INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student	:	Debasish Barman
Roll Number	:	166122005
Programme of Study	:	Ph.D.

Thesis Title: "Modulation of Ground and Excited State Dynamics in Donor-Acceptor Organic Functional Small Molecules for Photonics and Biomedical Applications"

Name of Thesis Supervisor(s)	:	Prof. Parameswar K. Iyer
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SHORT ABSTRACT

Organic photofunctional materials based on donor-acceptor (D-A) π-conjugated structures with ambient stable triplet-harvesting thermally activated delayed fluorescence (TADF), room temperature phosphorescence (RTP) and aggregation induced emission (AIE) have received immense attention on gathering momentum and rapidly progressing towards commercial application. Successful design strategies of these combined properties are resulted in thermal up-conversion of non-emissive triplets into emissive singlet excitons, increasing the maximum internal efficiency from 25 to 100 % in purely organic systems. Throughout the course of this thesis, design and development of new organic D-A and D-σ-A based molecules with their intrinsic structure-property functions along with ground and excited state kinetics are precisely elucidated. The exciting photophysical properties of AIE, TADF and RTP activity and associated mechanism carefully investigated in different new class of single component to multicomponent binary systems (co-crystals) respectively. With the finding of novel chemical structures, few important photophysical mechanism was elucidated towards the origin of multimode emission and white-light emission with the current aspects of excited-state mechanism for model TADF involving of higher-order vibronic coupling and "hot-excitons". In addition, complementary to TADF, RTP, another efficient triplet harvesting emitter has also been investigated for control release of excitons and to discriminate the individual and/or combined emission from TADF in a structurally rigid or flexible molecular skeleton. Besides, we could solved the dilemma of excited state quenching effect in aggregated or solid state by exploring Anti-Kasha mechanism as reason for AIE behavior. Moreover, it is discussed how to modulate and harvest the efficiency of the ambient triplets by varying different molecular conformers that show variant charge-transfer induced color-tunable emission, efficient photon transportation as optical wave-guiding activity in crystals and generation of toxic reactive oxygen species in aggregated state for image-guided cancer therapy.