INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Functionalization of Two-dimensional $Ti_3C_2T_x$ MXene and its Nanocomposites for Application in Catalysis and Optoelectronics

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SHORT ABSTRACT

This thesis explores the strategic modulation of surface defect states in $Ti_3C_2T_x$ MXenes and their hybrid architectures to advance catalytic wastewater treatment, electrochemical hydrogen production, and broadband photodetection. Controlled chemical etching was optimized to tailor low-valent Ti^{3+} or oxygen-vacancy-rich defect sites in accordion-like, multi-layered $Ti_3C_2T_x$ for efficient Fenton-based degradation of organic dyes. Phosphorus doping further enhanced the catalytic performance by suppressing nanosheet restacking and facilitating the formation of a porous aerogel, which promotes mass diffusion and the generation of reactive oxygen species. In addition, constructing $Ti_3C_2T_x/Bi_2S_3$ heterostructures enhanced interfacial charge transfer and light harvesting, enabling both catalytic reduction of organic contaminants and photoelectrochemical (PEC) hydrogen evolution. Furthermore, ultrasmall Ru nanoclusters anchored on N-doped, oxygen-vacancy-engineered $Ti_3C_2T_x$ nanoribbons exhibited strong electronic metal-support interactions, improved photothermal response, and superior alkaline PEC hydrogen evolution activity. Finally, MXene/Bi_2S_3 Schottky junction photodetectors demonstrated efficient carrier separation and transport, delivering broadband UV-Vis-NIR (300-1550 nm) detection capability. Overall, this work establishes MXene-based defect engineering and heterostructure design as powerful routes for multifunctional environmental remediation and sustainable energy applications.