Title:	Twisted Donor-Acceptor Fluorescent Molecular Rotors and Conjugates for Sensing, Photocatalytic and Electroluminescence Applications
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Abstract:	Twisted organic donor-acceptor (D-A) fluorescent molecular rotors (FMRs) are of great importance because of their photophysical properties that are tunable by variations in solvent polarity, temperature, viscosity, and pH. Accordingly, FMRs have found extensive applications as probes for sensing, bio-imaging, as well as in organic electronics and photocatalysis. In cellular microenvironment, an abnormality in viscosity, temperature and pH can lead to cellular malfunctions and various diseases. Fluorescent molecular rotors exhibit twisted intramolecular charge transfer (TICT) process resulting in multi-stimuli responsive dual emission and serve as efficient ratiometric sensors to detect the abnormalities in cellular microenvironment. Another class of twisted D-A molecules are characterized by their small singlet-triplet energy gaps that facilitate reverse intersystem crossing (RISC). Such molecules as a result of RISC can exhibit long-lived delayed fluorescence (DF) components and show thermally activated delayed fluorescence (TADF) process. Accordingly, TADF conjugates have found profound utilization as emitters in electroluminescence applications such as in organic light-emitting diodes (OLEDs). Owing to their long-lived DF components and suitable excited state redox potentials, TADF conjugates serve as photocatalysts for various organic transformations. This thesis intends to address the design, synthesis, and investigation of photophysical properties of twisted organic (1) D-A FMRs with TICT properties, and (2) D-A conjugates with TADF properties, and their utilization for sensing, bio-imaging, photocatalysis and OLEDs. The first chapter describes the design and synthesis of TICT-based three D-□-A rotors based on BODIPY and benzodithiophene chromophores utilized for ratiometric temperature sensing and viscosity sensing. Furthermore, the triplet states of regioisomeric BODIPYs and a triad rotor are populated via spin-orbit coupling ISC and CT-mediated ISC respectively as delineated by steady state and transient absorption spectroscopy. Accordingly, these rotors showed high singlet oxygen quantum yields and could catalyze the aerobic photooxidation of thioanisole to methyl phenyl sulfoxide with 99% selectivity. The second chapter discusses the synthesis of three D-A rotors functionalized with aminoindole and naphthalimide and their utilization for pH sensing and live cell imaging of A549 (lung cancer) and L929 (fibroblast) cell lines, thereby differentiating healthy and diseased cells using these rotors. In the third and fourth chapters, diindolocarbazole-based D-A conjugates with TADF properties are designed and synthesized for photocatalytic organic transformations and OLED applications. The photocatalytic transformations include energy transfer mediated isomerization of E-stilbene to Z-stilbene with up to 90% conversion and electron transfer mediated C-H arylation of heteroarenes with up to 86% yield. The thesis concludes with the major findings of all chapters and future perspectives of twisted D-A TICT rotors and TADF conjugates towards development of multifunctional sensors, imaging probes and broadening their scope as organic photocatalysts.
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