

**3rd International Conference
on
Recent Trends in Materials Science & Devices
(ICRTMD-2025)**

24 - 26 March, 2025



Organized by:

**Department of Physics,
J.V.M.G.R.R. College, Charkhi Dadri Haryana, India**

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Abstract Book

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Performance Analysis of Bare and Co-Doped Graphene Nanosheets towards Detection of Trimethylamine

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Abstract

This study critically examines the sensing performance of pristine and cobalt (Co) decorated graphene nanosheet in the sensing of trimethylamine ((CH₃)₃N) using the first principle computational method in the Gaussian 09W and Gauss View 6.0 simulation package. Trimethylamine (TMA) is produced by bacteria in the human gut, when the human body digests foods having high amounts of choline and carnitine. TMA is converted to trimethylamine N-oxide (TMAO) in the liver. It can result in a strong body odor known as trimethylaminuria, if the proper conversion of TMA does not take place in the body, which makes detection of trimethylamine a novel scope for research in recent times. TMA is chosen as an adsorbed molecule for both the nanosheets, creating two different setups viz. TMA adsorbed pristine graphene nanosheet (Setup-I), and TMA adsorbed Co-doped graphene nanosheet (Setup-II). The interaction between TMA and the considered nanosheets was thoroughly compared through various electronic parameters such as Mulliken charge analysis, molecular orbital analysis, molecular electrostatic potential (MEP), and density of state (DOS). It was observed that the Co-decorated graphene nanosheet in Setup-II proved itself to be a better sensing material for detecting TMA with an improved adsorption energy of (-2.993 eV), and a reduced adsorption distance of 2.58 Å as compared to that of Setup-I (bare case) with an adsorption energy of (-0.081 eV), and adsorption distance of 2.95 Å, respectively. This study outlined the importance of TMA detection in the body averting metabolic disorders and potential cardiovascular diseases caused by the elevated levels of TMA and improper conversion of TMAO. The introduction of the Co atom over the surface of the pristine graphene sheet increased the adsorption in the case of Setup-II because of cobalt's higher electron affinity and stronger interaction with nitrogen (N) atom of TMA, establishing Co-doped graphene as a promising sensing material for identifying TMA.

Keywords: Trimethylamine; Co-decorated graphene nanosheet; Molecular electrostatic potential; Gas sensing; Adsorption distance.

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