

Synergy Effect of the Bifunctional Molybdenum of Nickel-Iron Oxyhydroxide/Molybdenum Oxide/Molybdenum doped Bismuth Vanadate Composite Photoanode Enabled Boost Charge Transfer for Efficient Water Splitting

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Received: 12 October 2025; Revised: 15 December 2025; Accepted: 26 December 2025

Type: Research article.

Abstract

Bismuth vanadate (BiVO₄) has garnered significant interest as a promising photoelectrochemical (PEC) material for water splitting. However, its poor electron mobility, sluggish surface water oxidation kinetics, and high overpotential limit its PEC water splitting efficiency, making it significantly lower than its theoretical maximum. To address these challenges, a composite bifunctional molybdenum layer photoanode Nickel-Iron Oxyhydroxide/Molybdenum Oxide/Molybdenum doped Bismuth Vanadate (NiFe/MoO_x/Mo:BiVO₄) was designed, incorporating Mo doped and a MoO_x hole transfer layer (HTL) at the oxygen evolution catalyst (OEC)/BiVO₄ interface, for highly efficient PEC water splitting. The NiFe/MoO_x/Mo:BiVO₄ photoanode exhibited a photocurrent density of 5.29 mA cm⁻² at 1.23 V_{RHE}, approximately three times higher than that of pristine BiVO₄. It also achieves an applied bias photon to current conversion efficiency (ABPE) value of 1.83%, representing a significant improvement over the 0.37% observed for pristine BiVO₄. Electrochemical analyses and density functional theory (DFT) calculations indicate that Mo doping improves bulk charge transfer, while the incorporation of a MoO_x HTL facilitates interfacial charge

separation. Additionally, the synergistic effects of Mo doping and the MoO_x HTL contribute to accelerating the kinetics of water splitting. These findings provide valuable insights for the rational design and development of integrated photoanodes for efficient solar energy conversion.

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