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

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SHORT ABSTRACT

Short Abstract of the Thesis is checked for correctness. Recommended for submission.

Biosensors have emerged as powerful analytical tools for the rapid and sensitive detection of biomolecules, with gold nanoparticles (AuNPs) playing a crucial role due to their unique optical properties, high surface area, and excellent biocompatibility. This thesis focuses on understanding biomolecular interactions at gold nanoparticle interfaces through a combination of experimental investigations and molecular simulations to support the development of efficient biosensing platforms. The first part of the study investigates the adsorption behavior of the enzyme allantoinase, identifying the structural and spatial factors that influence protein adsorption. Computational analyses provided molecular-level insights into protein orientation, surface accessibility, and adsorption characteristics, contributing to a better understanding of enzyme–surface interactions.The second part examines the functionalization of citrate-stabilized AuNPs using two thiol-based crosslinkers, 3,3'-dithiobis(sulfosuccinimidyl propionate) (DTSSP) and dithiobis(succinimidyl propionate) (DSP). Successful surface modification was confirmed through UV–Visible spectroscopy and Fourier Transform Infrared (FTIR) spectroscopy. Adsorption isotherm models were employed to evaluate linker adsorption behavior and determine the thermodynamic parameters governing the interaction. Molecular dynamics simulations, including binding free energy, radial distribution function, mean residence time, and mean square displacement analyses, provided atomistic insights that complemented the experimental observations. Overall, the findings demonstrate that linker chemistry significantly influences nanoparticle surface functionalization and

adsorption behavior. By integrating experimental characterization with computational modelling, this work advances the understanding of AuNP-based biointerfaces and provides a foundation for the rational design of stable and sensitive nanomaterial-based biosensing systems.