



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS



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Programme of Study : Ph.D.

Thesis Title: Impact of Light-Matter Interactions in Mapping Ultrafast Excited-State Dynamics of GFP Chromophore Derivatives: A Theoretical Perspective

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SHORT ABSTRACT

The interaction of light with living and non-living systems is a complex phenomenon that converges the branches of chemistry, physics, and biology. Over the past few decades, quantum mechanics has helped in understanding the photochemical panorama that goes beyond the Born-Oppenheimer approximation to account for the strong nonadiabatic couplings between the electronic states. These optically active entities undergo photoreactions via either adiabatic or nonadiabatic pathways. Based on the quantum-mechanical and quantum-classical methods, we have investigated the photophysical and photochemical behaviour of the Green Fluorescent Protein (GFP) chromophore and its derivatives upon absorption of a photon. We implement quantum mechanical methods in combination with mixed quantum-classical dynamics to understand a detailed understanding of the structure and dynamics of GFP based chromophore and the factors affecting their photochemical mechanisms. Our studies demonstrate how the steric and electronic environments significantly influence the photophysics of GFP chromophore derivatives, resulting in different phenomena such as excited-state inter and intramolecular proton transfer (ESIPT), cis-trans isomerization, etc., thereby modulating their fluorescent behaviour. Thus, the thesis aims to provide a comprehensive perspective on leveraging light-matter interactions to biological and organic chromophores and control molecular events.