

Supporting information

CoP electrocatalysts embedded in nitrogen doped carbon as iodine host toward fast iodine conversions

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1. Experimental

1.1. Preparation of CoP@NC

Brief, 500 mg nitrogen doped porous carbon (C, 99.9%, Porous Carbon Co Ltd.), 100mg Cobalt nitrate hexahydrate ($\text{Co}(\text{NO})_2 \cdot 6\text{H}_2\text{O}$, 99.9%, Sigma-Aldrich Ltd.) were fully dissolved in 100 ml DI water under vigorous stirring for 5 hours at 90 °C. Then, the obtained precursor was transferred into tube furnace and heated at 800°C for 2 hours (5°C/min) with Ar atmosphere to get Co@NC. Finally, the Co@NC powders and sodium hypophosphite ($\text{NaH}_2\text{PO}_2 \cdot \text{H}_2\text{O}$, 99.9%, Sigma-Aldrich Co Ltd.) (weight%: 1:3) were placed downstream and upstream of the tube furnace, respectively, and treatment at 350 °C for 2 hours at 2 °C min⁻¹ in Ar gas to obtain CoP@NC.

1.2. Synthesis of CoP@NC/I₂ composites

The CoP@NC and iodine powder (I₂, 99.9%, Sigma-Aldrich Co Ltd.) were mixed in a weight ratio of 1:1. The mixture was sealed in an autoclave and heated at 90 °C for 12 h. The CoP@NC/I₂ were obtained after cooling to room temperature.

1.3. Materials characterization

The morphology and structure of the samples were evaluated by SEM (FEI Quanta 200) and TEM (JEM-2100F). EDS (Oxford XMax20) elemental mapping attached on the SEM was used to characterize the element distribution. Bruker Contour GT-K 3D optical microscope (3D optical profiler) was used to analysis the 3D optical photographs of all samples. The structure information and chemical status were evaluated by XRD (XRD Bruker D4 ENDEAVOR) with Cu K α radiation and XPS (K-Alpha) using an Al K α source, respectively. TGA (TGA 8000) were used to analyze iodine content in cathode in the cathode at 35-600°C. UV-vis spectroscopy (Agilent Cary 5000) was employed to record the type of iodine species from 250-500 wavelength (nm).

1.4. Electrochemical characterization

The CoP@NC active materials, conductive carbon black, and sodium carboxymethyl cellulose

were mixed with a weight ratio of 8:1:1 in DI water to form a slurry. Then, the uniform slurry was coating on graphite paper and an iodine loading of ~ 1.0 - 1.2 mg cm^{-2} . The CR2032-type coin cells were assembled using Zn foil, glass fiber membrane, and 2 M ZnSO_4 as the anode, separator, and electrolyte, respectively. The galvanostatic charge/discharge (GCD, 0.6-1.6 V vs. Zn/Zn^{2+}) performance was recorded on Neware Battery Testing System at different current density, Cyclic voltammetry (CV) in the range of 0.6~1.6 V with the scan rate of 0.2 mV s^{-1} and electrochemical impedance spectroscopy (EIS) were tested on a CHI 760E electrochemical workstation in a frequency range from 0.01 Hz to 100 kHz (5.0 mV).

1.5. Visualized iodine species adsorption experiments

To conduct the polyiodides adsorption tests, the CoP@NC or NC were soaked into $\text{Zn}(\text{I}_3)_2$ solution, respectively. Then it was tested to evaluate the polyiodide absorption ability of both samples. The material after reaction was dried at 60°C overnight and used for XPS testing and the supernatant before and after adsorption was used for UV testing.

Supplementary Figures and Tables

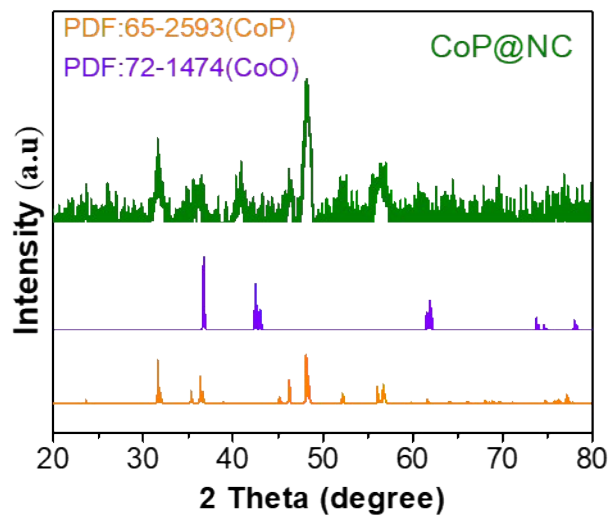


Fig. S1. XRD pattern of CoP@NC composite.

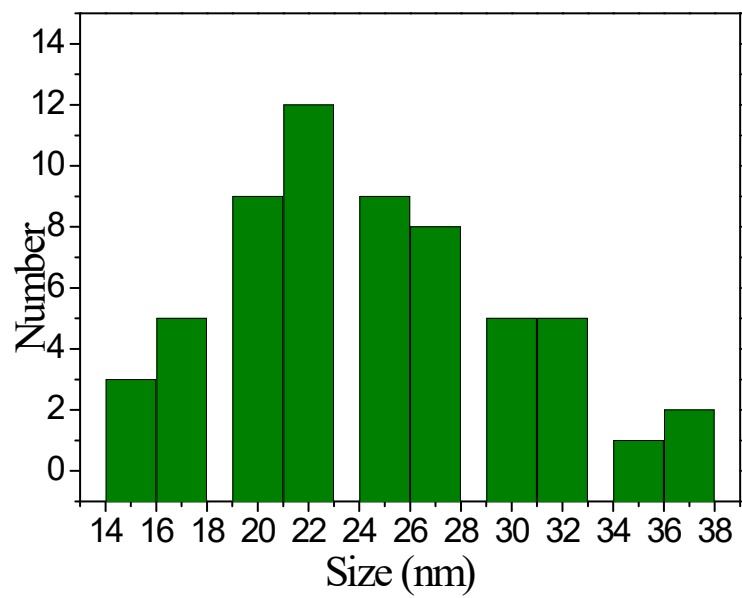


Fig. S2. The size statistics of CoP nanoparticles.

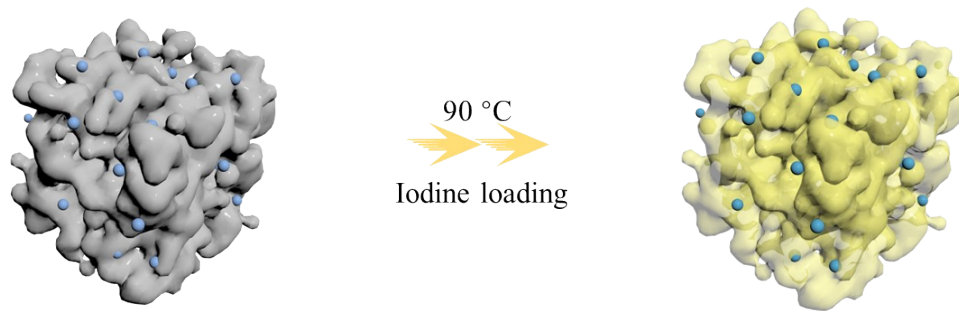


Fig. S3. Schematic illustration of the preparation of the CoP@NC/I₂ composite.

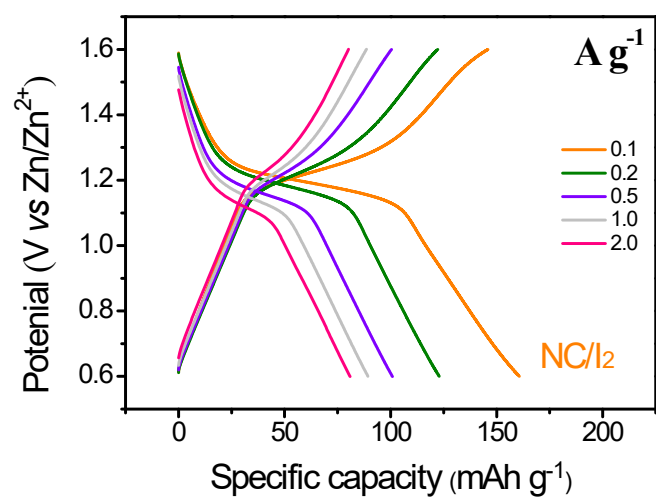


Fig. S4. Discharge/charge curves at various current density of NC/I₂.

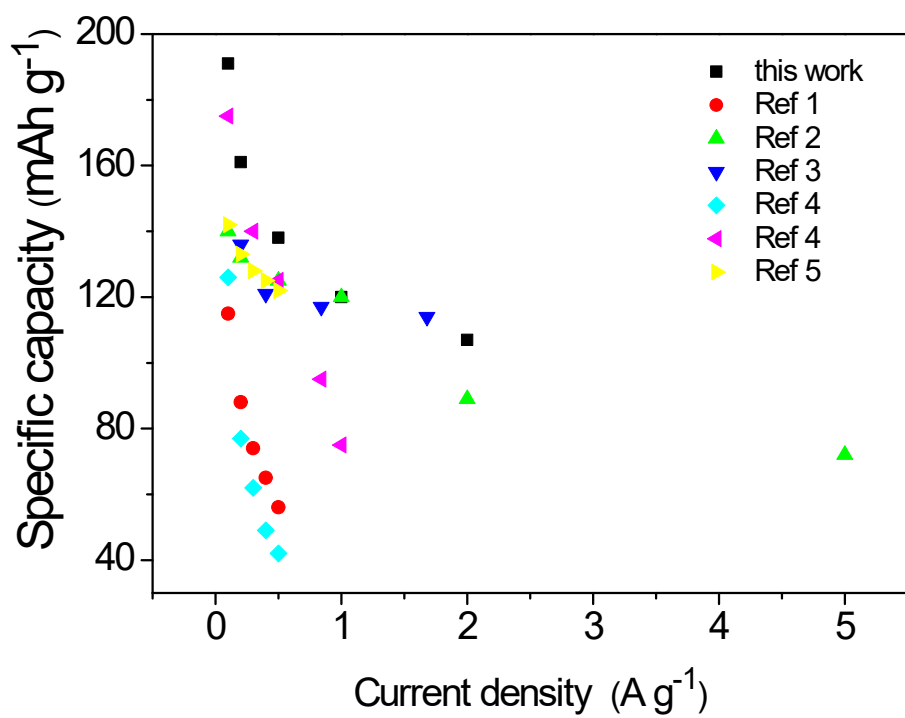


Fig. S5. Comparison of rate performance with reported zinc-iodine batteries.

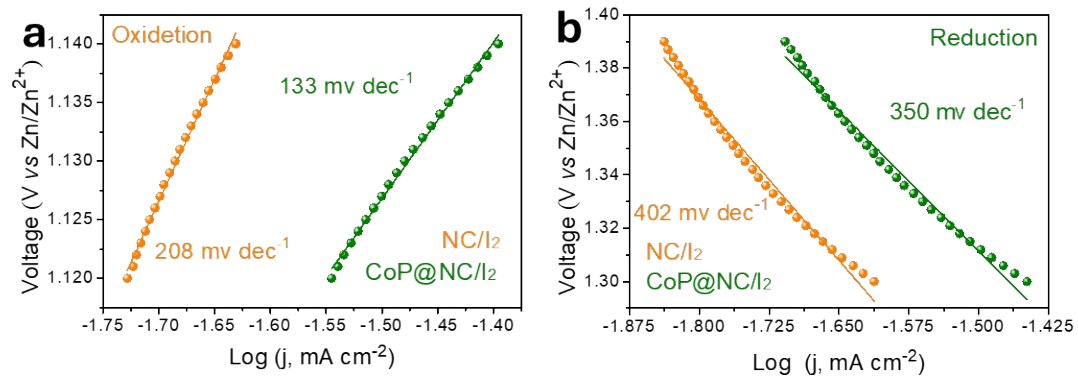


Fig. S6 (a, b) Tafel curves of CoP@NC/I₂ and NC/I₂ cathodes for oxidation and reduction reactions.

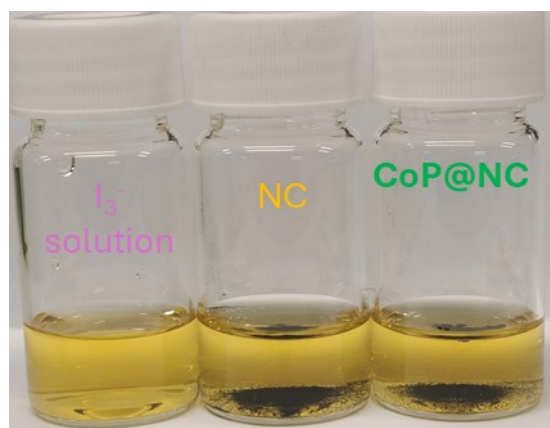


Fig. S7. Initial optical images of adsorption by CoP@NC and NC.

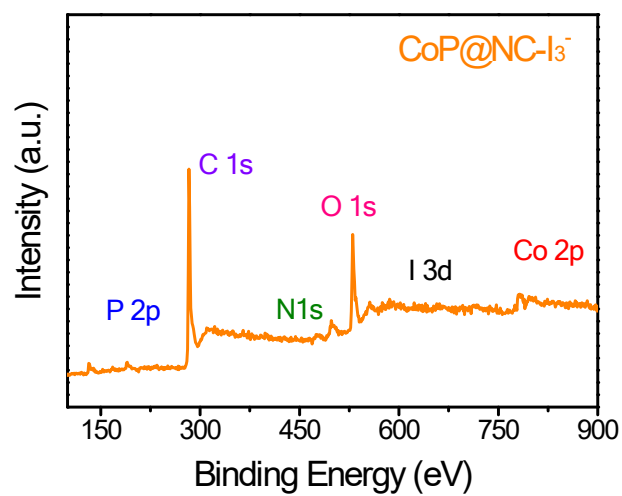


Fig S8. XPS survey spectrum of the CoP@NC after polyiodide adsorption.

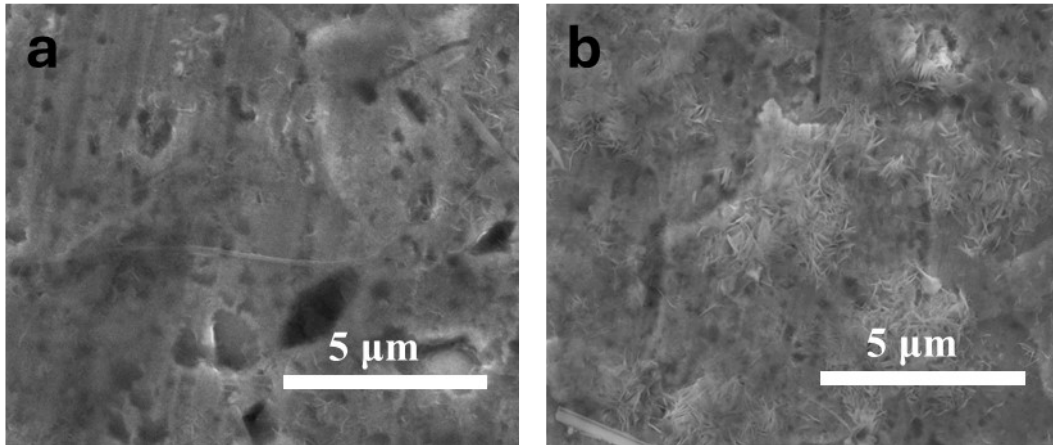


Fig. S9. SEM images of Zn anode after cycles in the Zn-I₂ battery with (a) CoP@NC/I₂ and (b) NC/I₂ cathode.

References

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