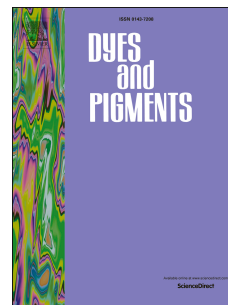


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Investigation on the effect of connected bridge on thermally activated delayed fluorescence property for DCBPy emitter

Ying Gao, Yun Geng, Yong Wu, Min Zhang, Zhong-Min Su



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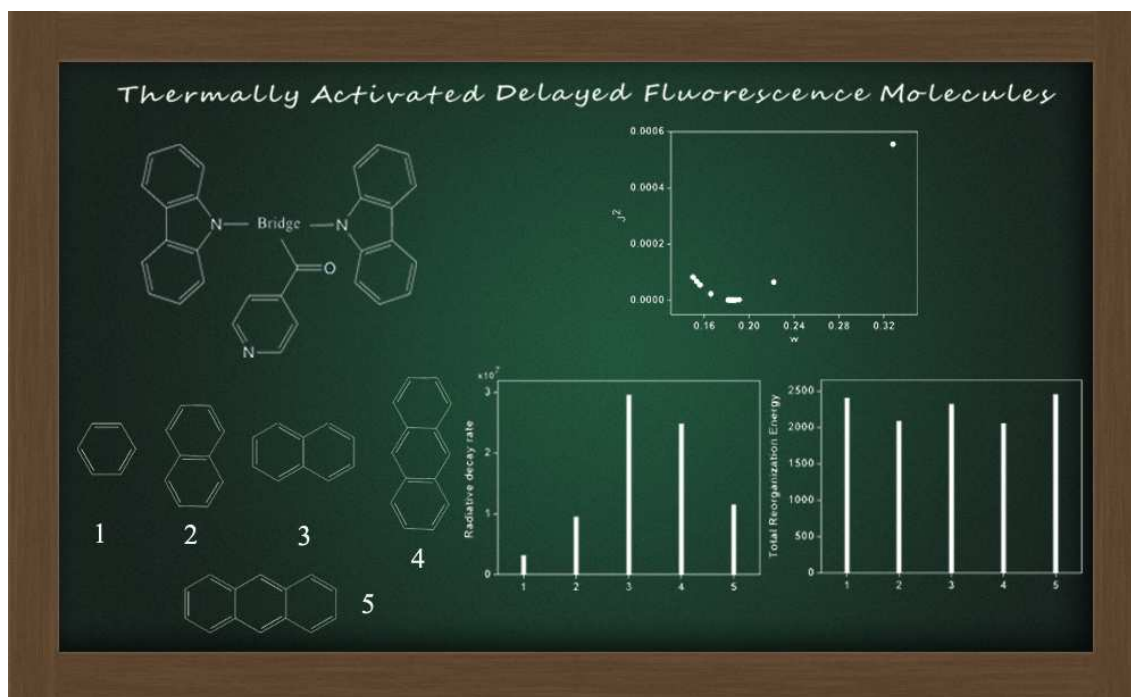
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Previously, extensive efforts have been devoted to designing highly performance TADF material via varying the electron-donor (D) and electron-acceptor (A) units and tried the best to find a matching combination of D and A units with high external quantum 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 ( $\Delta E_{ST}$ ), the tuning range-separated functional has been utilized to calculate  $\Delta E_{ST}$ . The calculated normal mode reorganization energy ( $\lambda$ ) for the non-radiative decay process displays that the  $\lambda$  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 ( $\langle S_n | H_{SOC} | T_n \rangle$ ) values, although the  $\Delta E_{ST}$  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.

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