

Supporting information

Fe₂O₃ microcubes derived from metal-organic frameworks for lithium-ion storage with excellent performance

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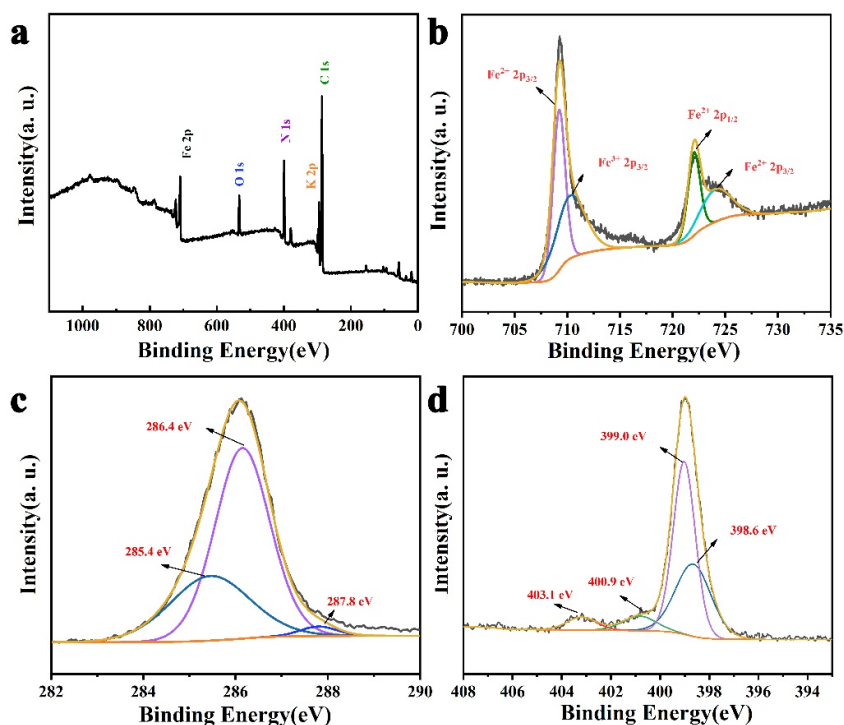


Figure S1. XPS spectra for PB precursor (a) XPS spectrum, (b) Fe 2p, (c) C 1s, (d) N 1s.

The elements in PB precursor were investigated via XPS. Fe, O, C, N and K elements were detected in the full XPS spectrum (Fig. S1a) of PB precursor, which the results is consistent with previous report [S.1]. Fig. S1b shows the high-resolution XPS spectrum of Fe 2p orbit, the two peaks at 709.3 and 722.1 eV are corresponding to Fe^{2+} ($2p_{3/2}$) and Fe^{2+} ($2p_{1/2}$), while the other two peaks at 710.5 and 724.3 eV correspond to Fe^{3+} ($2p_{3/2}$) and Fe^{3+} ($2p_{1/2}$). This result proves that part of Fe^{3+} is reduced. The Fig. S1c displays C 1s spectrum. Two peaks at 285.4 and 287.7 eV can be assigned to C-N bond, and the peak at 286.4 eV correspond to C-O bond. In Fig. S1d, the peaks situat at 398.6, 399.0, 400.9 and 403.1 eV reveal the presence of N in the $-(\text{CN})$ [S.2, 3].

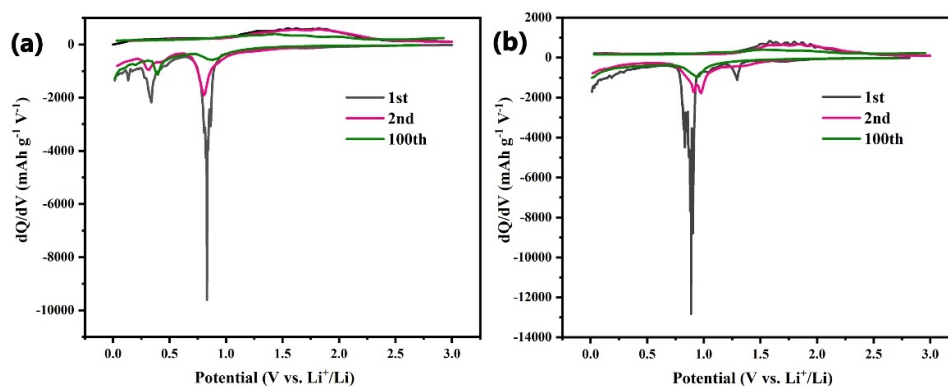


Figure S2 The Differential capacity plot of (a) Fe_2O_3 -500 and (b) Fe_2O_3 -700.

For two samples, it is obvious that the first cycle is distinct substantially from those of the subsequent ones, indicating a different Li^+ storage reaction taking place in the first cycle compared with the following cycles. During the first cycle of Fe_2O_3 -500 (

Fig. S2a), the cathodic peaks at about 0.82 and 0.35V can be ascribed to the reduction of Fe^{3+} to Fe^0 , with the decomposition of electrolyte to form a solid electrolyte interphase (SEI) film. In the follow cycles, the cathodic peaks are shifted, due to a structure rearrangement and associated with the reversible reduction of Fe^{3+} . The curves of Fe_2O_3 -700 re as similar as Fe_2O_3 -500 (Fig. S2b), but overlap parts are less than Fe_2O_3 -500. This means that the cycling stability of Fe_2O_3 -700 is worse than Fe_2O_3 -500.

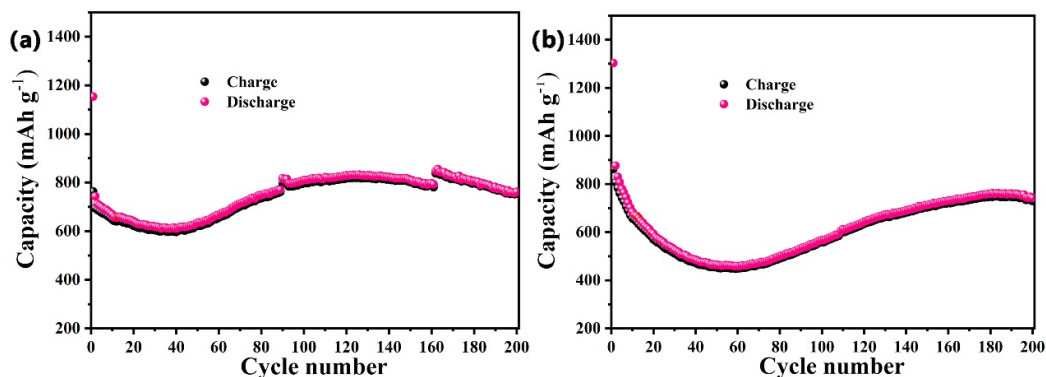


Figure S3 The Cycling performance of (a) Fe_2O_3 -400 and (b) Fe_2O_3 -600.

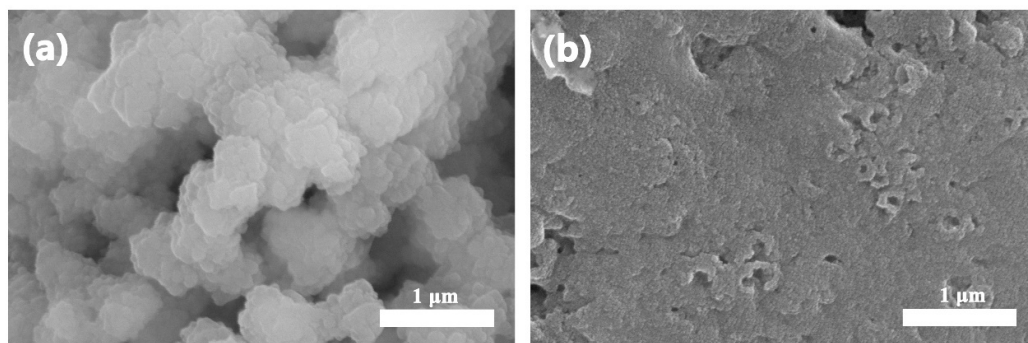


Figure S4 SEM images of (a) Fe_2O_3 -500 and (b) Fe_2O_3 -700 after 300 cycles at 1000 mA g^{-1} .

References

- S.1. He, X.; Tian, L.; Qiao, M.; Zhang, J.; Geng, W.; Zhang, Q. A novel highly crystalline $\text{Fe}_4(\text{Fe}(\text{CN})_6)_3$ concave cube anode material for Li-ion batteries with high capacity and long life. *J. Mater. Chem. A*, **2019**, 7, 11478-11486.
- S.2. Matienzo, J.; Yin L.I.; Grim, S.O.; William, E. X-ray photoelectron spectroscopy of nickel compounds. *Inorg. Chem.*, **1973**, 12, 2762-2769.
- S.3. Fluck, E.; Inoue, H.; Yanagisawa, S. Mössbauer and X - ray photoelectron spectroscopic studies of prussian blue and its related compounds. *Anorg. Allg. Chem.*, **1977**, 430, 241-249.