Prediction for photophysical properties of thermally activated delayed fluorescent emitters and application to carbazole-oxadiazole derivatives

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Highly efficient thermally activated delayed fluorescent (TADF) emitters have significant attention in the field of organic light-emitting diodes (OLEDs) to develop high performance. TADF emitters allow the internal quantum efficiency (IQE) theoretically up to 100% by harvesting both singlet and triplet through the reverse intersystem crossing (RISC). Prediction of energy difference between first excited singlet state (S_1) and first excited triplet state (T_1), ΔE_{ST}, is important to design highly efficient TADF emitters because ΔE_{ST} is highly related to reverse intersystem crossing rate (k_{RISC}). Here, we developed methods to predict ΔE_{ST} based on time-dependent density functional theory (TD-DFT). Moreover, k_{RISC} was computed by Fermi Golden rule [1] and Marcus theory [2]. We found that k_{RISC} is correlated with decay time of TADF emitters. We applied our methods to carbazole-oxadiazole derivatives, and TADF devices made from carbazole-oxadiazole-based materials were shown to small ΔE_{ST} with high external quantum efficiency of up to 24.4% [3]. These results demonstrate that prediction of energy differences and k_{RISC} are promising methods and parameters for application in developing highly efficient TADF system.

References

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