From triplet to singlet: exploring fluorescence enhancements in organic materials

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Energy transfer has been in the center of a manifold of optics, photonics and optoelectronic applications. Usually, triplet excitons contribute negatively to a device's efficiency, especially in organic light-emitting diodes (OLED). Experimental studies have been able to demonstrate simultaneous singlet-singlet (SS) and triplet-singlet (TTS) FRET from a single donor material (NPB) [1]. To explore this further, we used Density Functional Theory (DFT) to analyze the geometry and normal modes of NPB and the acceptor (DCJTB) molecules. By employing the nuclear ensemble method, we obtained the absorption and emission spectra for both materials. Additionally, we calculated the intersystem crossing (ISC) rates and phosphorescence spectra of NPB regarding the triplet excited state. In previous experimental studies, it has been observed that changes in the acceptor concentration can lead to alterations in the system's polarizability [2] . This effect influences fluorescence spectra due to their dependence on the dielectric constant, subsequently impacting how intersystem crossing, emission, and transfer rates are calculated. To gain further insights into these dynamics, we developed a Kinetic Monte Carlo (KMC) algorithm based on electronic structure parameters from differently polarized systems. Using this approach, we investigated energy transferring, internal conversion, and non-radiative contributions as the acceptor concentration increased. The first mentioned experimental work attributed the intense decay in exciton lifetime to non-radiative processes. Our results indicate that TTS does occur, which is in agreement with experimental results. The authors claim that the observed lifetime decay is mostly attributed to non-radiative decay in the donor. Nonetheless, the same decay was well reproduced without taking any form of non-radiative process into consideration. In conclusion, our study sheds light on the simultaneous SS and TTS transfers and provides valuable insights into energy transfer mechanisms. These findings contribute to the advancement of optics, photonics, and optoelectronics, particularly concerning organic light-emitting diodes.[1]

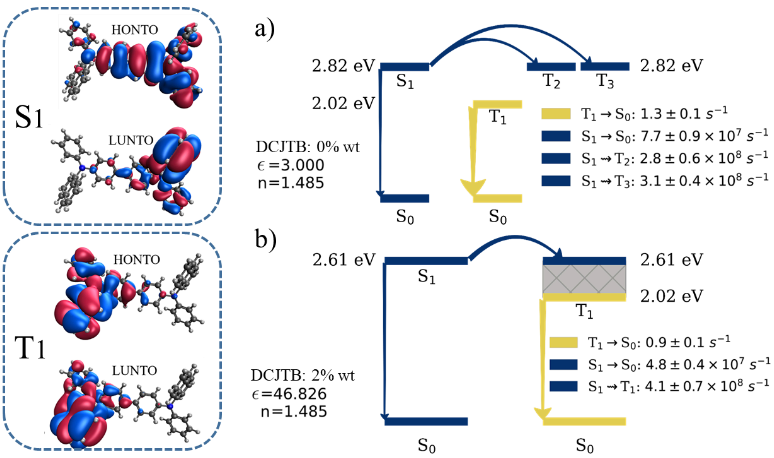

Figure 1: NTOS for the S_1 and T_1 states along with energy level diagrams of NPB with (a) 0\% DCJTB concentration and (b) 2% concentration. Curved and straight arrows represent ISC and emission, respectively.

Keywords: triplet to singlet, afterglow, delayed fluorescence, excitons

[1] Kirch, A. et. al. The journal of physical chemistry letters 10.2 (2019): 310-315.
[2] Bulović, V., et. al. Chemical Physics Letters 287.3-4 (1998): 455-460