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CuO/TiO_2/ZnO NPs Anchored Hydrogen Exfoliated Graphene: To Comprehend the Role of Graphene in Catalytic Reduction of p-Nitrophenol

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ABSTRACT: The present study deals with sonochemically in situ synthesis of a novel functional catalyst using hydrogen exfoliated graphene (HEG) supported titanium dioxide (TiO_2) and copper sulfate ($CuSO_4$) doped with zinc oxide (ZnO) (abbreviated as Ti/Cu/Zn-HEG). The synthesis of the Ti/Cu/Zn-HEG nanocomposite (NCs) catalyst was confirmed through its characterizations by XRD, SEM-EDX, TEM, XPS, FTIR, and BET methods. It was assessed for catalytic conversion of a model aromatic compound *para*-nitrophenol (p-NP) in an aqueous solution. The p-NP is a nitroaromatic compound that has a toxic and mutagenic effect. Its removal from the water system is necessary to protect the environment and living being. The newly synthesized Ti/Cu/Zn-HEG NCs were applied for their higher stability and catalytic activity as a potential candidate for reducing p-NP in practice. The operating parameters, such as p-NP concentration, catalyst dosage, and operating time were optimized for 150 ppm, 400 ppm, and 10 min through response surface methodology (RSM) in Design-Expert software to obtain the maximum reduction p-NP up to 98.4% at its normal pH of 7.1 against the controls (using HEG, Ti/Cu-HEG, and Zn-HEG). Analysis of variance of the response suggested the regression equation to be significant for the process with a major impact on catalyst concentration and operating time. The model prediction data (from RSM) and experimental data were corroborated well as reflected through model's low relative error (RE < 0.10), high regression coefficient (R^2 > 0.97), and Willmott *d*-index ($d_{will\text{-}index}$ > 0.95) values.

1. INTRODUCTION

Heterogeneouslycatalyzed reactions are crucial for producing commodities and consumer products, such as chemicals, pharmaceuticals, and polymers, accounting for approximately 25% of industrial energy usage.[1,2] In the future, most energy-intensive chemical industries will essentially count on heterogeneous catalysis to secure carbon-neutral operations and sustainable manufacturing.[3] Therefore, an increasing demand is for the development of more efficient and environmentally friendly industrial catalysts. It is possible, in theory, to design atomically precise materials with self-regenerating sites of activity for use as catalysts in selective chemical/biochemical reactions.[4] Noble metallic nanoparticles (NPs) have a large surface area, many functioning surface areas, and the potential for quantum confinement effects, making them a few of the most extensively studied heterogeneous catalysts.[5] In particular, the effectiveness of these new catalysts for the hydrogenation reaction is measured by how well they reduce p-nitrophenol (p-NP) by using $NaBH_4$ as a model reaction.[6]

Nitrophenols or nitroaromatic compounds are widely discharged in water bodies due to their overuse in

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