when compared with 1 (a) consists of a HIL in addition to the conventional OLED structure in 1 (a). For the simulation in this paper, MoO3 and HAT-CN materials are used as HIL to investigate the electro-optical properties of the devices. These two materials are selected for the said investigation because they are proved to be effective HILs in the literature [11], [13].

![Diagram of OLED structures with and without HIL](image-url)

Figure 1. (a) OLED structure without HIL (b) OLED structure with HIL inserted

Figure 2 shows the silvaco structure of all the devices simulated for the study. For the analysis, device 1 in figure 2 (a) is simulated with no HIL, device 2 in figure 2 (b) consists of MoO3 as one of the HIL.
and device 3 in figure 2(c) consists of HAT-CN layer as HIL. Simulation results of the three structures are compared for the study and analysis of the device.

Figure 2. (a) Silvaco structure with no HIL inserted (b) Silvaco structure with MoO3 as HIL (c) Silvaco structure with HAT-CN as HIL

3. MATHEMATICAL MODEL
As reported in ref. [14], amount of light that can be loosed while passing a substrate i.e. \( n_{cp,ext} \) is

\[
\frac{1}{2n_{org}^2} \approx n_{cp,ext}
\]

where \( n_{cp,ext} \) is external out-coupling efficiency. Amount of light bound in the substrate can be given as \( n_{cp,sub} \) and in the ITO/ organic layers as \( n_{cp,org} \) i.e.

\[
n_{cp,sub} = Cos\theta_{org,c1} - Cos\theta_{org,c2}
\]

Also,

\[
n_{cp,org} = Cos\theta_{org,c2}
\]

where \( \theta_{org,c1} \) is the critical angle between organic and air and \( \theta_{org,c2} \) is the critical angle between organic and substrate. According to this theory, a large amount of generated light is intent at the interfaces or emitted only from the boundaries of device. Most OLED manufacturers used micro-cavity concept to reduce these losses and enhance the device characteristics [14][15].

For current injection, Richardson Thermionic emission law is used. Current density can be given as

\[
J = A* e T^2 \exp\left(\frac{\phi}{kT}\right) - enS
\]

where

\[
A_n^* = \frac{4\pi qK^2m_n^*}{\hbar^3}
\]

\[
A_p^* = \frac{4\pi qK^2m_p^*}{\hbar^3}
\]

\( A_n^* \) and \( A_p^* \) denotes the constants for electrons and holes respectively, \( m_n^* \) and \( m_p^* \) are the electron and hole effective masses.
Generally, value of this constant is $1.18 \times 10^2 \text{ A/cm}^2\text{k}^2$.

$T$ is the temperature, $\phi$ is the barrier height over which the carriers have to be injected, $k$ is the Boltzmann constant, $e$ the electron charge, $n$ is the charge density at the contact, and $S$ is the surface recombination velocity [13][16].

At zero electric field, $S$ can be defined as

$$S(0) = 16\pi \varepsilon \varepsilon_0 (kT)^2 \mu / e^3$$

(8)

where $\mu$ is the charge mobility and $\varepsilon_0$ is the dielectric constant.

When we apply the electric field, recombination velocity will become

$$S(E) = S(0)(1 / \phi^2 - f) / 4$$

(9)

4. RESULTS AND DISCUSSION

In the structures shown in figure 1, multi-layered nano-structure has been designed and simulated and hence analysed to optimize the electrical and optical characteristics of the devices. Figure 1 (a) includes the structure of the device where multilayers comprise of HTL, ETL, EIL, EML, buffer layer along with the electrodes. Devices in figure 1 (b) consists of HIL in addition to all other layers that are mentioned for structure in figure 1 (a). Materials used for HIL are MoO$_3$ and HAT-CN. Device structures of both the OLEDs are shown in figure 2. Figure 3 shows I-V characteristics comparison of the three devices simulated and it can be analysed from the characteristics that the device without HIL has lowest value of the current reached as compared to the other two devices. This is because of the fact that presence of hole injection layer in the device tends to increase the hole transport efficiency of p-type organic materials. Also, among the three OLEDs, diode with HAT-CN as HIL has achieved the maximum value of the current at the applied voltage. This is attributed to the presence of six acetonitrile groups in HAT-CN material. These groups contribute towards the LUMO levels of the HIL material [11][12].

![Figure 3. I-V Characteristics comparison for simulated devices](image)

Figure 4 shows the current density characteristics for the three simulated devices with respect to the applied voltage and it can be inferred from the graph that current density for the device without HIL is almost negligible as compared to the others where HIL is inserted between HTL and EML. Also, it can be clearly seen from the inset figure that device without HIL has maximum value reached is only 3 A/m and after that the device saturated whereas the other two devices have reached to a value of 25 A/m approx. at the same voltage. The reason has already been mentioned above.
Figure 4. J-V Characteristics comparison for simulated devices

Figure 5 shows the variation of electric field with respect to the applied voltage and it can be seen from the characteristics that OLED without HIL between HTL and EML has the highest electric field reached as compared to other two devices. In contrast to this, the device where HAT-CN is inserted as HIL has achieved the lowest value of the electric field.

Figure 5. Electric Field variation with varying voltage

To analyse the optical properties of the OLED devices, figure shows the electroluminescence (EL) intensity characteristics when wavelength is varied across it. Characteristics reveal that devices exerts a peak of EL intensity at around a wavelength of about 320 nm. All the three devices show the intensity peak at the same wavelength.
5. Conclusion

Efficient multilayer OLED devices have been designed and simulated to achieve the best electrical and optical properties of the device with the optimized device structure. For this, three devices have been analysed and investigated with different HIL materials. There is a drastic enhancement found in the electro-optical characteristics of the device when HIL is inserted in the device as compared to when it is not. OLED with HAT-CN has achieved the maximum current and current density as its electrical properties. Device’s optical properties include the study of its EL intensity which has been achieved at around a wavelength of 320 nm approx. The device is found to be best optimized in terms of its layer thicknesses.

6. References

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