Fabrication of dual-functional $Cs_3Bi_2I_9$-WO_3 S-scheme heterojunction for photocatalytic H_2 production and polluted water treatment: Optimization, mechanism and toxicity evaluation

Author links open overlay panelMutairah.S. Alshammari [a], Waqed H. Hassan [b c], Murtadha M. Al-Zahiwat [d], Ibrahm Mahariq [e f k], Mohamed A. Ismail [g], Zukhra Atamuratova [i j], Sokhibjan Muminov [h], Abdelfattah Amari [g]

Abstract

Efficient interfacial charge transfer and robust interface interactions are critical for achieving superior separation of carriers and developing advanced heterogeneous photocatalysts. Herein, a novel S-scheme heterojunction of $Cs_3Bi_2I_9$-WO_3 (CBIW) was synthesized through a simple ultrasonic method. The optimized nanocomposite demonstrated exceptional photocatalytic performance, achieving a H_2 production rate of 750 µmol. $g^{-1}.h^{-1}$ and a degradation efficiency of 95 % for cefixime (CFX) under visible light irradiation. Various characterization techniques, including XRD, XPS, FTIR, Raman spectroscopy, SEM, TEM, and UV-Vis, confirmed the successful formation of the S-scheme heterojunction. Furthermore, ESR analysis and radical scavenging experiments revealed that hydroxyl radicals (•OH) and superoxide radicals ($•O_2^-$) played crucial roles in the photocatalytic degradation of CFX. Also, the formation of this S-scheme heterojunction, significantly enhanced interfacial charge transfer, improving carrier separation and reducing recombination as demonstrated by PL, photocurrent, and EIS analyses. LC-MS analysis was employed to identify intermediate products formed during the photodegradation of CFX, facilitating the development of plausible degradation pathways. The ecotoxicological impacts of these byproducts were further evaluated using the Toxicity Estimation Software Tool (T.E.S.T.) and QSAR analysis. The nanocomposites exhibited excellent stability, maintaining consistent photocatalytic activity over four consecutive cycles. These findings suggest that the $Cs_3Bi_2I_9$-WO_3 S-scheme heterojunction is a promising photocatalyst for environmental remediation and H_2 production applications.

DOI: https://doi.org/10.1016/j.jallcom.2025.179730