Molecular Energy Level Effect of the Hole Transport Layer in OLED
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Abstract
This work elucidates the impact of the molecular orbital energy level of the hole transport layer (HTL) on the electric-field, carrier accumulation and exciton generation in organic light emitting diodes using SETFOS. A deeper highest occupied molecular orbital energy level of HTL could reduce hole-injection-barrier between HTL and emissive layer, and hence enables high efficiency.

1. Introduction
The organic light emitting diodes (OLEDs) have been the most promising candidates in today's emerging high-quality flat panel display and solid state lighting technology. After the milestone study of OLEDs by Tang and VanSlyke in 1987, enormous efforts have been done on the improvement of devices in terms of their efficiency, stability and color tunability, making them ideal for the future display and ambient lighting.

In this article, we demonstrate a comprehensive model to quantitatively investigate the effect of highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) level of HTL on the electric field, charge drift and exciton recombination probability in the organic light emitting diode.

2. Multi-layered OLED Structure
2.1 Device designing
Electrical Simulation Moleccl-energy-level-dependent internal electric field and recombination zone in each organic layer of the studied OLEDs were performed using a commercial software package SETFOS. The setting parameters included hole mobility, electron mobility, lowest unoccupied molecular orbital (LUMO), and highest occupied molecular orbital (HOMO).

Figure 1 shows the studied OLED device structures and their corresponding energy level diagrams. The device structure consisted of an indium tin oxide (ITO) as the anode layer, a 3 nm 1,4,5,8,9,11-hexaazatriphenylene hexacarbonitrile (HAT-CN) as a hole injection layer, a 40 nm 4,4'-cyclohexylidenebis[N,N-bis(4-methyl phenyl)benzenamine] (TAPC) as a hole transporting layer, a 15 nm single emission layer (EML), a 40 nm 1,3,5-tris( N-phenyl-benzimidazol-2-yl) benzene (TPBi) as ETL, a 0.5 nm lithium fluoride (LiF) as electron injection layer, and a 100 nm aluminum as cathode. The employed light-emitting green dye was tris(2-phenylpyridine) iridium(III) (Ir(ppy)3). The employed host was 4,4'-bis(carbazol-9-yl)biphenyl (CBP) for Device I, and 4,4',4''-tri(N-carbazolyl) triphenylamine (TCTA) for Device II. The work function set was 5.2 eV for the anode and 4.3 eV for the cathode.

Fig. 1. Schematic energy-level diagrams of the OLED devices with CBP (Device-I) and TCTA (Device-II) hosts.

2.2 Electric field
In the OLEDs, holes are entered from the anode into the HOMO of HTL, while electrons are entered from the cathode into the LUMO of ETL. The electric field in EML and ETL is affected only by HOMO level, but remains unaffected by LUMO level of the HTL material. The reason beside this may be varying the LUMO level of HTL changes the electron density in HTL but the hole density remains the same.

Figures 2(a) and (b) show the HOMO-dependent internal electric fields of the CBP- and TCTA-host containing devices. As seen, the electric field distribution in EML is highly sensitive to the HOMO level of HTL, as compare to ETL. The electric field in EML markedly decreases as the HOMO level of HTL increases, indicating the tuning of HOMO levels of HTL to be a highly effective approach to prevent electric breakdown caused device failure, if any. Furthermore, Figures 2(a) and (b) also show that the electric field in ETL decreases as the HOMO level of HTL increases, when CBP is taken
as a host, but it remains unaffected, when TCTA is taken as a host.

Fig. 2. Electric field variation in EML and ETL at different HOMO values of HTL (TAPC) and (a) CBP as a host (b) TCTA as a host.

2.3 Recombination

We further investigated the effect of the different HOMO level of HTL on the spatial recombination distribution. Figure 3(a) show that as the HOMO level of HTL increases from 5.3 eV to 5.7 eV the recombination peak of Device-I with CBP host decreases at HTL/EML interface whereas increases at the interface of EML/ETL. Futhermore, Figure 3(b) shows that the recombination at EML/HTL interface independent with the HOMO level of the HTL, for the device having TCTA host. However, the recombination peak is higher for lower HOMO at HTL/EML interface. Figures 3(a) and (b) also show that the recombination of the entering holes and electrons would mainly occur within the emission layer, but be dispersed near the two interfaces for the CBP host composing device. Whilst, the recombination would still mainly occur within the emission layer, but concentrates near the interface between EML and ETL for the TCTA-host composing counterpart.

Fig. 3. Recombination distribution in device corresponding to different HOMO values of HTL (TAPC) and (a) CBP as a host (b) TCTA as a host.

3. Conclusions

In this study, we have demonstrated a computational model to analyze the effect of HOMO/LUMO levels on the electric field and recombination zone in the OLED. The simulations have shown that the electric field in EML is more sensitive to the HOMO level of the HTL, as compare to ETL. Moreover, spatial recombination distribution, hence efficiency and lifespan of OLEDs also depend on hole injection barrier between HTL and EML. The findings might help domain experts to carry out extensive studies to design and synthesize the suitable HTL materials for OLEDs.

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References
