

ABSTRACT

Thesis Title: Exploring Charge Transport Properties of Copper-based Chalcogenides and their Carbon Composites for Dye Wastewater Treatment

Dye wastewater discharged into water bodies, primarily by textile industries, is becoming an increasing environmental concern that leads to significant ecological issues. Previous efforts to address this problem through physicochemical and biological methods have been economically inefficient and often resulted in secondary pollutants. Photocatalysis using semiconducting materials has emerged as a promising method for wastewater decontamination. However, challenges such as wide bandgaps and short exciton lifespans limit the practical application of compound semiconductors. For example, TiO_2 , a potential material for pollutant decomposition, can only be activated by UV light due to its wide bandgap. In contrast, copper (II) sulfide (CuS) with a direct bandgap of ~ 2.29 eV and copper selenide (CuSe) having direct bandgap of ~ 2.60 eV for which it can efficiently capture visible light from the solar spectrum and make it practically functional to use as a 'visible-light-driven photocatalyst'. Copper-based chalcogenides especially when combined with carbon materials like carbon nano tube (CNT) or reduced graphene oxide (rGO) offering some excellent features, such as environmentally friendly, non-toxicity, low cost, large surface area, biocompatibility, higher physical and chemical stability and ease of recyclability which enhances its effectiveness for being a prospective photocatalyst. Despite these advantages, CuS, CuSe nanomaterials suffer from fast electron-hole recombination, which affects their photocatalytic performance. Concurrently, metal oxides such as CuO, ZnO, CdO, ZnTe, WO_3 , and CeO_2 have been utilized for treating industrial effluents through photocatalytic decomposition. However, they encounter limitations similar to those of single metal oxides.

This study aims to address these challenges through the synthesis of carbon-based composites of copper chalcogenides such as, carbon nanotube-copper sulfide (CNT-CuS) and reduced graphene oxide-copper selenide (rGO-CuSe) nanocomposite as photocatalyst. Both the CNT-CuS as well as rGO-CuSe nanocomposite exhibits enhanced photocatalytic activity, attributed to improved charge transfer facilitated by higher carrier mobility, strong interfacial contact, visible light absorption, and low electron-hole pair recombination. Firstly, charge transport phenomena of CuS are observed by different synthesis methods (hydrothermal and co-precipitation method). Further the CNT and rGO incorporation into the CuS and CuSe materials through a hydrothermal route, exploring their potential in azo dye degradation. My primary objective is to synthesize and evaluate the performance of carbon allotropes-semiconductor-based CNT-CuS and rGO-CuSe composites and the photocatalyst for wastewater treatment applications. This study also intends to explore the charge transfer mechanism and emphasize the potential of these composite materials in environmental remediation. Furthermore, my research seeks to extract the mobility of each catalyst using the space-charge-limited conduction (SCLC) theory of thermionic emission and comprehensively discuss how the mobility of charge carriers impacts the degradation efficiency of the photocatalysts.

In summary, this research seeks for the efficient and sustainable photocatalysts for dye wastewater treatment by examining microscopic parameters to improve their practical applications in environmental remediation.

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30/04/2025

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