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F-093

Distinguishable Improvement on Graphene Nanosheet via Foreign Ni-dopant towards Detection of Trimethylamine Gas

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Abstract

The present investigation focuses on a comparative analysis between various electrochemical sensing properties of pristine graphene nanosheet (NS), and Nickel (Ni)-doped graphene NS, having the dimension of 4×4 supercell, towards accurate sensing of the toxic trimethylamine (TMA) gas. First-principles-based computational approach was employed for obtaining optimized structures of TMA-adsorbed pristine graphene NS (Type I system), and TMA-adsorbed Ni-doped graphene NS (Type II system). Gaussian 09W, and GaussView 6.0 software aided in thorough calculations of the parameters, and 2D/3D visualization of the obtained results. Key gas sensing parameters, such as adsorption energy, binding distance, Frontier Molecular Orbitals (FMO), Electrostatic Potential (ESP), Density of States (DOS), and Infrared (IR) spectra were examined for elucidating the atomic-level interactions. Results revealed that nickel doping significantly enhanced the adsorption strength of the nanosheet. The detailed findings highlight the potential of Ni-doped graphene NS as a superior sensing material, for development of a high-performing TMA sensor in upcoming future.

Keywords: 2D Graphene, Nickel doping, TMA sensing, FMO, Adsorption characteristic.

Distinguishable Improvement on Graphene Nanosheet via Foreign Ni-dopant towards Detection of Trimethylamine Gas

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1 Introduction

Trimethylamine (TMA) is a volatile gas that belongs to the amine (C-N) group, with a relatively low molecular weight. It produces a fish-like odour at low concentration, while on the other hand, at higher concentrations, it gives a pungent odour like ammonia, often described as the smell of rotten eggs. Overexposure to TMA, leading to various skin disorders, like hyperemia, has been observed along with skin irritation and a feeling of burning sensation [1]. Excessive accumulation of TMA in the human body can indicate metabolic disorders such as trimethylaminuria and cardiovascular

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Thanks and Regards,

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