INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study	:	**Ph.D.**

Thesis Title: **Structural Effects, Solvent Interactions, and Machine Learning Potentials in Photochemistry of Cyclohexadiene and Hexatriene Derivatives: A Computational Investigation**

Name of Thesis Supervisor(s)	:	**Prof. Manabendra Sarma**
Thesis Submitted to the Academic Division	:	**Chemistry**
Date of completion of Thesis Viva-Voce Exam	:	**January 12, 2026**
Key words for description of Thesis Work	:	**Photochemistry, Nonadiabatic Effect, Conical Intersection, Mixed-Quantum Classical Dynamics, Surface-Hopping**

SHORT ABSTRACT

Photochemistry is a branch of chemistry that investigates how molecular systems absorb light and subsequently undergo chemical transformations. Among the most extensively studied photochemical processes is the ring-opening and ring-closure reaction of cyclohexadiene (CHD), which plays a crucial role in the photochemical synthesis of vitamin D_3 in human skin and is a core unit in various photoswitches and photoresponsive materials. Photochemical reactions can proceed through adiabatic or nonadiabatic pathways, depending on the nature of the electronic and nuclear dynamics involved. Understanding these pathways is essential for elucidating the complex excited-state dynamics that govern molecular reactivity. In the thesis, the role of internal conversion in controlling the ring-opening and ring-closure mechanisms of CHD and its derivatives is systematically investigated using advanced computational approaches based on quantum mechanical methods and machine-learning models. We explored substitution effects and solvent effects, examined one experimentally synthesized fulgide derivative for applications as a photoswitch, and evaluated the robustness of two machine learning potential variants: MS-ANI and SS-ANI, for exploring photochemical reactions. We believe that the investigations carried out will help researchers understand complex reaction mechanisms, which in turn can accelerate the innovation of potent functional materials.