

**THE ROLE OF HOSTS ON EFFICIENCY IN ORGANIC LIGHTING-EMITTING
DIODES WITH THERMALLY ACTIVATED DELAYED FLUORESCENCE
(TADF) MOLECULES**

Emmanuel Santos Moraes (emmanuel-moraes@hotmail.com)

José Carlos Germino (germino@ua.pt)

Lucas Scalon (scalon.chem@gmail.com)

Teresa Dib Zambon Atvars (atvars@unicamp.br)

Luiz F. R. Pereira (luiz@ua.pt)

Thermally activated delayed fluorescence (TADF) organic compounds represent an innovative approach when applied to organic light-emitting diodes (OLEDs) due to their ability to collect triplet excitons under electrical injection, leading to an internal quantum efficiency (IQE) of 100% without the use of heavy metals in the structure. Due to the role of triplet states in the process, the selection of host materials, with respect to energy levels and charge mobility, is fundamental to optimizing the charge-carrier balance in the active layer and achieving the device's maximum external quantum efficiency (EQE).¹ In this study, we investigated the influence of different host materials, mCP and DPEPO, along with a 1:1 mixture of both, with a blue TADF emitter, DMOC-DPS.^{2,3} Using steady-state spectroscopy and photoluminescence lifetime, corroborated by density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations, we demonstrate that host polarity and the alignment of triplet state energy levels significantly affect exciton recombination dynamics. Our results indicate that a

smaller singlet-triplet energy gap (ΔE_{ST}), less than 0.05 eV, increases the reverse intersystem conversion (RISC) in the electroluminescence process. Furthermore, based on spin-orbit coupling (SOC) calculations, both 3CT-1CT and 3LE-1CT pathways are viable with low ΔE_{ST} . The device layers were fabricated by solution processing via spin coating. The dual-host approach significantly increased the device EQE, rising from 3.0% in single-host devices (mCP and DPEPO) to 7.8% in dual-host devices (mCP:DPEPO). The final device color ranged from blue in mCP to cyan in DPEPO, and the 1:1 mCP-DPEPO mixture exhibited an intermediate blue color compared with the pure hosts. These results provide valuable insights into the optoelectronic properties operating in the TADF regime, offering guidelines for the rational design of high-performance OLEDs.

Reference

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Palavras-chave: oled; tadf; host; solution-processed.