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Catalytic Synergy via Optimized MoS₂-WS₂ Heterostructure Supported on Nitrogen-Doped Reduced Graphene Oxide for Enhanced Hydrogen Generation in Acidic Medium

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Abstract

Tungsten disulfide (WS₂) has shown promise as a catalyst for the hydrogen evolution reaction (HER), and doping it with transition metals (e.g., Mo) can further boost its activity. In this study, we synthesized MoS2-WS2 heterostructure supported on nitrogen-doped reduced graphene oxide (N-rGO) using a hydrothermal method, testing MoS₂ concentration(w/w) levels at 5%, 10%, and 20% to optimize HER performance. Raman spectroscopy and SEM confirmed the successful formation of MoS₂-WS₂/N-rGO composites, with Raman spectra revealing four characteristic peaks: 420 cm⁻¹ (A_{1g} mode of WS₂), 380 cm⁻¹ (E¹_{2g} mode of MoS₂), and D and G bands of N-rGO at 1,360 cm⁻¹ and 1,600 cm⁻¹, respectively. Additionally, the peak heights of MoS₂ and WS₂ are influenced by the incorporating concentration of MoS₂. SEM images showed a structural shift from irregular flakes to granular and flower-like particles with increased MoS₂ concentration, and the presence of MoS₂ is responsible for the formation of flower-like particles. Electrochemical HER testing in 0.5 M H₂SO₄ demonstrated that 10% MoS₂-WS₂/N-rGO achieved the lowest overpotential (-177.6 mV at -10 mA cm⁻²) and smallest Tafel slope (73.40 mV dec⁻¹), compared to 5% (-292.3 mV; 101.8 mV dec⁻¹) and 20% (-284.9 mV; 92.9 mV dec⁻¹). The Tafel slope of 10% MoS₂-WS₂/N-rGO suggests balanced Volmer and Tafel contributions. Double layer capacitance (C_{dl}) of 5%, 10%, and 20% MoS₂-WS₂/NrGO, as determined by the CV method, is 2.72, 5.71, and 1.17 mF cm⁻², respectively. The corresponding electrochemical active surface areas (ECSAs) measured are 136, 285.5, and 58.5 cm². This indicates that a 10% (w/w) concentration of MoS₂ provides optimal active surface area, highlighting its superior HER performance in acidic media.

Keywords: Hydrogen evolution reaction, Water splitting, MoS₂ doping, WS₂, Electrocatalyst