

Theoretical and experimental study of highly efficient blue emitters for organic light-emitting diodes

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Although organic light-emitting diodes (OLEDs) using phosphorescent emitters (PhOLEDs) have shown ~20% external quantum efficiency (EQE), the efficiency roll-off at high current density is severe, which limits their application when high brightness is required, such as for outdoor lighting. On the other hand, OLEDs using fluorescent emitters (FOLEDs) exhibit better efficiency roll-off due to shorter exciton lifetime and less bimolecular quenching. However, the FOLEDs can only use singlet excitons, to convert electrical energy to light, which imposes a limit of the EQE of 5%. Conversely, recent theoretical studies indicate that it is possible to achieve highly efficient FOLEDs because the singlet generation fraction can be higher than indicated by the classical statistical limit.

To obtain this goal, we designed and synthesized organic molecules bearing electron-donating and/or electron-withdrawing fragments. By optimizing the molecular structures via incorporating both electron-donating and electron-withdrawing groups to the molecules, we attain a remarkable improvement in the maximum EQE of undoped device from 2.0% to 4.99%. Additional optimization of the thickness of emitting layer and applying thermal annealing treatments led to a very high maximum EQE of 7.40% for the undoped sky-blue device. In order to improve the efficiency as well as the color purity, we doped the emitter in a suitable host material, 4,4'-bis(carbazol-9-yl)biphenyl (CBP) at an optimized concentration of 4%, to achieved pure blue emission with extremely high maximum EQE of 8.60% and CIE coordinates of (0.149, 0.132).

Our theoretical study indicates that designed molecules possessing both electron-donating and electron withdrawing fragments have lower carrier injection barriers and more balanced hole-electron transport properties. Furthermore, using a simplified model and density functional theory (DFT) calculations, the singlet generation fraction of the emitters was calculated to be about 50%, much higher than the 25% from simple classical statistics.

Our efforts indicate that it is possible to obtain FOLEDs with efficiency higher than 5% limit, by optimizing molecular structures and device designs.