INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
PhD-17 SHORT ABSTRACT OF THESIS

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Thesis Title: **Development of Bioinspired Nanostructured Materials for Photocatalytic CO_2 Reduction to Value-added Chemicals**

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SHORT ABSTRACT

The global energy crisis and greenhouse gas emissions arising from excessive fossil fuel consumption demand sustainable and environmentally benign solutions. Photocatalytic CO_2 reduction (PCO_2R) offers a promising pathway to simultaneously address energy scarcity and CO_2 mitigation by converting CO_2 into value-added chemicals such as methanol (CH_3OH), ethanol (C_2H_5OH), formic acid (HCOOH), and carbon monoxide (CO) under solar irradiation in aqueous media. Developing green synthetic routes for nanomaterials further enhances the sustainability of this approach. This doctoral research focuses on environmentally friendly synthesis of CdS nanostructures—nanorods, nanoparticles, and quantum dots (QDs)—and their bio-inspired modifications for enhanced visible-light-driven PCO_2R. In the first study, bio-based CdS nanorods were synthesized using phytochemicals from *Aegle marmelos*, while carbon quantum dots (CQDs) were derived from orange peels. The optimized 0.50 wt% CQDs/CdS(bio) composite exhibited a fourfold enhancement in photocurrent and CO_2 adsorption, achieving the CH_3OH production rate of 1060.52 μmol/g.h (apparent quantum yield (AQY) 7%) without sacrificial reagents, along with excellent stability over 25 h. Subsequently, Z-scheme In_2O_3/CdS(bio) heterostructures demonstrated enhanced charge separation, suppressed photocorrosion, and superior CO_2 conversion to HCOOH/CO (514.4/162μmol/g·h; 4.44/2.45%). Density functional theory (DFT) analysis confirmed electronic structure modulation and improved interfacial charge transfer. Similarly, biomass-derived carbon dots embedded in CdS QDs promoted sulfur vacancies and favored HCOOH formation (439.51 μmol/g·h; AQY 3.81%), with DFT revealing HCOO* as the key intermediate. Further, Z-scheme SnO_2/CdS QDs(bio) and p–n CuO/CdS QDs(bio) heterojunctions enhanced internal electric fields, charge dynamics, and CO_2 adsorption. The optimized SnO_2/CdS system achieved CH_3OH/hydrogen production of 675.9/139.5 μmol/g·h; AQY 3.51/0.24%), while CuO/CdS enabled selective C_2H_5OH/CO formation (158.48/182.68 μmol/g·h; AQY 8.24/1.58%). Overall, this work provides integrated experimental and theoretical insights into bio-based CdS heterostructures for efficient, stable, and selective PCO_2R toward sustainable fuel production.