

Supporting information

One-step synthesis of MOF-derived Ga/Ga₂O₃@C dodecahedron as a anode for high-performance lithium-ion batteries

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Experimental

1 Preparation of Ga-MOF (MIL-96)

Ga-MOF (MIL-96) was prepared by a facile synthesis route with a little modification. 0.222g Ga(NO₃)₃ • xH₂O and 0.112g 1,3,5-benzenetricarboxylic acid (BTC) were added in 5 mL of deionized water and seal in a 25 mL Teflon-lined autoclave at 200 °C for 5h. After the hydrothermal treatment, the pale yellow powder was collected by centrifugation and washed with deionized water and ethanol for several times. It was dried at 60 °C for 24 h under vacuum to obtain the final product.

2 Preparation of Ga/Ga₂O₃@C and Ga@C

The Ga-MOF powder was firstly placed in a tube furnace and passed a mixed gas of Hydrogen and Argon (R_{H₂}:R_{Ar} = 1:9) for 1h at room temperature. And then, program temperature to 400 °C for 3h with a heating rate of 2 °C min⁻¹. Finally, the product was collected. (This process was completed in a fume hood)

The Ga@C was prepared by the same method as the Ga/Ga₂O₃@C products. The only difference was that the temperature was maintained in 600 °C for 3h.

3 Preparation of Ga₂O₃@C

The Ga₂O₃@C was prepared by the same method as the Ga/Ga₂O₃@C products. The only difference was that Ga-MOF powder was processed under Argon (Ar) atmosphere.

4 Characterization and electrochemical testing

The composition of all products was investigated by X-ray diffraction (XRD, Bruker D₂ Phaser X-Ray Diffractometer, Cu K α radiation). Hydrogen temperature programmed reduction (H₂-TPR) was performed on a Micromeritics Autochem II 2920 to calculate the H₂ consumption from 50 to 600 °C in 10% H₂/Ar (30 mL min⁻¹) with a ramp rate of 10 °C min⁻¹. The micromorphologies and nanostructures of composites were further investigated using a Hitachi S4800 scanning electron microscopy (SEM) and a Hitachi H-800 transmission electron microscopy (TEM). Elemental mapping was carried out by the X-ray spectroscopy on the Hitachi H-800. The N₂ adsorption-desorption isotherms were performed by liquid N₂ by Micromeritics ASAP 2460 analyzer with a degassing temperature of 473 K. The specific surface area and porosity analysis were used the Brunauer-Emmett-Teller (BET) equation and the Barrett-Joyner-Halenda (BJH) model, respectively. The samples were also examined by X-ray photoelectron spectroscopy (XPS, Thermo ESCALAB 250XI equipped with an Al K α X-ray source).

To prepare the electrode, active materials, conductive materials (acetylene black) and binders (polyvinylidene difluoride, PVDF) at a weight percent ratio of 7:2:1 were mixed and then pasted onto a Cu foil (1.1 cm²), the loading amount of the anode was kept at 1.15 mg. Lithium foil was used as the counter electrode. The electrolyte was 1

M LiPF₆ dissolved in dimethyl carbonate (DMC) and ethylene carbonate (EC). (1:1, v/v).

Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) curves were tested by CHI660D electrochemical workstation at room temperature. The charge/discharge measurements were carried out on NEWARE CT-3008 instrument and the voltage range was 0.01-3.0 V for lithium ion battery.

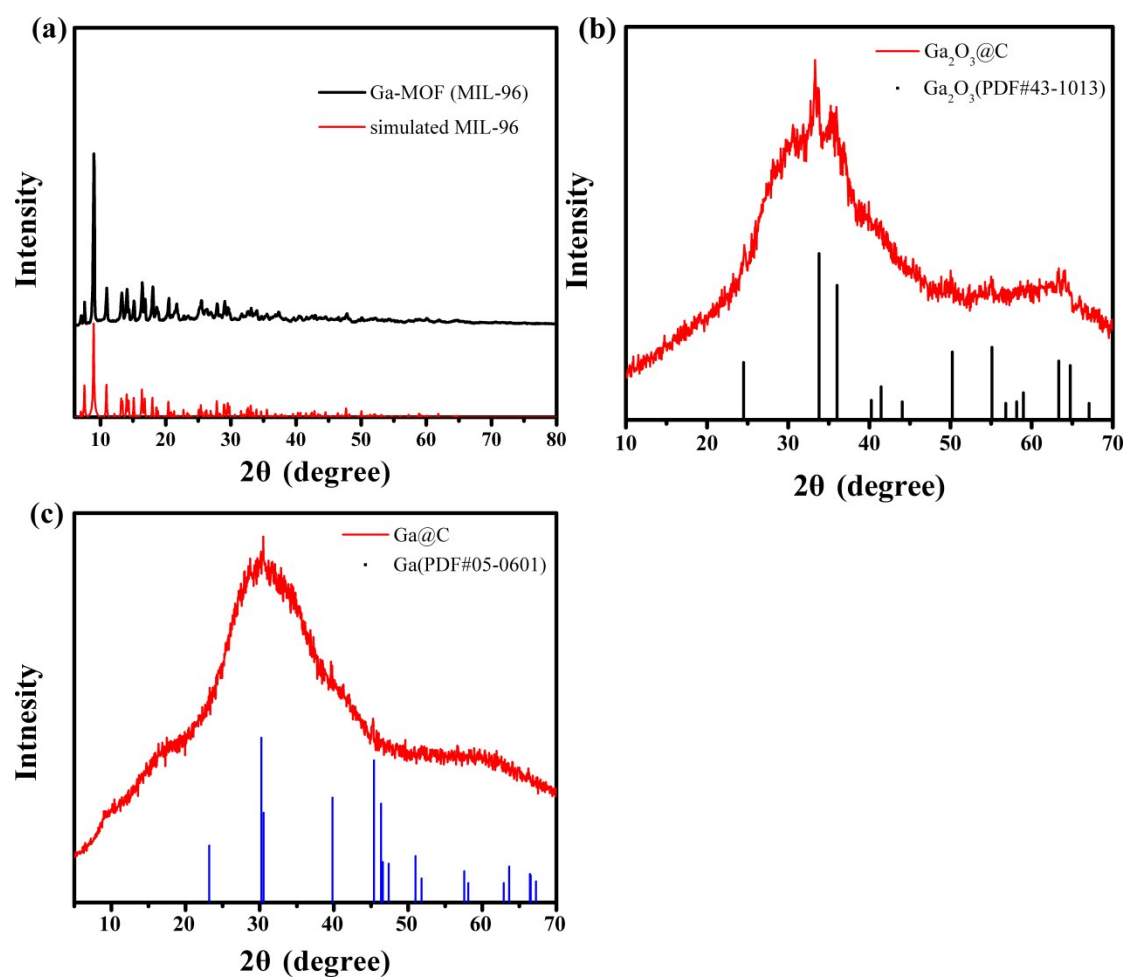


Fig.S1 XRD patterns of Ga-MOF (a), Ga₂O₃@C composite(b) and Ga@C composite(c).

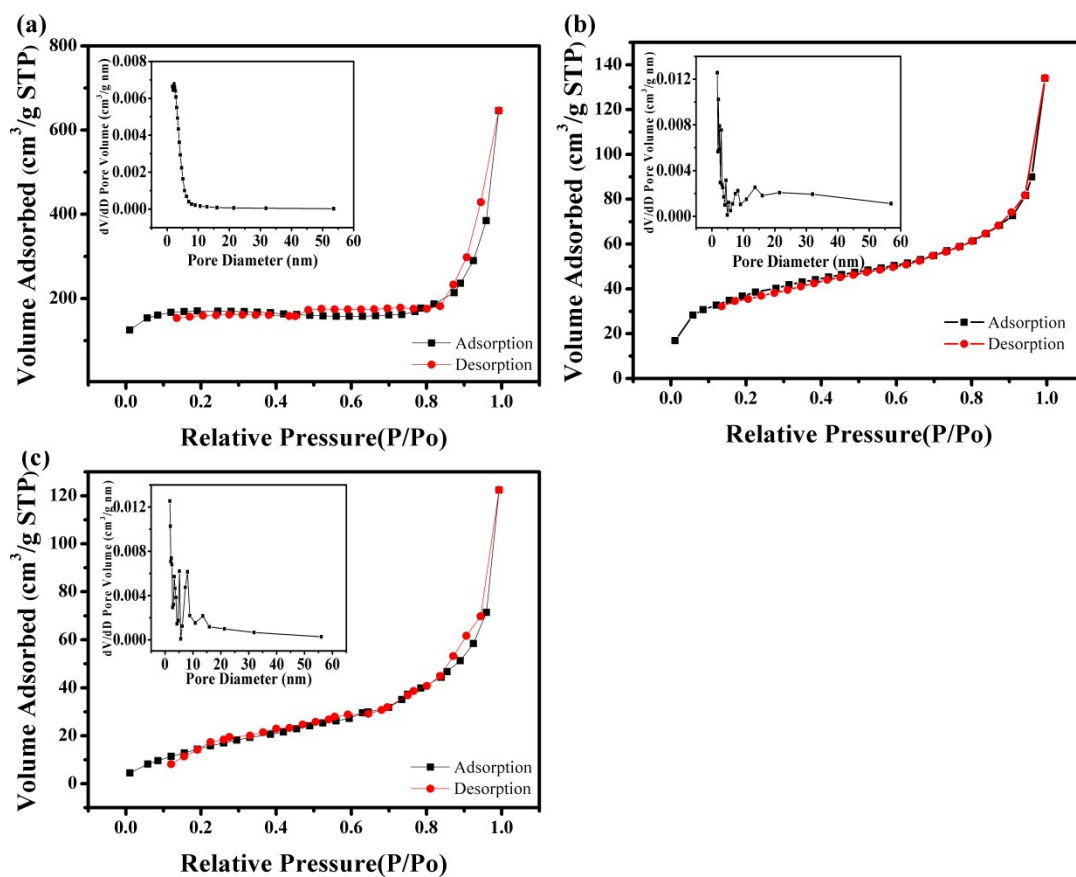


Fig.S2 N_2 adsorption-desorption isotherms and pore size distributions of Ga-MOF (a), Ga/Ga₂O₃@C (b), and Ga₂O₃@C (c) materials

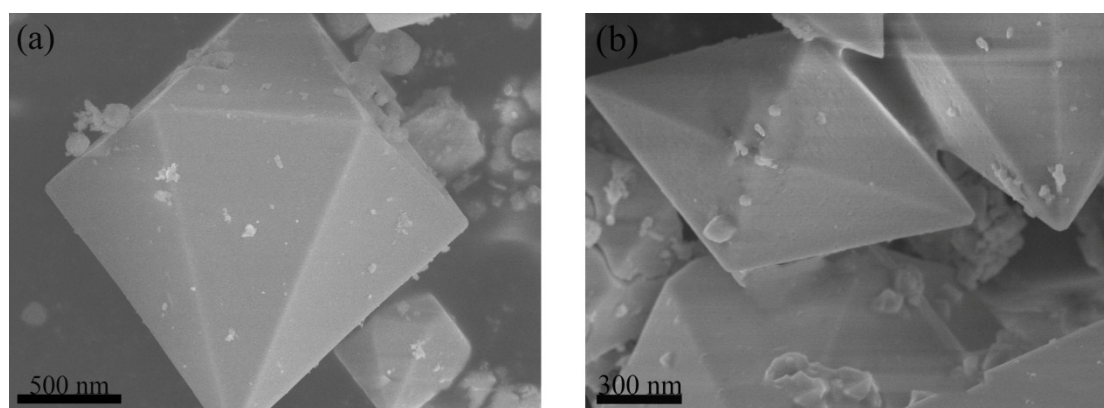


Fig.S3 SEM images of Ga-MOF (MIL-96)(a), and Ga₂O₃@C(b).

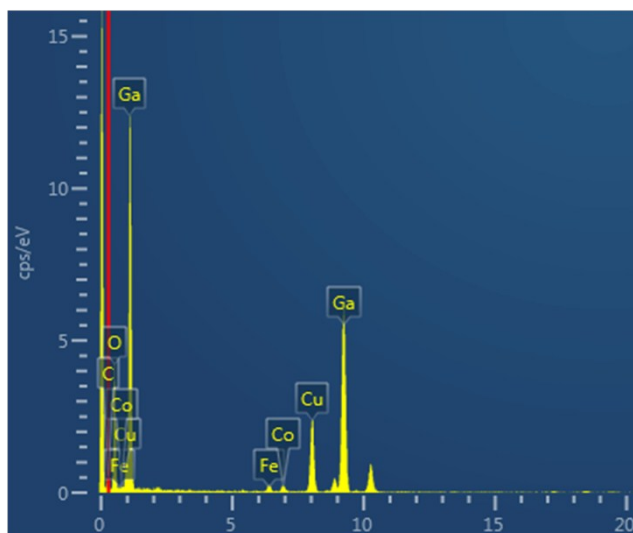


Fig.S4 EDX image of Ga/Ga₂O₃@C composite.

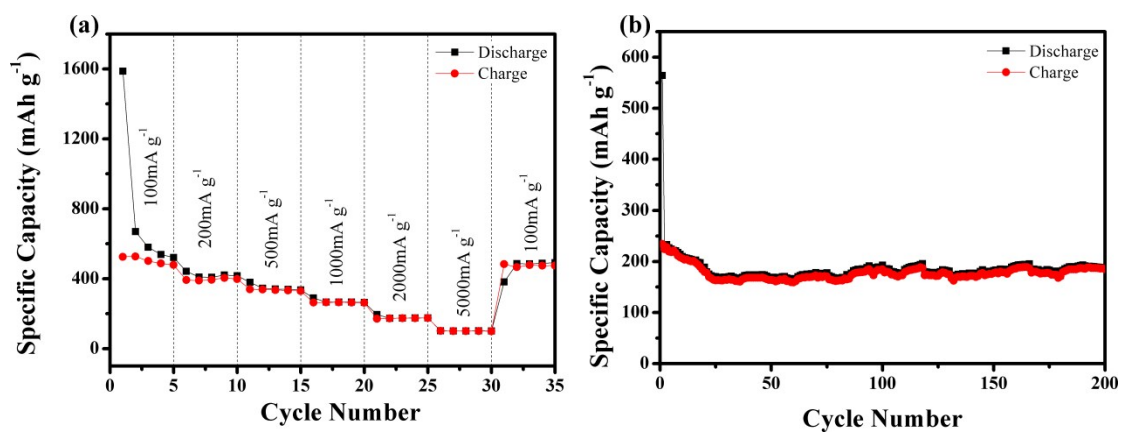


Fig.S5 (a) Rate performance tests of Ga@C electrode, (b) Cycling tests of the Ga@C electrode at a current density of 1000mA g⁻¹ for 200 cycles.

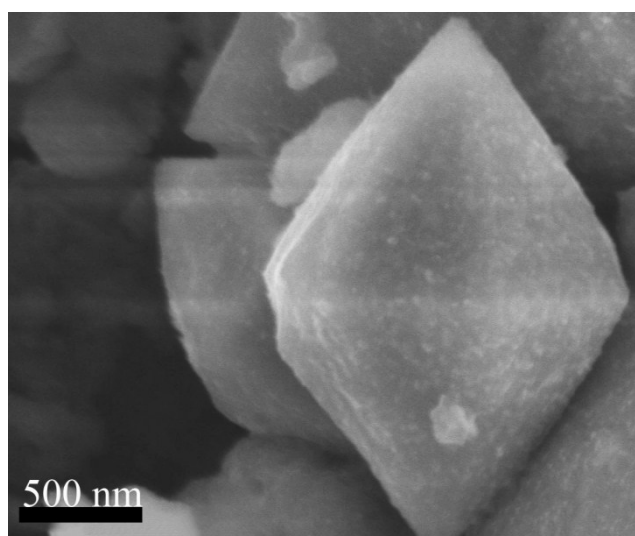


Fig.S6 SEM image of the Ga/Ga₂O₃@C composite after 150 cycles.

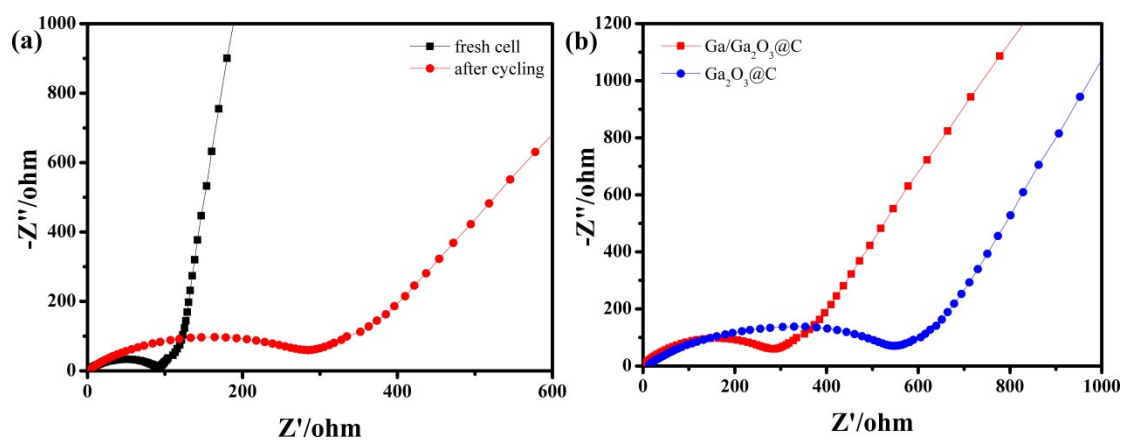


Fig.S7 (a) Electrochemical impedance spectra of the Ga/Ga₂O₃@C electrode before and after cycling. (b) Electrochemical impedance spectra of the Ga/Ga₂O₃@C and Ga₂O₃@C electrodes after cycling.

TableS1

The N₂ adsorption–desorption test results of Ga-MOF, Ga/Ga₂O₃@C, and Ga₂O₃@C materials

sample	Specific surface area (m ² g ⁻¹)	Pore size (nm)
Ga-MOF	522	3.1
Ga/Ga ₂ O ₃ @C	93	7.2
Ga ₂ O ₃ @C	64	11.2

Table S2

A comparison of the electrochemical performance of our sample with reported Ga-based samples.

Materials	Current density mA g ⁻¹	Cycle number	Specific capacity mAh g ⁻¹	References
Ga-C	100	20	300	1
Ga ₂ O ₃ /rGO	50	40	770	2
carbon-coated Ga ₂ O ₃	500	200	721	3
Ga ₂ O ₃ nanorods	400	150	200	4
Ga ₂ O ₃ @carbon@ graphene	100	50	458	5
Ga/Ga ₂ O ₃ @C	100	150	987	This work
	1000	200	542	

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