Intra- vs. intermolecular charge transfer in substituted 1,4-Distyrylbeneze: A quantum mechanical and photophysical approach

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Purely organic materials with π-conjugation have garnered significant interest in fundamental and applied research due to their versatile applications. These materials find use in various fields such as organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), organic light emitting transistors (OLET), and organic lasers.[1-3] Understanding the intramolecular (ICT) and intermolecular (InCT) charge transfer processes of these materials is crucial for their aforementioned applications. In this talk, I will present a detailed photophysical and quantum-mechanical analysis of various Donor-substituted (D), Accepter-substituted (A), co-crystal of various D and A (D:A), and donor-acceptor (DA) based distyrylbenzene (DA-DSB) molecule (Figure 1).

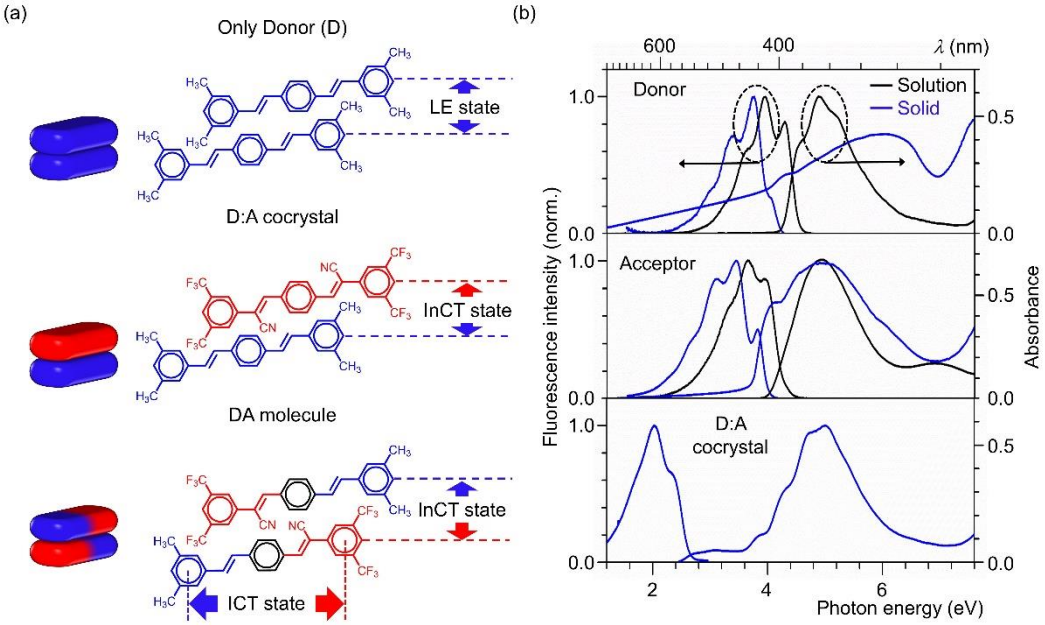

Figure 1: (a) Schematic representation of the studied molecules, (b) absorption and emission spectra of these molecules.

Reference:

[1] Gierschner, J.; Shi, J.; Milián-Medina, B.; Roca-Sanjuán, D.; Varghese, S.; Park, S. *Adv. Optical Mater.* **2021**, *9*(13), 2002251.
[2] Varghese. S. *et. al. Adv. Mater*. **2012**, *24*, 6473.
[3] Kwon. Y. *et. al. Nat. Commun*. **2023**, *14*, 92.