INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Heterocyclic conjugated polymers are potential candidates for a number of organic devices, including OLEDs, OFETs and OPVs, owing to their interesting optical, electronic and electrochemical properties. In order to improve efficiency and stability of these devices, many theoretical/computational studies have been carried out to explore varieties of conjugated polymers and to gain an understanding of their properties. This dissertation begins with the study of optoelectronic and charge transport properties of thiophene–azomethine–pyrrole-based oligomers, which points out that few of these azomethines are suitable for applications such as light absorption, hole injection and hole transport in organic devices. Our study on the stabilities and optoelectronic properties of different conformers of π-spaced heterocyclic oligomers shows that helical conformers of vinylene-linked systems are the most stable conformers, and their properties are quite different than their respective linear conformers. A detailed study on pyridine-furan, pyridine-pyrrole and pyridine-thiophene oligomers shows that their helical conformers are feasible, and the absorption spectra of these oligomers are composed of multiple electronic transitions having significant oscillator strengths. Finally, our *ab-initio* investigation on pyridine-pyrrole based cross-conjugated systems indicates that electronic and optical properties of these oligomers can be tuned effectively by introducing π-spacers in the main chain.