Electronic Supplementary Information

Porous Fe_2O_3 nanocubes derived from MOFs for highly reversible lithium storage

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Experimental Section

Materials Synthesis. In a typical procedure, polyvineypirrolydone (PVP, K30, MW ~ 40000, 3.0 g) and $K_4Fe(CN)_6 \cdot 3H_2O$ (0.226 g) were added to a HCl solution (0.01 M, 40 mL) under magnetic stirring. After stirring for 30 min, a clear solution was obtained. The reaction mixture was then transferred into a 100 mL polytetrafluoroethylene (Teflon)-lined stainless-steel autoclave and kept in an electric oven at 80 °C for 24 h. The autoclave was then taken out from the oven and left to cool to room temperature. The obtained blue product was filtered and washed several times with distilled water and absolute ethanol and finally dried in a vacuum oven at 25 ^{o}C for 12 h. To convert the Prussian blue nanocubes into porous Fe_2O_3 nanocubes, the as-synthesized Prussian blue product was heated at a temperature of 350 ºC with a heating rate of 1 ºC min^{-1} for 6 h in air. The α-Fe_2O_3 microparticles are synthesized by adding 90 mL of 6 M NaOH into 100 mL of 2 M $FeCl_3$ under vigorous stirring, followed by the addition of 10 mL of 0.6 M Na_2SO_4. The solution was then heated at 102 ^{o}C for 4 days in an air-flow electric oven.

Materials Characterization. X-ray diffraction (XRD) patterns were collected on a Bruker D8 Advanced X-Ray Diffractometer with Ni filtered Cu Kα radiation (λ=1.5406 Å) at a voltage of 40 kV and a current of 40 mA. Field-emission scanning electron microscopy (FESEM) images were acquired on a JEOL JSM 6700F microscope operated at 5 kV. Transmission electron microscopy (TEM) images were taken on JEOL 2010 and JEOL 2100F microscopes. Thermogravimetric analysis (TGA) was carried out under air flow with a temperature ramp of 10 ^{o}C min^{-1}. Nitrogen sorption measurement was performed on Autosorb 6B at liquid N_2 temperature.

Electrochemical Measurements. The electrochemical tests were carried out in two-electrode Swagelok cells. The working electrodes consist of 70% of active material, 20% of conductive carbon black (Super-P-Li), and 10% of polymer binder (polyvinylidene fluoride, PVDF). The electrolyte is 1

M $LiPF_6$ in a mixture of ethylene carbonate and diethyl carbonate (1:1 by weight). Lithium foil was used as the counter and reference electrode. Cell assembly was carried out in an Ar-filled glovebox with moisture and oxygen concentrations below 1.0 ppm. The charge-discharge tests were performed on a NEWARE battery tester.

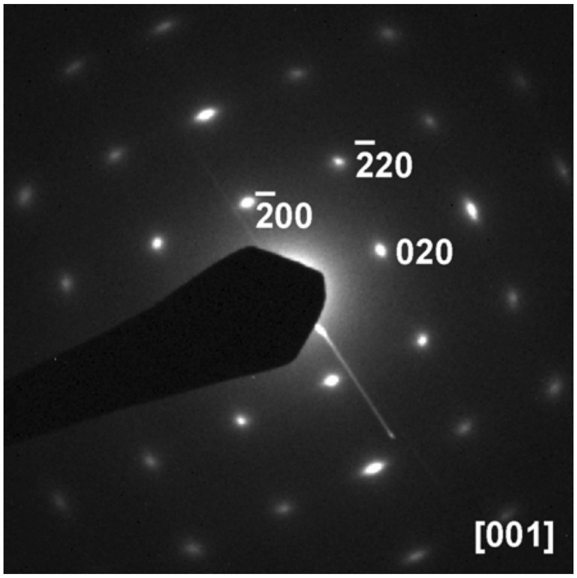

Fig. S1 Selected-area electron diffraction (SAED) pattern of a $Fe_4[Fe(CN)_6]_3$ nanocube.

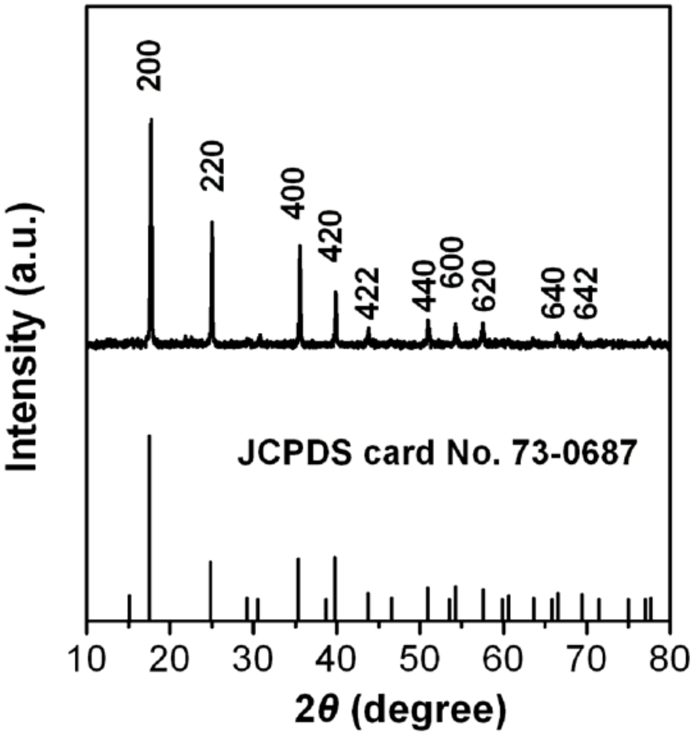

Fig. S2 XRD pattern of $Fe_4[Fe(CN)_6]_3$ nanocubes.

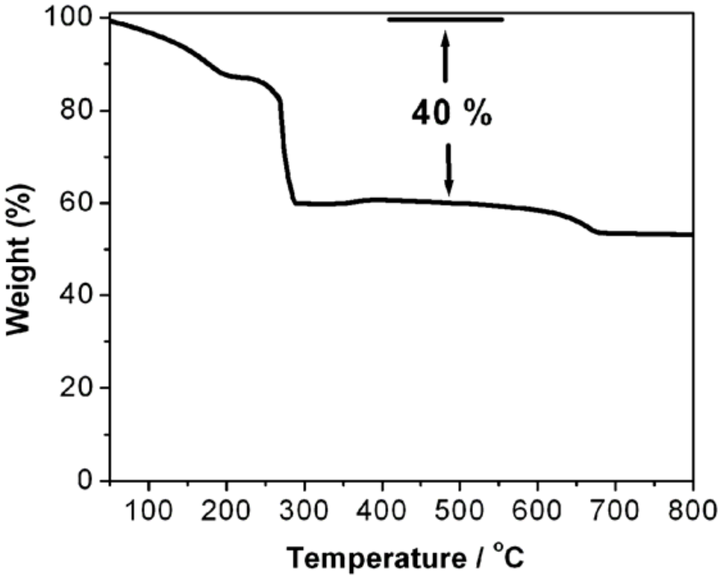

Fig. S3 TGA curve of $Fe_4[Fe(CN)_6]_3$ nanocubes in air flow.

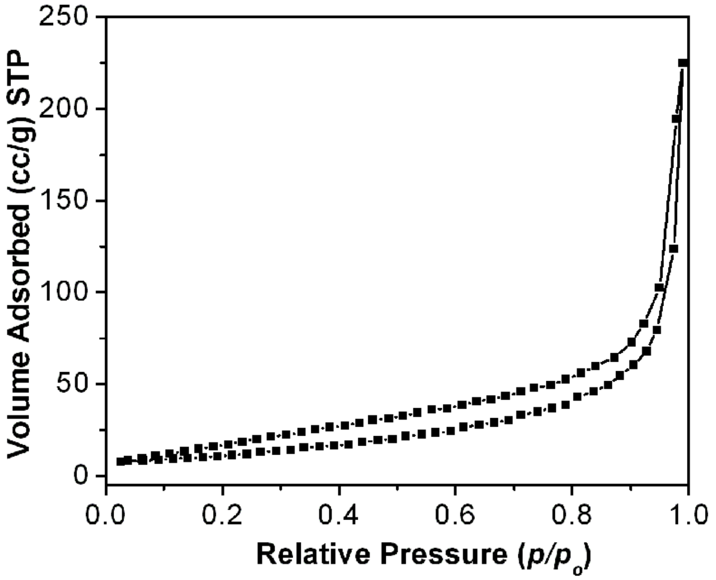

Fig. S4 N_2 adsorption-desorption isotherm of porous Fe_2O_3 nanocubes.

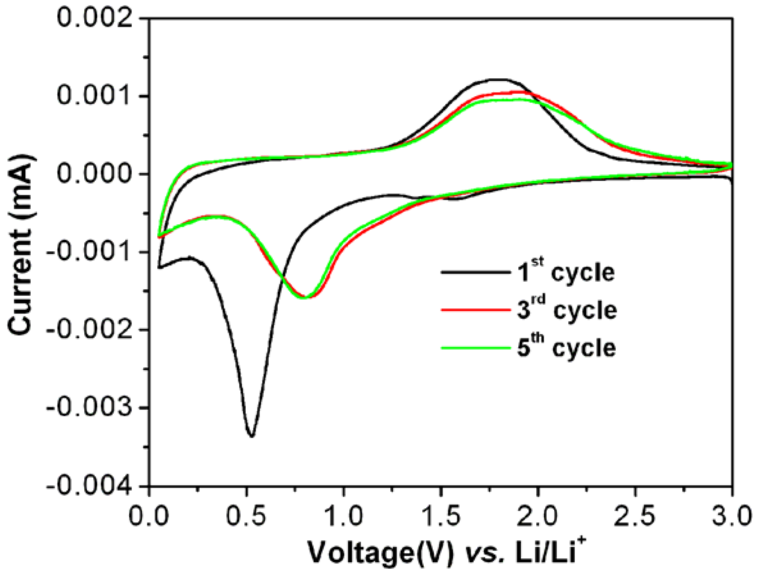

Fig. S5 CV profiles of porous Fe_2O_3 nanocubes showing the 1st, 3rd and 5th cycles between 0.05 and 3.0 V at a scan rate of 0.5 mV s^{-1}.

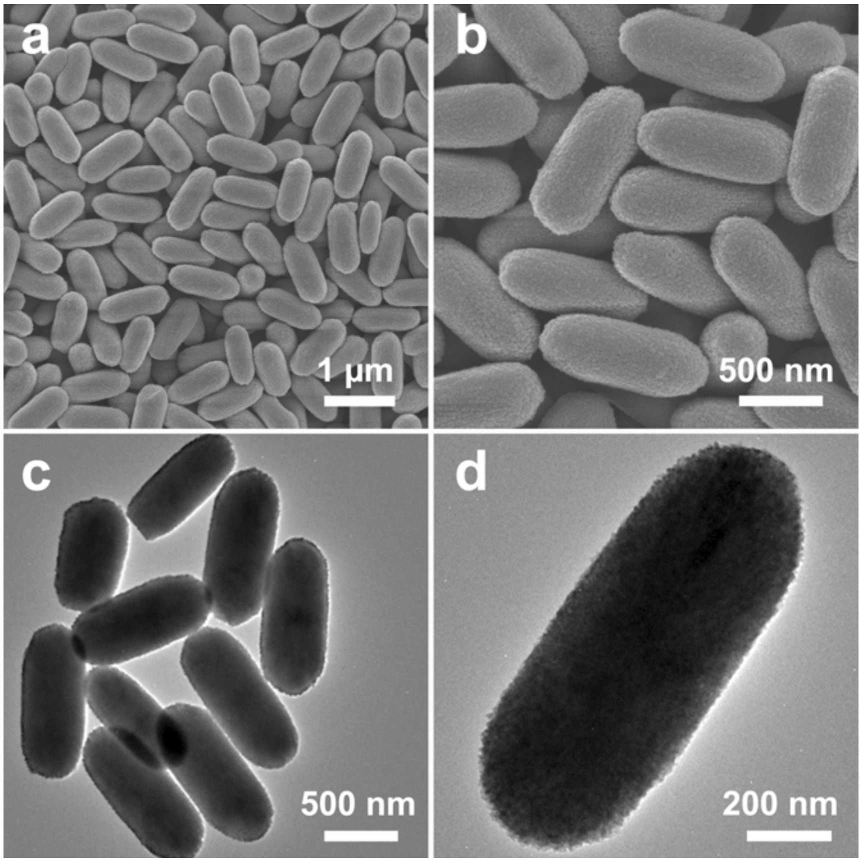

Fig. S6 (a, b) FESEM and (c, d) TEM images of α-Fe_2O_3 microparticles.

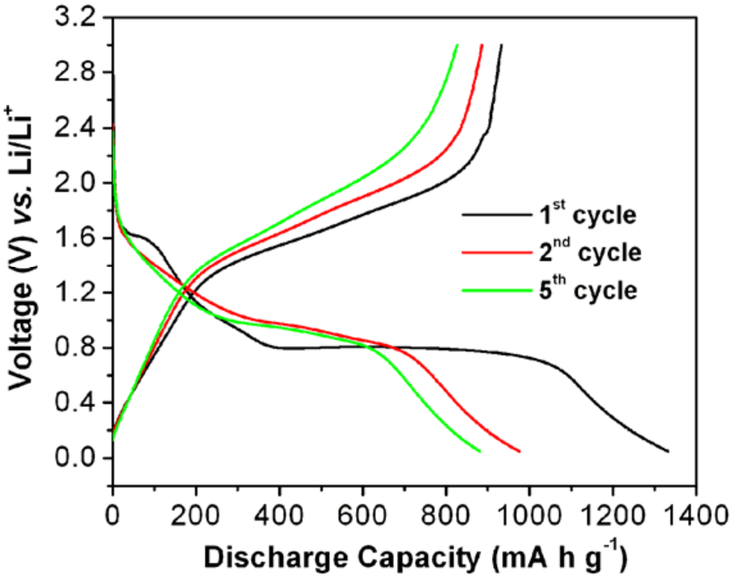

Fig. S7 Discharge/charge voltage profiles of α-Fe_2O_3 microparticles in the voltage window of 0.05 – 3.0 V *vs.* Li/Li^+ at the same current density of 200 mA g^{-1}.

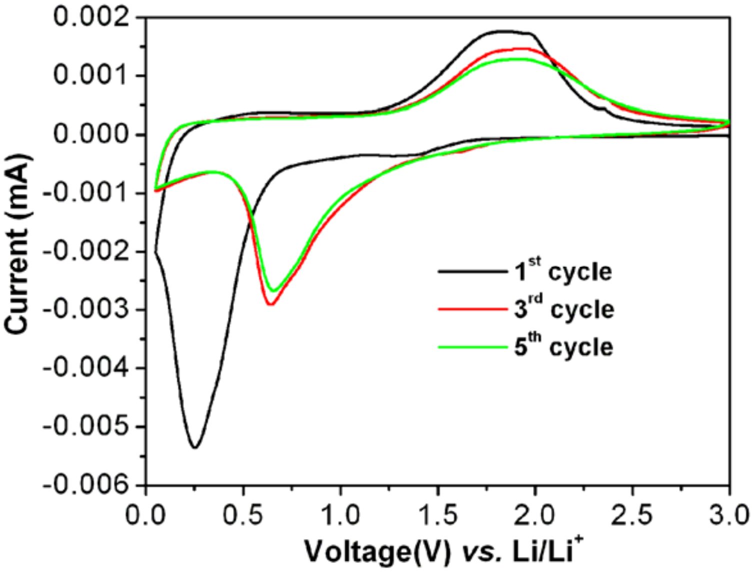

Fig. S8 CV profiles of α-Fe_2O_3 microparticles showing the 1st, 3rd and 5th cycles between 0.05 and 3.0 V at a scan rate of 0.5 mV s^{-1}.