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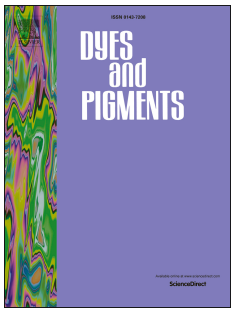

Investigation on the effect of connected bridge on thermally activated delayed fluorescence property for DCBPy emitter

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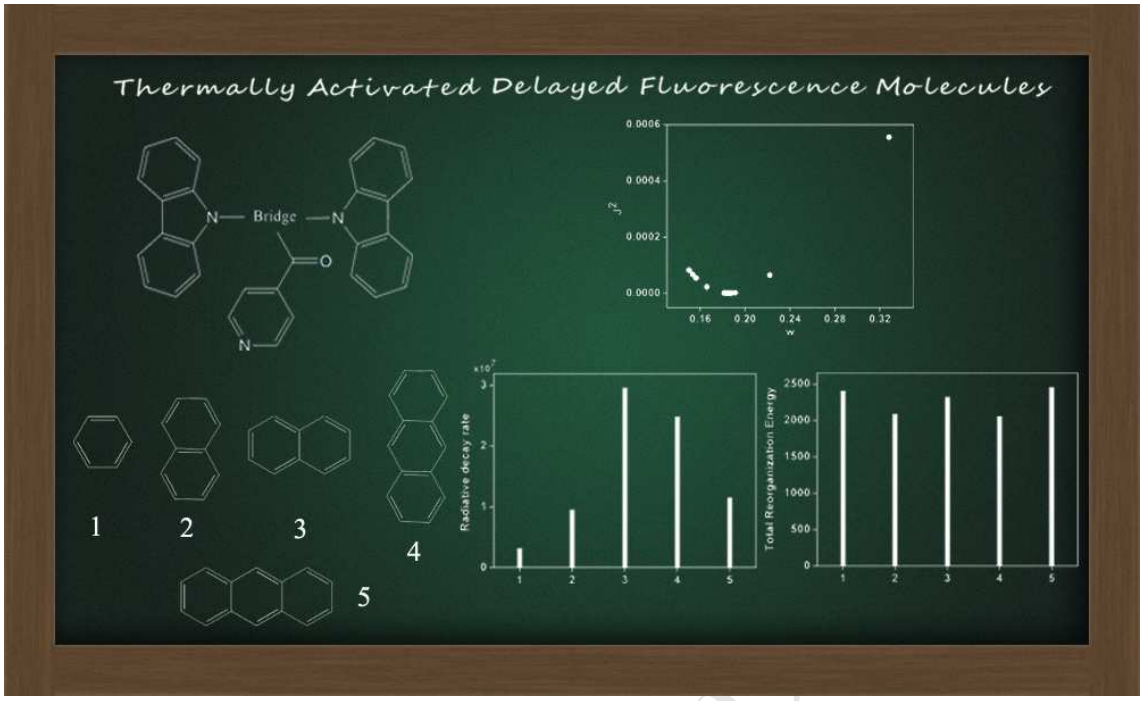

Previously, extensive efforts have been devoted to designing highly performance TADF material via varying the electron-donator (D) and electron-acceptor (A) units and tried the best to find a matching combination of D and A units with high external quantum efficiency. In present work, we have investigated the effect of modifying the connected bridge between D and A units on their electronic properties. Based on the reported thermally activated delayed fluorescence (TADF) molecule DCBPy (compound **1**), four compounds **2-5** have been designed by modifying the connected bridge between D and A units. For predicting the accurate singlet-triplet energy gap (ΔE_{ST}), the tuning range-separated functional has been utilized to calculate ΔE_{ST}. The calculated normal mode reorganization energy (λ) for the non-radiative decay process displays that the λ of compounds **2-5** in the high-frequency region is noticeably reduced compared with compound **1**, suggesting that the high-frequency C=O stretching vibration is hindered through modifying the connected bridge between D and A units. Moreover, the radiative decay rate constant (k_r) values of compound **2-5** are one order of magnitude higher than that of pristine compound **1.** Besides, for our designed molecules, modifying the connected bridges noticeably increase their spin-orbital coupling matrix element ($<S_n|H_{SOC}|T_n>$) values, although the ΔE_{ST} values of compound **2-5** are greater than that of compound **1**. As a consequence, for this kind of DCBPy compounds, modifying the connected bridge between D and A units maybe a valid approach to improve their TADF performances.