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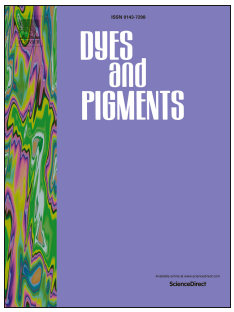

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Boron-Based TADF Emitters with Improved OLED Device Efficiency Roll-Off and Long Lifetime

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Abstract

A class of four-coordinate boron complexes is reported that contain both electron-rich and electron-poor functional groups. Judicious selection of donor and acceptor moieties with the use of a boron atom as a separating node yields charge transfer complexes capable of thermally activated delayed fluorescence (TADF). Complexes were prepared by a modular method providing access to a wide range of emission colors. The singlet (S1) and triplet (T1) energies are independently tuned to achieve a small S_1-T_1 gap. Raising and lowering of S_1 and T_1 states can be predicted using cyclic voltammetry, NTO analysis, and spin density distribution as determined using Density Functional Theory; separation of the hole and electron wavefunction for S_1 excitation and delocalization of spin density distribution in the T_1 state can help in achieving negligible S_1-T_1 gap. Although photoluminescent quantum yields of the boron complexes in a host matrix are less than 65%, OLED device external quantum efficiencies of up to 8.1% have been achieved at a luminance of 1000 cd/m^2. Selection of a