



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
PhD-17 SHORT ABSTRACT OF THESIS

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**SHORT ABSTRACT**

In recent years, conjugated oligomers and polymers have attracted significant attention as promising alternatives to inorganic materials for electronic devices (such as in photovoltaic cells, light-emitting diodes, and field-effect transistors), primarily because of their distinctive optoelectronic properties. These organic materials are lightweight, inexpensive to process, and mechanically flexible; however, their performance and efficiency are still behind those of inorganic electronic devices. The performance and efficiency of organic-based electronic devices are governed by several factors, notably the molecular architecture, which influences excited-state phenomena such as charge separation, energy transfer, exciton localization and delocalization, and charge recombination. Therefore, understanding molecular-level structure-property relationships is essential for designing materials with improved performance for efficient organic electronics. Computational explorations are of great help at this point to have a good molecular-level understanding of the statics and dynamics of the underlying processes. Keeping this in mind, in this thesis, we report on excited-state processes, including exciton localization and delocalization, intra- and inter-molecular charge transfer (CT), and excimer formation, which are examined for different conformational isomers of specific molecular systems using computational approaches. For the investigation of exciton localization and delocalization, two conformers of 2-Phenylpyridine oligomers, namely linear and helical structures, are analyzed. Non-adiabatic surface-hopping dynamics simulations are performed using the semiempirical time-dependent density functional tight-binding (TD-DFTB) method to investigate localization and delocalization. Additionally, static electronic-structure calculations are carried out using the algebraic diagrammatic construction to the second order (ADC(2)) method for the three distinct isomers of 2-Phenylpyridine oligomers. Following 2-Phenylpyridine, the next chapter reports on the differences in the excited states of trans and cis-2,2' -bipyridine oligomers. In another case, analysis of intra- and inter-molecular CT is performed on four

conformers of azulene-fused anthracene and naphthalene and their  $\pi$ -stacked dimers. This part of the work involves excited-state characterization at the ADC(2) level, followed by time-dependent density functional theory (TD-DFT) studies employing DFT functionals such as CAM-B3LYP, SCS- $\omega$ B2GP-PLYP, and SCS-RSX-QIDH. Excimer formation is explored in covalently linked azulene-fused anthracene by considering two conformers that differ in the mode of fusion of the azulene units with the anthracene cores.

