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ARTICLE

Optimization of ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al Layers Configuration for OLED and Study of Its Optical and Electrical Characteristics

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ABSTRACT

Nowadays, OLEDs have shown aesthetic potential in smart cards, sensor displays, other electronic devices, sensitive medical devices and signal monitoring etc. due to their wide range of applications like low power consumption, high contrast ratio, speed highly electroluminescent, wide viewing angle and fast response time. In this paper, a highly efficient organic LED ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al with low turn-on voltage and high optically efficiency is presented including electrical and optical characteristics. The simulation of electrical characteristics like current versus applied voltage, current density versus applied voltage, recombination prefactor versus excess carrier density characteristics and optical characteristics like light flux versus current density, light flux versus applied voltage and optical efficiency versus applied voltage has been explained. The physical design, working principle and thickness of different layers along with the process of formation of singlet and triplet excitons are discussed in detail. Here double electron transport layer (ETL), cathode layers are used to enhance the electrical and optical efficiency of OLED. The operating voltage is found to be ~ 3.2 V for the ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al heterostructure based OLED. The designed organic LED has achieved the maximum optical efficiency at 3 V.

Keywords: OLED; Alq_3; BPhen; TPBi; I-V characteristics

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1. Introduction

Organic LED has attracted a lot of attention owing to its many advantages like flat display panels, ecological lighting sources, tuneability, flexibility, wide viewing angle and fast response time [1-4]. Researchers and scholars are making a great deal of effort to fabricate OLEDs that have good stability, picture quality, durability, low operating voltage and the materials used to design them are cheap and easily available [5,6]. Recently, OLED has been industrialized as indoor lighting, bio-sensors, digital camera and mobile phones. However, fabricating OLED with good electrical and optical characteristics to be used as lighting source and large display panel is still challenging [7].

Vanadium oxide (V_2O_5) is readily accessible, earth abundant and nontoxic. Vanadium oxide, a versatile substance that improves device performance, is essential in OLED technology. In OLEDs, it can be typically utilized as a hole transport layer (HTL). Without HTL there is carrier recombination on the surface of Alq_3 and bad ohmic contact between metal electrode and Alq_3. The influence of vanadium oxide (V_2O_5) as HTL on the performance of OLED has been investigated. For example, the operating voltage of OLED has been lowered by using vanadium oxide (V_2O_5). The effect of V_2O_5 on the device performance was investigated theoretically to provide complete future guidelines. For the eco-friendly, low cost vanadium oxide could be used as a good and promising candidate [8]. Vanadium oxide (V_2O_5) improves the exciton generation and suppresses the charge recombination [9]. It exhibits high charge carrier mobility and charge carrier transport capability. The work function of vanadium oxide is found to be comparable to that of Alq_3. The obstacle in the path of commercialization of OLED is the unavailability of ambient stable and efficient HTL material. Each layer present in OLED has its impact on the device's efficiency and power output. The HTLs and ETLs are critical for various reasons: (1) these are in direct contact with the emissive layer. (2) These layers are usually having thermal stability as compared to other layers in the heterostructure. (3) These layers play a pivotal role in increasing the charge transport properties.

There is a need of imminent research to design and develop highly reliable, long lasting and flexible lighting sources. In this paper, we focus on improving the efficiency of the device by using HTL (V_2O_5) and ETL (TPBi and Bphen) layers to provide better functionality and bypass the negative effects from OLED. Alq_3 (Tris(8-hydroxyquinolinato)aluminum) as an EML (emissive layer) has made a momentous contribution to improving optical efficiency and lowering its operating voltage. Alq_3 has been used as EML and ETL in the first commercial OLED produced by Tang. Alq_3 reacts immediately on coming in contact with the environment and water [10-12].

2. Structure configuration and working principle

OLED is a thin film optoelectronic device composed of organic semiconductors based on the principle of electroluminescence instead of LED technology composed of semiconductor material [13-15]. The organic semiconductors, in the form of semiconducting polymeric materials or organic molecules, are composed of hydrocarbon chain having properties like mechanical flexibility, highly efficient and highly feasible [16-22]. Initially, OLED consisted of single layer/monolayer and was less efficient because the injection of electrons and holes did not take place at the same time. Gradually double, triple and multi-layer OLEDs were developed to increase the efficiency [23]. Here, the four-layer OLED has been designed, as shown in **Figure 1**. The organic materials "BPhen and TPBi" has been used in ETLs; for EML purpose the organic material "Alq_3" has been utilized. For the purpose of HTL, a unique material V_2O_5 has been used. The HTL (V_2O_5) and ETL (TPBi/BPhen) play an important role in confining electrons and holes in active layers so that there is no quenching of excitons at the layer interface. All the layer specifications (materials along with their role and layer size) for the ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al heterostructure OLED have been illustrated in **Table 1**.

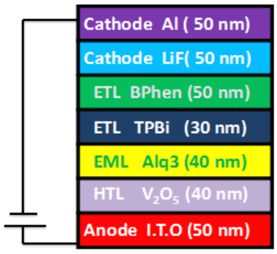

Figure 1. Layered structure of the ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al heterostructure OLED.

In this case, when a voltage is applied to oppositely charged electrodes i.e. anode and cathode, the electrons and holes are injected into the active layer from the cathode (LiF/Al) and anode (ITO), respectively. See **Figure 2**. The work function of adjacent layers is so low that there is ohmic contact between two different layers that can support the transportation of carriers. Hence, the transportation of carriers could take place readily without any barrier. The recombination of electrons and holes takes place in the emissive layer results the formation of singlet and triplet exciplex/excitons. The ratio in which singlet and triplet excitons are produced is 3:1 [24,25]. The emission of light takes place from the emissive layer and color of light or wavelength of light depends on the difference between the energy gap of the uppermost occupied molecular orbital (HOMO) and the lowest vacant molecular orbital (LUMO).

Table 1. Layers specification for the ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al OLED.

S. No.	Layer specifications	Thickness (nm)	Materials used
1	Anode	50	ITO (indium titanium oxide)
2	Cathode	50	Al (Aluminium)
3	Cathode	50	LiF (Lithium Fluoride)
4	HTL	40	Vanadium (V) oxide
5	EML	40	Alq_3 (tri-(8-hydroxyquinoline))
6	ETL	50	TPBi (2,2',2"-(1,3,5-Benzyinetriyl)-tris(1-phenyl-H-benzimidazole)
7	ETL	30	Bphen (Bathophenanthroline)

The brightness or luminescence of light depends on the amplitude of the voltage applied. It is very difficult to control the amount of charge carriers reach at the emissive layer; it should be equal in number so that recombination results in the emission of light. The mobility of holes is more than that of electrons inside the active layer [26,27]. ITO has high work function, good optical transparency, excellent hole injection properties, ease of patterning and high electrical conductivity. Further, ITO is a well-known n-type degenerate semiconductor with an optical band gap of 3.5-4.3 eV and has high transmission in the near infrared and visible regions of the electromagnetic spectrum [28]. These properties of ITO influence the optical and electrical characteristics of OLED [29]. LiF plays a crucial role in improving OLED durability and efficiency. It has been used widely to modify chemical reactivity at interface, electrode work function and contact adhesion [30-36]. It can be kept on the top as well as the bottom of the device as the electrodes as well as the substrate. The energy band diagram of the design with the layer specifications ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al OLED has been illustrated in **Figure 2**.

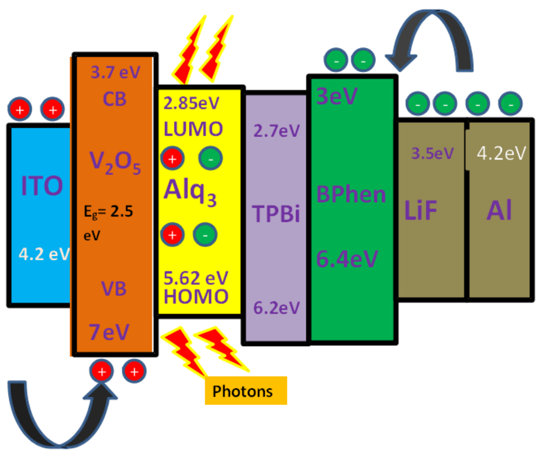

Figure 2. Layer specification in ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al OLED.

3. Simulation results and discussion

Understanding OLEDs' electrical behaviour and efficiency requires an understanding of their I-V (current-voltage) properties. These qualities aid engineers in fine-tuning OLED devices, guaranteeing effective control over power usage and brightness. Studying I-V curves also helps with problem-solving and diagnosis, which enhances the performance and lifespan of OLED displays.

To calculate the value of the potential profile i.e. φ Poisson Equation (1) has been used. Further, to study the motion of free electrons and holes within the OLED of ITO/V_2O_5/Alq_3/TPBi/LiF/Al, both electron and hole drift diffusion Equations (2) and (3) are used. Carrier continuity Equations (4) and (5) are solved to calculate the recombination and generation rate of electrons and holes inside the device [37-40].

$$\frac{d}{dx}\epsilon_0\epsilon_r\frac{\partial\varphi}{\partial x} = q(n-p) \tag{1}$$

$$J_n = q\mu_c n\frac{\partial E_c}{\partial x} + qD_n\frac{\partial n}{\partial x} \tag{2}$$

$$J_p = q\mu_n p\frac{\partial E_p}{\partial x} - qD_p\frac{\partial p}{\partial x} \tag{3}$$

$$\frac{\partial J_n}{\partial x} = q(R_n - G + \frac{\partial n}{\partial x}) \tag{4}$$

$$\frac{\partial J_p}{\partial x} =- q(R_p - G + \frac{\partial p}{\partial x}) \tag{5}$$

where, the terms used in Equations (1)-(5) have been explained as follows:

ϵ_0 = Electrical permittivity of free medium
μ_n = hole mobility
ϵ_r = Relative electrical permittivity
E_c = free electron mobility edge
φ = Voltage profile
E_p = free hole mobility edge
q = elementary charge on an electron
D_n = electron diffusion coefficient
n = free electron concentration
D_p = hole diffusion coefficient
p = free hole generation rate
R_n = electron recombination rate
J_n = electron current flux density
R_p = hole recombination rate
J_p = hole current flux density
G = free carrier generation rate
μ_c = electron mobility

With the help of simulation, we have determined the I-V characteristics of the designed OLED. **Figure 3** shows the current versus voltage characteristics of ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al-based heterostructure OLED. There is no variation in current with the increase in applied voltage till ~3.5 V. Further increase in bias voltage results in an exponential increase of current. On increasing the biased voltage applied between ITO and LiF/Al, there is an increase in the concentration of carriers, which are transported to the emissive layer with the help of TPBi/BPhen (ETL) and V_2O_5 (HTL). The recombination of electron and holes takes place in the emissive layer i.e. Alq_3 which result in the formation of exciplexes. There is the emission of light from the emissive layer. The upsurge of exciplexes results in an increment in the outflow of light. The turn-on voltage of the diode also depends on the energy gap between LUMO and HOMO of the emissive layer [41]. **Figure 4** shows the J-V characteristics of the designed heterostructure OLED. From 0 to 3.25 V, there is a minimal increase in current density with the applied biased voltage which is similar to that of a resistive diode. One can see from the graph that increasing the voltage after 3.2 V results in an exponential increase of current density. The obtained results for J-V characteristics completely agree with the I-V characteristics result. The efficiency of OLED estimated by most of the special technology and scientific interest is calculated from the luminescence/light flux multiplied by a factor of π, rather than from a value of light flux only [42]. Light flux is defined as the amount of light emitted per unit cross section area of the device [43]. There is a non-linear relationship between light flux and applied voltage in the low voltage region, it increases superlinearly from 2.5 V to 3.5 V and further increases i.e. above the operating voltage resulting in an exponential increase of light flux with the applied voltage. See **Figure 5**.

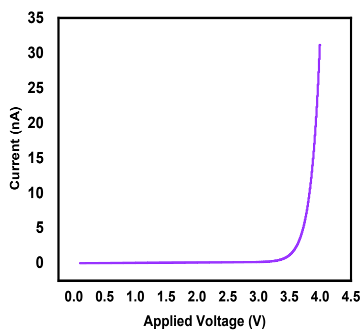

Figure 3. Current-voltage (I-V) characteristics of ITO/V_2O_5/Alq_3/TPBi/BPhen/LiF/Al OLED.

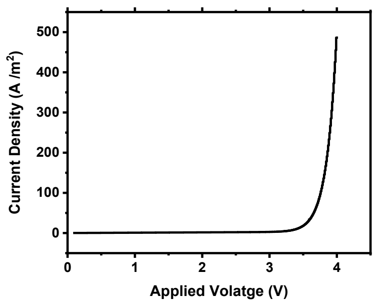

Figure 4. Current density-voltage (J-V) characteristics of ITO/ V_2O_5/Alq_3/TPBi/BPhen/LiF/Al OLED.

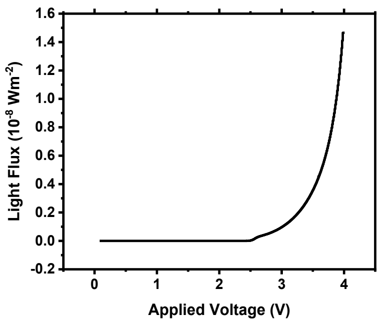

Figure 5. Plot of light flux vs applied voltage for ITO/V_2O_5/ Alq_3/TPBi/BPhen/LiF/Al OLED.

Refer to **Figure 6**, which shows the plot of light flux Vs current density for the designed OLED. The light flux increases linearly after 75 A/m^2 value of current density. It means that the light radiated per unit area per unit time from the device increases with the increase in the current applied between the oppositely charged electrodes. The optical efficiency is defined as the amount of light radiated by OLED to the amount of voltage applied to device for this irradiance. For the designed organic LED, the peak value of optical efficiency is found to be at an applied voltage of 3.25 V which is very low. It means that organic LED starts to operate/glow at such a low voltage. At this voltage, maximum numbers of excitons i.e. electron and hole pairs bounded by coulombic forces of attraction are converted into photons. See **Figure 7**.

The recombination prefactor of the ITO/V_2O_5/ Alq_3/TPBi/LiF/Al OLED has also been thoroughly studied. Bimolecular recombination is a fundamental phenomenon that controls how much light is generated, which has an impact on the effectiveness of organic optoelectronic devices like OLEDs. The recombination prefactor indicates the rate at which electron and holes are recombining to emit light. To determine the quantities (such as the generation of light and efficiency), the recombination prefactor is necessary. As shown in **Figure 8**, with the increase in excess charge carrier density, there is an exponential increase in the value of the recombination prefactor. Refer to **Figure 8**, up to 1.0×10^{22} excess carrier density, no recombination prefactor occurs, because such amount of excess carriers is not enough to produce the recombination. The probability of recombination increases with the increase in the carrier concentration of electrons and holes beyond the 1.0×10^{22} excess carrier density.

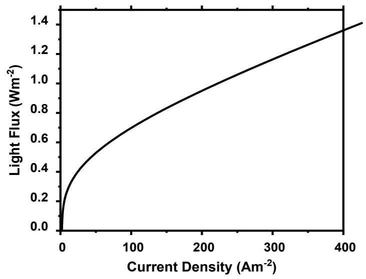

Figure 6. Plot of light flux vs current density for ITO/V_2O_5/Alq_3/ TPBi/BPhen/LiF/Al OLED.

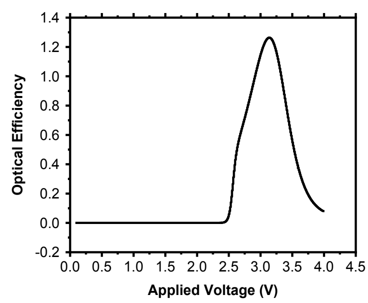

Figure 7. Plot of optical efficiency Vs applied voltage.

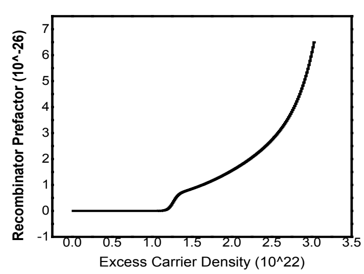

Figure 8. Plot of recombination prefactor Vs excess carrier density.

4. Conclusions

The structure optimization, as well as the optical and electrical properties of the ITO/V_2O_5/Alq_3/TPBi/LiF/Al OLED, has been studied using Poisson, bipolar drift diffusion and continuity equations. The operating voltage was found to be to be approx. 3.2 V. The optical efficiency of the device has been achieved to be optimum at 3.2 V. Definitely, the work reported will be an input for lowering the operation power and boosting the stability of OLEDs which are most weakest points of OLEDs for practical applications.

Author Contributions

All authors contributed to the study conception and design. Data generation, collection and analysis were performed by [Ritu], and [P. A. Alvi]. The first draft of the manuscript was written by [Ritu], [P. A. Alvi], [S. Z. Hashmi], [Jasgurpreet Singh] and [Sandhya Kattayt], commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Conflict of Interest

There is no conflict of interest.

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