Enhanced Exciplex Formation on Triphenylamine-Benzothiazole (TPA-BT) Derivatives

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This study designed and synthesized a series of donor (D) molecules in an attempt to form exciplexes with known acceptor (A) molecules and to investigate the influence of the chemical structure of monomers on the photophysical properties of exciplexes. The five synthesized donor molecules exhibit intramolecular charge transfer effects. Changes in transition dipole moments were analyzed using the Lippert-Mataga model. Moreover, the electronic energy levels of these five molecules were estimated through molecular simulations and electrochemical potential measurements, providing the ground-state energies of the D molecules, which lie between the ground and excited-state energies of the A molecules, thus enabling the formation of exciplexes. The aggregation of D-A pair molecules resulted in the formation of a new emission band, indicating the presence of exciplexes. Controlling the electronic energy levels of electron donor molecules can regulate the emission wavelength of the formed exciplexes. Furthermore, the D molecules with a triangular-like structure are more likely to form exciplex than rod-like molecules. These triangular-like donors were selected to assemble solid films, and then, a preliminary optoelectronic device was fabricated. This report provides insights into monomer design and its impact on the desired photophysical properties of exciplexes, serving as a blueprint and guidance for molecular design in application-oriented product development.

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