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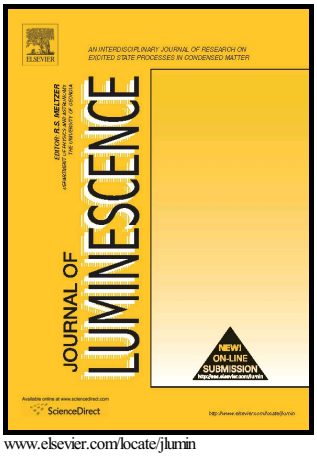

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Excited state properties of two unusual thermally activated delayed fluorescence molecules: A theoretical investigation

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Abstract

High efficient thermally activated delayed fluorescence (TADF) emitters containing 2,4-bis(3-(9H-carbazol-9-yl)-9H-carbazol-9-yl)-6-phenyl-1,3,5-triazine (CC2TA) and 2-biphenyl -4,6-bis(12-phenylindolo[2,3-a] carbazole-11-yl)-1,3,5-triazine (PIC-TRZ) exhibit an internal quantum efficiency (η_{int}) of 56% and 34% respectively, which breaks the traditional limitation of 25%. CC2TA and PIC-TRZ are two special cases in Adachi's work and they are not in accordance with their proposed regulations. Based on the newly-proposed optimal Hartree–Fock percentage (OHF) method, we investigate the adiabatic energy gap (ΔEst) between the first singlet (S_1) and triplet (T_1) excited state as well as the absorption and emission spectra for CC2TA and PIC-TRZ. Moreover, we investigate the intersystem crossing (ISC) and reverse intersystem crossing (RISC) processes to illustrate the internal transfer mechanism of singlet and triplet excitons. Results show that our calculated data are consistent with the experimental values. RMSD and Huang-Rhys factor are smaller for PIC-TRZ than these for CC2TA, this results the non-radiative decay rate from S_1 to ground state (S_0) is decreased for PIC-TRZ. Moreover, the ISC and RISC processes are multi-step processes with the incorporation of intermediate energy level between S_1 and T_1. Our work could provide a clear guidance for molecular luminescence simulations and the design of high efficient TADF molecules.