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

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Thesis Title: Synthesis and Characterization of Doping Modulated Graphene-based materials for Device applications

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SHORT ABSTRACT

The growing demand for sustainable energy solutions necessitates the development of advanced materials for efficient energy generation and storage. Graphene, a two-dimensional carbon material with exceptional electrical, mechanical, and optical properties, emerges as a promising candidate; however, its zero bandgap and limited tunability restrict direct device applications. This work addresses these challenges through controlled doping and process engineering to tailor the electronic properties of graphene-based materials for supercapacitor and photovoltaic applications.

Graphene oxide (GO) is synthesized and reduced to reduced graphene oxide (rGO), providing a scalable route to graphene-like materials. Controlled heteroatom doping with boron and nitrogen enables stable p-type and n-type modulation, facilitating band structure tuning and enhanced carrier transport. Systematic structural, electrical, thermal, and electrochemical characterization establishes strong correlations between synthesis methods, doping, and performance. Boron-doped rGO demonstrates significantly enhanced specific capacitance (~326.56 F/g), indicating its suitability for high-performance energy storage applications.

Graphene films are synthesized using Hot Wire Chemical Vapor Deposition (HWCVD) on nickel substrates, where deposition parameters enable control over layer number, uniformity, and structural quality. To overcome limitations associated with transfer processes, direct growth of graphene on silicon substrates is achieved using HWCVD and Plasma Enhanced Chemical Vapor Deposition (PECVD), eliminating the need for metal catalysts and enabling improved interface quality. The work function of graphene is systematically tuned (≈4.15–4.54 eV) through control of deposition conditions and layer thickness, providing a critical parameter for optimizing device performance.

Graphene–silicon heterojunction solar cells are fabricated using directly grown graphene, demonstrating practical device feasibility. The fabricated devices exhibit an efficiency of ~1%, with a short-circuit current density of 25.52 mA/cm^2, open-circuit voltage of 0.13 V, and fill factor of 0.29, confirming the effectiveness of direct graphene growth and work function engineering.

Further insight into device performance is obtained through simulation using AFORS-HET, where the influence of graphene doping concentration, intrinsic layer thickness, and structural parameters is systematically analyzed. Optimized conditions predict a power conversion efficiency of 18.59%, highlighting significant potential for performance enhancement.

Overall, this work establishes doping-modulated graphene-based materials as versatile and scalable candidates for energy applications. The integration of controlled synthesis, direct growth on silicon, and work function tuning provides a comprehensive pathway for advancing high-performance supercapacitors and next-generation photovoltaic devices.