

Developing a light weight lithium ion battery - an effective material and electrode design for high performance conversion anodes

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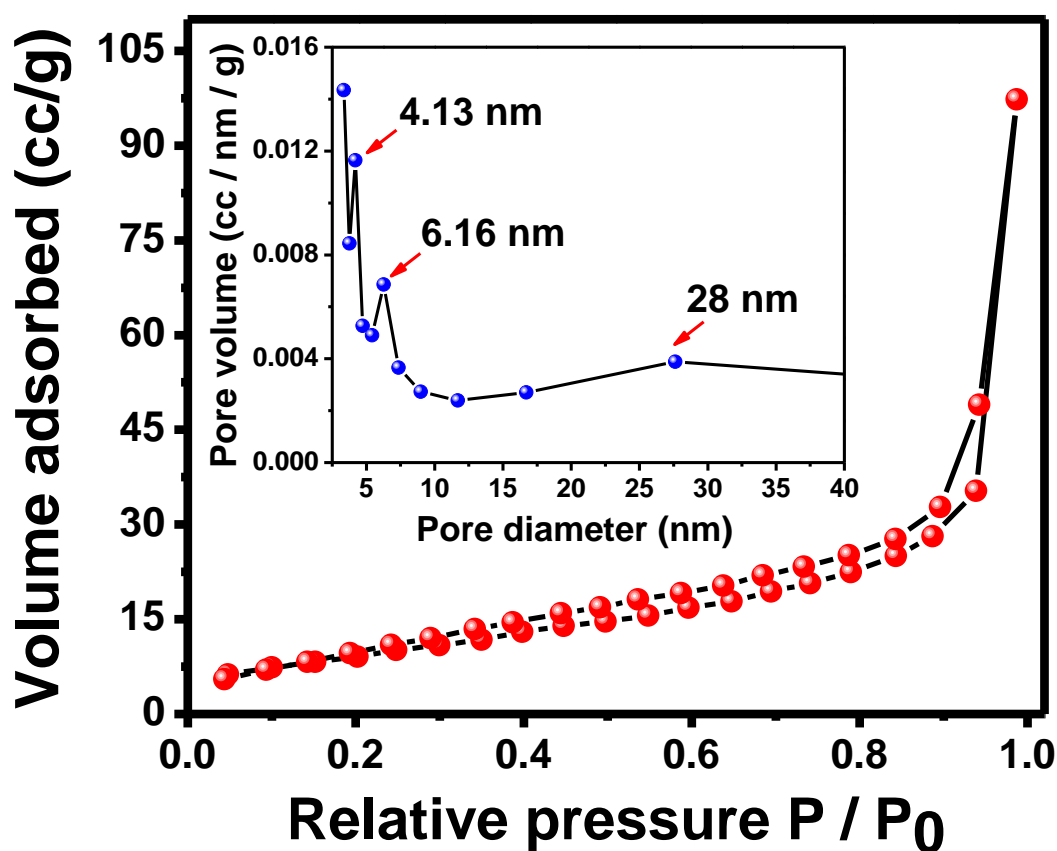


Fig. S1. N₂ sorption isotherm of the synthesized α -Fe₂O₃. Inset showing BJH pore size distribution

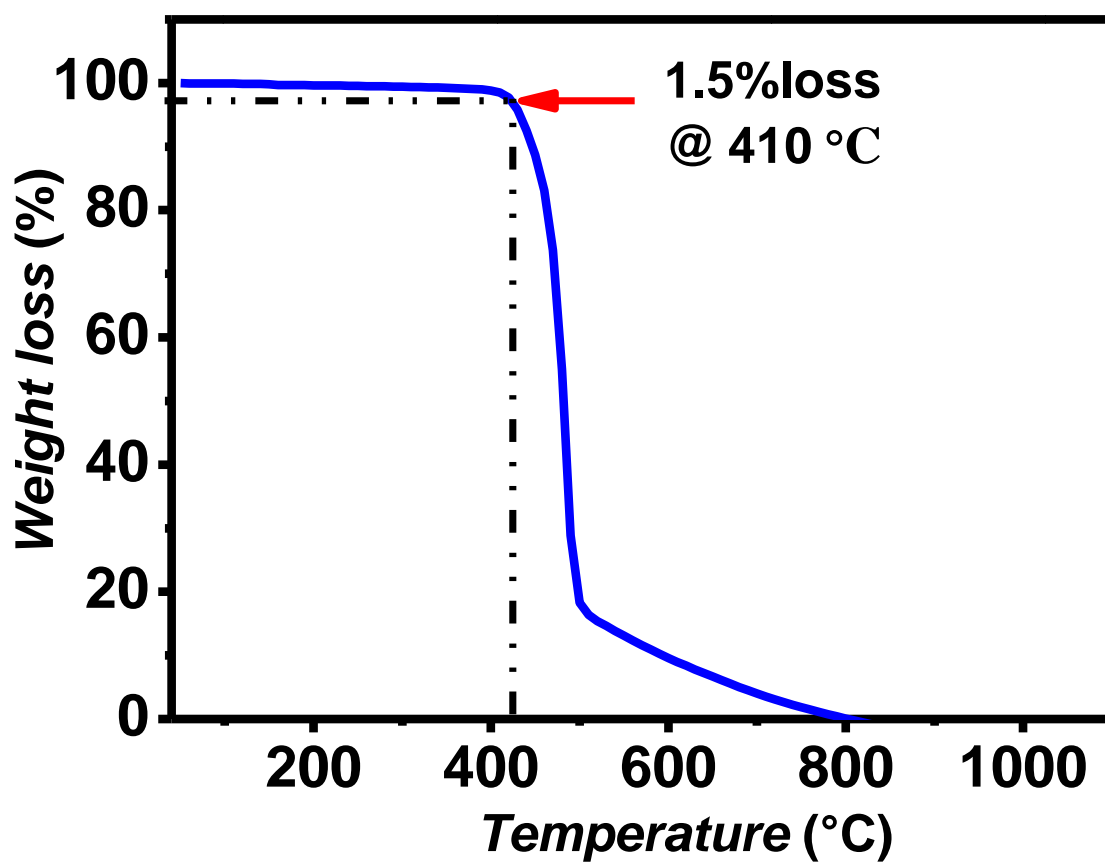


Fig. S2. TGA of the PVDF sample recorded from room temperature to 800 °C under inert atmosphere.

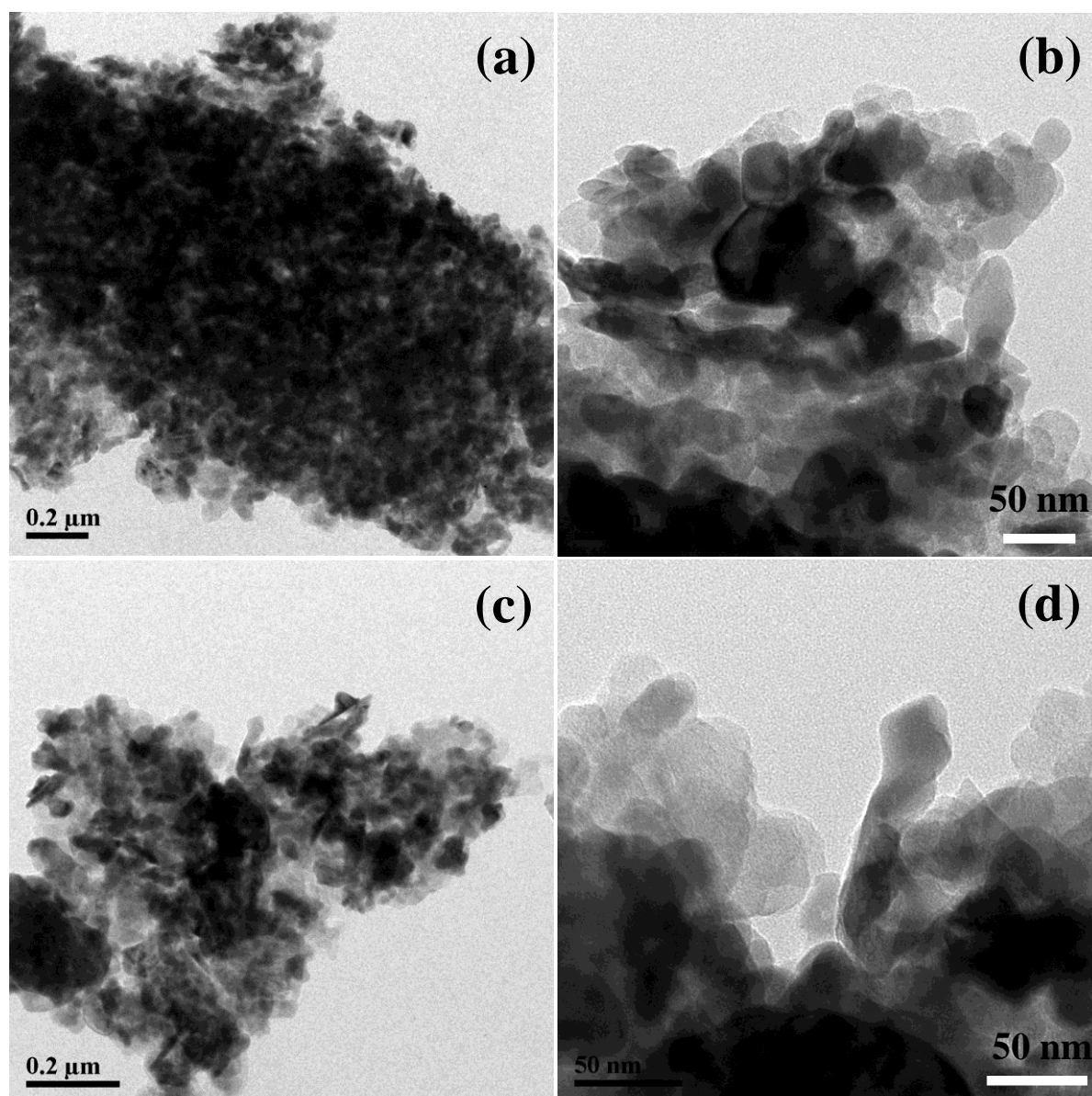


Fig. S3. (a) and (b) TEM images of the high temperature heated electrodes recorded at different magnifications. (c) and (d) TEM images of the conventionally dried electrodes at different magnifications.

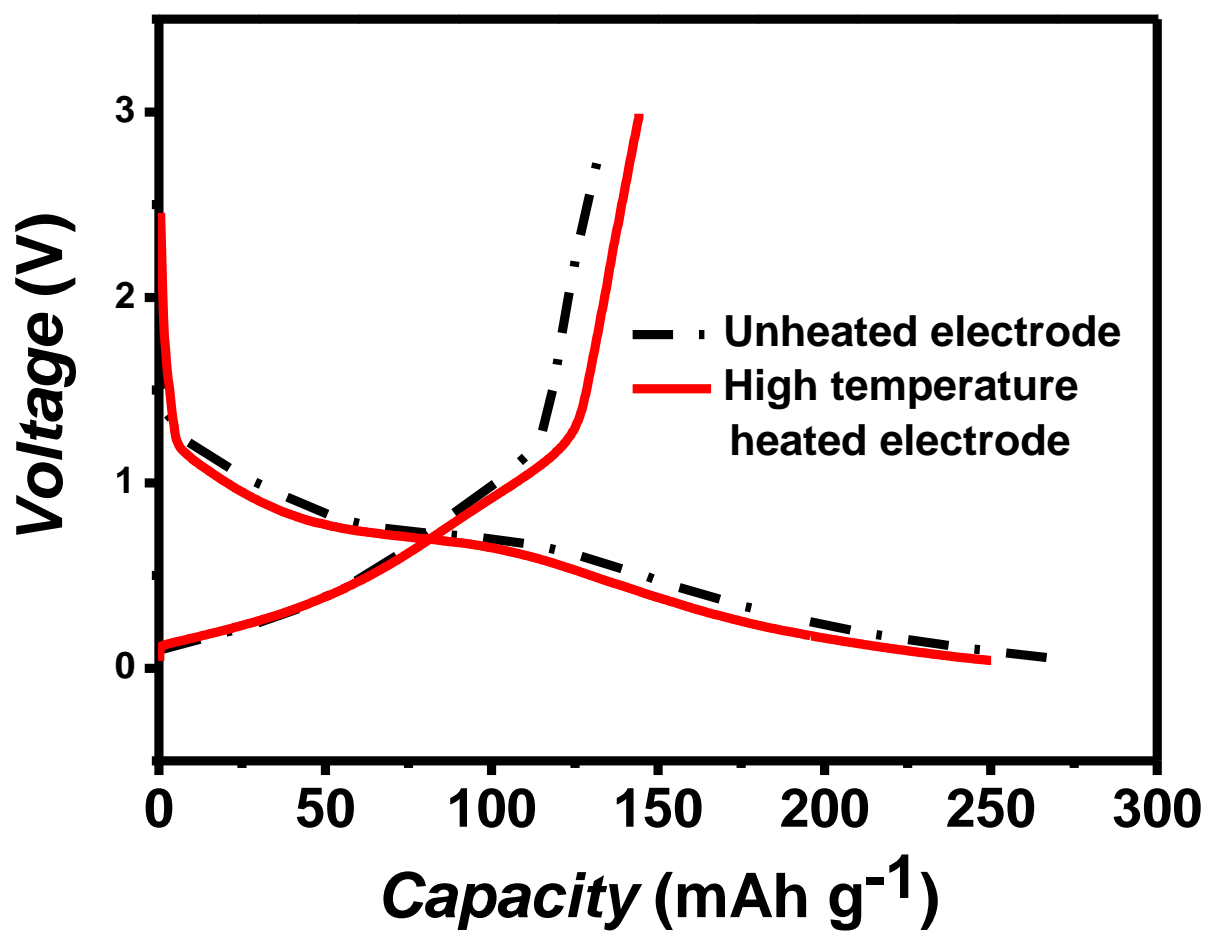


Fig. S4. Comparison of the first cycle reversibility of the unheated and high temperature heated composite electrodes. Note these electrodes contain carbon and PVDF in the weight ratio 90:10

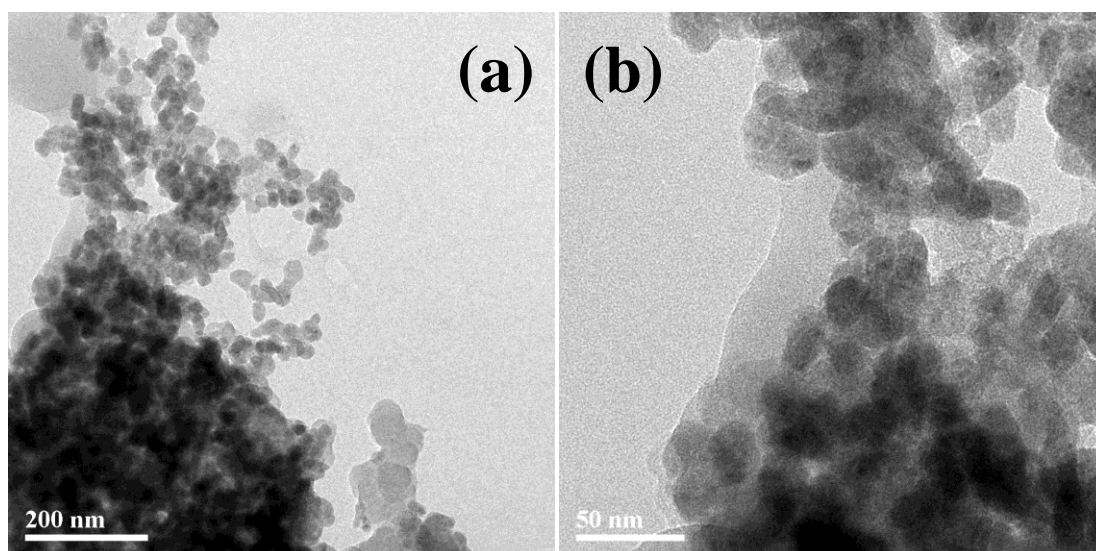


Fig. S5 (a) and (b) TEM images of the electrodes taken after the first cycle of conversion reaction showing grain size reduction.

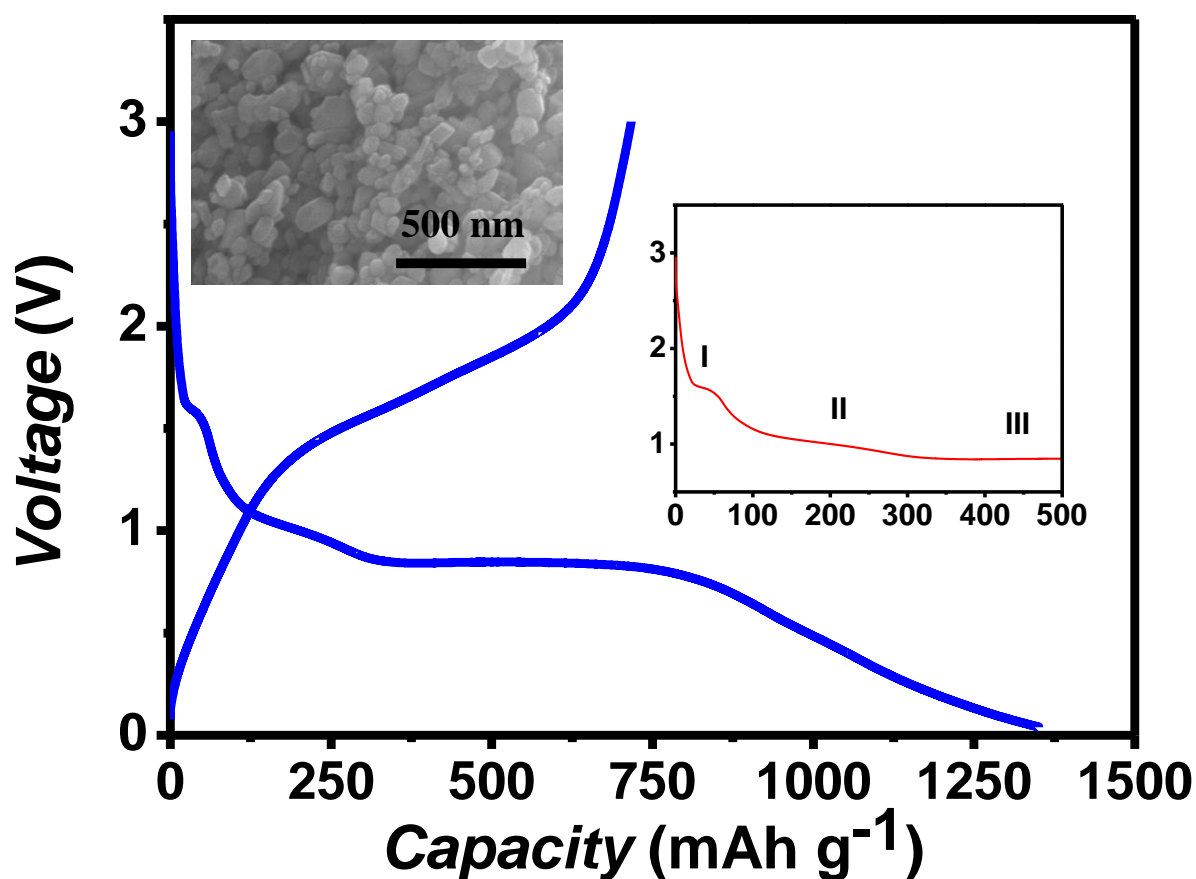


Fig. S6 First cycle voltage profile of commercial α -Fe₂O₃ sample. Inset of this figure shows the FESEM image of the commercial sample and the magnified view of the first discharge profile with three distinct plateaus. Plateaus I and II represent the lithium insertion in Fe₂O₃ while plateau III represents the conversion reaction.

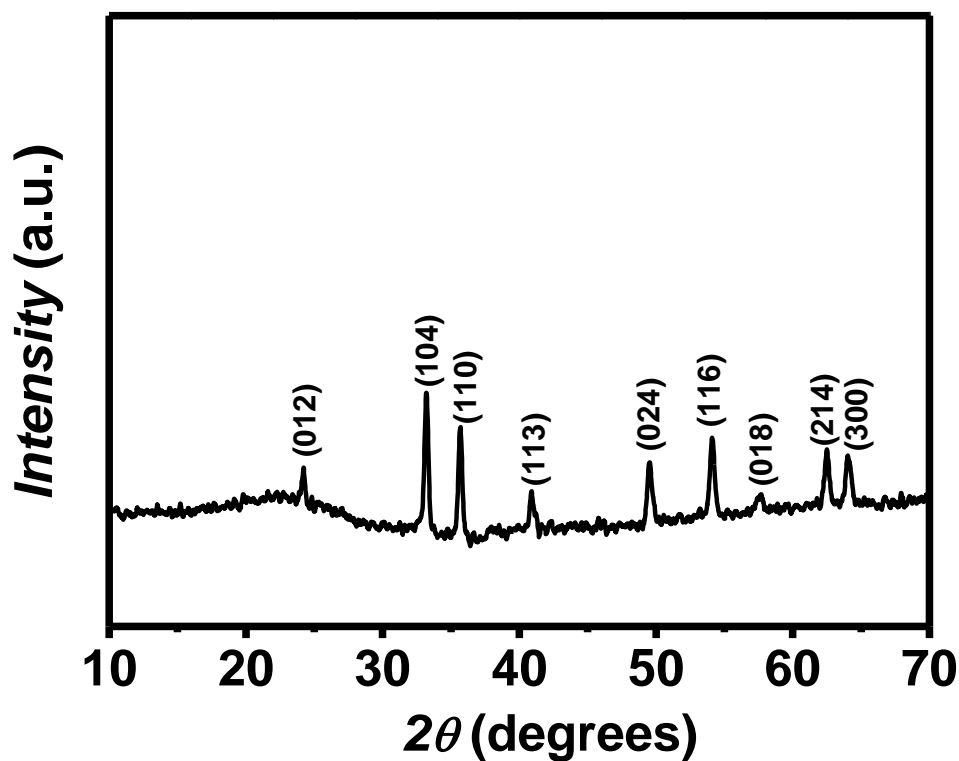


Fig. S7 XRD pattern of the commercial α - Fe_2O_3 sample.

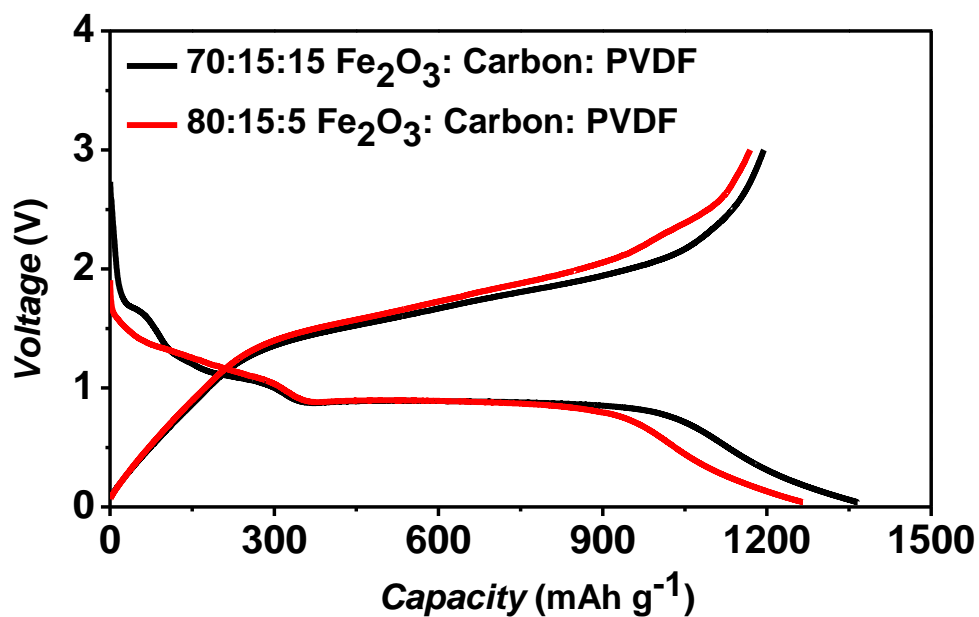


Fig. S8 First cycle galvanostatic voltage profile of the synthesized α - Fe_2O_3 with different active material, carbon and binder composition.

The first cycle coulombic efficiency of 70:15:15 and 80:15:5 compositions (active material: carbon: binder) were found to be 91% and 88% respectively.

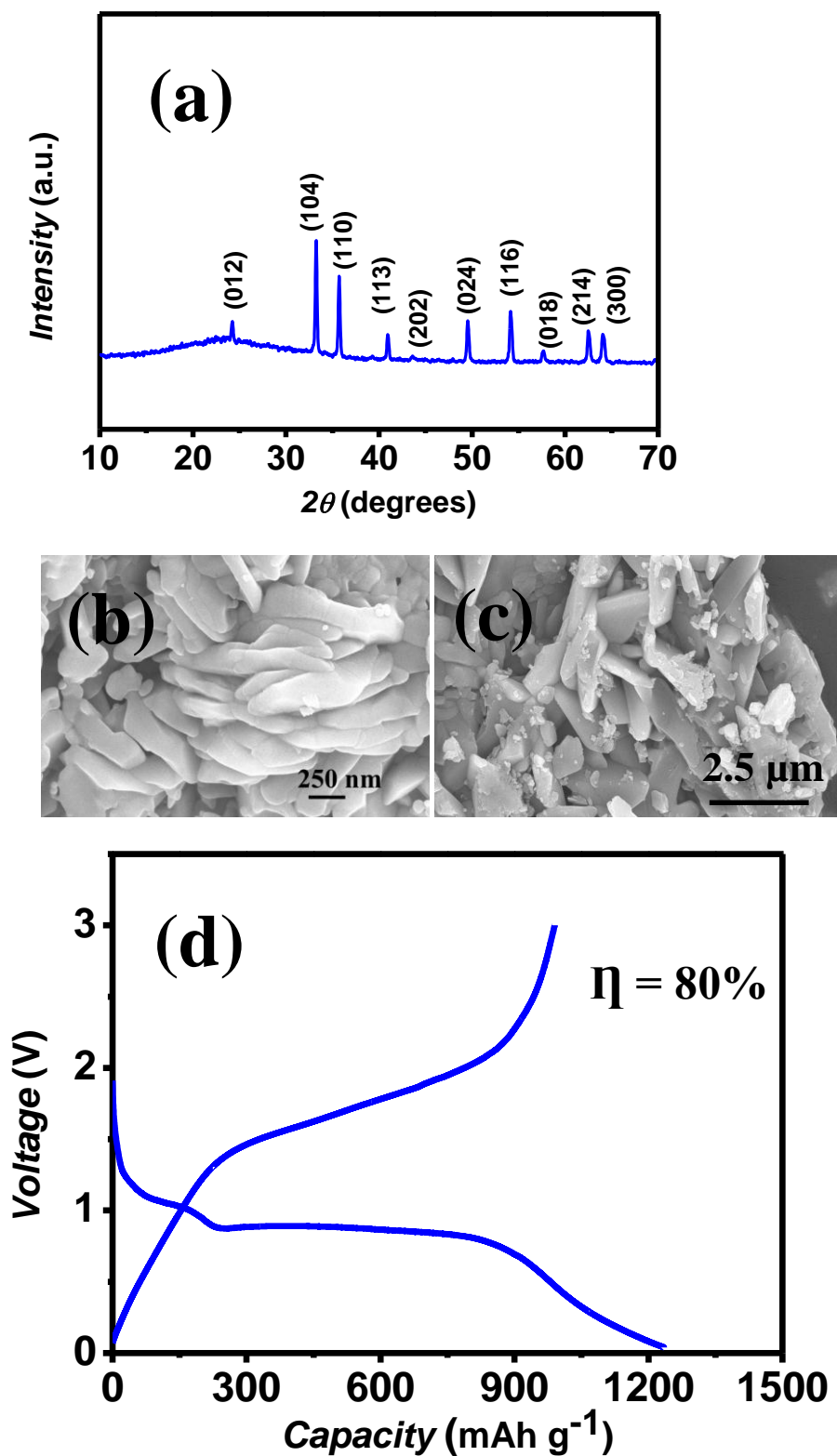


Fig. S9 (a) XRD pattern of α -Fe₂O₃-micron sample, (b) and (c) FESEM images, (d) First cycle voltage profile showing coulombic efficiency of 80%.

α -Fe₂O₃-micron was obtained by the soft template approach mentioned in the experimental section, except that the iron precursor was iron citrate.

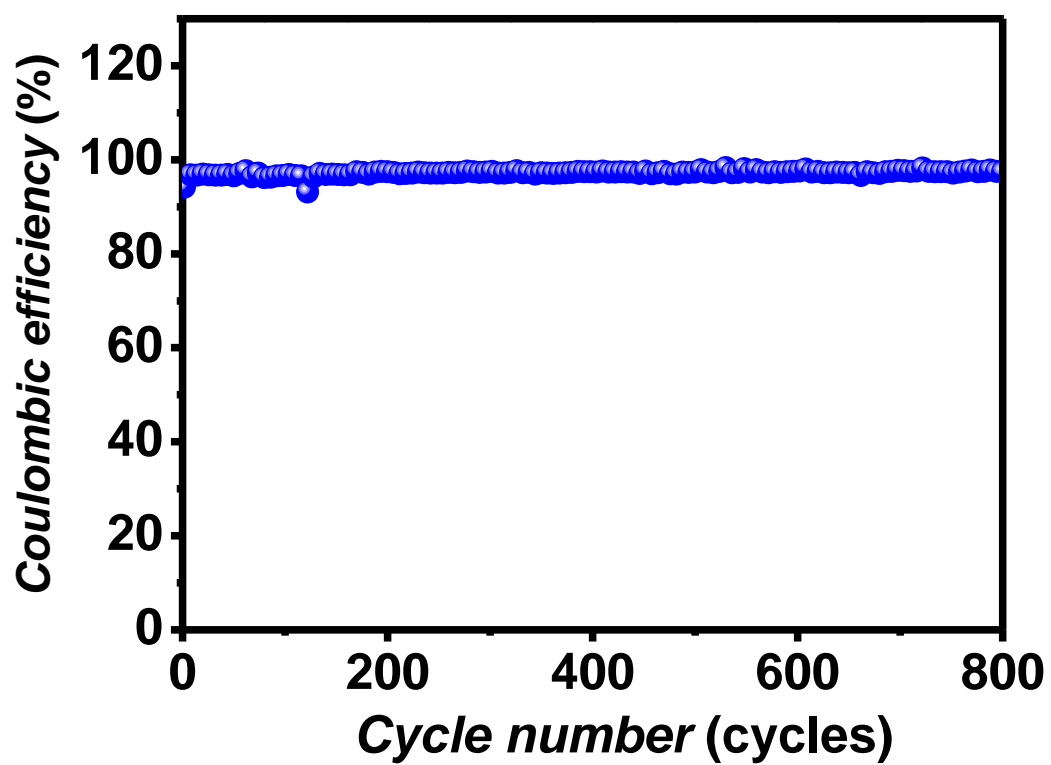


Fig. S10 Variation of coulombic efficiency as a function of cycle number during the long term cycling of α - Fe_2O_3

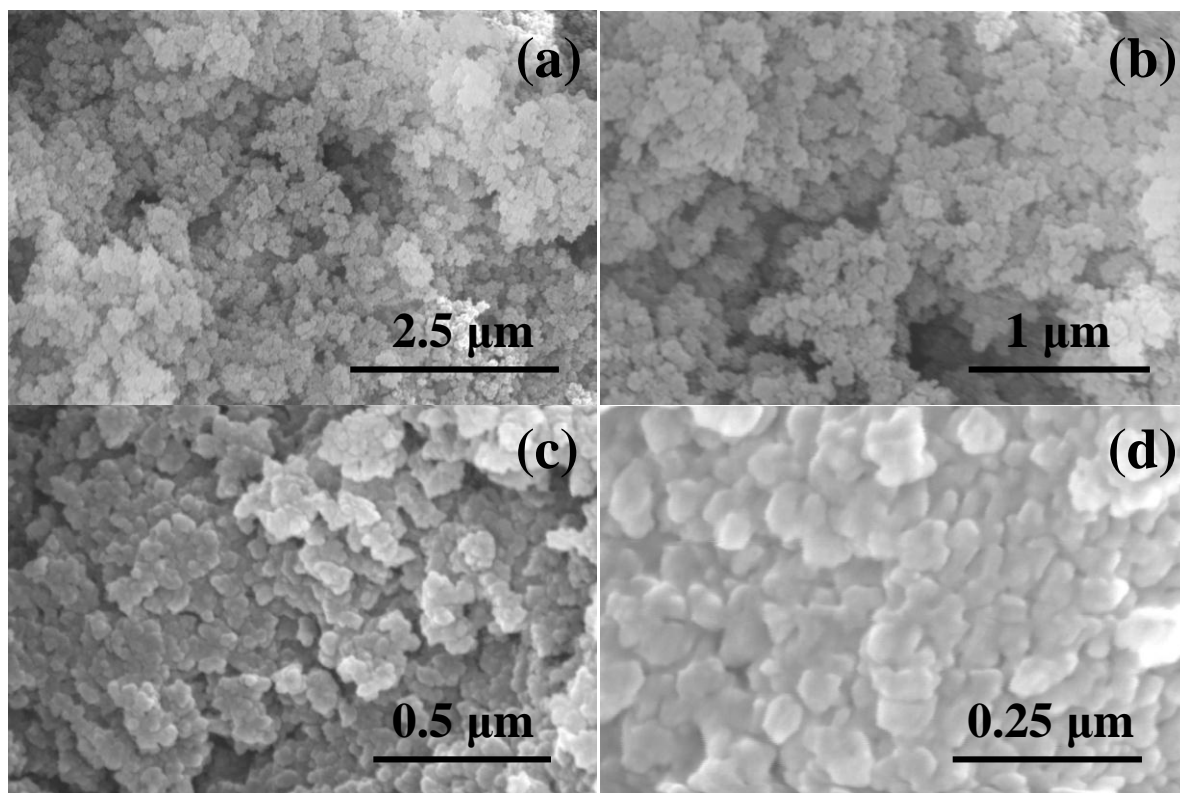


Fig. S11 (a)-(d) FESEM images recorded on the α - Fe_2O_3 electrodes after long term cycling. The images displayed here are recorded at different magnifications.

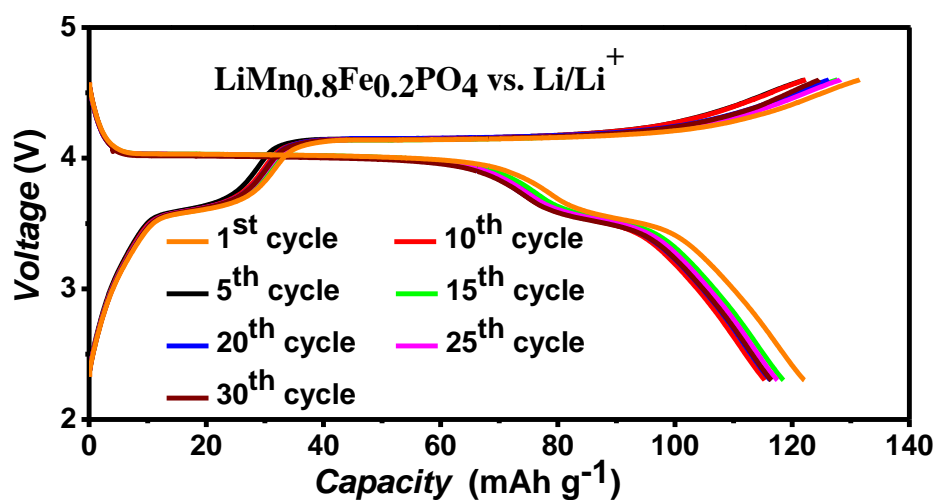


Fig. S12 Voltage profiles of LiMn_{0.8}Fe_{0.2}PO₄ vs. Li/Li⁺ in the voltage window 2.3-4.5 V at a current rate of 0.2C.

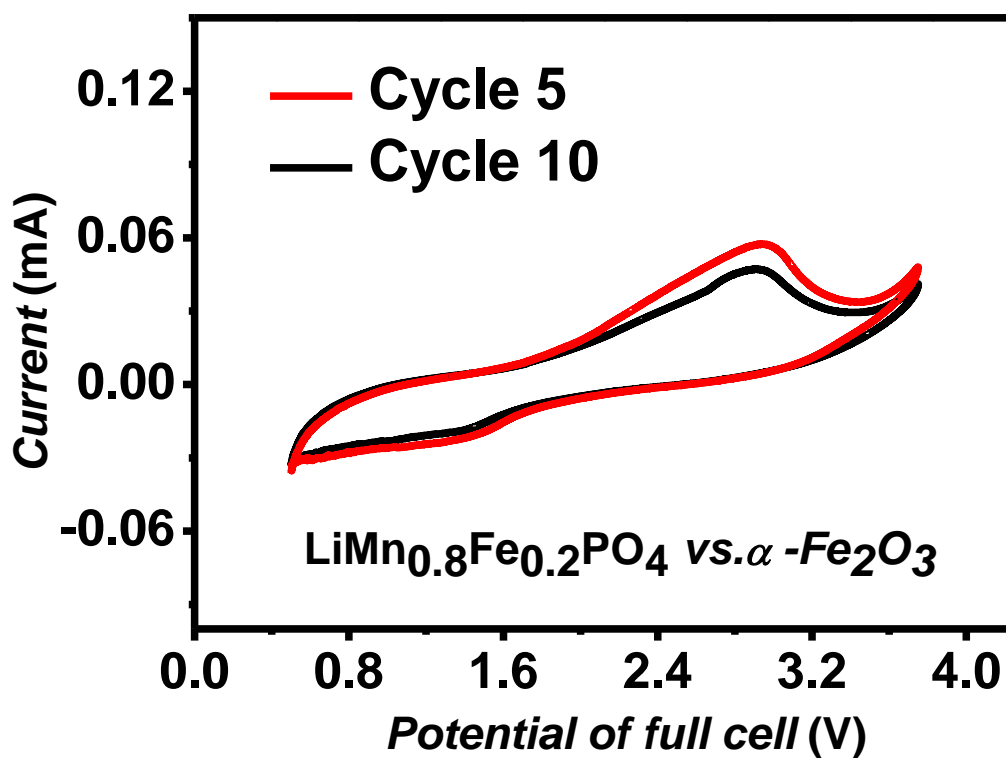


Fig. S13 Cyclic voltammogram of LiMn_{0.8}Fe_{0.2}PO₄ vs. Fe₂O₃ recorded in the voltage window 0.5-3.75 V at a scan rate of 0.2 mV s⁻¹.

Table S1. Assignment of the bands present in the FTIR spectrum

Sample	Fe-O (cm^{-1})	O-H stretching from surface hydroxyl groups (cm^{-1})	O-H bending from molecular water (cm^{-1})	C-H (cm^{-1})	C=O (cm^{-1})	PVDF (cm^{-1})
Fe ₂ O ₃ powder	451, 533	-	-	-	-	-
Electrode before heat treatment	451, 547	3300-3600	1638	2852, 2951	2340, 2362	840-1400
Electrode after heat treatment	449, 531	3317-3354	-	-	2341- 2361	840-1400

Table S2. Comparison of the coulombic efficiency obtained in this work with some literature reports

Sample/synthesis methodology	Current density [mA g ⁻¹]	Voltage window [V]	1 st discharge & charge capacities [mAh g ⁻¹]	1 st cycle coulombic efficiency [%]	Reference
Well-connected α -Fe ₂ O ₃ by soft template approach assisted with high temperature electrode heat treatment	100	0.04-3 V	1349/1221	90.5	This work
Commercial nano α -Fe ₂ O ₃	100	0.04-3 V	1340/716	53.4	Figure S6
Sub-micron sized Fe ₂ O ₃ cubes by hydrothermal synthesis	40	0.01-3 V	1089/900	82.65	1
α -Fe ₂ O ₃ Nano rods/ hydrothermal synthesis	201	0.005-3 V	1191/908	76.24	2
α -Fe ₂ O ₃ reduced graphene oxide	100	0.005-3 V	1693/1227	72.47	3
Porous α -Fe ₂ O ₃	100	0.01-3 V	1647/1163	70.6	4
Mesoporous α -Fe ₂ O ₃	200	0.005-3 V	1730/1200	69.36	5
Fe ₂ O ₃ nanosheets-G	0.2C	0.005-3.0 V	1416/1196	84.5	6

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