

Tuning palladium nickel phosphide toward efficient oxygen evolution performance

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ABSTRACT

Highly efficient and durable catalysts are increasingly sought in water electrolysis, particularly for resolving the sluggish oxygen evolution reaction (OER) kinetics. Herein, ternary phosphides in the palladium-nickel-phosphorus system developed via a simple reduction approach as hollow and dense nanostructures (PdNiP-H and PdNiP-D, respectively) are shown to overcome the kinetic drawbacks of Pd and deliver superior alkaline OER activity. The PdNiP-H showed OER activity at a significantly lower overpotential (300 mV) and Tafel slope (48 mV dec⁻¹) in addition to having a longer stability than the corresponding dense particles (PdNiP-D) (330 mV and 49 mV dec⁻¹) and the commercial benchmark, RuO₂ (360 mV and 67 mV dec⁻¹), in half-cell conditions. While combining experiments and density functional theory (DFT) calculations, these enhancements are shown to arise from surface properties and the modified electronic environment of the ternary phosphide as well as by the enhanced charge transfer sites due to the hollow architecture. DFT calculations identify the density of states (DOS) and support Pd lattice alteration, the shift in the d band center, and the subsequent modification in electronic properties of Pd that is favorable for OER. The phosphodization methodology adopted here highlights an efficient strategy for generating a range of morphologies of ternary phosphides as sustainable and stable energy conversion/storage materials.

KEYWORDS

Hollow structures; Kirkendall effect; Palladium nickel phosphide; Phosphodization; Oxygen evolution reaction; Water electrolysis

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