INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Theoretical and Experimental Investigation of Graphene based Devices for Bio-Sensing Applications**

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SHORT ABSTRACT

Biosensors are widely used to expedite the estimation of vital health signatures and provide techniques that aid in the continuous health monitoring of patients. Over the last few decades, the advancement in the silicon industry caused significant improvement in the development of sensing devices, marketing sensitive and robust sensors. However, multidisciplinary expertise is needed for the furtherance of developed biosensors. Biotechnology provides simple yet efficient assays to detect biomarkers and hence plays an imperative role in sensor development. Recent developments in two-dimensional nanomaterials such as graphene have also proved to be of great importance to achieve better sensor performances. However, the estimation and modelling of the interaction between the biomarkers and newly discovered nanomaterials are not yet matured, which is indispensable for developing a new generation of sensors. The traditional methods to evaluate these interactions are based on experimentally determined parameters that are difficult to estimate. Therefore, methods for electronic structure calculation, such as density functional theory (DFT), can be a good candidature for the study of interactions between biomarkers and nanomaterials. The primary research objective of this thesis is to employ DFT for estimating the electronic structure of pristine graphene and doped graphene nanostructures and evaluating their interactions with numerous gaseous molecules and biomarkers by calculating binding energies, electronic structures, and charge transfer. The doped nanostructures exhibit superior sensing capabilities over pristine nanostructures. Further, the synthesis of graphene and its functionalization routes to employ them as Glutathione and Lactate sensors are explored. Later, for experimental proof, the chem-resistive-based sensing devices were fabricated, and sensor parameters were estimated. The high sensitivity and better limit of detection of the fabricated devices make them suitable for devices for point of care applications for detecting various health disorders.