Journal of Environmental Chemical Engineering 11 (2023) 110867

Contents lists available at ScienceDirect

Journal of Environmental Chemical Engineering

journal homepage: www.elsevier.com/locate/jece

Tailoring the bandgap of zinc indium sulfide/boroncarbonitride heterostructure for efficient photocatalytic CO_2 reduction

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ARTICLE INFO

Editor: Zacharias Frontistis

Keywords:
$ZnIn_2S_4$
BCN
CO_2 reduction
Photocatalysis
Heterostructure
Mechanism

ABSTRACT

Many efforts have been devoted to the reduction of atmospheric CO_2 and the development of a route map for sustainability in the energy and environmental sectors. The present work describes the bandgap tailoring of the ternary metal sulfide $ZnIn_2S_4$ (ZIS) with two-dimensional (2D) boroncarbonitride (BCN) and a constructed heterostructure. The ratio of BCN to ZIS has been varied in different ratios and examined for morphological, structural, and optical characterization. The crystalline structure of the synthesized materials was subjected to Materials Studio software, which examined the geometry, stacking, and interaction between ZIS and layered BCN. ZIS/BCN-1 is found to be efficient compared to all other counter catalysts under study. Diffuse reflectance infrared Fourier transform (DRIFT) and Gas Chromatography Mass spectrophotometry (GC-MS) analysis confirm the formation of carbon monoxide and methane gas. In the presence of ZIS/BCN-1, it was found to produce 158 and 57 μmol $g^{-1}h^{-1}$ of CO and CH_4, respectively, during CO_2 reduction under visible light. The effect of sacrificial agents has been investigated, and found that triethanolamine (TEOA) showed enhanced activity compared to others. The mechanism of photocatalysis has been discussed in detail and found to form type-II heterostructure through the interface between ZIS and BCN. The stability of ZIS/BCN-1 is good even after 5 cycles of the CO_2 reduction experiment, and no structural changes were found.

1. Introduction

Continuous and excessive use of fossil fuels across the globe leads to the accumulation of enormous amounts of atmospheric CO_2. This leads to serious issues like global warming, imbalances in natural carbon, environmental pollution, and destruction of the ecological system [1–3]. Ever-increasing energy and environmental concerns have encouraged massive research efforts to harness renewable energy and reduce CO_2 in the atmosphere. Nature's photosynthesis inspired researchers to mimic it for other artificial photosynthetic systems in energy and environmental-related issues. Hence, light-driven CO_2 reduction is gaining high importance to overcome air pollution and increase the availability of carbon-based raw materials for the energy sector [4–6]. Reduction of linear CO_2 into value-added products still remains a challenge due to its high stability and high dissociation energy of the C═O bond of around 750 kJ mol^{-1} [7]. The degree of photoreduction of inert CO_2 into value-added products depends on the ability of the catalyst to harness the light and photoexcited electrons and holes to cleave the bond. Nevertheless, most of the known photocatalysts still face difficulties due to the poor separation efficiency of photogenerated carriers, the involvement of multiple electrons and protons, and their low transfer rate kinetics to the catalytically reactive sites [8,9]. Hence, increasing the efficiency of charge separation, prolonging light absorption, and increasing CO_2 adsorption ability by building reactive sites could be the solution to overcome the ambiguities associated with light-driven catalysis [10,11].

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https://doi.org/10.1016/j.jece.2023.110867
Received 8 July 2023; Received in revised form 12 August 2023; Accepted 26 August 2023
Available online 28 August 2023