

Book of Abstracts

39th



Indian Engineering Congress

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Theme

Irresistible India -
a Global Engineering Powerhouse

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Interaction Dynamics of Pristine and Pt-decorated ZnO Nanosheet during Cytosine Adsorption: A Robust Electro-Chemical Analysis of Biosensor

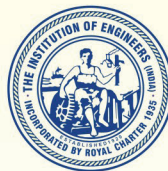
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Abstract: The performance of pristine and platinum (Pt) decorated ZnO nanosheets in detecting cytosine (C) nucleobase was compared in the current study, using a first principle computational study with Gaussian 09W and Gauss View 6.0 package. Cytosine, a pyrimidine nitrogenous base, was selected as the adsorbed biomolecule for both nanosheets. Two systems were involved: cytosine-adsorbed pristine ZnO nanosheet (case-A) and cytosine-adsorbed Pt-doped ZnO nanosheet (case-B). The interaction between the sensed molecule and the sensing material was analyzed using various electronic parameters such as molecular electrostatic potential, the total density of states, the lowest unoccupied molecular orbital (LUMO), the highest occupied molecular orbital (HOMO), and Mulliken charge analysis. It was inferred that the Pt-doped ZnO nanosheet was a better sensing material, exhibiting strong adsorption energy (-1.421 eV) and a decreased binding distance (2.215 Å) compared to the pristine ZnO nanosheet, which had an adsorption energy of -0.377 eV and a binding distance of 2.707 Å. The importance of accurate detection and sensing of cytosine in our body was elucidated, helping in coding for proteins and regulating gene expression.

Keywords: Cytosine; Pt-ZnO Nanosheet; Density of State (DOS); Mulliken Charge; Molecular Electrostatic Potential (MEP)



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Interaction Dynamics of Pristine and Pt-decorated ZnO Nanosheet during Cytosine Adsorption: A Robust Electro Chemical Analysis of Biosensor

Theme: Biomedical Science & Technology

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