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MULTIFUNCTIONAL APPLICATION OF PLANAR 2D MOLECULE FOR LIGHT-EMITTING HETEROSTRUCTURES

TThe object of research is the donor-acceptor compound, organic and hybrid heterostructures based on it. The paper is focused on a comprehensive approach to solving the problem of the efficiency of light-emitting devices, finding new technological and design solutions for the use of organic compounds as multifunctional materials for various types of light-emitting devices.

The paper presents the multifunctional application of a planar 2D molecule as an emission layer for typical and inverted types of light-emitting heterostructures, as well as a matrix for a host-guest system using inorganic quantum dots. The developed light-emitting structures are characterized by external quantum efficiency typical for fluorescent devices, but good stability over the entire length of the consumption voltage. QLED brightness is 1600 cd·m^{-2} and EQE 1.4 %, which are good parameters for use in display technology.

Organic LEDs based on planar molecules are promising candidates for use in modern lighting systems. A separate advantage of these light-emitting structures is the multifunctionality of using one compound for different types of light-emitting structures, including inverted heterostructures. Special attention is paid to the technological and design implementation of invert structures, since their geometry allows direct connection to the back board of the n-channel transistor on the substrate. In addition, organic LEDs have low energy consumption and are environmentally friendly due to the absence of toxic substances in their architecture, which creates the prerequisites for saving energy resources and reducing the industrial burden on the environment.

Keywords: *organic light-emitting diodes, OLED, inverted OLED, quantum dots, electron-hole emissive recombination.*

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1. Introduction

The development of new molecules and materials that can function as blue light-emitting components in organic light-emitting diodes (OLEDs) remains a challenge in both materials' science and organic chemistry. In the molecular design of light-emitting materials, various parameters such as chemical stability, solubility, aggregation and color purity must be taken into account. To further exploit the attractive optical properties of planar 2D molecules. Finally, organic light-emitting diodes using novel compounds as light-emitting layers have been fabricated and characterized, revealing the potential applications of planar 2D molecule as green-emitting electroluminescent semiconductors [1, 2].

Inverted OLEDs have attracted considerable attention due to the demand for active-matrix OLED display panels as their geometry allows direct coupling to the *n*-channel transistor backplane on the substrate. One of the main challenges for high-performance inverted OLEDs is an efficient electron injection layer with excellent electrical and optical properties compatible with the indium tin oxide cathode on the substrate [3].

Quantum dot QLEDs are attracting attention as a next-generation display alternative to liquid crystal displays (LCDs) and organic light emitting diodes (OLEDs). QDs used in electroluminescent (EL) devices can tune the emission color by changing the QD size1 and have a narrow full width at half maximum (FWHM) of 18–25 nm in the visible range, which increases color purity. These QLEDs are fabricated using the traditional architecture of OLEDs [4]. They are usually composed of materials such as organic monomers and metal oxides.

In this paper, let's investigate the planar 2D molecules and emission mechanisms occurring in OLEDs, inverted OLEDs and quantum dot-based OLEDs. The emerging luminescence properties of OLEDs and the various functions that planar 2D molecules can perform in OLEDs suggest that these new compounds are promising materials for organic electronics applications [5]. Special attention is paid to the technological and design implementation of invert structures, since their geometry allows direct connection to the back board of the *n*-channel transistor on the substrate.

The aim of this research is to study the multifunctionality of the planar 2D molecule in conventional and inverted organic light-emitting devices. We propose a synergistic electron injection architecture using surface modification of the ZnO layer to enhance electron injection into the organic emitter and simultaneously enhance the outward coupling of the directed light. Efficient inverted OLEDs are achieved by introducing a nanoimprinted non-periodic nanostructure of ZnO for broadband and angle-dependent light output and an n-type doped interlayer for energy level tuning and lowering of the injection barrier.

In addition, the transfer of energy from an organic compound to inorganic quantum dots is study. This would indicate that efficient forster resonance energy transfer (FRET) can take place when *Em1* is doped with CdSeS/ZnS alloy quantum dots. Therefore, the possibility of using planar 2D molecule as the host component of guest CdSeS/ZnS core-shell quantum dots in the fabrication of the corresponding QLEDs will be found.

2. Materials and Methods

Fabrication of conventional and inverted OLEDs. Devices with conventional electroluminescent structures using planar 2D molecules emitters were made by thermal vacuum evaporation of organic compounds and metal electrodes. The layers were deposited on pre-cleaned ITO (Indium Tin Oxide) glass substrates at base pressures below 10^5 Torr. CuI, an amorphous, optically transparent and highly conductive p-type semiconductor, was used as the hole injection layer in conventional OLED systems, while the TPBi layer (2,2′,2″-(1,3,5-benzintriyl)-tris(1-phenyl-1-benzimidazole)) served the dual function of electron transport and hole blocking. It fulfills the dual functions of electron transport and hole blocking. Various efficient cathode structures can be achieved in inverted organic light emitting diodes (IOLEDs). In this work, *n*-type semiconductor zinc oxide (ZnO) deposited by spin-coating on pre-cleaned ITO was used [6]. The TPBi layer promotes electron injection from the ZnO layer to the circulating emitter layer of the IOLED while effectively blocking hole injection [7]. Functional layers other than ZnO were deposited by thermal vacuum evaporation, and the IOLED was fabricated using a step-by-step method. Furthermore, MoO_3 was used as the hole injection layer in the IOLED [8]. Since Ca is highly reactive and corrodes rapidly in air, a Ca layer covered with a 200 nm aluminum (Al) layer was used as the cathode in the conventional OLED, while a pure Al layer was used as the anode material in the IOLED. The active area of both devices obtained was 2*3 mm^2. The intensity-voltage and luminance-voltage dependence were recorded using the HP4145A semiconductor parameter analyzer (USA). Calibrated photodiodes were used to measure brightness. Electroluminescence (EL) spectra were recorded using an Ocean Optics USB 2000 spectrometer (USA). The general configuration of the two fabricated devices corresponds to the following scheme (Fig. 1):

1) Conventional OLED: (An+)ITO/CuI/4/TPBI/Ca/Al(Cat-).

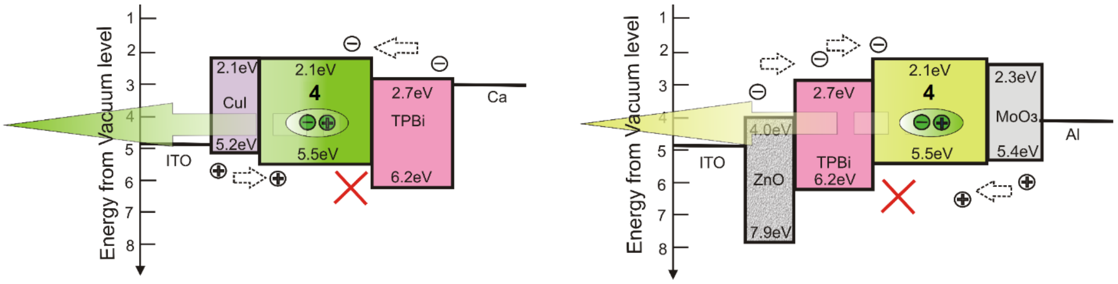
2) Inverted OLED: (Cat-)ITO/ZnO/TPBI/4/MoO_3/Al(An+).

Fig. 1 presents energy diagrams of developed conventional and inverted light-emitting devices. Functional layers are selected with insignificant, but present energy barriers to ensure recombination and balance of charge carriers in the emissive layers.

3. Results and Discussions

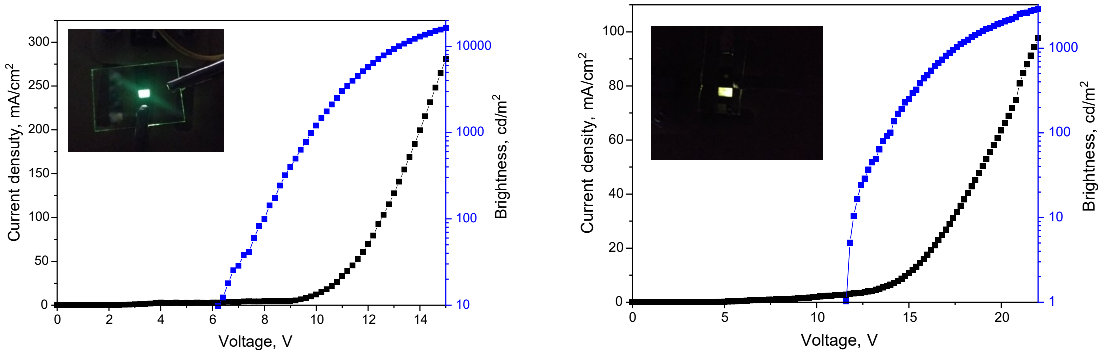
3.1. Fabrication and characterization conventional and inverted OLEDs. Fig. 2, *a*, *b* shows the brightness characteristics of conventional OLEDs structure and electroluminescence (EL) spectra.

Short wavelength emission band (about 515 nm) in the photoluminescence (PL) spectrum of solid-state films and the EL spectrum of conventional organic ELs (Fig. 3, *a*). Short-wavelength emission band in the photoluminescence (PL) spectrum of solid films and the EL spectrum of conventional OLEDs (approximately 51 nm) is due to the recombination of singlet excitons within the emission layer of compound 4.



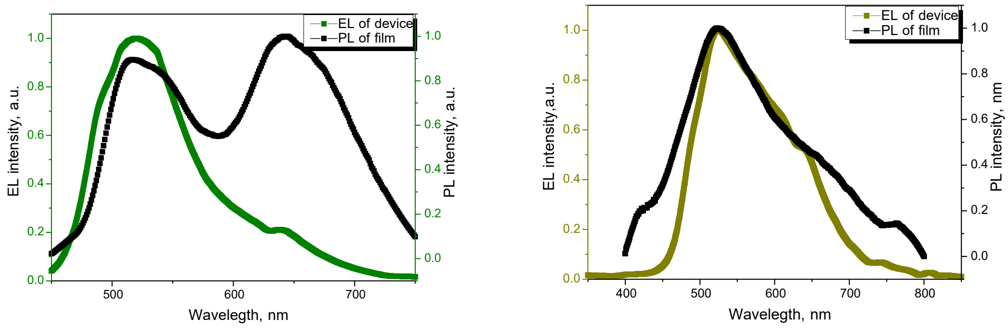
a *b*

Fig. 1. The energy diagrams of OLEDs: *a* – conventional; *b* – inverted



a *b*

Fig. 2. The current density/luminance vs. voltage characteristics of OLEDs based on the planar 2D molecules emitter: *a* – conventional; *b* – inverted



a *b*

Fig. 3. The EL spectra of OLED vs. PL spectra of: *a* – compound solid film; *b* – ZnO/compound heterostructure

The PL and EL spectra in Fig. 3 are both red-shifted relative to the fluorescence spectrum in solution. This is most likely due to the aggregation behavior of 4. This is supported by the appearance of low energy bands (around 650 nm wavelength) in the PL and EL spectra.

Low energy bands (around 650 nm wavelength) due to excimer emission from stacked excited state dimers were observed in the PL and EL spectra. However, there is a significant difference in the ratio of band intensities at short (515 nm) and long (650 nm) wavelengths. This was observed in the PL and EL spectra. This is due to the predominance of single-molecule (i. e. localized) exciton emission pathways due to the good excimer channel. Conventional OLED structures have a good electron-hole balance, which traditional OLED structure.

The EL spectra of IOLED devices are similar to the PL spectra of ZnO/4 bilayer structures and are also similar to the EL spectra of conventional OLEDs.

A major emission band is observed around 515 nm wavelength and a weak emission band is observed around 650 nm (Fig. 3, *b*). Comparing the PL spectra of the pure compound 4 thin film and the ZnO/4 structure, a large difference in the intensity of the long wavelength band at 650 nm is observed.

The reason for the quenching of this excimer band in the composite ZnO/4 film is probably the energy transfer from circulene to ZnO/4. It is likely that the energy transfer from the circulene to the ZnO layer. The higher excimer emission intensity under the influence of applied bias in the inverted structure (compared to conventional (compared to conventional ones) originates from the secondary Stark effect. Table 1 shows the lighting characteristics of conventional and inverted OLEDs using planar 2D molecule as the emitter.

Table 1

Lightning characteristics of conventional and inverted OLEDs based on the planar 2D molecule emitter

Device	V_{on}, V	Maximum brightness, cd·m^{-2}	Current efficiency, cd·A^{-1}	Power efficiency, lm·W^{-1}	*EQE*, %
			at 100/max. cd·m^{-2}		
conventional	5.8	16000	2.1/10.0	0.86/3.2	0.7/3.3
inverted	11.4	2800	1.5/3.0	0.3/0.5	0.5/1.1

Notes: V_{on} – turn-on voltage, *EQE* – external quantum efficiency

It should be emphasized that the use of planar 2D molecule 4 as an emitter for inverse OLEDs is practically convenient for future OLEDs. When the cathode of the IOLED is turned on (leaks) to the *n*-channel TFT of the printed TFT, it is practically convenient to use such an IOLED in an active-matrix OLED panel.

3.2. Fabrication and characterization of QLED. Considering that compound 4 is an amphipolar semiconductor, it is possible to use it as a hole transport layer in an OLED based on CdSeS/ZnS alloyed red-emissive quantum dots. The obtained devices (so-called QLEDs) consisted of the ITO/CuI/4/QD/TSPO1/TPBI/Ca/Al (energy diagram is shown in Fig. 4).

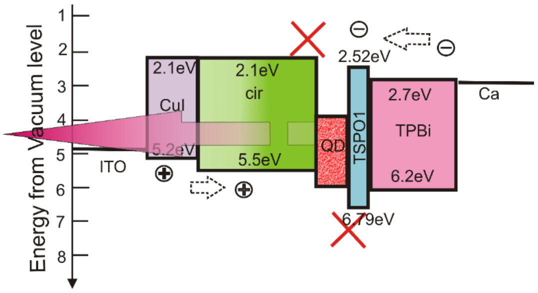


Fig. 4. QLED The energy diagram of fabricated in this work

This QLED used spin-coating and thermovacuum deposition techniques were used. As the first step an organic heterostructure, ITO/CuI/4, was formed by stepwise thermal vacuum deposition. Next, CdSeS/ZnS alloy quantum dots were deposited on ITO/CuI/4. They were deposited on ITO/CuI/circulene substrates by spin-coating technique. Finally, a hole-blocking TSPO1 layer, an electron transporting TPBi layer and Ca/Al cathode were deposited by thermo-vacuum deposition. The films were deposited by vapor deposition. The resulting QLEDs are characterized by vivid red electroluminescence, with an EL maximum (630 nm) and FWHM of the EL spectrum (30 nm) are exactly the same as those observed in photoluminescence. The EL spectrum of the CdSeS/ZnS alloy quantum dots is identical to that of the photoluminescence spectrum of the CdSeS/ZnS alloy quantum dots. The photoluminescence spectrum of λ_{em}=630 nm, FWHM=30 nm (Fig. 5, 6). The efficient transfer of charge carriers to the emission layer supports the use of compound 4 as a suitable hole transport material.

The illumination characteristics of the manufactured QLEDs are shown in Table 2.

Table 2 shows the luminance of 1600 cd·m^{-2} and an external quantum efficiency (*EQE*) of 1.4 % were achieved. The energy diagram of QLEDs (Fig. 4) shows that the valence band (*VB*) end (5.5 eV) of compound 4 was at the same energy as the hole-injected CuI (5.2 eV) and the corresponding VB levels of the luminescent QD (6.0 eV) layers.

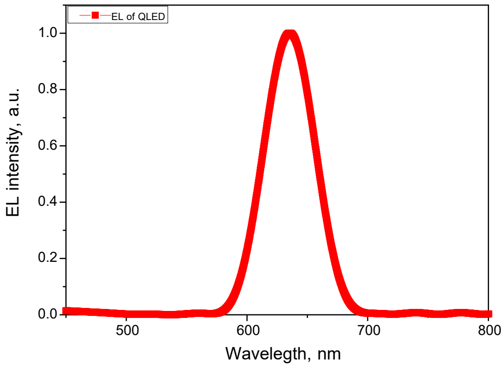


Fig. 5. EL spectrum of the fabricated QLED

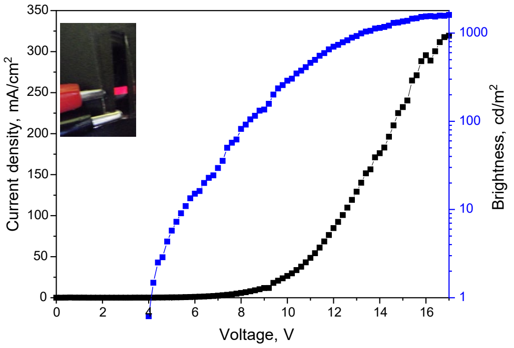


Fig. 6. The current density/luminance vs. voltage characteristics for the QLED

Table 2

Lightning characteristics of QLEDs based on the CdSeS/ZnS alloyed red-emissive quantum dots and compound 4 as hole-transporting material

Device	V_{on}, V	Maximum brightness, cd·m^{-2}	Current efficiency, cd·A^{-1}	Power efficiency, Lm·W^{-1}	*EQE*, %
			at 100/max. cd·m^{-2}		
QLED	4.0	1600	1.33/1.51	0.37/0.55	1.3/1.5

Notes: V_{on} – turn-on voltage, *EQE* – external quantum efficiency

The use of compound 4 as a hole transport layer enables the smoothing of the energy barrier for hole injection between the CuI and QD layers and the electron injection from the QD layer into the circulene conduction band (the energy barrier for such an injection is about 2 eV). Blocking electron-hole emission recombination, which occurs only in the QD bulk [9].

The final illumination characteristics of this OLED are similar to those published in a recent report [10]. The final illumination properties of the fabricated OLED are similar to those presented in a recent report [10]. The same type of red emissive CdSe/ZnS is a technical investigation of the appropriate conditions to achieve distinct narrow electroluminescence from the same type of red emissive CdSe/ZnS quantum dots.

3.3. Discussion. In recent years, OLED manufacturing technology has reached the stage of practical application, and methods to optimize emission color quality continue to evolve, creating new device architecture approaches to improve energy efficiency and color quality. In this context, the use of OLED technology with its simplified structure is extremely promising.

The devices exhibit efficient emission characteristics and high color stability, making them very useful for use in modern lighting systems and display technology.

The main limitation of the applicability of the results obtained is the high cost of introducing lighting systems based on the studied compounds into mass production.

Also, the gradual degradation of light-emitting layers during operation leads to a decrease in efficiency and changes in spectral characteristics.

It should be noted that for the further introduction of the obtained OLEDs as key elements of modern lighting systems, complex work needs to be carried out. In particular, it is necessary to fulfill such complex tasks as the development of the technology of thermal vacuum application of functional light-emitting structures at industrial facilities and obtaining large-area OLED matrices. Another conditions to increase stability and roll-off of devices are the technology of incapsulate or passivate of these devices.

Power outages caused by the war in Ukraine may have affected the production technology of light-emitting devices and led to the deterioration of the output parameters of OLEDs.

4. Conclusions

This paper reports the multifunctional application of a simple donor-acceptor organic compound, as emissive material in the emission layer of organic light emitting devices. Compound 4 has been used as active components in OLEDs, where compound 4 is the emitter (Device A) in conventional and inverted OLED and the transport layer of the CdSeS/ZnS alloy quantum dot. The external quantum efficiencies of devices A-C are characterized by values common to pure fluorescent OLEDs (up to 5 % of the theoretical limit). These devices sustain low-efficiency roll-off of electroluminescence over a wide range of current densities. The brightness of QLED is 1600 cd·m^{-2} and EQE 1.4 % which are good parameters to application for displays technology.

Conflict of interest

The authors declare that they have no conflict of interest concerning this research, whether financial, personal, authorship or otherwise, that could affect the study and its results presented in this paper.

Financing

The study was performed without financial support.

Data availability

The paper has no associated data.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating this work.

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