Facilely Fabricating F-Doped Fe_3N Nanoellipsoids Grown on 3D N-Doped Porous Carbon Framework as a Preeminent Negative Material

Dan Zhang [1,*], Chunyan Zhang [1], Huishi Xu[1], Zhe Huo[1], Xinyu Shi[1], Xiaodi Liu[1], Guangyin Liu[1] and Chuang Yu[2,*]

[1] College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, PR China; zhangchunyanny@163.com (C.Z.); x3243536058@163.com (H.X.); imkc62@163.com (Z.H.); sxy021112@163.com (X.S.); liuxiaodiny@126.com (X.L.); liugy13@163.com (G.L.)

[2] State Key Laboratory of Advanced Electromagnetic Engineering and Technology, School of Electrical and Electronic Engineering, Huazhong University of Science and Technology, Wuhan 430074, PR China

* Correspondence: danzhangny@163.com (D.Z.); cyu2020@hust.edu.cn (C.Y.)

Electrochemical measurements

The electrochemical performance of the samples was tested using CR2025-type coin cell. The test electrodes were prepared by mixing the samples, carbon black, and binder (polyvinylidene fluoride (PVDF)) at a weight ratio of 7:2:1 in N-methyl-2-pyrrolidinone (NMP). The resulting slurries were coated onto a copper foil and then dried under vacuum at 80 ^{o}C for 12 h. Coin cells were assembled in an argon-filled glovebox (H_2O and O_2 < 0.1 ppm) using lithium foil as the counter and reference electrode, a polymer separator (Celgard 2500), and 1 M $LiPF_6$ in EC:DMC:DEC (1:1:1 in volume) as the electrolyte. The cells were tested using a LANHE Battery Test System in the potential range between 0.01 and 3 V at room temperature. Cyclic voltammetry (CV) was measured using an electrochemical workstation (CHI660C). Electrochemical impedance spectra (EIS) were characterized by the same instrument over a frequency range of 100 kHz to 0.01 Hz.

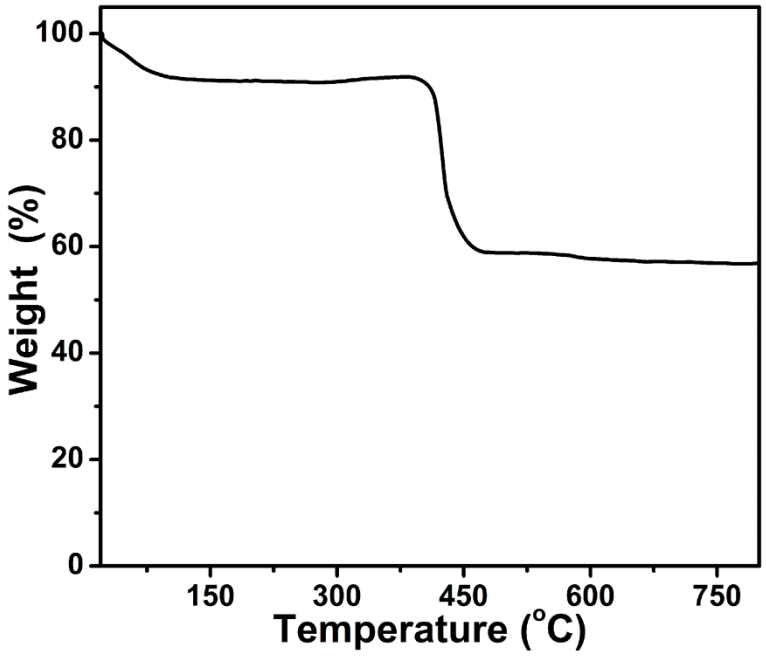

Figure S1 TG curve of F-Fe_3N/NPCF composite.

TGA curve for F-Fe_3N/NPCF composite can be divided into two parts: from 20 °C to 200 °C and from 200 °C to 800 °C. In the first part, a mass loss of approximately 8.9% (wt %) is observed below 200 °C on the TG curve, which can be attributed to the desorption of adsorbed molecules (e.g., CO_2, H_2O). In the second part, from 200 °C to 800 °C, the Fe_3N phase was oxidized into Fe_2O_3, accompanying the complete removal of carbon. Based on the remaining weight percent of Fe_2O_3, we can calculate the weight percent of 43.2% for Fe_3N. Thus, the carbon content for the F-Fe_3N/NPCF composite is approximately 47.9% (1-8.9%-43.2%).

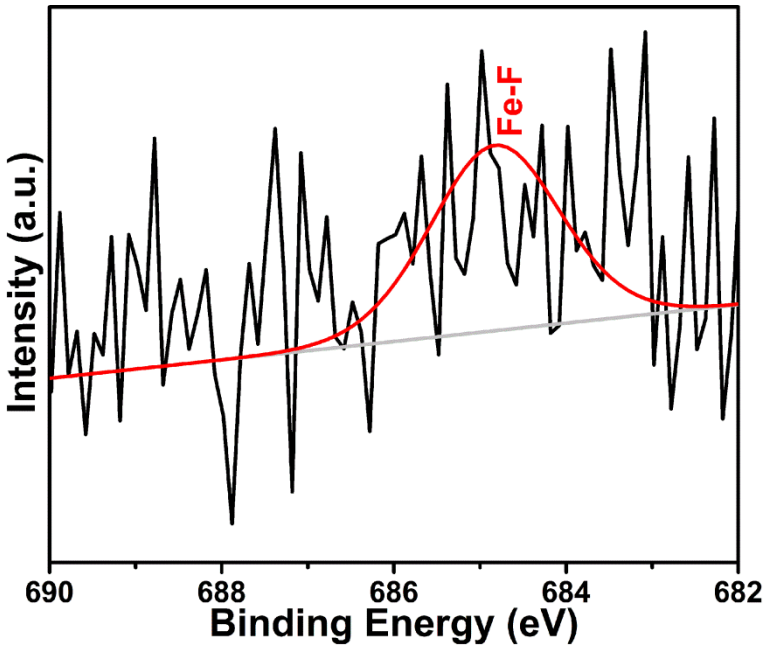

Figure S2 XPS spectrum of the F 1s region for F-Fe_3N/NPCF composite.

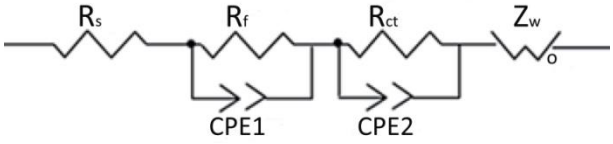

Figure S3 Equivalent circuit.

Table S1 Electrochemical impedance parameters of the F-Fe_3N/NPCF, Fe_3N/NPCF and Fe_xN/Fe/NPCF electrodes obtained from equivalent circuit fitting of experimental data.

Sample	Cycle number	R_s/Ohm	R_f/Ohm	R_{ct}/Ohm
F-Fe_3N/NPCF	after five cycles	4	34	65
Fe_3N/NPCF	after five cycles	4	50	74
Fe_xN/Fe/NPCF	after five cycles	4	65	86