

# Modulating Surface Reconstruction of Nickel Cobalt Phosphide by Iron Incorporation Enhancing ORR/OER for Hybrid Sodium–air Battery

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The design of highly efficient and inexpensive bifunctional electrocatalysts that possess highly catalytic activity towards oxygen reduction reaction and oxygen evolution reaction is desirable for boosting the performance of hybrid sodium–air batteries (HSABs). Herein, Fe regulated NiCoP nanoflowers embedded by nanoporous carbon layer (Fe-NiCoP@C) are synthesized as bifunctional ORR/OER catalysts for HSABs. The amorphous carbon layer can effectively improve the electron conductivity of the Fe-NiCoP and stabilize the electrolyte at the Fe-NiCoP interface, thus improve the electrochemical activity and stability. The surface charge distribution of catalysts can also be modulated by introducing foreign-metal cations to enrich the catalytic sites and reduce the thermodynamic energy barrier of proton-coupled electron pre-equilibrium by assisting O–O bond formation, leading to enhanced catalytic activity. Compared to catalysts without incorporation of Fe or integration with carbon layer (NiCoP and Fe-NiCoP), Fe-NiCoP@C shows the highest onset potential of 0.81 V for ORR, lowest onset potential of 1.42 V, an low overpotential of 196 mV at 10 mA cm<sup>-2</sup>, the smallest Tafel slope of 36 mV dec<sup>-1</sup> for OER and highest Electrochemically active surface area (ECSA) of 100.1 mF cm<sup>-2</sup>. HSABs employing the Fe-NiCoP@C catalyst as the air cathode display a low overpotential of 0.14 V at the current density of 0.01 mA cm<sup>-2</sup>, the highest power density of 621 mW g<sup>-1</sup> and a superb stability of no significant degradation is observed after 500 cycles with the roundtrip efficiency remains 95.1%. Fe-NiCoP@C achieves superior catalytic activity and excellent stability as electrocatalyst in HSABs and is promising to resolve current limitations in TMPs and eventually scale up the applications of HSABs.