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## Spectroscopic and theoretical investigations on intramolecular charge transfer phenomenon in 1-3-dioxolane derivative

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### Abstract

High fluorescence quantum yield (FQY) and large Stokes shift (SS) cannot be easily achieved simultaneously by traditional PICT or TICT fluorescent probe. However, an 1-3-dioxolane derivative named 5-methyl-8,9-dihydro-5H-[1,3]dioxolo[4,5-b]carbazol-6(7H)-one (MDDCO) features both high FQY and large SS. The purpose of this study is to search the mechanism behind this phenomenon by theoretical method. Simulated structure changes and charge transfer suggest ICT process in MDDCO is similar to PLICT (Planarized Intramolecular Charge Transfer) process. Calculated UV-Vis spectra and fluorescence spectra show that PLICT-like state ( $S_1$  state) of MDDCO leads to large SS. Computed transient-absorption spectra and radiative decay rates indicate that PLICT-like state is key factor for high FQY of MDDCO. These findings suggest that PLICT-like state in 1,3-dioxolane derivatives can achieve both large SS and high FQY, which presents a new method for high-performance fluorescent probe design.

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