Emerging Materials for High-Efficiency Blue Organic Light-Emitting Diodes (OLEDs)

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Abstract. OLED plays a vital role in the realization of full-color display and lighting solutions. However, the development of blue OLED faces many challenges, such as energy gap issues, stability, and efficiency. This paper aims to explore the key role that advances in materials science and physics have played in the improvement of blue OLED technology. Firstly, the importance of the HOMO-LUMO energy gap in blue OLEDs for luminescence color is illustrated by explaining the electroluminescence process in organic compounds, with special attention to exciton formation and recombination mechanism. Subsequently, advances in light-emitting materials in blue OLED, including the development of phosphorescent materials and TADF materials, are discussed in depth, and examples from recent research papers are cited. In addition, strategies of molecular design in improving the stability of blue luminescent materials are discussed, and case studies of relevant research papers are provided. In terms of device structure and material selection, this paper analyzes the development of host materials and transport materials and introduces the influence on the performance optimization of blue OLED. Finally, the challenges faced by blue OLED materials and possible breakthrough directions for future materials science research are discussed.

Keywords: Blue OLED, Phosphorescent material, TADF.

1. Introduction

OLED technology has become a prominent player in the display and lighting industries thanks to its many advantages, including thinness, energy efficiency, and bright colors. The global market has seen the successful introduction of numerous OLED displays, and the development of lighting products has progressed quickly. Mobile phones, TVs, multimedia players, digital cameras, vehicle meters, smart bracelet wearables, and other electronic products are just a few of the many products that use OLED technology. Currently, it is deeply ingrained in materials science, health science, energy science, artificial intelligence, and other industry directions, driving breakthroughs in related fields such as information technology, healthcare, aerospace, and renewable energy while also reversing the direction of these fields to drive OLED [1]. Although it has the technical basis of industrialization, OLED technology has not reached perfection, and it still needs to be improved in some technical links, which has also attracted the interest of many researchers [2]. The purpose of this review is to discuss the progress of blue OLED technology. By studying the basic principles of OLED, including the electroluminescence process and the importance of energy levels and band gaps in blue OLED. In addition, this article will also introduce the latest advances in blue OLED light-emitting materials, including phosphorescence and TADF materials, host materials, charge transport layers, and device architecture design. Finally, the current challenges and future directions of blue OLED materials will be discussed.

2. Fundamentals of OLED Operation

2.1. The basic structure of OLED

Figure 1 in the following illustrates the fundamental construction of an OLED. On the substrate are all the functional layers. The substrate can be made of materials such as plastic or glass. The

functional layer consists of three parts, the anode, the cathode, and the organic material wrapped between the electrodes [3].

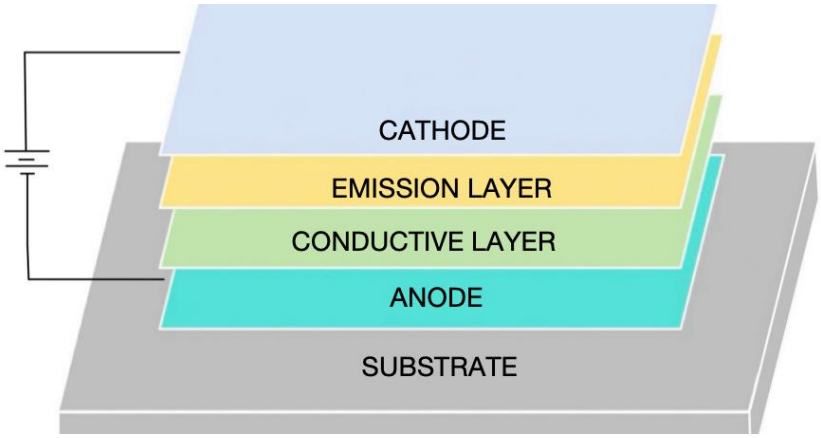

Fig. 1 Fundamental Structure of OLED (Picture credit: Original)

2.2. Electroluminescence in Organic Materials

The hole carrier is injected via the anode into the adjacent organic functional layer's Highest Occupied Molecular Orbital (HOMO) when a forward bias is given to the flexible OLED device. The neighboring organic functional layer's Lowest Unoccupied Molecular Orbital (LUMO) is injected with electron carriers via the cathode. Furthermore, when an electric field is provided, the injected holes and electrons go in the direction of the electrode that is oppositely charged.

An exciton is a localized pair of electrons and holes with an excited energy state that is created when electrons and holes locate on the same molecule and are spatially close to each other in the organic emissive layer. Following their relaxation through a photoemissive process, a portion of these excitons spontaneously emit light and radiatively decay to the ground state. Recombination releases energy in the form of light [4]. Figure 2 depicts the electroluminescence mechanism of an OLED.

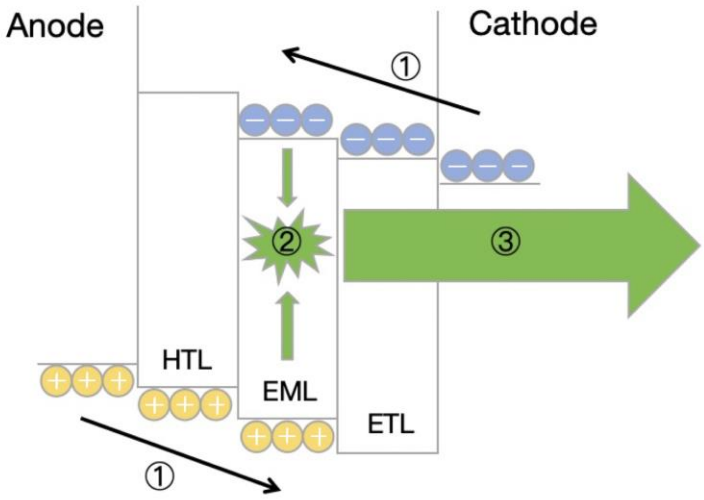

Fig. 2 Diagram of an OLED's electroluminescence mechanism: Following the injection of electrons (blue) and holes (yellow) from the electrodes into the emission layer, an exciton (green) is formed. This exciton then undergoes radiative recombination, which releases photons. (Picture credit: Original)

2.3. Energy Levels and Bandgap in Blue OLED

In organic semiconductors, HOMO is the highest occupied electron orbital and LUMO is the lowest occupied electron orbital [5]. Between these two energy levels, there is an energy differential, which determines the photoelectric properties of organic materials. The wavelength of the light that

is emitted is directly determined by the HOMO-LUMO gap and is directly correlated with its color. For blue OLEDs, a smaller energy gap is needed to produce high-energy photons to achieve blue emission. In addition, the size of the HOMO-LUMO band gap also affects the stability of organic materials. In general, smaller energy gaps are more likely to lead to intermolecular interactions, which affect the stability of the material.

3. Advancements in Emissive Materials for Blue OLEDs

3.1. High-Efficiency Blue Emissive Materials

3.1.1 Phosphorescent materials

When electrons and holes recombine in an organic luminescent layer, two different forms of excitons are generated due to different spin modes. A singlet exciton is one kind that deactivates to the S0 state and releases energy as fluorescence. An additional variety is the triplet exciton, which deactivates to the S0 state and releases energy as phosphorescence. Fluorescence is an allowed transition between the same multiple states, and the entire process is very rapid. When transition metal atoms are involved, the singlet excited state can undergo non radiative inter system transitions to triplet excited states with different spin intensities. The radiative transition from the lowest vibrational level of the triplet excited state back to the S0 state is known as phosphorescence [6].

The participation of these transition metal atoms will enhance the spin orbit coupling (SOC) effect between singlet excitons and triplet excitons, enhance the inter system crossing phenomenon, and break through the traditional 25% internal quantum efficiency limit based on fluorescent materials, thereby achieving 100% internal quantum efficiency luminescence [7]. In order to obtain high external electron efficiency in blue phosphorescent OLEDs, T.J. et al. designed the core structure of a carbazoledibenzothiophene molecule as a hole-transporting high-triplet energy host. The CzThTh host with a carbazoledibenzothiophene core and dibenzothiophene functional group efficiently harvested triplet excitons from Ir(dbi)3 triplet emitters and exhibited high EQE (22.8%) through carrier balancing [8].

3.1.2 Thermally activated delayed fluorescence (TADF)

Because phosphorescent materials require the addition of precious metals and are susceptible to concentration quenching effects, their large-scale applications are limited. In 2021, Wang et al. reported a third-generation electroluminescent material (TADF) that can produce efficient OLED. Similar to phosphorescent materials, TADF materials possess the capacity to reach internal quantum efficiency of 100% by using the reverse intersystem crossing (RISC) method that is thermally activated to transfer triplet excited states to singlet states and emit fluorescence [7].

3.2. Stability Enhancements in Blue Emissive Materials

Organic fluorescent materials have a maximum internal quantum efficiency of no more than 25% because spin confinement restricts their triplet excitons, which means that they can only emit light through radiative transitions from singlet to ground states. Heterocyclic or polycyclic aromatic functional groups are typically added to increase luminescence efficiency and stability, and conjugated molecular structures with twisted spatial configurations are created and manufactured to lessen the effects of molecular aggregation. Small molecule materials have a clear structure and are easy to purify, such as the D-π-A anthracene derivative fluorescent material synthesized by Hu et al. with cyanide and methoxy groups at both ends, which has high color purity and stability, and its power efficiency can reach 5.6l m/W [9].

4. Advancements in Host Materials and Device Architecture Design

4.1. Host and Transport Materials in Blue OLEDs

High triplet energy, appropriate HOMO and LUMO, broad bandgap, bipolar transmission properties, and good solubility in organic solvents should all be considered when choosing the primary material [10]. Wang et al. employed a unique type of thermally stimulated delayed fluorescence material (4- (3,3 ", 6,6" - tera pert butyl-9'H - [9,3 ': 6', 9 "- tercarbazol]) to produce excellent performance and minimal roll-off blue OLEDs. TPPOCz, or -9 '-yl) phenyl) phosphineoxide, the main component of blue dopants. The maximum brightness and current efficiency of the OLEDs were 13235cd/m2 and 43.6cd/A, respectively.

Through the energy level design of carrier transport materials, charges and excitons are contained in the luminous layer, allowing for high quantum efficiency in OLEDs. Transport materials in OLEDs can be categorized into two groups based on their distinct functions: materials for transporting holes and electrons [11].

Hole transport materials can increase the transfer rate of holes, block electron leakage from the luminescent layer, and achieve maximum carrier recombination [11]. On the basis of CDBP (29) material, Wang et al. [12] constructed a large molecule blue phosphorescent hole transport material by reintroducing a carbazole group onto the carbazole group. The quantum efficiency outside the system of the prepared deep blue phosphorescent device can reach 18.2%.

Electronic transfer materials should have strong electron affinity and large ionization energy, which is conducive to electron injection [13,14]. A high migration rate can reduce the driving voltage of OLED and improve power efficiency. Suitable electron transfer materials can improve the electron transfer rate, block hole leakage from the luminescent layer, and enhance exciton recombination. By modifying the electron transport material's HOMO energy level to stop holes from leaking into the luminescent layer and by modifying the LUMO energy level to introduce electrons into the luminescent layer [11]. Shih et al. synthesized a novel electron transport type host material TPOTP (31) by combining triphenyl and a diazole group with high electron withdrawing ability, wide energy gap, and planar structure [15]. The Tg of TPOTP (31) reached 220 ℃, and the triplet energy level was 2.76 eV.

4.2. Device Architecture and its Impact on Blue OLED Performance

Many factors affect the performance of blue OLED, such as the design of the optical cavity and layer structure optimization.

4.2.1 Layer structure optimization

The emission layer is the core part of OLED. This involves selecting the appropriate blue emitter and body material, whose energy levels and triplet energies need to be suitable. In addition, controlling the doping concentration and thickness of the emission layer is essential to maximize the radiative recombination of excitons and minimize non-radiative decay pathways.

The layer that connects the luminous layer to the cathode, which is primarily utilized for electron transport, is known as the charge transport layer. An electron injection is more advantageous the smaller the barrier between the cathode material's and the electron transport material's LUMO levels. In addition, there should not be a significant difference between the LUMO levels of the components in the light-emitting layer and the electron transport layer [16].

The blocking layer generally selects materials with higher trilinear energy levels to prevent exciton diffusion in the emission layer and improve the exciton usage rate. Second, the material of the hole blocking layer has a higher LUMO level than the electron transport layer and a lower HOMO level than the hole transport layer to prevent electrons from being transferred to the hole transport layer [17].

4.2.2 Optical cavity design

The luminous color and color purity of organic electroluminescent devices are largely limited by the characteristics of organic materials themselves, and the color purity can be adjusted by the change of device structure through the optical microcavity effect [18]. Among them, three crucial characteristics are the absorption coefficient of HTL and ETL, the thickness of the material, and the refractive index. Regarding the microcavity structure, the device's microcavity length is primarily adjusted theoretically in order to modify the thickness of the organic structure layer and produce microcavities of various modules. This allows the device to be in various microcavity strengthening areas and enhances the device's performance [18].

More specifically, the gain impact of the first-order and second-order micro-cavity OLED structures is comparable, but the device's short-circuit issue may be successfully avoided by extending the distance between the two electrodes. However, altering HTL thickness has little effect on the electrical properties of the device since hole mobility is bigger than electron mobility. Because of this, the optical microcavity of the device is usually created using thinner ETL and thicker HTL. Regarding the choice of the transport layer's refractive index, Fuchs et al. have documented the effects of HTL materials with varying refractive indices on TE-OLED efficiency. Greater deposition thickness is necessary for materials with lower refractive void for fixed optical cavity length. This increases the distance between the metal electrode and the luminescent layer and boosts device efficiency [19].

5. Challenges and Future Directions in Blue OLED Materials

The stability of blue OLEDs has been a matter of close attention. First of all, phosphorescence devices have the characteristics of using trilinear excitons to emit light, and the longer lifetime of trilinear excitons will greatly improve the possibility of exciton accumulation. Second, the airborne water and oxygen seriously harm the device, causing a rapid decrease in its life and effectiveness. Generally, the device packaging can lessen the harm that water and oxygen do to the device while also enhancing its stability.

The performance of blue organic luminescent devices is affected by factors such as organic luminescent materials [20]. Therefore, improving blue OLED materials will be an important development direction in the future. First, the performance of blue OLED materials can be improved by synthesizing and designing new organic molecules. For instance, reliance on pricey metals can be decreased by using the TADF (Thermally Activated Delayed Fluorescence) molecular design technique. In addition, future research may focus on the development of more stable and durable organic materials by synthesizing specific structures of organic molecules, which can reduce the material's susceptibility to degradation, thereby improving the long-term stability of the device. However, by improving charge injection and transport efficiency and achieving new breakthroughs in blue OLED stability and efficiency, the design and synthesis of new carrier transport materials—particularly electronic transport materials for blue OLEDs—is anticipated to boost the device's efficiency and stability.

6. Conclusion

Looking back, the continuous development and improvement of blue OLED technology has had a huge impact on the field of display and lighting technology. Electroluminescence in organic materials and the importance of energy levels and band gaps in blue OLEDs have laid the foundation for researchers to improve device performance. Recent research results show that the exploration of highly efficient emission materials such as phosphorescence and TADF materials opens up new ways to achieve stable and efficient blue emission. In addition, efforts to improve the stability of blue-emitting materials through molecular design strategies have shown promising results. By optimizing the host and transport materials and device structure, significant improvements in charge balance, recombination efficiency and overall device performance are achieved. However, challenges such as

energy gaps, stability issues and efficiency constraints remain. However, with the continuous advancement of materials science and the exploration of next-generation material innovations, such as environmentally friendly and multifunctional materials, it is evident that there is great potential for increasing the stability and efficiency of blue OLEDs.

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