Numerical Analysis on the Electrical and Optical Properties in Multilayer OLED Device

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ABSTRACT
In this paper, we report our numerical study on the electrical and optical properties in multilayer organic light emitting diode (OLED) device structure. Our finite element method (FEM) model includes the transport behavior of electrons and holes, the generation and decay of excitons, and emission and extinction properties of excitons. We made a focus on the charge balance in host material comprising a phosphorescent OLED (PHOLED). Finally, we investigated the variation of charge density and recombination density, which affect exciton density.

NUMERICAL MODEL
The electrical and optical characteristics of multilayer OLEDs critically depend on the device structure, which includes the species of LUMO and HOMO, the thicknesses of each layer, and sequence of layers. In order to analyze each element, we need to employ a numerical model which allows us to optimize the OLED structure.

\[
\frac{\partial E(x)}{\partial x} = \frac{e}{\varepsilon_0} (p(x) - n(x) + p_i - n_i - A^{\text{Doping}} - D^{\text{Doping}}) \quad (1)
\]

Equation (1) is the Poisson equation that yields the electric field distribution. \( n(x) \) is the density of electrons, \( p(x) \) is density of holes, and \( E(x) \) is the electric field.

\[
\frac{\partial n(x)}{\partial t} = \frac{1}{e} \frac{\partial J_n(x)}{\partial x} - r(x) \cdot p(x) \cdot n(x) \quad (2)
\]

Equation (2) is continuity equation for electrons determines the time evolution of the system. \( r(x) \) means Langevin recombination rate coefficient.

SIMULATION RESULTS
We use the multilayer structure that consists of 1,1-bis[(di-4-tolylamino) phenyl] cyclohexane (TAPC); 4,4'-bis[N-(1-naphthyl)-N-phenylamino] bipheryl (\( \alpha \)-NPD); 4,4'-bis[N-(p-tolyl)-N-phenylamino] bipheryl (TPD) as a hole transport layer, 3,5'-N,N'-dicarbazole-benzene (mCP) as an emissive layer, 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP); 4,7-diphenyl-1,10-phenanthroline (BPhen) as an electron transport layer. Fig. 1 is a schematic diagram illustrating the multilayer structure for organic light emitting diodes under this work. Referring to Figs. 2 (a) and (b), we can see how the density of carriers change as time continues. Fig. 3 (a), (b) are plots in case when the energy level of HTL and ETL has been changed. Keeping the energy level of the other layers unaltered, we varied the HOMO energy level of TAPC from 5.3eV to 5.7eV and LUMO energy level of BPhen from 3.0eV to 3.4eV. While the injection barrier height is raised by the increment of the HOMO energy level of TAPC, the internal barrier height is reduced. Fig. 4 shows a plot illustrating the recombination density for the wide range of devices.

CONCLUSION
Our simulation exhibits that the recombination density varies with the energy level. Furthermore, we could demonstrate that the charge balance has a strong effect on the recombination density profile.

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REFERENCES
Fig. 1. Schematic diagram illustrating the multilayer structure under this study.

Fig. 2. (a) Calculated electron density profile in OLED after turn-on [10μs]
(b) Calculated hole density profile in OLED after turn-on [10μs].

Fig. 3. (a) Recombination density profile for different HOMO energy level of TAPC [eV].
(b) Recombination density profile for different LUMO energy level of BPhen [eV].

Fig. 4. Calculated recombination density profile for the variation of material.