Electronic Supplementary Information

NiFe saponite as a new anode material for high-performance lithium-ion batteries

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Materials characterizations

XRD patterns were obtained on Shimadzu X-ray diffraction (XRD)-6000 with Cu Ka radiation at 40 kV, 30 mA. SEM and HRTEM images were collected on Zeiss Supra 55 scanning electron microscope and JEOL JEM-2010 high-resolution transmission electron microscope, combined with energy disperse spectroscopy (EDS) for determination of metal composition. A Vector 22 (Bruker) spectrophotometer was used to achieve Fourier transform infrared (FTIR) spectra under 2 cm⁻¹ resolutions. X-ray photoelectron spectra (XPS) were collected on Thermo VG Escalab 250 instrument with Al 193 Ka exciting illuminant. A CHI 660C type electrochemical workstation was implemented for the cyclic voltammetry (CV) test. Galvanostatic charging-discharging test was implemented using a LAND battery test system. Extend X-ray absorption fine structure spectroscopy (EXAFS) for the Fe and Ni K-edge was performed at the beamline 1W1B of the Beijing Synchrotron Radiation Facility (BSRF), Institute of High Energy Physics (IHEP), Chinese Academy of Sciences (CAS). Thermogravimetry and derivative thermogravimetry (TG-DTG) analysis were carried out on a PCT-1A thermal analysis system to obtain the water content of NiFe saponite under Ar atmosphere with a heating rate of 10 °C/min. Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) was used to determine the elementary composition of NiFe saponite, by dissolving the sample in agua regia with moderate hydrofluoric acid.

Supplementary Figures



Fig. S1 A digital photograph of the as-synthesized NF-SAP sample.



Fig. S2 EDS mapping results of the NF-SAP sample.



Fig. S3 FTIR spectrum of the NF-SAP sample.

Table S1 FTIR peaks attribution of NF-SAP in Fig. S3.

Wavenumber (cm ⁻¹)	Attribution
3610	M(II)–O–H stretching vibration of the trioctahedral
	character
3450	absorbed water stretching mode
3220	O-H stretching mode of H-bridged OH groups
1642	absorbed water bending mode
1015	Si-O-Si stretching mode
708	M(II)–OH stretching mode
670	Si–O–M(II) bending mode



Fig. S4 TG-DTG of NF-SAP from room temperature to 900°C.



Fig. S5 (a) CV curves of Al/Li cell at 50 mV s⁻¹. (b) Constant current charging-discharging test of Al/Li cell at 40 mA g⁻¹. (c) CV curves of Cu/Li cell at 50 mV s⁻¹. (d) Constant current charging-discharging test of Cu/Li cell at 20 mA g⁻¹. These tests show the current collectors Cu and Al foils nearly have no capacity.



Fig. S6 CV curve of the NF-SAP/Li half cell at 0.5 mV s⁻¹.



Fig. S7 (a) The first cycle discharging curve of NF-SAP indicates activation of saponite. (b) A demo charging-discharging curve in a common cycle of NF-SAP half cell.



Fig. S8 HRTEM images of NF-SAP at (a) 3.0 V and (b) 0.01 V.



Fig. S9 XPS spectra of Na at different voltage in the NF-SAP electrode (C and D mean charge and discharge, respectively).



Fig. S10 X-ray absorption fine structure (XAFS) spectra of Fe in the NF-SAP electrode.



Fig. S11 X-ray absorption fine structure (XAFS) spectra of Ni in the NF-SAP electrode.



Fig. S12 XANES spectra of (a) Fe and (b) Ni in a whole charge/discharge cycle (C and D mean charge and discharge, respectively).



Fig. S13 Charging and discharging curve exhibition for a single step of GITT tests: (a) charging (b) discharging.

Galvanostatic intermittent titration technique (GITT) measurement was used to calculate the diffusion coefficient of organic cation (D_s) in the NF-SAP/Li half cell based on the following equation:

$$D_s = \frac{4}{\pi \tau} \frac{mV}{(MA)^2} (\frac{\Delta Es}{\Delta Et})^2$$
(1)

where *m* (g) and *M* (g mol⁻¹) are loading mass and molecular weight of NF-SAP; τ (s) is constant current pulse time; *V* (cm³ mol⁻¹) denotes the molar volume; *A* (cm²) is the surface area of the electrode; ΔE_s (V) and ΔE_t (V) are assigned to the voltage change between the two relaxations and voltage change caused by the pulse. Pulse current density is 50 mA g⁻¹ with τ = 10 min, and relax time of 1 h.

Material	$Log (D_s/m^2 s^{-1})$	Reference
TiNb ₆ O ₁₇	-13.5 ~ -12	43
TiNb ₂ O ₇	$-14.7 \sim -13$	43
$\alpha @\beta$ -FeC ₂ O ₄	-17.0	44
β-FeC ₂ O ₄	-17.3	44
α -FeC ₂ O ₄	-17.1	44
ZnMoO ₄	-21.6 ~ -20.5	45
H-NiO	-15.1	46
C-NiO	-15.3	46
TNO	-20.5	47
Ar-TNO	-20.4	47
S-TNO	-20.0	47
HfNb ₂₄ O ₆₂	-15.8	48
VG-MS-80%	-17.9	49
VPO_4	-18.5	49
MoS_2	-21.2	50
MoS ₂ @C	-21.4	50
V ₄ C ₃ -MXene/MoS ₂	-20.7	50
V ₄ C ₃ -MXene/MoS ₂ /C	-19.9	50
NiFe saponite	$-14 \sim -12$	this work

Table S2 Comparison study on the lithium-ion diffusion coefficients (D_s) of some anodematerials with this work.



Fig. S14 Cycling performance of NF-SAP/Na half cell at 200 mA g^{-1} with a voltage window of 0.01 V to 3.0 V using NaClO₄ as electrolyte.



Fig. S15 (a) CV curve of the $LiMn_2O_4/Li$ half cell at 0.5 mV s⁻¹. (b) Cycling performance of the $LiMn_2O_4/Li$ half cell at a current density of 100 mA g⁻¹ with a voltage window from 3.0 V to 4.3 V.