

Electronic supplementary information (ESI)

Investigation of Fe₂N@Carbon encapsulated in N-doped graphene-like carbon as a catalyst in sustainable zinc-air batteries

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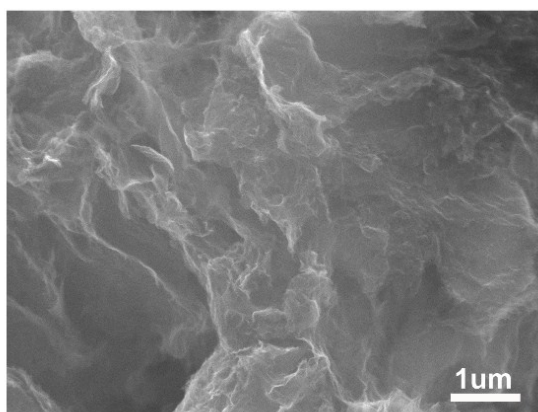


Fig. S1 FESEM images of NG.

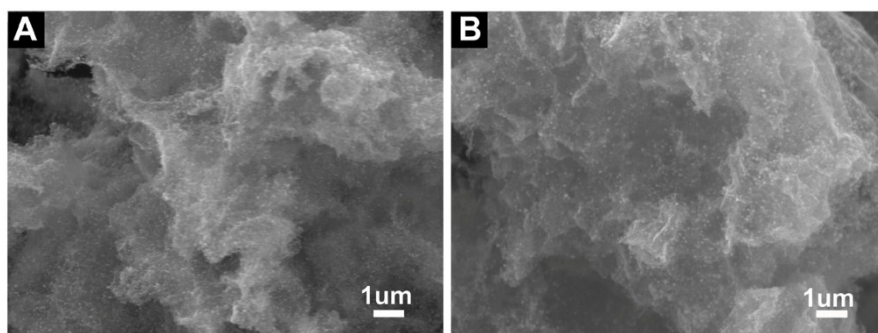


Fig. S2 FESEM images of $\text{Fe}_3\text{C}/\text{NG}$.

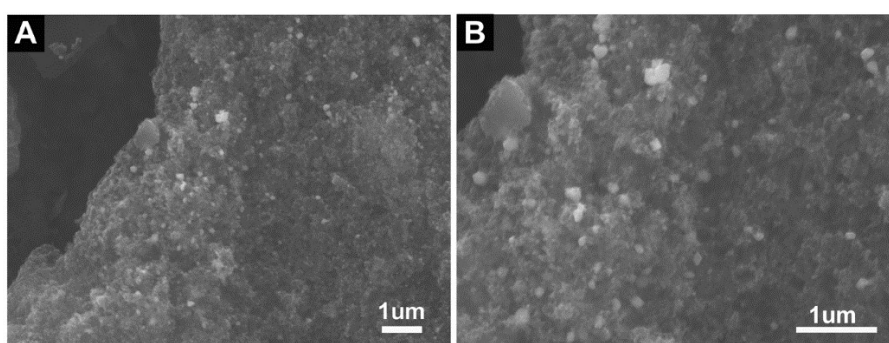


Fig. S3 FESEM images of $\text{Fe}_2\text{N}/\text{NG}$ without adding melamine.

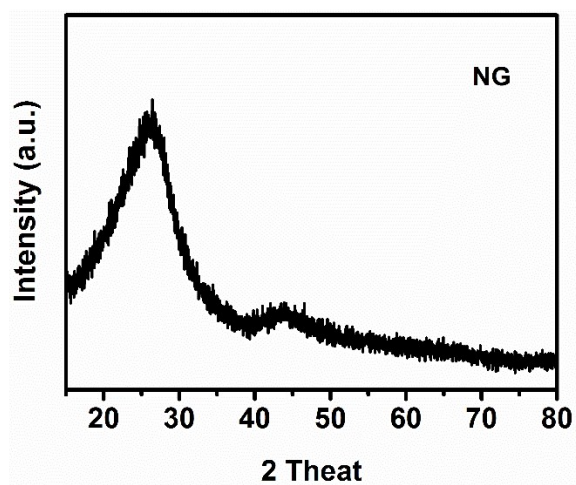


Fig. S4 XRD patterns of NG.

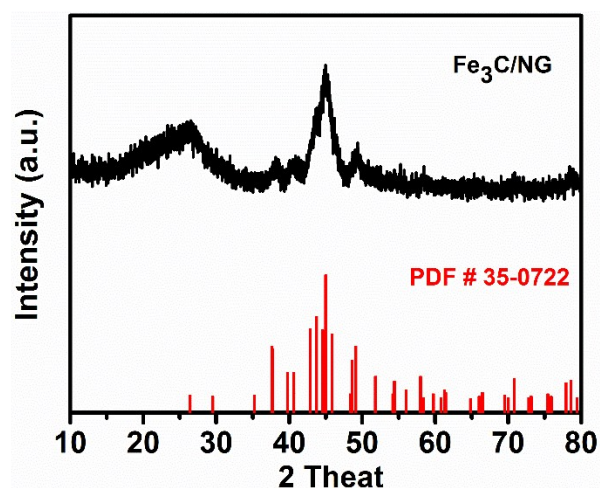


Fig. S5 XRD patterns of Fe₃C/NG.

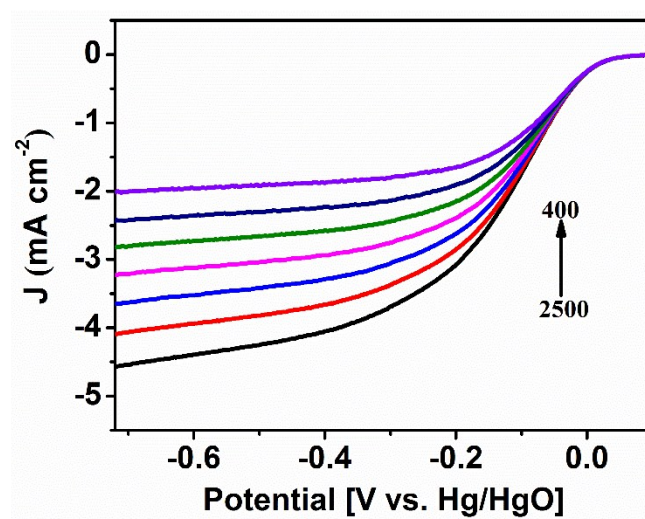


Fig. S6 The different rotation rates of Fe₃C/NG.

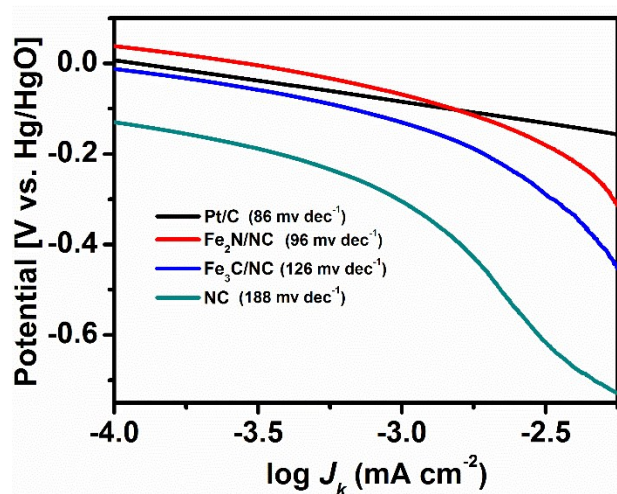


Fig. S7. Tafel plots of the four samples.

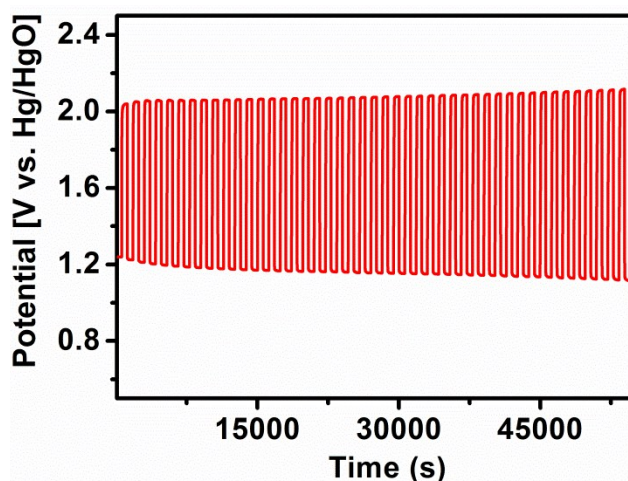


Fig. S8. The discharge and charge voltage of profiles of Zn-air batteries with $\text{Fe}_2\text{N/NC}$.

Material characterizations and electrochemical measurements

The crystal structure of the prepared catalysts were characterized by powder X-ray diffractometer (XRD, Shimadzu XRD-7000). Transmission electron microscopy (TEM, Jeol-2100, Japan) and field emission scanning electron microscopy (FESEM, JSM-7800F, Japan) were used to characterize the physical morphology of the catalysts. X-ray photoelectron spectroscopy (XPS, Escalab 250xi, USA) was used to analyze the surface properties. Raman spectra were obtained with a LabRAM HR Evolution. The thermal properties analysis of the samples was studied by a Thermo Gravimetric Analyzer(TGA,Q50,USA). The electrochemical measurements were

performed in a three-electrode system by using a CHI 660 electrochemical workstation (CHI Instruments Inc.) and Autolab potentiostat (PGSTAT302N) system coupled with a Pinerotator (AFMS-LXF) in 0.1 M KOH with Hg/HgO and Pt foils as reference electrode and counter electrode. For Cyclic voltammetry (CV) experiment, 5 uL catalysts ink (2mg mL⁻¹) was loaded on a modified glassy carbon electrode(GCE) (diameter 3.0 mm) substrate as the working electrode. For the rotating ring disk electrode (RRDE) test, 25 uL catalysts ink (2mg mL⁻¹) was dropped onto the RRDE of 5.6 mm in diameter. After drying at room temperature, it was coated with a thin film of 0.5 % of Nafion solution. All the electrochemical tests were conducted at room temperature.

Koutecky-Levich (K-L) equations:

$$J^{-1} = J_L^{-1} + J_K^{-1} = (B\omega^{1/2})^{-1} + J_K^{-1} \quad (1)$$

$$B = 0.62nFC_0(D_0)^{2/3}\nu^{-1/6} \quad (2)$$

where J is the measured kinetic density, J_k is the kinetic current density, J_d is the diffusion-limiting current density, ω is the angular velocity of the disk in rad s⁻¹ ($\omega = 2\pi N/60$, N = rotation speed in rpm), F is the Faraday constant (96485 C mol⁻¹), D is the diffusion coefficient of O₂ in the electrolyte (1.90×10⁻⁵ cm² s⁻¹), ν is the kinematic viscosity of the electrolyte (0.01 cm² s⁻¹), C_0 is the bulk concentration of O₂ in the electrolyte (1.20 × 10⁻⁶ mol cm⁻³).

The electron transfer number (n) calculated from the RRDE measurement was based on the disk current (J_{Disk}) and ring current (J_{Ring}) via the following equation^[1]:

$$n = 4I_{\text{Disk}}/(I_{\text{Disk}} + I_{\text{Ring}}/N)$$

where N = 0.37 is the current collection efficiency of Pt ring