

## Supporting Information

### **Al-doped Fe<sub>2</sub>O<sub>3</sub> nanoparticles: advanced anode materials for high capacity lithium ion batteries**

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## Experimental Section

### 1. Materials

All reagents in this study were of analytical grade and were used without further purification and displayed in

Table S1.

Table S1. Chemicals, agents and materials used in the study.

<b>Chemicals, Agents and Materials</b>	<b>Type</b>	<b>Company</b>	<b>Characteristics</b>
<b>Fe(NO<sub>3</sub>)<sub>3</sub>•9H<sub>2</sub>O</b>	AR	SinoPharm	purity≥98.0%
<b>Al(NO<sub>3</sub>)<sub>3</sub>•9H<sub>2</sub>O</b>	AR	SinoPharm	purity≥99.0%
<b>AB</b>	Battery grade		/
<b>NMP</b>	AR	Kermel	purity≥99.0%
<b>PVDF</b>	Battery grade		/
<b>Electrolytes</b>	LBC-305-01	CAPCHEM	1 M LiPF <sub>6</sub> /EC:EMC:DMC (1:1:1) /1% VC
<b>Li plate</b>	15.6*0.45 mm	China Energy	15.6*0.45 mm
<b>Foam nickel</b>	Battery grade	Tianjin Aiweixin Chemical Technology	Thickness: 1.5 mm
<b>Cu foil</b>	200*0.015	GuangZhou JiaYuan	Total thickness: 15 μm; weight: 87 g m <sup>-2</sup>
<b>Glass microfiber filters</b>	GF/D 2.7 μm; 1823-090	Whatman	Diameter: 25 mm; Thickness: 675 μm; weight: 121 g m <sup>-2</sup>
<b>Cell components</b>	CR-2025	ShenZhen TianChenHe	/

## ***2. Synthesis of Al doped Fe<sub>2</sub>O<sub>3</sub>(Al-Fe<sub>2</sub>O<sub>3</sub>) and Fe<sub>2</sub>O<sub>3</sub> nanoparticles.***

The chemicals and reagents used in this paper are of analytical level (A.R.) and are used without further treatment. Dissolve 0.270 g of Fe(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O (1 mmol) and 0.029 g of Al(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O (0.1 mmol) in into 50 mL solvents of deionized water. The solution was stirred for 30 min and transferred into a 100 mL Teflon-lined stainless steel autoclave and kept at 140 °C for 25 h, and cooling at room temperature subsequently. The obtained precipitate was purified by dispersing in deionized (DI) water and ethanol respectively following centrifugal separation for three times. After dried at 90 °C about 24 hours, the reddish-brown precursor was calcined at 500 °C in air atmosphere for 7 hours, the muffle furnace was taken out until cooling to 100 °C or below, and then the Al-doped Fe<sub>2</sub>O<sub>3</sub> nanomaterial was obtained. Pure Fe<sub>2</sub>O<sub>3</sub> are also synthesized by the same route without Al(NO<sub>3</sub>)<sub>3</sub> adding as the original stocks.

The phase structure and ingredient of the obtained mesoporous composite were assessed by X-ray diffraction (XRD, Rigaku, D/max-A, Cu K<sub>α</sub>, λ = 1.5406 Å) and X-ray photoelectron spectra (XPS). The morphology was identified by scanning electron microscopy (SEM, JEM-6700F) and Transmission electron microscopy (TEM, JEM2100F). The element contents were further examined by energy-dispersive X-ray spectroscopy (EDS). In order to get more information of their specific surface area and mesoporous nature, Surface Area and Pore Size Analyzers (Tristar-II 3020) were utilized, which using high-quality surface area with gas adsorption technology and solid material porosity measurement.

## ***3. Electrochemical measurements***

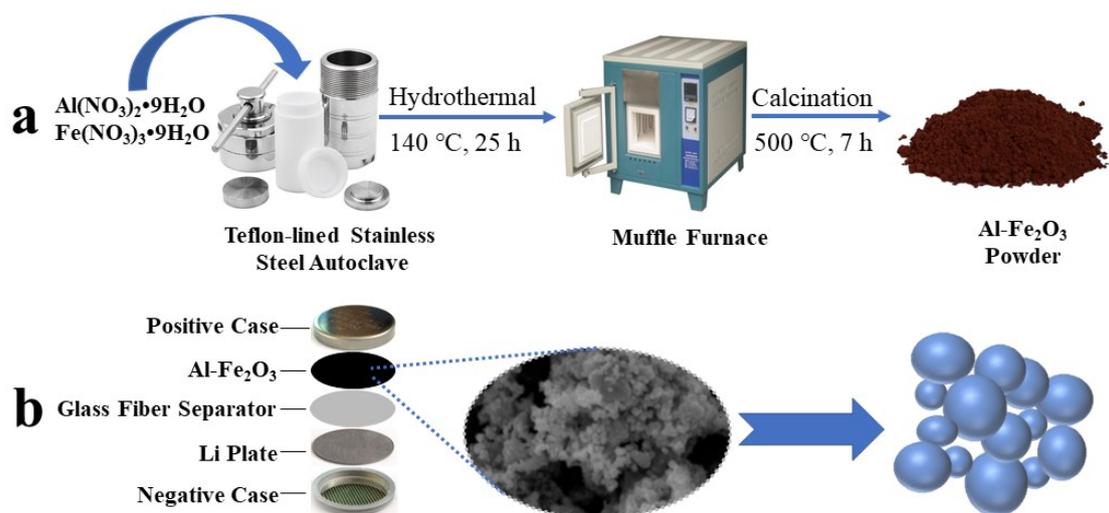
The as-prepared Al-Fe<sub>2</sub>O<sub>3</sub> nanoparticles were evaluated as an anode material for LIBs (Fig.S1b). The anode was prepared by mixing the active Al-Fe<sub>2</sub>O<sub>3</sub> particle, carbon black and polyvinyl fluoride (PVDF) in a mass ratio of 7:2:1, all of them were dissolved in N-methyl-2-pyrrolidone (NMP) solvent together to form homogeneous slurry.

The slurry was coated on the copper foil, and then the copper foil was placed in a vacuum drying oven at 110 °C

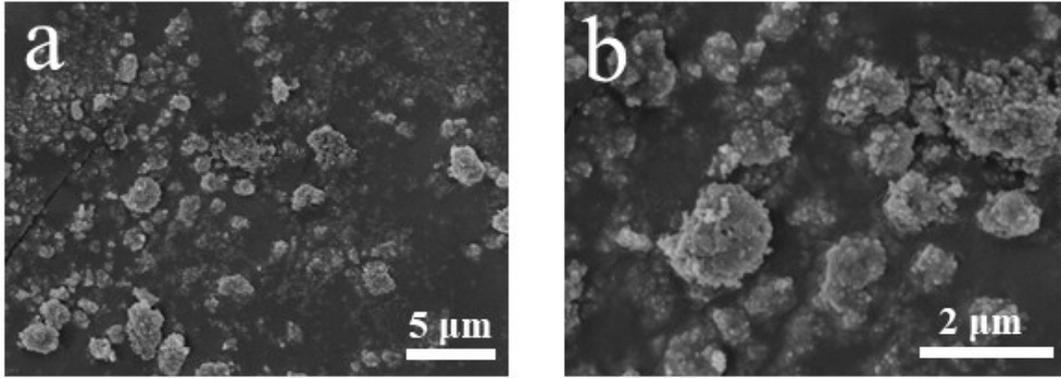
for 12 h. Cut them into disks with diameter of 12 mm with the active materials mass loading of about 1.0-1.2 mg

cm<sup>-2</sup>. The electrochemical measurements of the anode were carried out by CR2025-type coin cells, consisting of the Al-Fe<sub>2</sub>O<sub>3</sub> electrode, Cellgard 2400 micromesoporous polypropylene(separator), lithium metal (counter electrode) and 1 M LiPF<sub>6</sub> in a mixture of ethylene carbonate (EC) and diethyl carbonate (DEC) (1:1:1 in vol%) as the electrolyte. Galvanostatic charge-discharge (GCD) tests were performed in the voltage range of 0.01-3 V with a multichannel battery test system (LAND CT2001A) at room temperature. Electrochemical impedance spectra (EIS) measurements of the half-cell were carried out in a CHI660A electrochemical work station at the frequencies ranging from 10<sup>-2</sup> to 10<sup>4</sup> Hz combined with the cyclic voltammetry (CV) at a scan rate of 0.1-1.0 mV s<sup>-1</sup>.

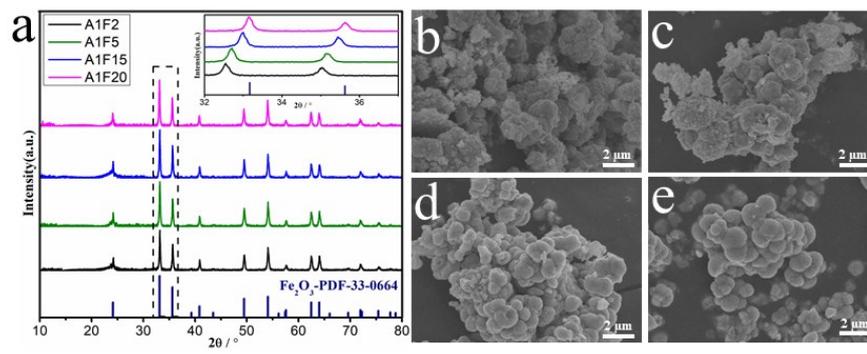
<sup>1</sup>. All currents and specific capacity presented in this work were calculated based on the total mass of the active particles.



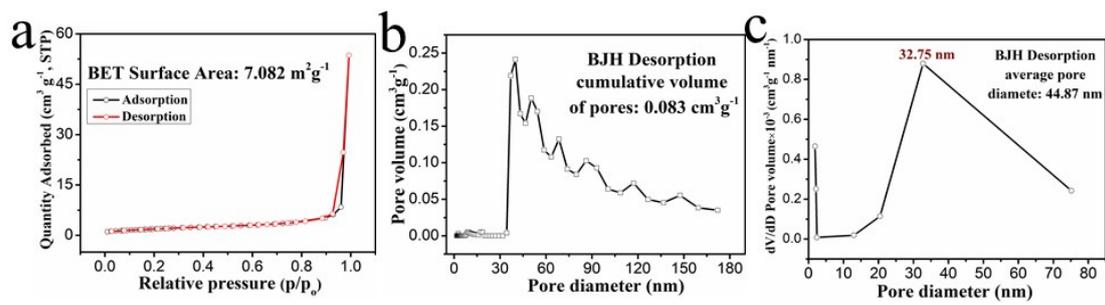
**Fig. S1.** (a) Schematic illustration of the synthesis procedure of  $\text{Al-Fe}_2\text{O}_3$ . (b) the composition of coin cell.



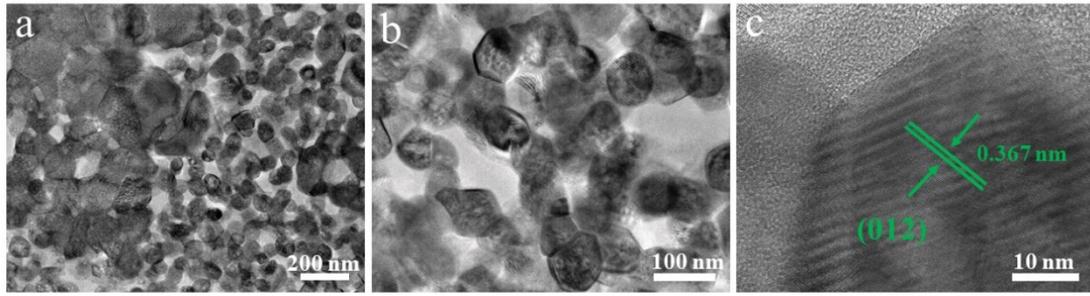
**Fig. S2.** The SEM images of pure Fe<sub>2</sub>O<sub>3</sub>.



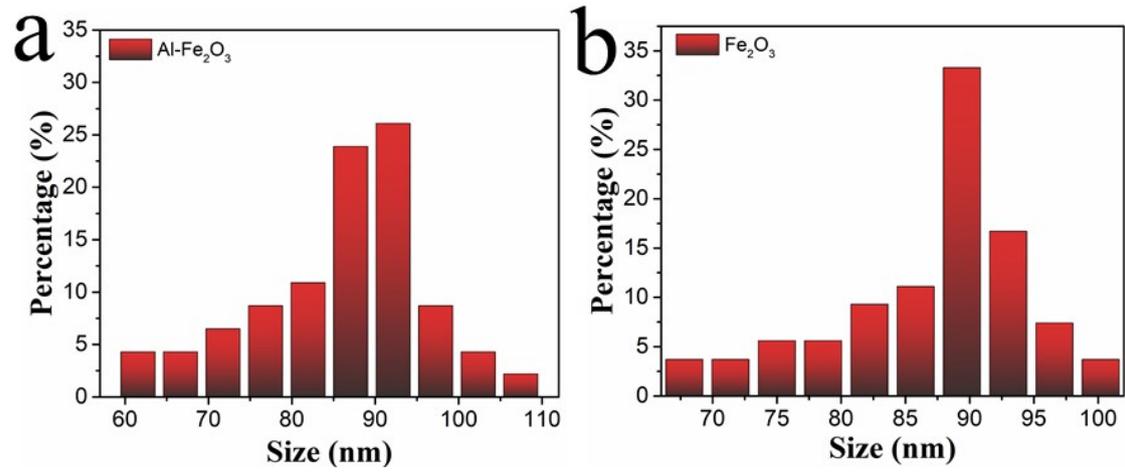
**Fig.3.** (a) XRD patterns of Al doped Fe<sub>2</sub>O<sub>3</sub> with various Al doping level and the corresponding SEM images (b-d).



**Fig. S4.** (a) The  $\text{N}_2$  sorption isotherms. (b) pore volumes. (c) pore size distributions of  $\text{Fe}_2\text{O}_3$ .



**Fig. S5.** The TEM images (a-b) and HRTEM (c) of  $\text{Fe}_2\text{O}_3$ .



**Fig. S6.** Al-Fe<sub>2</sub>O<sub>3</sub> particle size distribution (a) and (b) the particle size distribution of Fe<sub>2</sub>O<sub>3</sub>.

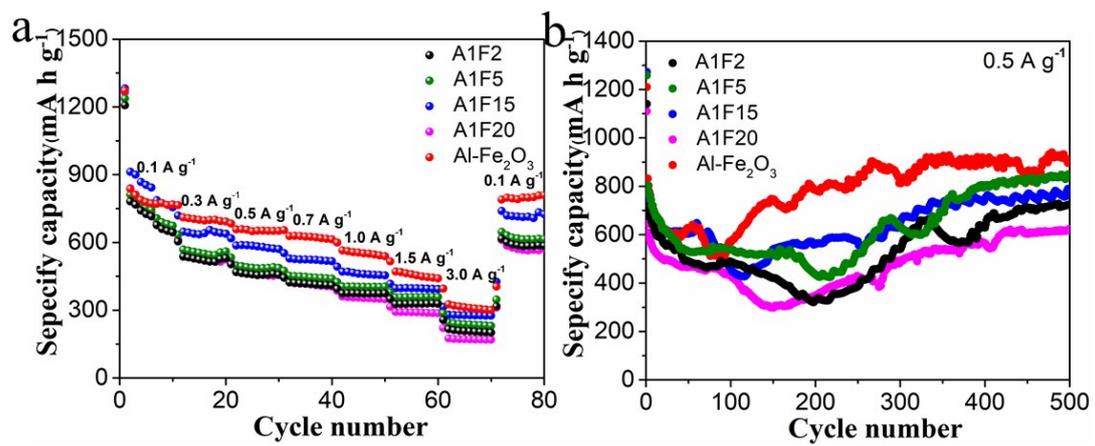
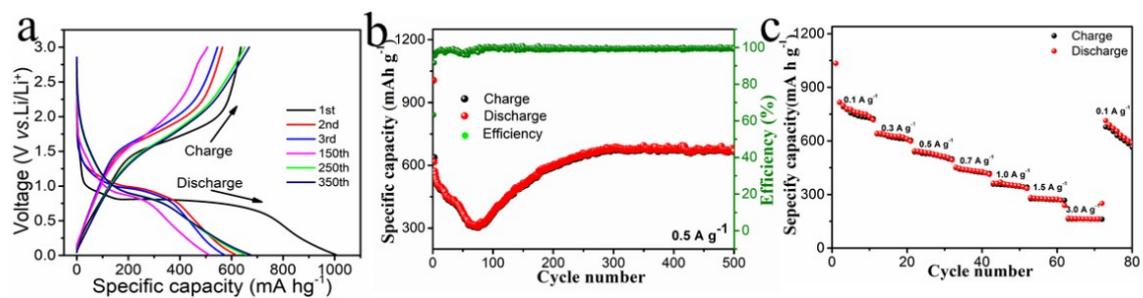
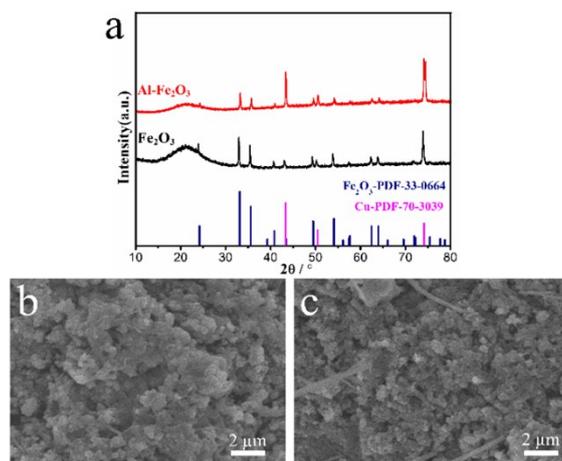


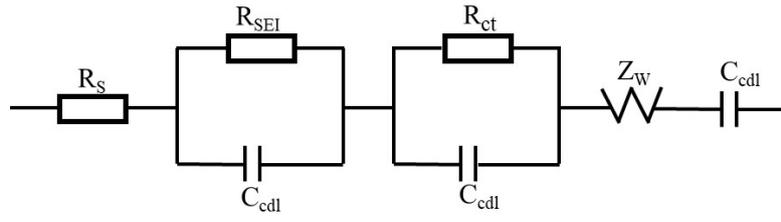
Fig. S7. (a) rate performance and (b) cycling behaviors of Al doped Fe<sub>2</sub>O<sub>3</sub>.



**Fig. S8.** Electrochemical performances of pure Fe<sub>2</sub>O<sub>3</sub> electrode (a) GCD curves at a current density of 0.5 A g<sup>-1</sup>. (b) Cycling behaviours at 0.5 A g<sup>-1</sup>. (c) The rate performance of pure Fe<sub>2</sub>O<sub>3</sub> electrode from current density of 0.1 to 3 A g<sup>-1</sup>.



**Fig. S9.** (a) XRD patterns and SEM images of (b)  $\text{Al-Fe}_2\text{O}_3$  and (c)  $\text{Fe}_2\text{O}_3$  after cycling.



**Fig. S10.** The equivalent circuit model.

**Table S2.** A comparison for the performance of Al-Fe<sub>2</sub>O<sub>3</sub> in the study with some reported materials.

Materials	Specific capacitance /mAh g <sup>-1</sup>	Rate capability /mAh g <sup>-1</sup>	Cycling behavior	Refs.
α-Fe <sub>2</sub> O <sub>3</sub>	800/0.1 A g <sup>-1</sup>	350/3.0 A g <sup>-1</sup>	459/mAh g <sup>-1</sup> after 500 cycles at 0.5 A g <sup>-1</sup>	1
α-Fe <sub>2</sub> O <sub>3</sub>	567/0.05 C	52/4 C	601/mAh g <sup>-1</sup> after 300 cycles at 0.1 C	2
α-Fe <sub>2</sub> O <sub>3</sub>	895/0.1 A g <sup>-1</sup>	285/3.0 A g <sup>-1</sup>	880/mAh g <sup>-1</sup> after 800 cycles at 1.0 A g <sup>-1</sup>	3
Fe <sub>2</sub> O <sub>3</sub>	/	/	705/mAh•g <sup>-1</sup> after 430 cycles at 0.1 A g <sup>-1</sup>	4
Ni and Co doped Fe <sub>2</sub> O <sub>3</sub>	819/0.1 A g <sup>-1</sup>	61.6/3.0 A g <sup>-1</sup>	415.7/mAh g <sup>-1</sup> after 200 cycles at 0.2 A g <sup>-1</sup>	5
α-Fe <sub>2</sub> O <sub>3</sub> /Spherical graphite	519/0.1 A g <sup>-1</sup>	202/5.0 A g <sup>-1</sup>	540/mAh g <sup>-1</sup> after 200 cycles at 0.5 A g <sup>-1</sup>	6
SiO <sub>2</sub> @Fe <sub>2</sub> O <sub>3</sub>	437/0.06 C	310/1 C	770/mAh g <sup>-1</sup> after 550 cycles at 0.1 C	7
Ag-Fe <sub>2</sub> O <sub>3</sub>	938/0.1 A g <sup>-1</sup>	650/5.0 A g <sup>-1</sup>	678/mAh g <sup>-1</sup> after 250 cycles at 1.0 A g <sup>-1</sup>	8
Titanium-doped Fe <sub>2</sub> O <sub>3</sub>	447/0.1 A g <sup>-1</sup>	175/1.0 A g <sup>-1</sup>	454/mAh g <sup>-1</sup> after 500 cycles at 0.1 A g <sup>-1</sup>	9
<b>Al-Fe<sub>2</sub>O<sub>3</sub></b>	<b>833/0.1 A g<sup>-1</sup></b>	<b>320/3 A g<sup>-1</sup></b>	<b>902 mAh g<sup>-1</sup> after 500 cycles at 0.5 A g<sup>-1</sup></b> <b>777 mAh g<sup>-1</sup> after 500 cycles at 1.0 A g<sup>-1</sup></b>	<b>This work</b>

## References

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**Table S3.** EIS parameters of Al-Fe<sub>2</sub>O<sub>3</sub> before (a) and after (b) cycling.

	Before CT	After CT	
Model	$R_s(CR_{SEI})(CR_{ct})WC$		
	$R_s$	4.831	5.079
	$C_{dl,1}$	$4.918 \times 10^{-6}$	$3.193 \times 10^{-6}$
	$R_{SEI}$	33.19	15.02
	$C_{dl,2}$	$1.938 \times 10^{-6}$	$1.17 \times 10^{-5}$
EIS parameters	$R_{ct}$	14.49	44.83
	$W$	$6.655 \times 10^{-3}$	$5.783 \times 10^{-3}$
	$C_{int}$	$1.509 \times 10^{-3}$	$2.276 \times 10^{-3}$
	$\chi^2$	$3.357 \times 10^{-3}$	$3.276 \times 10^{-3}$