

The FDTD Simulation of QDLED Performance Dependency on the Location of Colloidal Quantum Dots

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Received: March 2020

Revised: May 2020

Accepted: July 2020

ABSTRACT:

All types of Light Emitting Diodes (LEDs) are desirable because of their widespread applications. The Quantum Dot-Based Light Emitting Diodes (QDLEDs) have a lot of unique properties attracting more attention. Predicting performance of QDLEDs can lead to a better and more efficient design of the device. In this paper, we have attempted to investigate the dependency of the device performance on the location of Quantum Dots (QDs) and determine the best location for the QDs in the QDLEDs. We use FDTD method to simulate and analysis the QDLEDs structure. The QDs are located in five different positions in TPBi layer then results are compared with each other. The results show that the closer the QDs to the hole transport layer (HTL), the better the luminescence. This improvement would be explained by two charge transport mechanisms including direct charge injection and exciton energy transfer. The results show that when the QDs are closer to the HTL, the device performance is better due to the greater balance of carriers. In this condition holes can transfer from the HTL to the valence band easier.

KEYWORDS: Quantum dot, Efficiency, Light Emitting Diode, Location.

1. INTRODUCTION

The distinguished properties of quantum dots make them a very useful choice in the fabrication of next-generation displays. The advantages of using quantum dots in displays include the ability to solubility, easy colour tunability and narrow bandwidth. Because of these advantages, scientists currently working in the field of displays technology are looking for procedures to improve the performance of light emitting diode based on quantum dots (QDLED) [1-4].

Quantum dots are used in displays for two purposes. One as a self-emitting layer in electroluminescence structures and the other as a colour conversion layer on liquid crystal or LED displays [5]. Scientists are trying to improve the features of both types. The structure engineering of the quantum dots and diodes are two key points in improving the performance of QDLEDs. Existence of the exciton can improve the characteristics of the QLEDs. Excitons in quantum dots are created by two mechanisms: One by direct injection of carriers and the other by Froster resonance.

One of the disadvantages of QDLEDs is the low efficiency due to the large alignment between the energy levels of the quantum dots and the material of the hole and electron transfer layers. Especially the energy levels of the Hole Transfer Layer (HTL) are very unbalanced compared to the valence band of the QDs. This ultimately makes it difficult to directly inject the holes into QDs. As a result, the charge balance is disrupted and the concentration of electrons is increased compared to the holes and auger recombination will be occurred.

Generally, by choosing appropriate energy levels, direct injection of the carriers into the valence and conduction band of the quantum dots would be improved. In the Froster resonance method, the excitons are formed in the organic layer surrounding the quantum dots and then resonantly transferred to the quantum dots.

The first commercial use of QDLEDs occurred in 2013 [6]. This technology brings possibility to make wide colour gamut displays at affordable prices. To date, Organic Light Emitting Diodes (OLEDs) based on CdSe quantum dots have been developed, reaching an EQE of over 20% for green and red light. The lifespan of

QDLEDs based on CdSe quantum dots has reached an acceptable level for commercial use [7].

Today, the efficiency of QDLEDs is greatly improved due to the upgrade synthesis methods. EQE above 30% has recently been introduced for a QDLED based on CdSe quantum dots [8]. They have been able to achieve these results by using the structural device and quantum dot engineering.

So far, scientists have been obtained EQE equal to 30.9% [8], 25.04% [9] and 19.8% [10] for red, green and blue light, respectively. Matvienko et al. in 2012, investigated influence of morphology of hybrid QD-polymer active layer and the QDLED architectures on their electroluminescent intensity and efficiency. They investigated QDLEDs in bulk heterojunction and quantum dot bilayer conditions [11].

P. O. Anikeeva et al. in 2008, studied some variety of QDLED structure to survey fundamental processes that govern the operation of QDLEDs. They fabricated the set of the devices to vary the position of the emissive QD monolayer to investigate the contribution of the direct charge injection and exciton energy transfer to QDLED. They found that the QD monolayer should be deposited into a HTL ≤ 10 nm away from exciton generation interface for improving the performance of the devices [12]. Their conclusion are completely in consistent with our results.

Hossein Zamani Siboni et al. in 2015, enhanced the efficiency of QDLEDs by using a thermal annealed sensitizer that transfers the excitation energy to the QDs via Forester Resonance Energy Transfer (FRET) [13]. Kheng Swee Leek in 2013, deposited QDs in HTL layer and controlled the nonradiative recombination happen by balance of the electron and hole injected into QDs but the FRET was in minimum quantity [14].

Aiwei Tang et al. in 2008, fabricated a hybrid QDLED with the blends of different sized of CdSe and PVK. They concluded that the FRET for smaller size had better results. They also showed that the EL spectra of the PVK reduced when the size of QDs decreased and the colour of the EL emission was almost located in the white region [15]. They also studied the effects of the different applied voltages and the different mass ratio of CdSe to PVK of the device performance. Their results show that the ratio of EL from CdSe QDs and PVK decreased with enhancing applied voltage. Also, the colour of emission spectra could be tuned from yellow to white. They could obtain a pure white colour by optimizing the mass ratios of CdSe to PVK and applied voltage [16].

There are many factors influencing the final performance of QDLEDs, such as the size of the QDs, the layer deposition methods and the synthesis method of QDs. As reviewed in this section most of those methods have been studied to date. Although one important factor that has not been fully explored is the

placement of quantum dots in a blend organic layer. This parameter can significantly influence on the device performance. In this paper, we try to predict the best location for quantum dots in the structure of QDLEDs by SILVACO simulation software using FDTD method. The FDTD method is a powerful tool for integrated and diffractive optics device simulations. This method can model light propagation, scattering and diffraction, and reflection and polarization effects. It can model the effective and powerful simulation and analysis of sub-micron devices with very fine structural details. The FDTD approach is based on a direct numerical solution of the time-dependent Maxwell's curl equations.

2. QDLED STRUCTURE

In this survey, we study dependency of the device performance on the location of quantum dots. As a result, the best location for the quantum dots in the QDLEDs is determined. An inverted structure of a hybrid organic-inorganic led by means of quantum dots and organic materials are chosen for this purpose. In this paper, the structural characteristics of QDLEDs with different locations of QDs are compared.

The device cross-sections and the energy band diagram of the QDLED discussed in this paper are shown in Fig. 1. The energy diagram of QDLED is plotted in Fig. 1 (a).

The External Quantum Efficiency (EQE) of QDLEDs strongly depends on injection of holes from the Hole Injector Layer (HIL) into the valence band of the quantum dots and the injection of the electron from the Electron Injector Layer (EIL) into conduction band of the quantum dots. Therefore, the lower the energy level of the material used as the HIL, the better the efficiency of the device.

In order to increase exciton production of the first method, the highest occupied molecular orbital (HOMO) of HIL would be less than the valence level of the QDs. The transferred energy by the Froster resonance mechanism is dependent on the size of the quantum dots and is less effective for larger size quantum dots due to the greater receiver-acceptor distance.

If the QDs are blended in the polymer, most of the electroluminescence contribution of the quantum dots are related to the transferred energy through the second mechanism and the direct electric excitation has less role. However, for a monolayer of quantum dots, most of the electroluminescence contribution is due to the direct charge transfer.

The size of the CdSe quantum dots is 4 nm and the band gap of them is about 2.1 eV (The energy of the valence level is 4.3 eV and the conduction band is about 6.4 eV).

Because of the good spectral overlap between TPBi PL and quantum dots absorption, this organic material is

used as an electron transport layer in this study [17]. Quantum dots are blended into TPBi in different locations and their results are compared together.

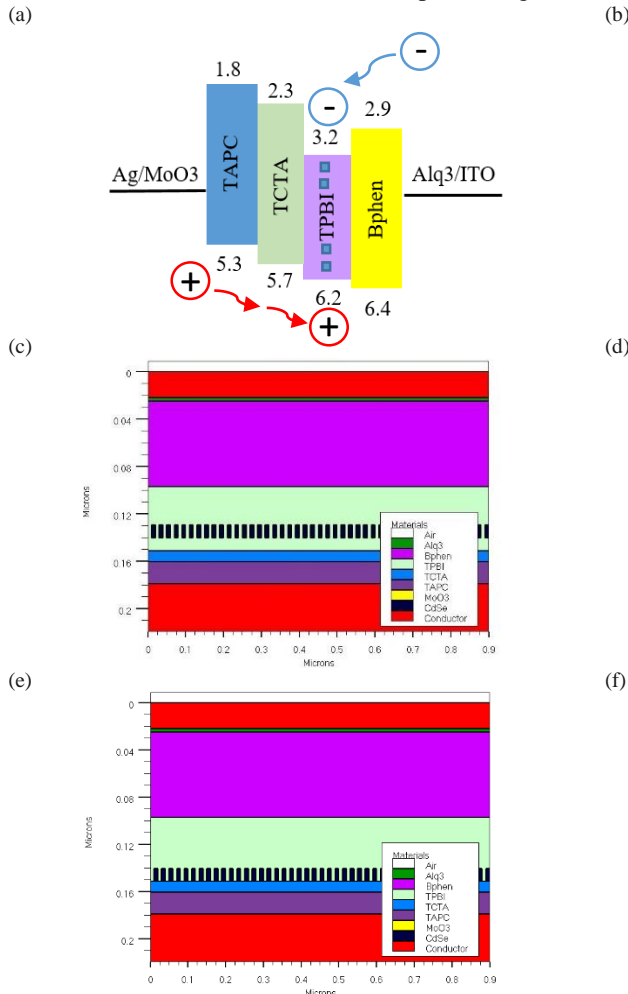


Fig. 1. Schematic display of the device configuration and the energy levels of the structures. (a) The energy diagram of QDOLED, (b) The structure of IH-QDOLED when QDs are in the TPBi/2, (c) QDs are in the 3TPBi/4, (d) QDs are in the TPBi/4, (e) QDs are in the 7TPBi/8, (f) QDs are in the TPBi/8.

3. RESULTS AND DISCUSSION

All the results of simulated structures are presented and compared together in this section. The anode current of QLED versus the applied voltage (I-V) is shown in

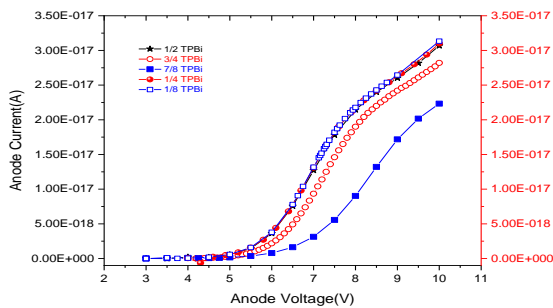


Fig. 2. Current-voltage characteristics.

Obviously, quantum dots are located in TPBi/2, 3TPBi/4, TPBi/4, 7TPBi/8, TPBi/8.

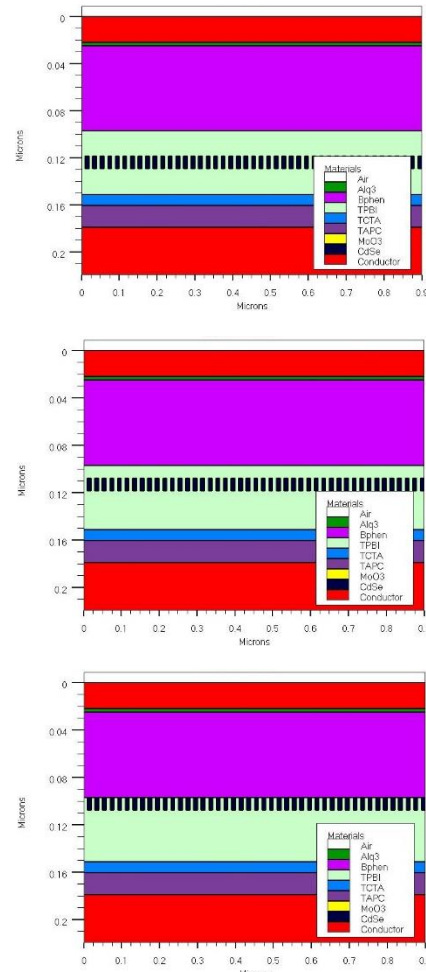


Fig. 3. luminescence of the five different structures.

Fig. 2. It is obvious that the closer QDs to HTL, the less turn on voltage (V). In fact, whenever QDs are closer to HTL, the holes can inject to QDs more facile. Therefore, the carriers will be in more balance condition and as a result, the device will work in better performance.

In Fig. 3 the luminance-voltage ($L-V$) curves of the all five structures are shown and compared with each

other. As expected, the luminance also shows improvement where QDs are located closer to the HTL.

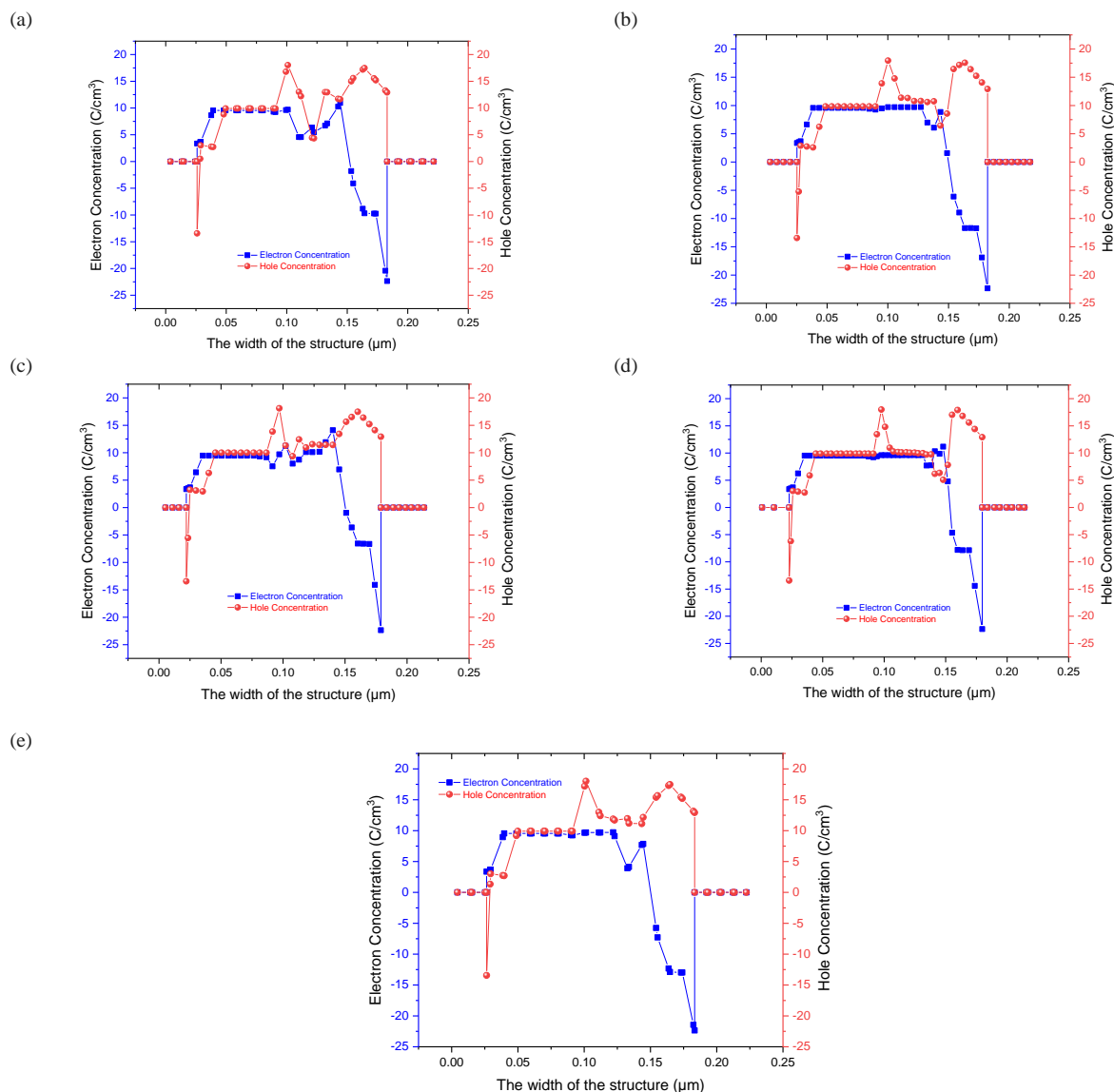


Fig. 4. The concentration of the carrier when (a) QDs are in the TPBi/4, (b) QDs are in the 3TPBi/4, (c) QDs are in the TPBi/8, (d) QDs are in the 7TPBi/8, (e) QDs are in the TPBi/2.

In fact, each QD has a role like a potential well where holes are injected from HTL and electrons are transferred from the ETL to QDs. Therefore, the more adjustment between energy levels of ETL, HTL and band energy of QDs, the more suitable results.

Fig. 4. shows the carrier's concentration of each structure, and it is completely obvious where QDs are located in 7TPBi/8, carriers have better equilibrium. These curves confirmed the results of luminescence in Fig. 3.

The electron's concentration is usually more than hole concentration in Organic Light Emitting Diodes

(OLEDs) and this unbalanced condition increases the auger recombination probability which is considered as nonradiative recombination. The shorter distance makes holes easier transfer where QDs are as near as possible to HTL layer. It would increase the equilibrium of the electrons and holes in emissive layer especially QDs. This continues in other part of Fig. 4. Fig. 4 (b) also shows a relatively suitable balance between the electron and the hole but as the QDs move away from the HTL layer, this balance becomes less and less, which is not usually desirable.

Nonradiative recombination causes a great reduction of the device lifetime by increasing the temperature of the device due to the generating phonon. The total radiative recombination is drawn in Fig. 5. As it is shown, the most radiative recombination occurs where the QDs are in the 7TPBi/8. This figure is expected from Fig. 4.

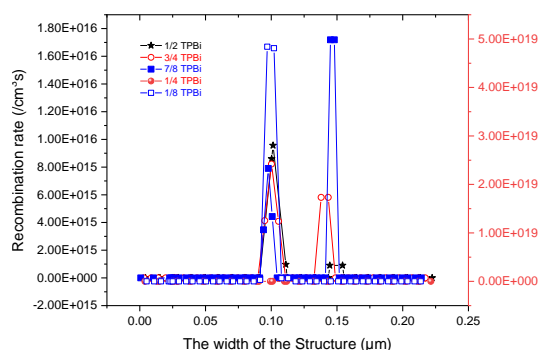


Fig. 5. Recombination rate in all structure versus the width of the structure.

There are two kinds of excitons called singlet and triplet. They are formed when electron and holes meet each other. The total amount of spin of singlet and triplet excitons are zero and one, respectively. Unfortunately, the triplet exciton mostly recombine non-irradiated. So the singlet one is desirable in QDLEDs.

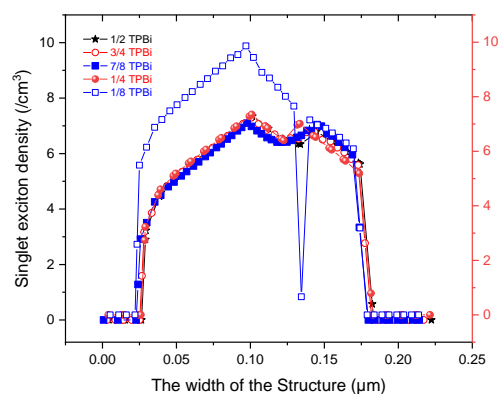


Fig. 6. The singlet exciton density versus the width of the structure.

The singlet exciton density versus the width of the structure is shown in Fig. 6 for all structures. As it is expected, the amount of singlet exciton density for the structure that QDs are located in 7TPBi/8 is more compared to other structures.

4. CONCLUSION

The location of QDs in the QDLED structure is investigated to improve the electrical and optical characteristics of the device. The QDs are located in five

different positions and results are compared with each other. The results proposed that the closer the quantum dots to the HTL, the better device performance.

The results were justified by two mechanisms related to charge transfer, direct injection of carriers and the other exciton energy transfer by Froster resonance. It was shown that when the QDs are closer to the HTL, the direct transfer of the holes from the HTL to the valence band of the QDs is performed better and faster. Since the number of electrons are usually more than the holes in the radiation layer, this improvement in holes transport creates a greater equilibrium between the charge carriers. Balance between carriers will improve the overall performance of the device by reducing nonradiative recombination inside the device.

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