Article

Theoretical Investigation of Triscarbazole Derivatives As Host Materials for Blue Electrophosphorescence: Effects of Topology

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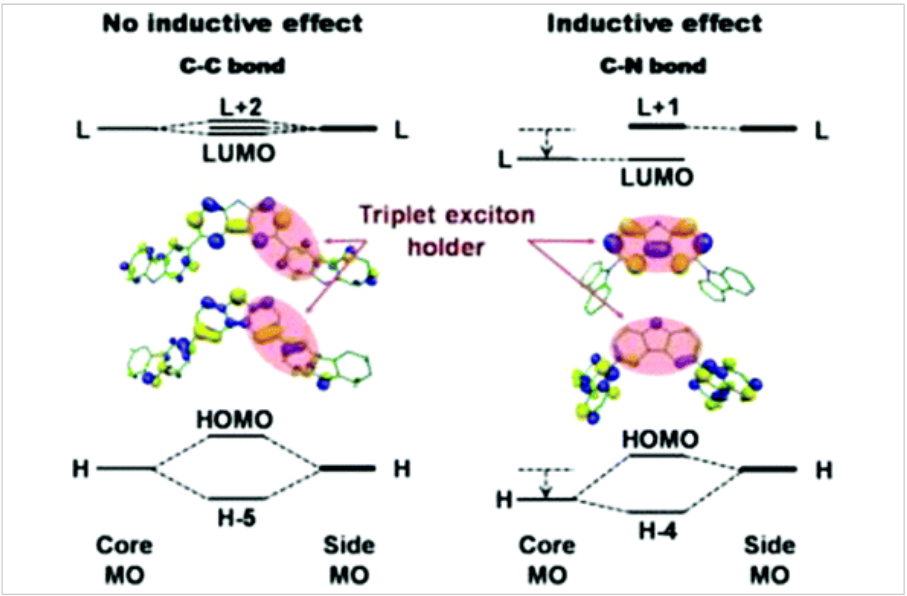
Abstract



We have investigated the electronic structure of triscarbazole derivatives used as host materials in blue phosphorescent organic light-emitting diodes. The results of density functional theory calculations show that, in the case of triscarbazole derivatives where the carbazole units are linked via C–C bonds, the frontier molecular orbital energies are modulated by strong molecular orbital interactions between the central and side carbazole

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units. On the other hand, in the case of triscarbazoles linked via C–N bonds, the combination of inductive effects and molecular orbital interactions tunes the frontier level energies and, interestingly, gives rise to an ambipolar character. In the C–N linked systems, the lowest triplet states are characterized mainly by an electronic transition localized within the central carbazole, while in the C–C linked compounds it is the longest oligo-*para*-phenyl segment to be found in the chemical structure that defines the lowest triplet transition. When the N–H group of the central carbazole unit is replaced by other groups [O, S, CH_2, $C(CH_3)_2$, $C(CH_3)(CF_3)$, and $C(CF_3)_2$], the HOMO/LUMO energies fluctuate substantially in the absence of the side carbazoles, but these variations are significantly reduced in their presence; also, the singlet–triplet energy differences decrease substantially when going from the isolated central unit to the triscarbazole-like derivatives.

Keywords: blue OLEDs; ambipolar hosts; triscarbazoles; singlet−triplet energy differences; density functional theory (DFT) calculations