

Dual-functional Pd Metallene for Boosted Photocatalytic H₂ Evolution Coupled with Lactic Acid Oxidation over ZnCdS

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Abstract

Constructing highly efficient active sites is fundamental to advancing photocatalytic performance. However, the fabrication of stable bifunctional catalytic interfaces capable of sustaining concurrent redox reactions remains a significant challenge. Herein, we rationally design Pd metallene-decorated ZnCdS photocatalysts (PZCS) featuring electronic metal-support interaction (EMSI) interfacial architecture, which enables the synchronous photocatalytic H₂ evolution and selective lactic acid (LA) oxidation. Owing to the dynamically modulated interfacial electronic environment and the optimized adsorption configurations for H₂O and LA substrates, the optimal 10PZCS catalyst achieves an H₂ evolution rate of 22.4 mmol g⁻¹ h⁻¹ and a LA-to-pyruvic acid conversion rate of 6.7 mmol g⁻¹ h⁻¹, substantially outperforming pristine ZnCdS. A synergistic combination of comprehensive spectroscopic characterizations, photoelectrochemical measurements, and density functional theory (DFT) calculations unravels the origins of the markedly enhanced dual-redox activity, which are attributed to the spatially coupled yet functionally differentiated Pd metallene active sites. Specifically, Pd sites reinforce H₂O adsorption, disrupt the rigid hydrogen-bonding network on ZnCdS surface, and lower the dissociation energy barrier of H₂O. Meanwhile, the reversible Pd²⁺/Pd⁰ redox cycle ensures continuous regeneration of active centers, thereby accelerating the reduction half-reaction toward efficient H₂ generation. Driven by the EMSI effect, photogenerated electrons spontaneously migrate from ZnCdS to Pd metallene, substantially suppressing charge-carrier recombination, while the hole-enriched ZnCdS selectively oxidizes the adsorbed LA into high-value pyruvic acid with negligible over-oxidation. This work not only elucidates the atomic-scale kinetic mechanism underlying the bifunctionality of Pd metallene cocatalysts in integrated photocatalytic water splitting and organic valorization, but also offers a versatile interfacial engineering paradigm for development of high-performance sulfide-based photocatalysts toward synergistic clean H₂ production and value-added chemical synthesis.

Keywords

Pd Metallene, Photocatalytic, ZnCdS, EMSI, LA Oxidation, H₂ Evolution