Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Three-dimensional iron oxyfluoride/N-doped carbon hybrid nanocomposites as high-performance cathodes for rechargeable Li-ion batteries

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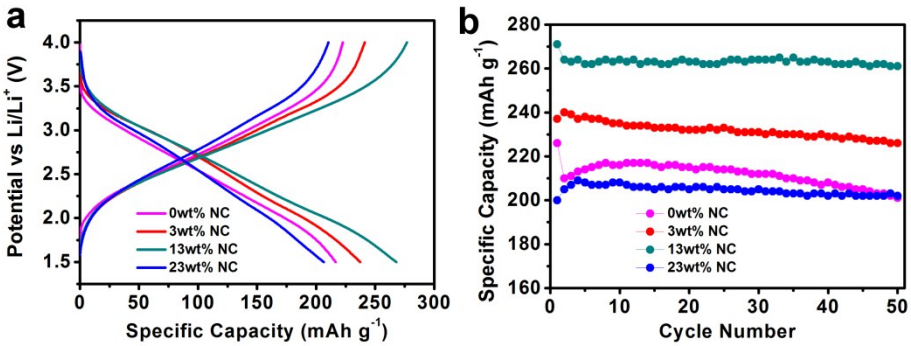

Fig. S1 (a) Charge/discharge curves of the FeOF/NC electrode with different contents of NC at a constant current density of 0.2 A g^{-1} in the voltage range of 1.5-4.0 V at room temperature. (b) Corresponding specific capacity vs. cycle number.

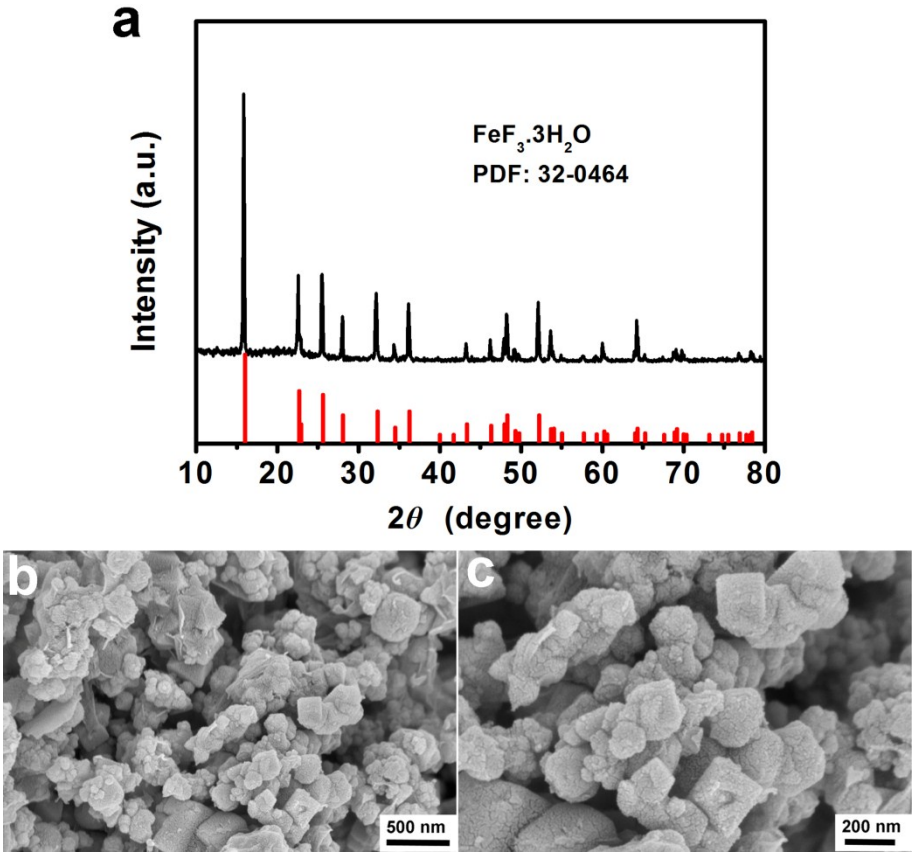

Fig. S2 (a) XRD pattern of the $FeF_3 \cdot 3H_2O$ precursors. (b, c) SEM images of the $FeF_3 \cdot 3H_2O$ precursors.

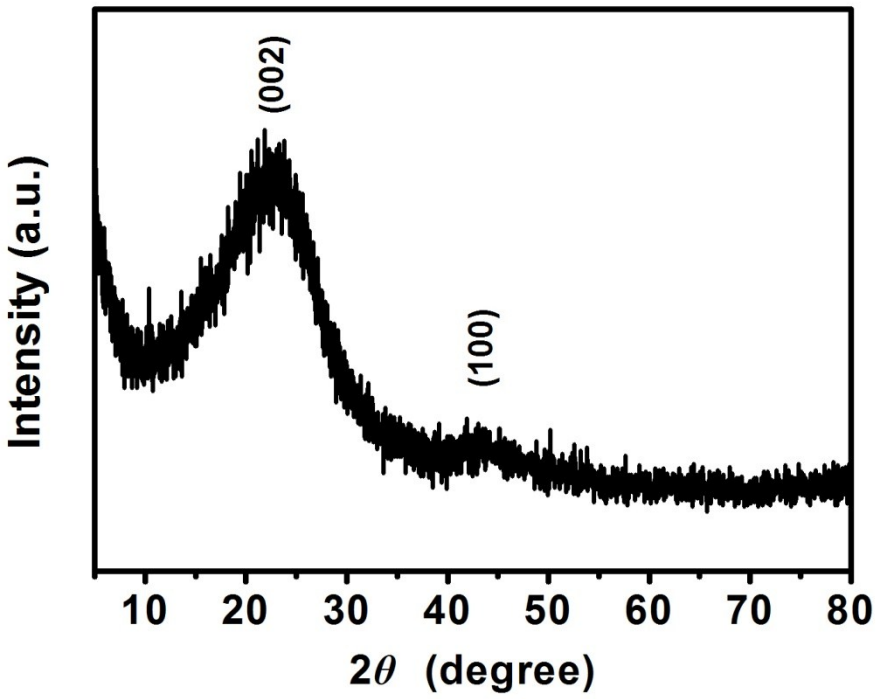

Fig. S3 XRD pattern of the as-prepared porous NC matrix. It can be obviously seen that the NC is a typical amorphous carbon.

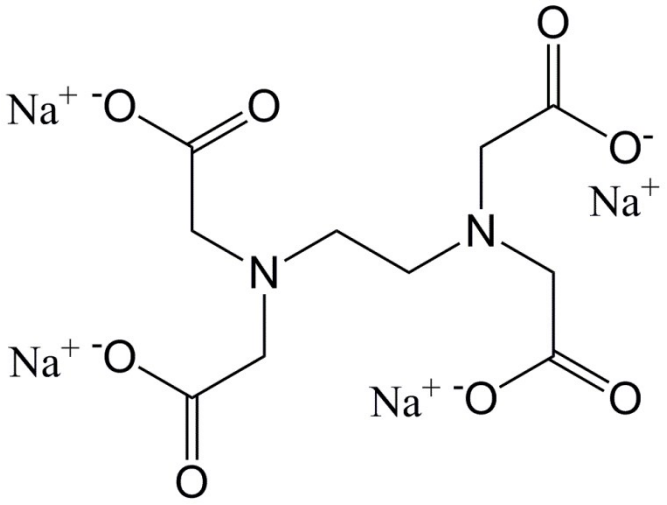

Fig. S4 The molecular structure of the Na_4EDTA. It can be seen that the nitrogen atoms exist in its structure.

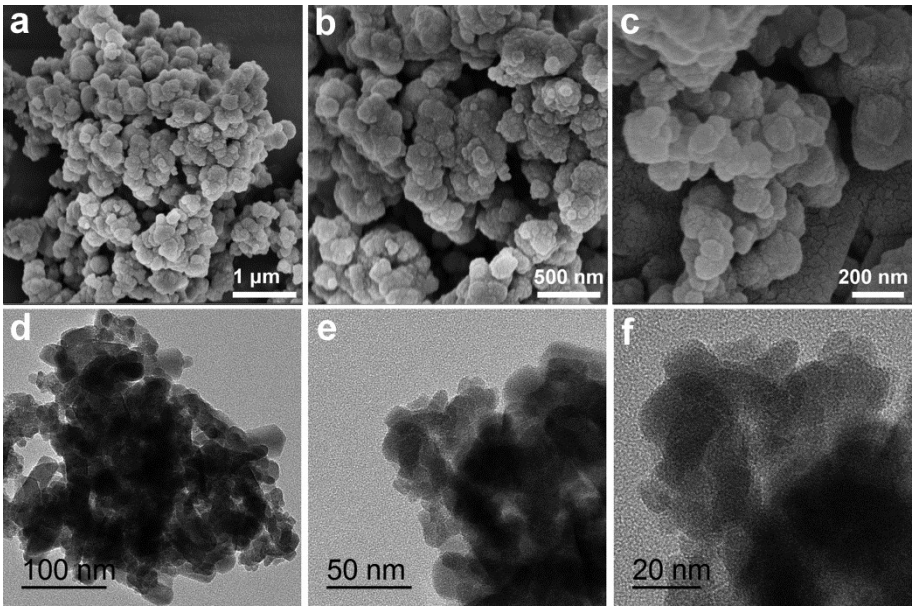

Fig. S5 (a-c) SEM images of the as-synthesized bare FeOF. (d-f) TEM images of the as-synthesized bare FeOF. From the above SEM and TEM images, it can be clearly seen that these bare FeOF particles are aggregating together, which is due to the absence of porous NC matrix to disperse FeOF nanoparticles.

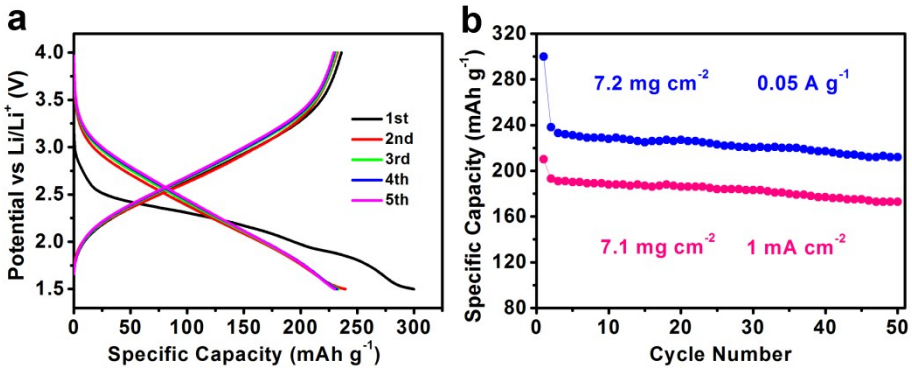

Fig. S6 (a) Discharge/charge curves of the 3D FeOF/NC electrode with a high mass loading of 7.2 mg cm^{-2} at a constant current density of 0.05 A g^{-1} in the voltage range of 1.5-4.0 V at room temperature. (b) The cycling performance of the electrodes at 0.05 A g^{-1} and 1 mA cm^{-2}.

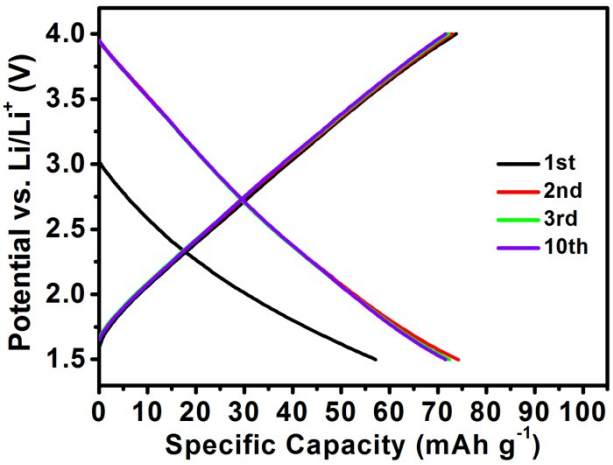

Fig. S7 Discharge/charge curves of the NC electrode at a constant current density of 0.2 A g^{-1} in the voltage range of 1.5-4.0 V at room temperature. Considering the weight ratio of NC is 13 wt% in the nanocomposites, therefore, it could contribute about 3.5% to the overall electrode capacity.

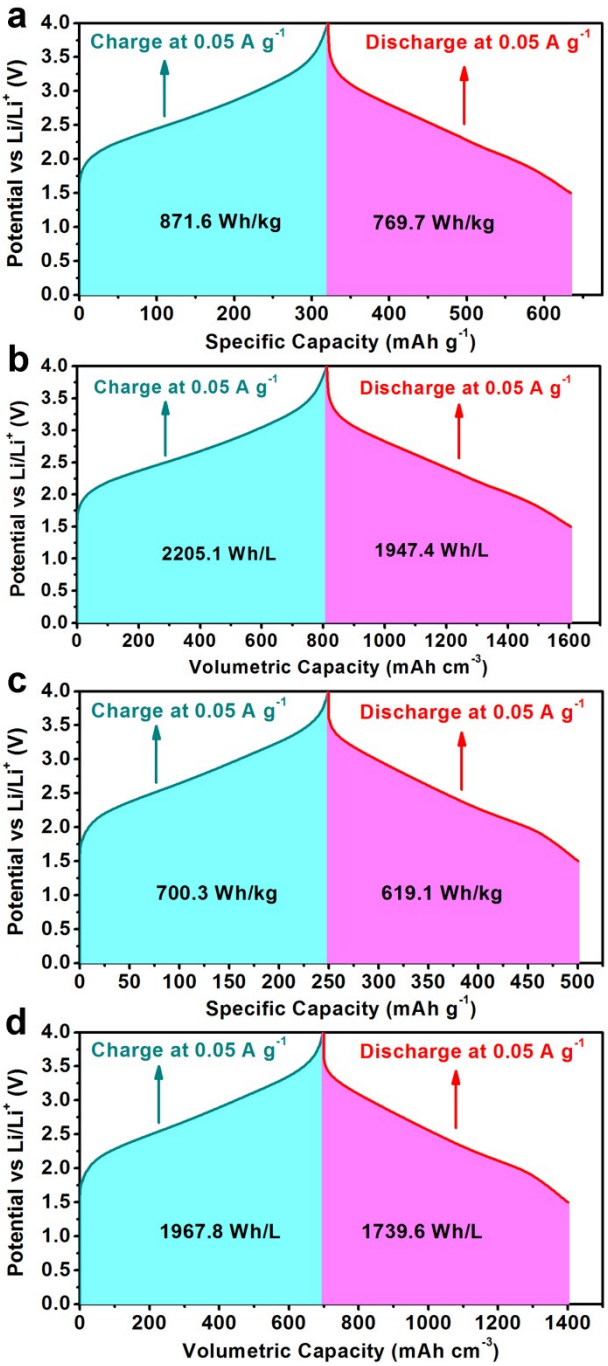

Fig. S8 Comparison of gravimetric energy densities and volumetric energy densities for (a, b) FeOF/NC and (c, d) FeOF based on their charge/discharge curves at 0.05 A g^{-1}.

Table S1 Comparison of the electrochemical performance of 3D FeOF/NC with other iron oxyfluoride/fluoride cathode electrodes based on conversion reaction process.

Materials	Voltage range (V)	Rate capacity (mAh g^{-1})	Rate (mA g^{-1})	Cycling capacity (mAh g^{-1})/Current density (mA g^{-1})/(Cycle number)	Ref.
FeOF@PEDOT	1.2-4.0	230	400	407/50/150th	[S1]
LiPON/FeOF	1.2-4.0	250	300	222/300/100th	[S2]
C/FeOF/FeF_3	1.5-4.5	70	200	130/20/50th	[S3]
FeF_2@CNT	1.3-4.3	133	1000	181/100/50th	[S4]
FeF_3@GF–$scCO_2$	1.4-4.5	130	1000	145/200/30th	[S5]
FeF_3/C	1.5-4.5	71	1040	198.9/20.8/50th	[S6]
FeF_3/G	1.5-4.5	73	1040	119.9/208/100th	[S7]
$FeF_3 \cdot xH_2O$/G	1.5-4.5	130	1185	183/237/100th	[S8]
FeF_3@NAN	1.0-4.5	79	1780	215/71/110th	[S9]
$FeF_3(H_2O)_3$/C	1.5-4.5	210	70	200/70/30th	[S10]
3D FeOF/NC	1.5-4.0	241 213 184	500 1000 2000	246/200/100th 191/1000/300th	This Work

References

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