

Supplementary Information

Porous CaFe_2O_4 as a promising lithium ion battery anode: a trade-off between high capacity and long-term stability

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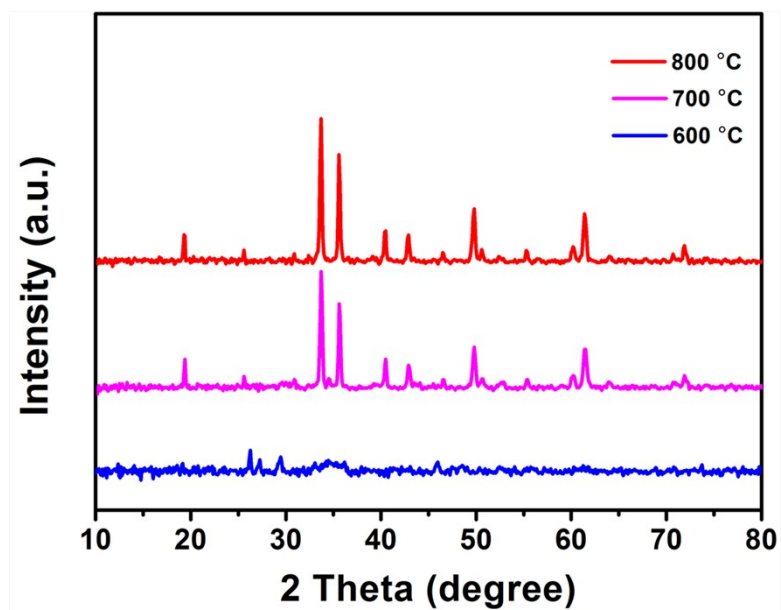


Fig. S1 XRD patterns of the CaFe_2O_4 calcined at different temperatures for 5 h in air.

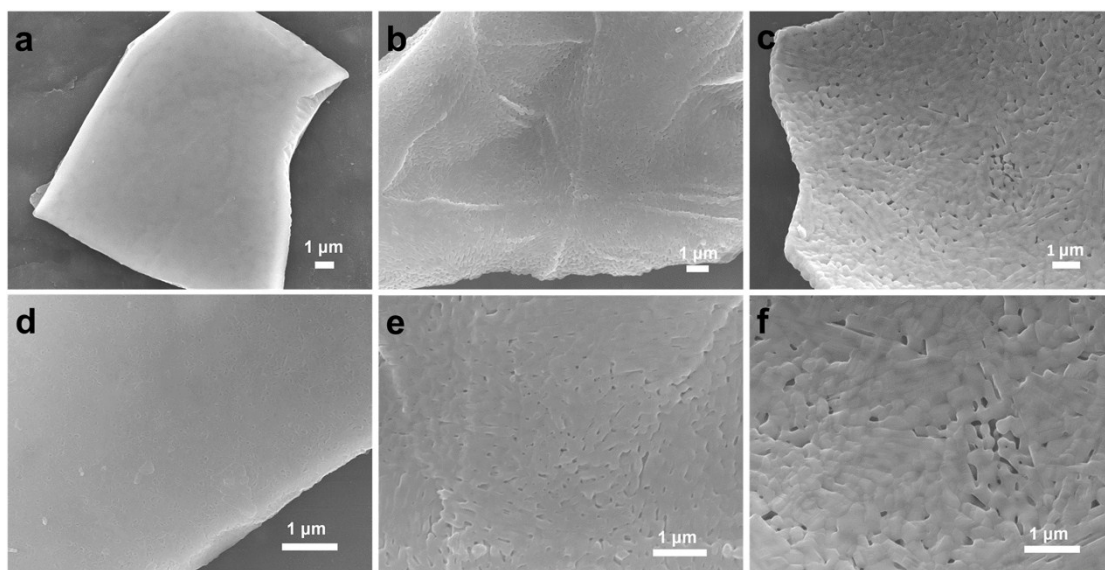


Fig. S2 SEM images of the CaFe_2O_4 calcined at 600 °C (a, d), 700 °C (b, e), 800 °C (c, f) for 5 h in air.

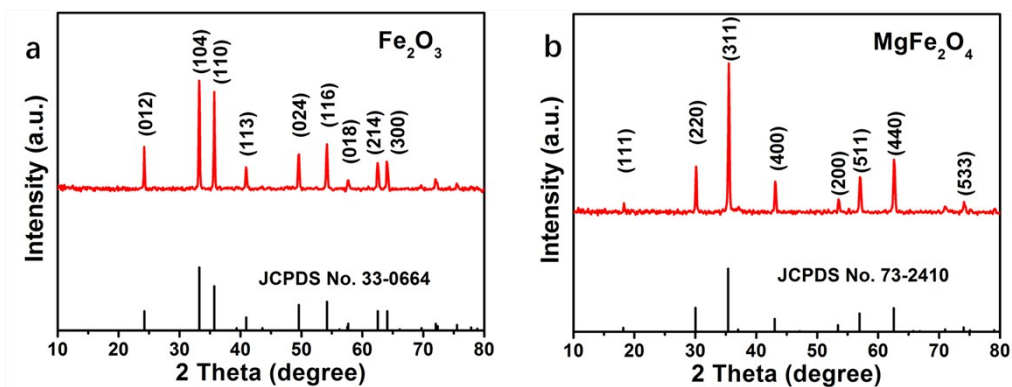


Fig. S3 XRD patterns of the Fe_2O_3 (a) and MgFe_2O_4 (b) calcined at $800\text{ }^\circ\text{C}$ for 5 h in air.

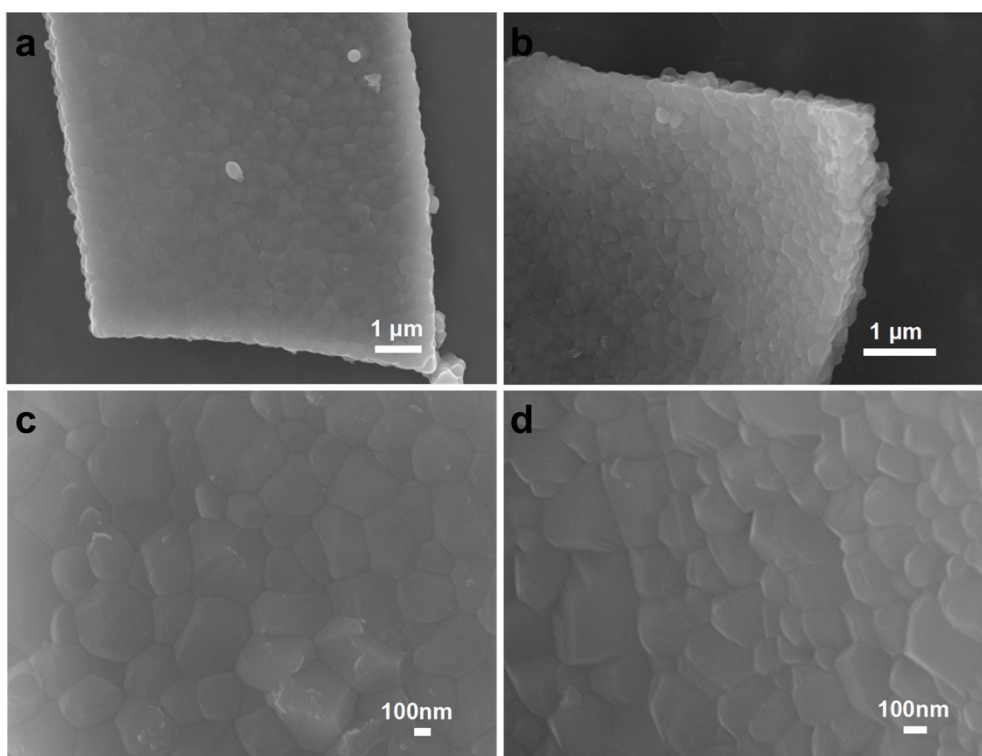


Fig. S4 SEM images of the Fe_2O_3 (a, c) and MgFe_2O_4 (b, d) calcined at $800\text{ }^\circ\text{C}$ for 5 h in air.

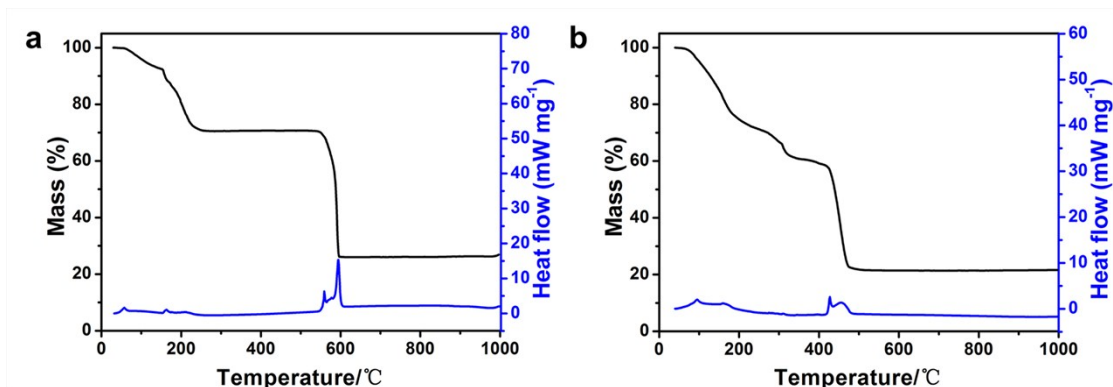


Fig. S5 TGA and DSC curves of the commercial $\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ (a) and $\text{Mg}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (b).

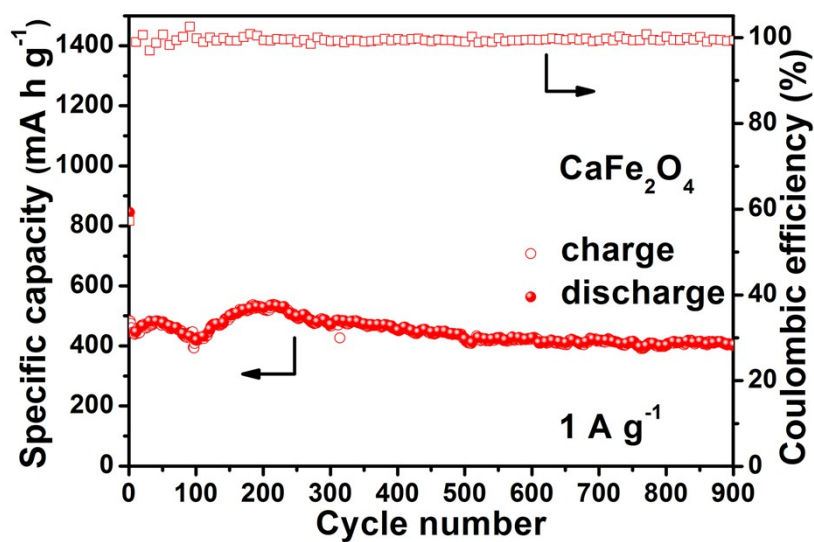


Fig. S6 Cycling performance of the CaFe_2O_4 calcined at 800 °C for 5 h tested at a current density of 1 A g^{-1} .

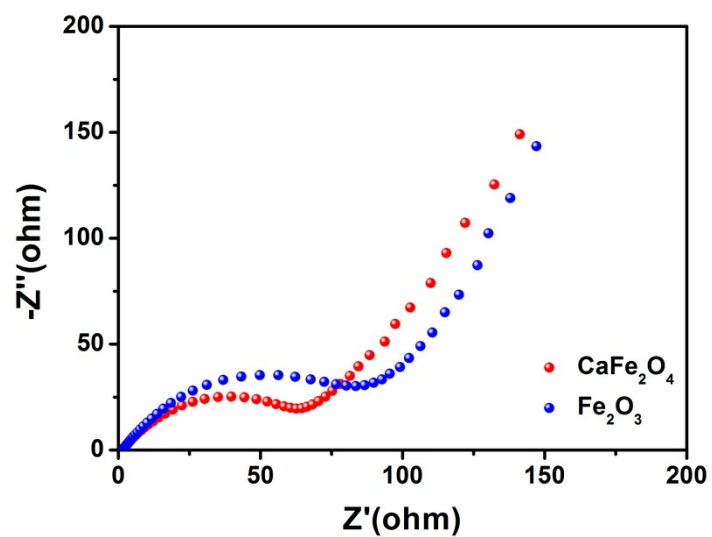


Fig. S7 Nyquist plots of CaFe_2O_4 and Fe_2O_3 after 5 cycles.

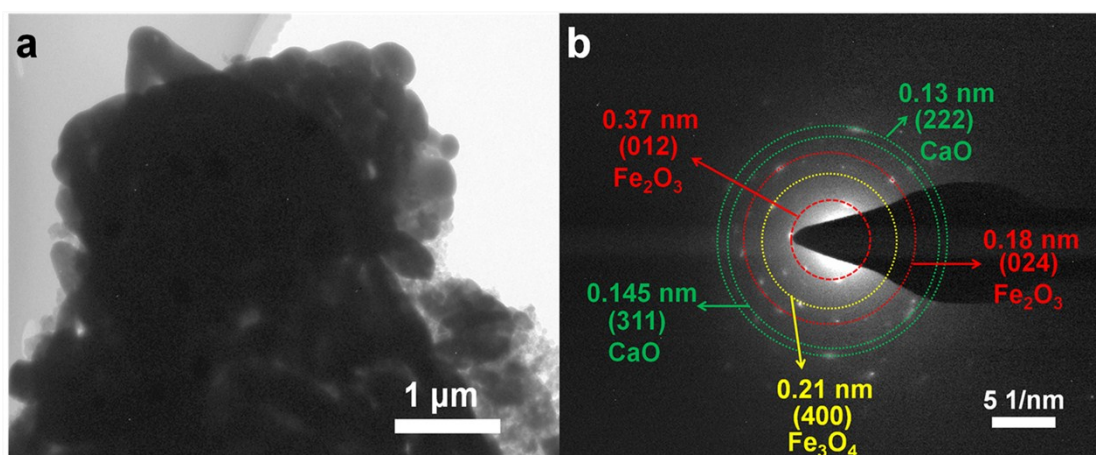


Fig. S8 (a) TEM image, (b) SAED pattern of CaFe_2O_4 at the delithiation state at 0.5 A g^{-1} after 5 cycles.

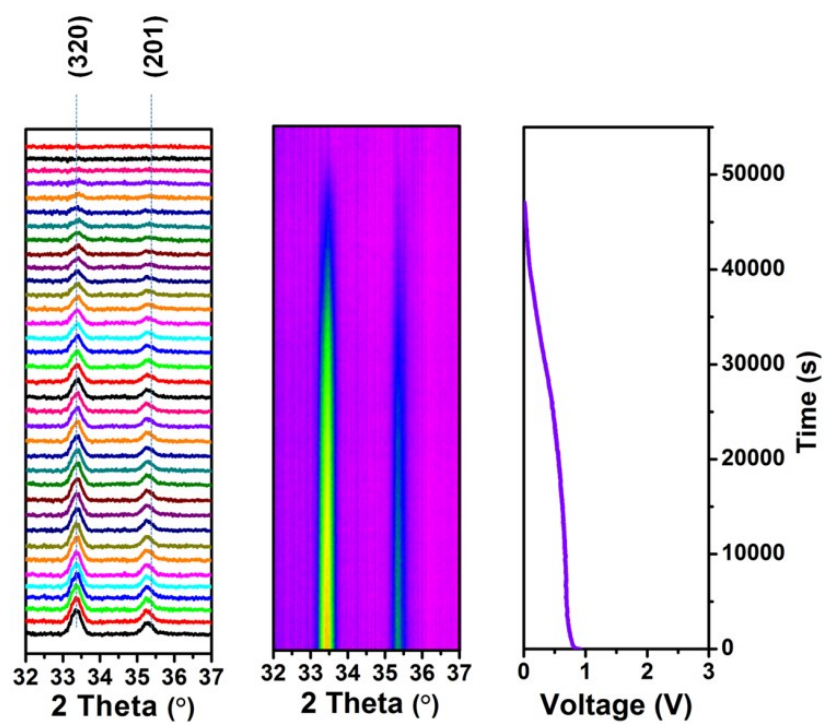


Fig. S9 *In situ* XRD results of CaFe_2O_4 during the initial discharge process.

Tab. S1 Comparison of properties between the CaFe_2O_4 (this work), graphite, Fe_2O_3 and Silicon.

	Graphite	CaFe_2O_4	Fe_2O_3	Silicon
Theoretical capacity (mA h g^{-1})	372	770	1007	4200
Reaction mechanism	Insertion	Conversion	Conversion	Alloying
Density(g cm^{-3})	2.25	4.8	5.26	2.34
Volume change	~10%	<96%	~96%	~400%
Price	Commercial	Low preparation cost	Low preparation cost	High preparation cost
Cycling performance without modification	excellent	excellent	Significant capacity decay	Significant capacity decay

Tab. S2 Electrochemical performance comparison of the porous CaFe_2O_4 (this work) with various Fe-based anodes.

Morphologies	Voltage range (V)	Current density (A g^{-1})	Retained capacity (mA h g^{-1})	Reference
		0.1	816 (100 cycles)	
Porous CaFe_2O_4	0.01-3	0.5	532 (1000 cycles)	Our work
		1	404 (900 cycles)	
Mesoporous Fe_2O_3	0.05-3	0.1	1176 (200 cycles)	[1]
		1	744 (500 cycles)	
3D net-like FeO_x/C	0.01-3	0.2	851 (50 cycles)	[2]
		1	714 (300 cycles)	
$\alpha\text{-Fe}_2\text{O}_3$ void@frame microframes	0.05-3	0.2	700 (550 cycles)	[3]
porous $\alpha\text{-Fe}_2\text{O}_3$ nanorods	0.01-3	0.2	740 (300 cycles)	[4]
		1	600 (300 cycles)	
Core-Shell $\text{Fe}/\text{Fe}_2\text{O}_3$ Nanowire	0.01-3	0.1	872 (100 cycles)	[5]
		0.5	767 (200 cycles)	
$\alpha\text{-Fe}_2\text{O}_3$	0.01-3	0.1	617 (100 cycles)	[6]
		0.1	968 (100 cycles)	
Ultrathin Fe_2O_3 nanoflakes	0.05-3	0.1	1043 (100 cycles)	[7]
		5	578 (500 cycles)	

References

- [1] W. Guo, W. Sun, L.-P. Lv, S. Kong, Y. Wang, *ACS Nano*, 2017, 11, 4198-4205.
- [2] M. Li, H. Du, L. Kuai, K. Huang, Y. Xia, B. Geng, *Angew. Chem., Int. Ed.*, 2017, 129, 12823-12827.
- [3] J. Zhu, D. Deng, *J. Mater. Chem. A*, 2016, 4, 4425-4432.
- [4] Y. Zhu, Q. Wang, X. Zhao, B. Yuan, *RSC Adv.*, 2016, 6, 97385-97390.
- [5] Z. Na, G. Huang, F. Liang, D. Yin, L. Wang, *Chem.–Eur. J.*, 2016, 22, 12081-12087.
- [6] P. Santhoshkumar, K. Prasanna, Y.N. Jo, I.N. Sivagami, S.H. Kang, C.W. Lee, *J. Mater. Chem. A*, 2017, 5, 16712-16721.
- [7] Y. Wang, J. Han, X. Gu, S. Dimitrijević, Y. Hou, S. Zhang, *J. Mater. Chem. A*, 2017, 5, 18737-18743.