



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph.D.

Thesis Title : **Atomistic Modelling of Structurally Engineered 2D Materials for Enhanced Gas Sensing and CO₂ Conversion**

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Thesis Submitted to the Academic Division : Department of Chemistry

Date of completion of Thesis Viva-Voce Exam : 30 October 2025

Key words for description of Thesis Work : 2D Materials, Gas Sensor, CO₂ activation, Electrocatalyst, Density functional theory

SHORT ABSTRACT

This thesis highlights the advancements in gas-sensing and electrocatalytic performance of two-dimensional (2D) materials through strategic structural engineering. Introducing various atomic-scale structural modifications, such as doping, defect, functionalization, the properties of the 2D materials (graphene, oxygen functionalized boron sulfide monolayer, bilayer borophene) are optimized, and show their application towards SO₂, NO, and NO₂ sensing and electrocatalytic CO₂ conversion. Thus, this thesis is an effort toward energy and environmental sustainability, addressing global air pollution and bridging first-principles computational chemistry with materials design for energy-efficient and sustainable technologies.