Supporting Information

Topochemical Pyrolytic Synthesis of Quasi-Mxene Hybrids via Ionic Liquid-Iron Phthalocyanine as Self-template

EXPERIMENTAL SECTIONS

Materials and reagents

Iron phthalocyanine (Fe-Pc) was purchased from TGI (Tokyo Chemical Industry) and 1-ethyl-3-methylimidazolium dicyanamide ([emim][DCA]) was purchased from CJC (Cheng Jie Chemical). All reagents were of analytical grade and applied without further purification.

Synthesis of quasi-Mxene structure C/Fe_3C/Fe composite

Ionic liquid used here was 1-ethyl-3-methylimidazolium dicyanamide ([emim][DCA]). Firstly, [emim][DCA] and Fe-Pc were homogeneously mixed in an agate mortar with the mass ratio of 10:2 (250 mg:50 mg). Then, the uniform reagents were transferred into a crucible for heat treatment. After the sample were calcined in a tube furnace at 900 ^{o}C via heating rate of 5 ^{o}C/min for 3h in nitrogen atmosphere, C/Fe_3C/Fe hybrids in quasi-Mxene structures were obtained and marked as QMxene-2. 50 mg of pure Fe-Pc, standing for mass ratio of 0:1, was treated through the same procedure to get QMxene-0 as control group. Maintained the dosage of Fe-Pc invariant, QMxene-1 (10:4) and QMxene-3 (10:1) were synthesized by halved or doubled the amount of [emim][DCA].

Beyond that, a series of temperatures were examined for mass ratio of 10:2 (QMxene-2) to investigate morphological transformations at different durations. 250 mg [emim][DCA] and 50 mg Fe-Pc were heated in nitrogen atmosphere for 3h at 300 ^{o}C, 500 ^{o}C, and 900 ^{o}C to generate QMxene-300, QMxene-500, and QMxene-900 respectively. In addition, 50 mg Fe-Pc without [emim][DCA] was also heated in nitrogen atmosphere for 3h at 300 ^{o}C as a contrastive sample to prove that crystal structure change from room temperature to 300 ^{o}C was the result of intercalation of [emim][DCA].

Characterization

All morphologies were got from a field emission scanning electron microscope (FE-SEM, JEOL, Model JSM-7600F) and lattice information was obtained through transmission electron microscope (TEM, JEOL, Model JEM-2100) at 200 kV for further micro-structure. X-ray diffraction (XRD) was brought out by a Scintag PAD-V X-ray diffractometer with Cu Kα irradiation for crystal and component information. Thermo gravimetric analysis (TGA, Q500) was delivered in temperature range of 25-900^{o}C under air flow via heating rate of 5 ^{o}C min^{-1} to confirm precise content of Fe element in the as-synthetic composite. Raman measurements (Renishaw in Via Raman Spectroscope) were performed using a green laser (532 nm) . And X-ray photoelectron spectroscopy (XPS, PHI Quantera) was applied for information about more element and bonding details.

Electrochemical measurements

For preparation of electrode, the obtained quasi-Mxene composite, carbon black, and PVDF binder were homogenously mixed in NMP with mass ratio of 8:1:1. Coating the slurry we gained on a copper foil with active materials approximate 1 mg cm^{-1}, working electrode was produced, which was then put into a vacuum oven at 50 ^{o}C for 12h to remove the solvent. Taking lithium metal as reference electrode in $LiPF_6$ electrolyte (1 M $LiPF_6$ in volume ratio of 1:1 mixture of ethylene carbonate and dimethyl carbonate) with Celgard 2400 membrane as separator, the electrochemical performance was measured. All rating and cycling ability was tested using a NEWARE battery tester and electrochemical impedance spectroscopy was carried out through a CHI 660C electrochemical workstation after the battery went through several cycles.

Figures referred in this paper:

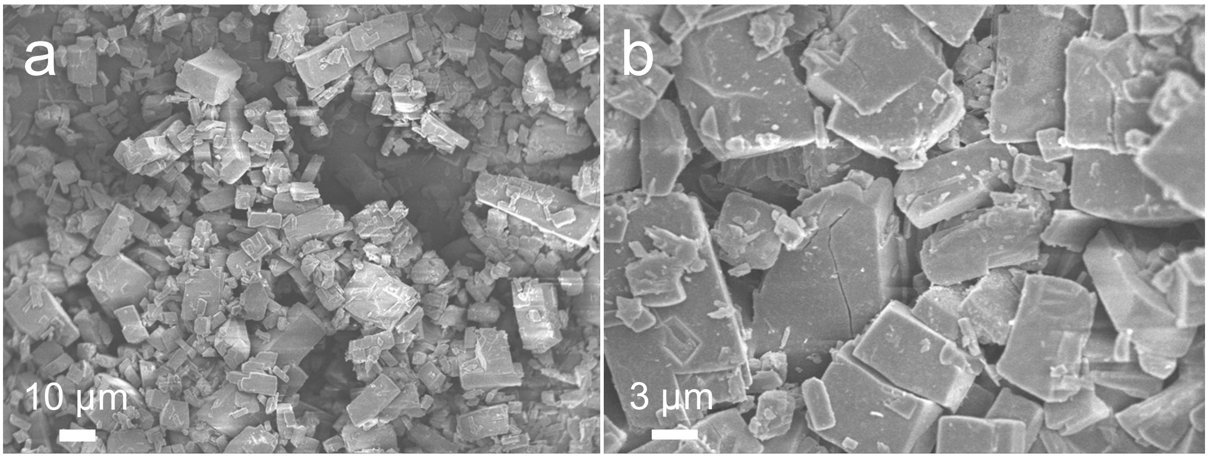

Fig. S1 SEM images of commercially available iron phthalocyanine (Fe-Pc) without any treatments.

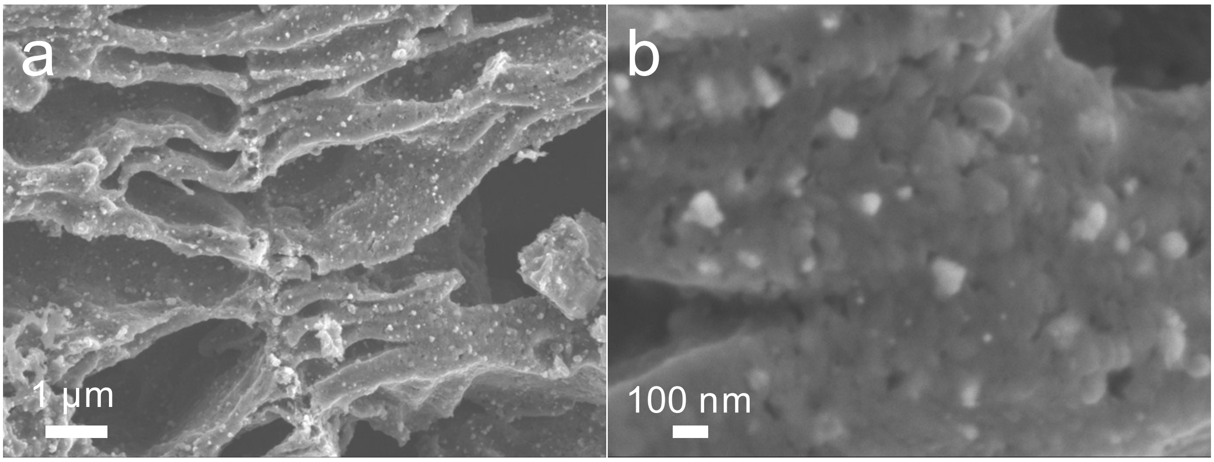

Fig. S2 Magnified SEM images of synthetic quasi-Mxene structure C/Fe_3C/Fe hybrid.

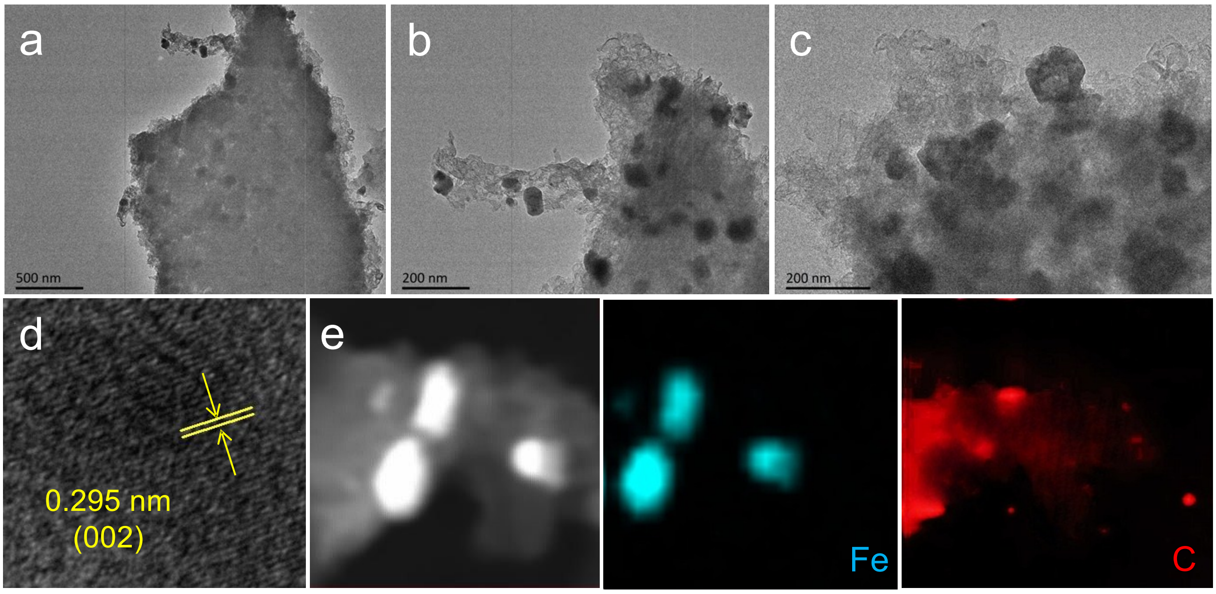

Fig. S3 TEM and corresponding high resolution TEM (HRTEM) images of microstructures of quasi-Mxene C/Fe_3C/Fe hybrid: (a-c) TEM images, (d) HRTEM image, (e) Element images, confiming the existence of Fe_3C/Fe nanoballs.

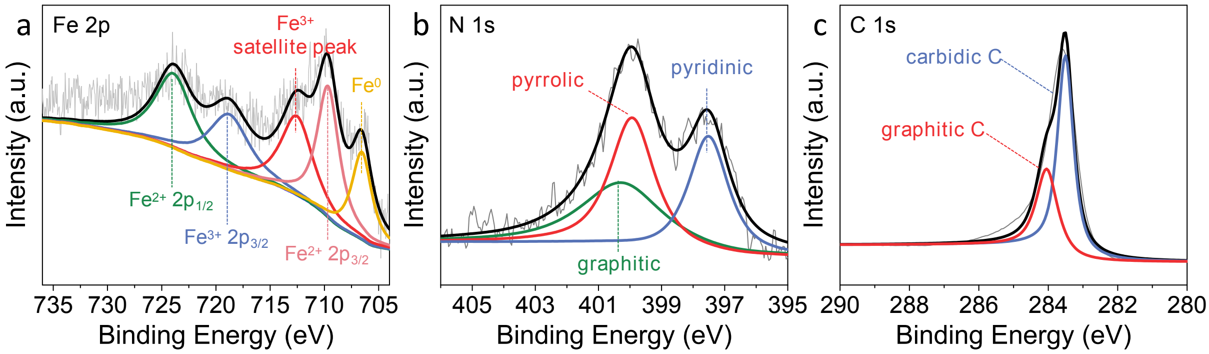

Fig. S4 XPS of quasi-Mxene structure C/Fe_3C/Fe hybrid of (a) Fe 2p orbitals, (b) N 1s orbitals, and (c) C 1s orbitals.

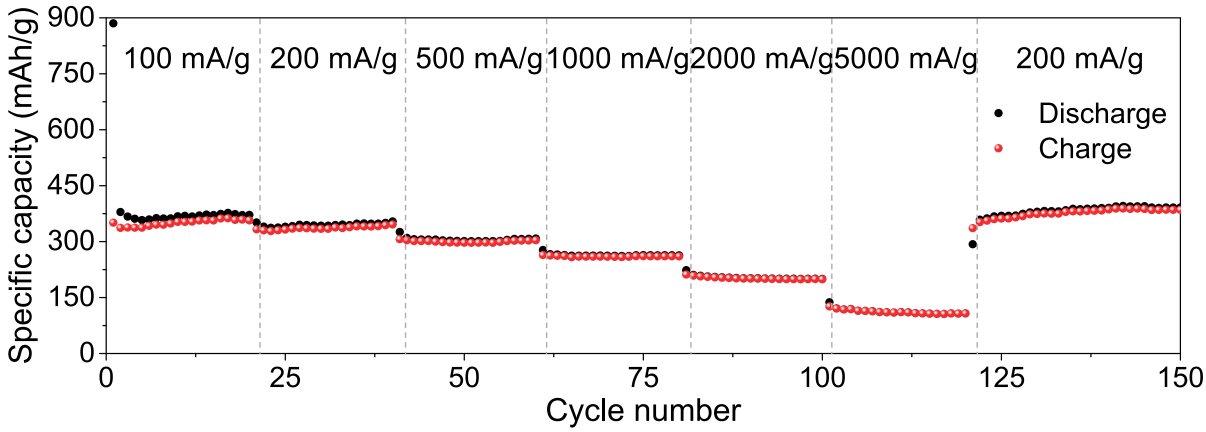

Fig. S5 Rate capability of quasi-Mxene structure C/Fe_3C/Fe hybrid at different current densities of 100, 200, 500, 1000, 2000, 5000 mA g^{-1}.

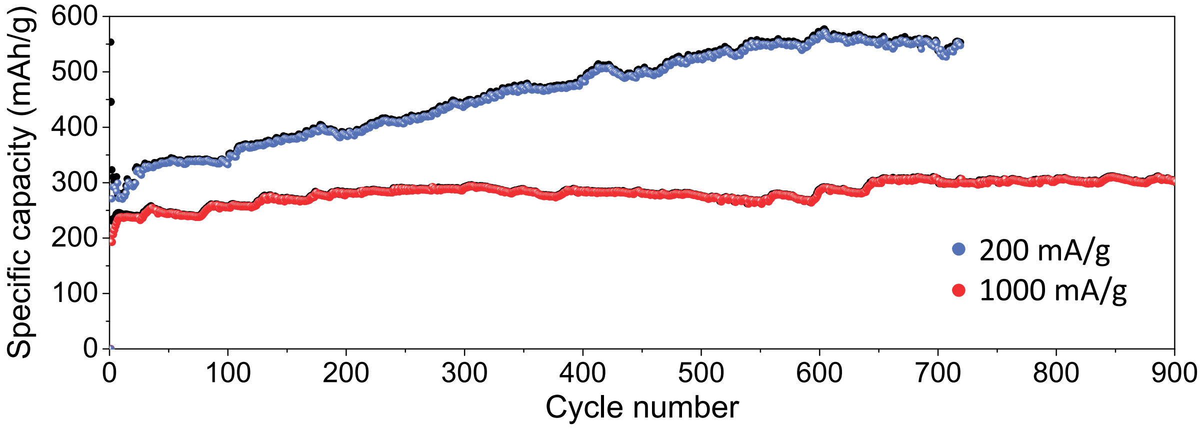

Fig. S6 Cycling stability of quasi-Mxene structure C/Fe_3C/Fe hybrid at current density of 200 mA g^{-1} and 1000 mA g^{-1}.

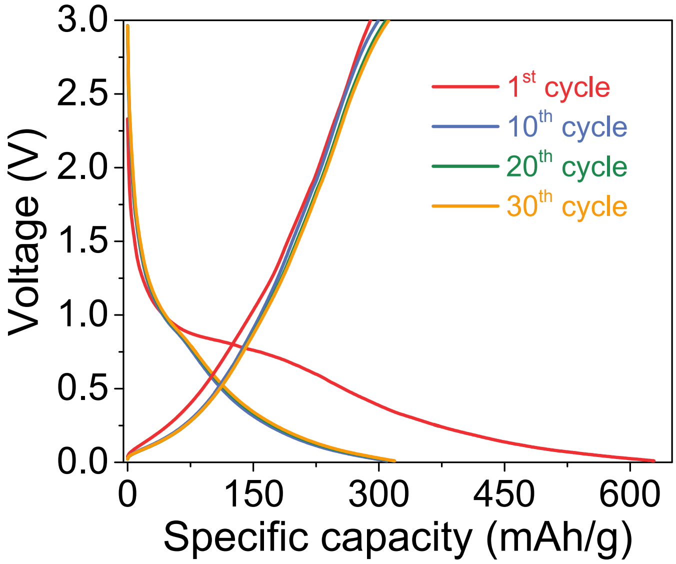

Fig. S7 Charge-discharge profiles of quasi-Mxene structure C/Fe_3C/Fe hybrid under current density of 200 mA g^{-1} at 1st, 10th, 20th and 30th cycles.

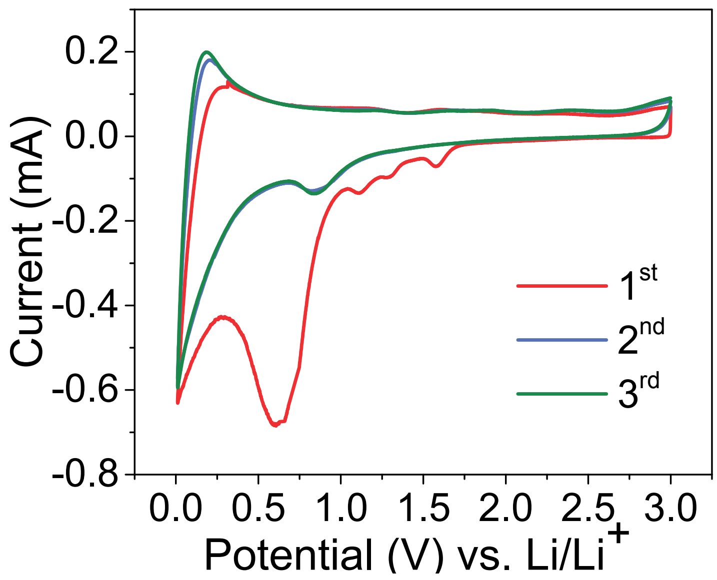

Fig. S8 Cyclic voltammetry curves of quasi-Mxene structure C/Fe_3C/Fe hybrid for the first three cycles.

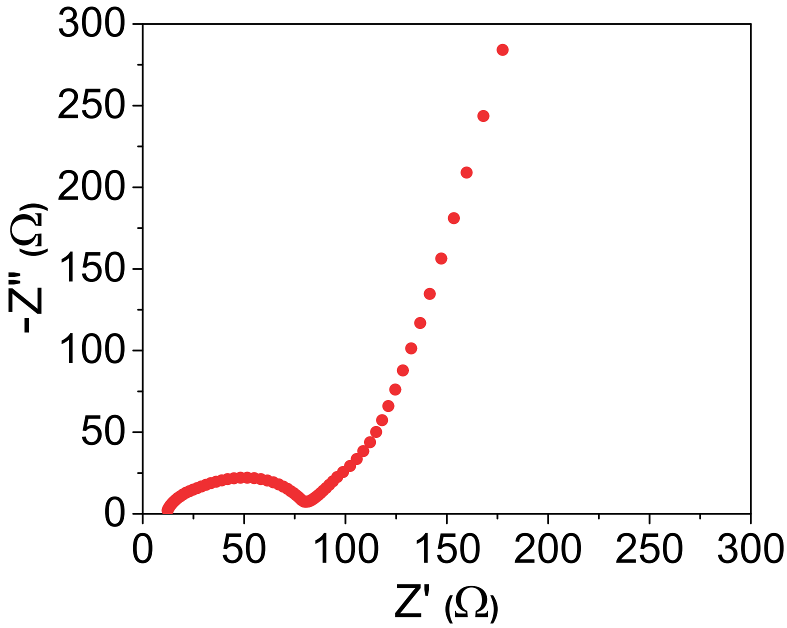

Fig. S9 Nyquist plots of quasi-Mxene structure C/Fe_3C/Fe hybrid after three cycles.