Zeolitic Imidazolate Framework Derived-cobalt Phosphosulfide Nanoparticles Encapsulated into P, S, N Tri-doped Carbon as Highly Active Bifunctional Oxygen Electrocatalyst for Zn-Air Battery

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Zinc-air batteries (ZABs) have recently drawn wide interest in electrochemistry because of their high energy density, low cost, and environmental friendliness compared to the lithium-ion batteries which have been applied ubiquitously in contemporary society. To commercialize zinc-air batteries, a highly active electrode catalyst for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) is essential owing to its critical role in the operation of rechargeable and primary metal-air batteries. In this paper, we propose a high-performance electrocatalyst consists of cobalt phosphosulfide (CoPS) nanoparticles encapsulated with S, P, N-tri-doped carbon (CoPS@SPNC) derived from zeolitic imidazolate framework-67 (ZIF-67) by a sulfidation and phosphating process of the optimized carbonized Co nanoparticles embedded N-doped carbon (Co@NC). The as-obtained CoPS@SPNC displays a regular polyhedral crystal structure with CoPS nanoparticles embedded in the typical mesoporous carbon and a hierarchical pore structure of 1.7–53.5 nm. CoPS@SPNC is used as an air electrode in Zn-air battery and exhibits the highest discharge voltage of 1.415 V at 1 mA cm-2 , the lowest overpotential of 0.20 V with the discharge voltage of 1.36 V at 2 mA cm−2, the highest current density and peak power density of 20 mA cm-2 at 1.0 V and 25.9 mW cm-2 at 0.518 V and a superb stability which the highest discharge voltage of 0.91 V and lowest charge voltage of 2.34 V are delivered without obvious performance degradation for 12h during long-term operation(36 cycles, 20 min for each cycle) at 20 mA cm-2. CoPS@SPNC-600 also possesses .