INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title : Computational investigation of excited state processes in ESIPT-based systems and vinylene-linked thiophene pyrrole

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Thesis Submitted to the Department/ Center	:	Chemistry
Date of completion of Thesis Viva-Voce Exam	:	19-01-2024
Key words for description of Thesis Work	:	Excited state process; non-adiabatic dynamics; proton transfer.

SHORT ABSTRACT

The thesis focuses on understanding the mechanistic pathway in systems undergoing excited state intramolecular proton transfer and cis-trans isomerization. Unveiling the mechanism of these processes at an atomistic scale is of utmost importance as it would add to our understanding and assist in designing materials with better performance. These kinds of processes are observed in our everyday life such as the vision process in retinal chromophores, vitamin D production in humans on exposure to sunlight and mutation during DNA replication, etc. The application part of systems undergoing photoinduced processes are realized in the design and development of certain materials such as optoelectronic devices. The thesis has three working chapters. The first work is based on 1-hydroxy-2-acetonaphthone (HAN) due to the unsettled issues regarding the proton transfer process. In addition, the process of full photocycle including the non-radiative relaxation pathways is proposed. The second work highlights the effect of implicit solvents on the photoinduced processes in nitrile-substituted 2-(oxazolinyl)-phenols. Additionally, the mechanisms behind these two regiomers' weakly emissive properties in the solvent phases are investigated. My last work involves the exploration of photoisomerization pathways in vinylene-linked thiophene-pyrrole system. Considering the computational cost for the dynamics study in the excited state, we have employed single-reference method such as time-dependent density functional theory (TDDFT) and algebraic diagrammatic construction scheme of second order (ADC(2)). However, multi-reference studies are also incorporated in our study wherever the single-reference methods fail.