Title:	Band Gap Modulated Donor-Acceptor Small Molecules for Efficient Charge Transport Properties and as Metal- free Visible Light Photocatalysts
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Abstract:	Donor-acceptor (D-A) □-conjugated small molecules and polymers have witnessed substantial advancements in optoelectronic applications over the past several decades. Such materials are well-studied for their exceptional optical and electronic properties resulting from the favourable interactions between D and A moieties within a conjugated framework. Optoelectronic device performances are largely governed by the mobility of charge carriers and thus, an in-depth understanding of charge transport properties of such D-A molecules is of paramount importance. Another emerging application of D-A □-conjugated small molecules has been in the realm of visible light photocatalysis which is rarely addressed and explored in literature. In this thesis, three distinct sets of D-A π-conjugated molecules have been designed and synthesized and their optical and redox characterization have been performed. Their charge transport properties have been investigated using space-charge limited current (SCLC) technique. Subsequently, the applications of these molecules as visible light, metal-free photocatalysts in various organic transformations have been explored. In the first chapter, tripodal D-A small molecules, Tr-Np3 and Tr-T-Np3, composed of 2,4,6-triphenyl-1,3,5- triazine and naphthalimides, without and with thiophene spacer were synthesized. These molecules displayed broad absorption in the visible range and appropriate energy levels for efficient electron transfer processes. Tr-Np3 and Tr-T-Np3 exhibited appreciable electron mobilities of 5.24 × 10 − 4 and 6.14 × 10 − 4 cm 2 /V s, respectively. These molecules demonstrated remarkable photocatalytic abilities for metal-free condensation cyclization reactions of aromatic aldehydes and o-phenylenediamine under blue light, yielding pharmaceutically relevant benzimidazole derivatives (conversion up to 99%). In the second chapter, A-D-A π- conjugated small molecules triad 1 and triad 2 composed of dithienopyrrolobenzothiadiazole (DPBT) and naphthalimide, without and with thiophene spacer, were synthesized. These triads exhibited broad absorption (300-600 nm) and narrow electrochemical bandgaps. Furthermore, their hole mobilities were obtained as 1.26 × 10 − 3 and 8.38 × 10 − 4 cm 2 /V s, for triad 1 and triad 2, respectively. Likewise, the electron mobilities were obtained as 6.73 × 10 − 4 and 4.18 × 10 − 4 cm 2 /V s for triad 1 and triad 2, respectively. Additionally, their applications as photocatalysts for the condensation of o-phenylenediamine/1,2-diamino-4,5-difluorobenzene and aromatic aldehydes under blue light, with broad substrate scope (yields up to 94%), were explored. The third chapter discusses the design and synthesis of three non-fused A-D-A'-D- A systems, namely, BT-IT1, BT-IBT2, and BT2F-IBT3. These molecules exhibited broad absorption spectra in both solutions and thin films and narrow bandgaps. Moreover, BT-IBT2 and BT2F-IBT3 demonstrated appreciable electron mobilities of 4.56 × 10 − 3 and 1.12 × 10 − 3 cm 2 /V s, respectively. Furthermore, they showed excellent photocatalytic performances for the selective oxidation of thioanisole to sulfoxides (conversion up to 99%) under visible light irradiation. The thesis will conclude with the major structure-property correlations delineated in this thesis and future perspectives of such D-A molecules for their incorporation in organic optoelectronic devices and as photocatalysts in a broad range of organic transformations.
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