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Supporting Information

A Wadsley-Roth crystallographic shear phase $SrNb_6O_{16}$ anode for fast Li-ion storage

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Experimental section

Material preparation. $SrNb_6O_{16}$ was prepared through a one-step solid-state reaction procedure. Briefly, $SrCO_3$ (Aladdin, 99.99%) and Nb_2O_5 (Aladdin, 99.5%) powders with a molar ratio of 1:3 were ball-milled for 2h using a SPEX-8000M ball apparatus, and then heated to 1000°C for 10h in a box furnace with a ramp of 10°C min^{-1} to obtain the pure white $SrNb_6O_{16}$ powders.

Material characterization. The powder X-ray diffraction (XRD) test was performed on Brucker D8 advance diffractometer. The Rietveld refinement was performed using the Materials Studio software with the corresponding crystallographic CIF file. In situ XRD measurements were analyzed by using the aforementioned XRD equipment. Scanning electron microscopy (SEM) images were collected with a Hitachi SU-70 microscope with an energy dispersive X-ray spectrometer (EDS) at an operating voltage of 5 kV and 15 kV.

Electrochemical test. For electrochemical tests, the anode consisted of 80wt% active substance ($SrNb_6O_{16}$ powder), 10wt% conductivity agent (carbon black), and 10wt% polyvinylidenefluoride (PVDF) dispersed in N-methyl-2-pyrrolidone (NMP, Macklin) to generate a slurry. This slurry was coated on copper foil by a tablet machine, dried at 80°C overnight to ensure removal of the NMP. Its loading mass was about 2.0 mg for each electrode. The Swagelok batteries were assembled in an argon-filled glove box using the as-prepared film as the working electrode, Li metal foil as the counter electrode, glass fiber as the separator and 1mol L^{-1} $LiPF_6$ dissolved in a mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC) (1:1 in volume) as the electrolyte. The sodium ion batteries are also assembled using the $SrNb_6O_{16}$ powder as the working electrode, Na metal foil as the counter electrode, glass fiber as the separator and 1 mol L^{-1} $NaPF_6$ dissolved in a mixture of EC and DMC (1:1 in volume) as the electrolyte. The charge-discharge performance was evaluated by multichannel LANHE battery tester at a constant current density of 50mAg^{-1}. Cyclic voltammetry (CV) was carried out at a scan rate of 0.1 mV s^{-1} between 1.0 and 3.0 V on a CHI1000B electrochemical workstation.

$SrNb_6O_{16}$ crystal model building, lithiation and sodiation behavior analysis. The VESTA (Visualization for Electronic and STructural Analysis) system has been developed for the 3D visualization of crystal structures, volumetric data and crystal morphologies. Amongst available softwares, VESTA is easy to use and allows importing of data from a large variety of formats.VESTA utilizes RIETAN-FP to simulate powder X-ray diffraction pattern from lattice and structure parameters. VESTA represents crystal structures by the five different models: ball-and-stick, space-filling, polyhedral, wireframe, stick models.

Capacity calculation. The theoretical capacity of $SrNb_6O_{16}$ was calculated according to the following formula:

$$C = \frac{n \times F \times 1000}{Mr \times 3600}$$

In the formula, *C* is the theoretical specific capacity, n means the molar number of intercalated lithium ions, F refers to the Faraday constant, and *M*r is the relative molecular mass. For $SrNb_6O_{16}$, its relative molecular mass is 901 g mol^{-1}. In addition, there are 12 intercalated lithium ions per unit during the discharge process based on theoretical calculations. Therefore, the theoretical capacity of

$SrNb_6O_{16}$ is 357 mAh g^{-1} between 1-3 V (versus Li^+/Li).

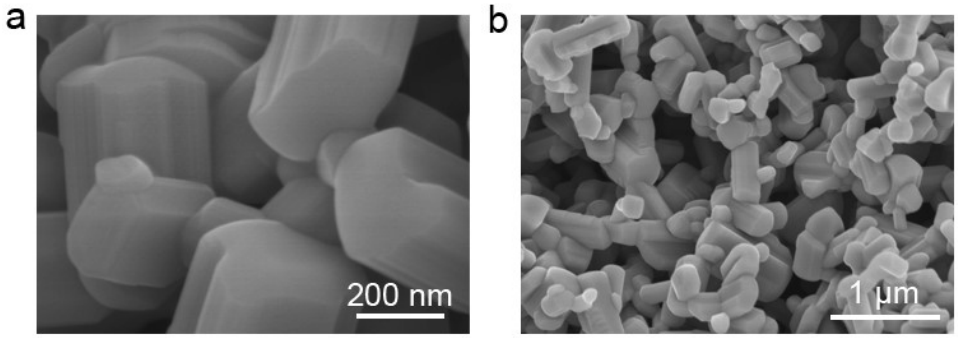

Fig. S1. (a) High-magnification SEM, and (b) Low-magnification SEM image of $SrNb_6O_{16}$.

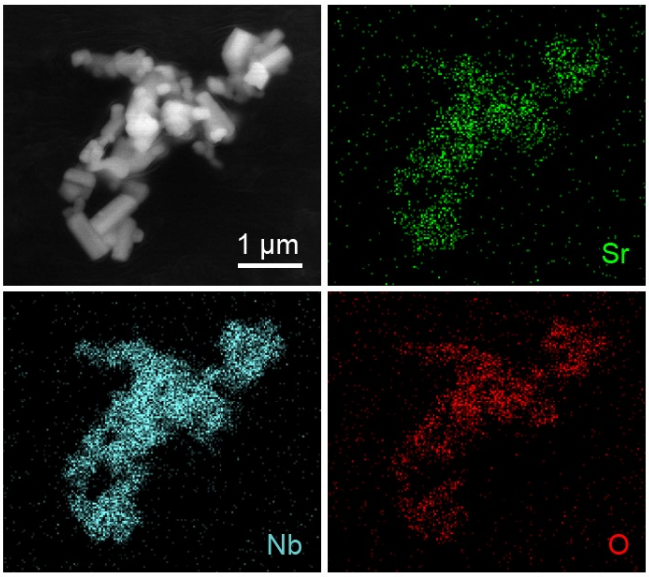

Fig. S2. EDS elemental mapping images of $SrNb_6O_{16}$.

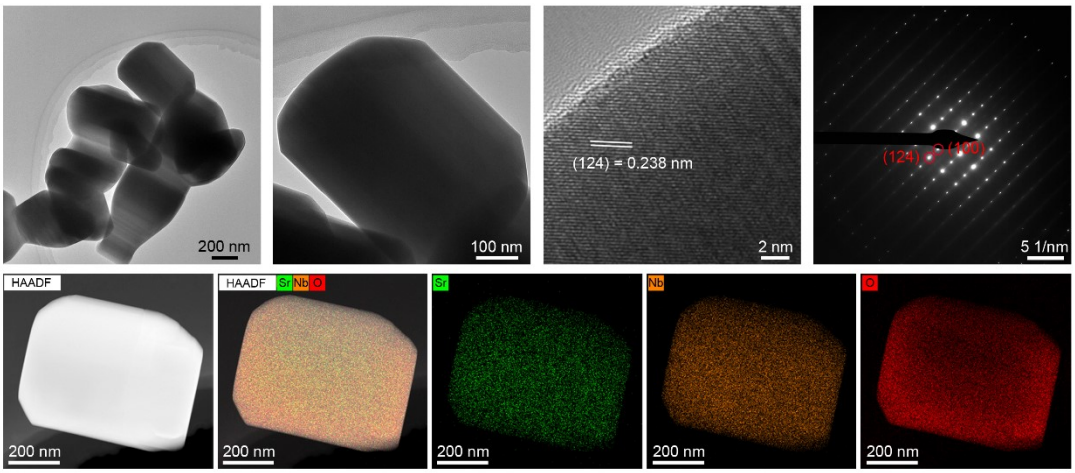

Fig. S3. HRTEM and SAED images of $SrNb_6O_{16}$.

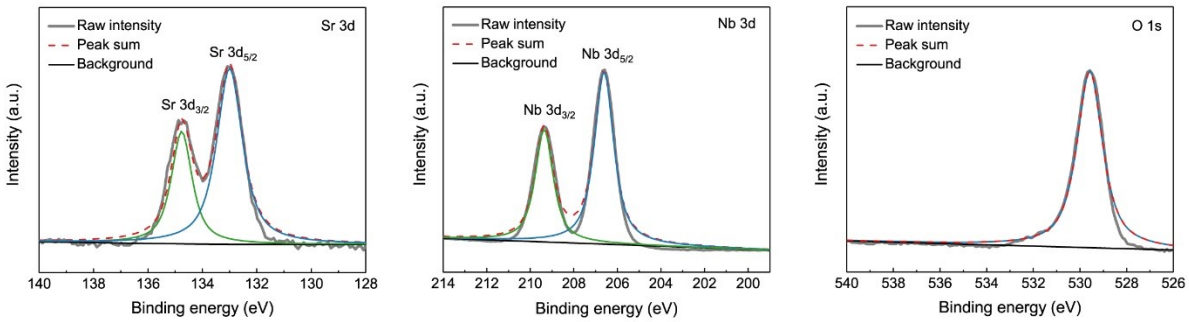

Fig. S4. High-resolution XPS spectra of Sr, Nb, and O on $SrNb_6O_{16}$.

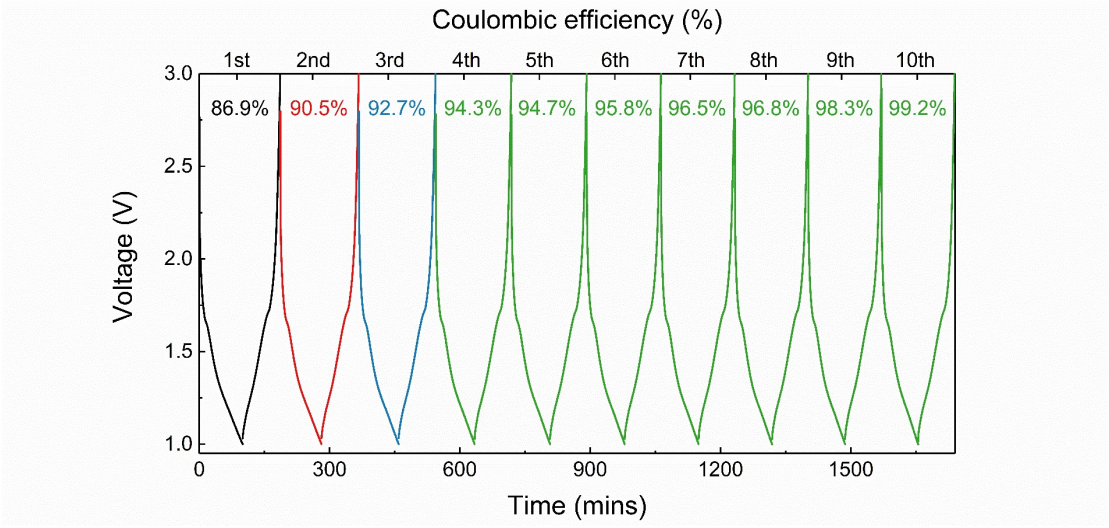

Fig. S5. Voltage profiles and corresponding coulombic efficiencies of $SrNb_6O_{16}$ for half cell.

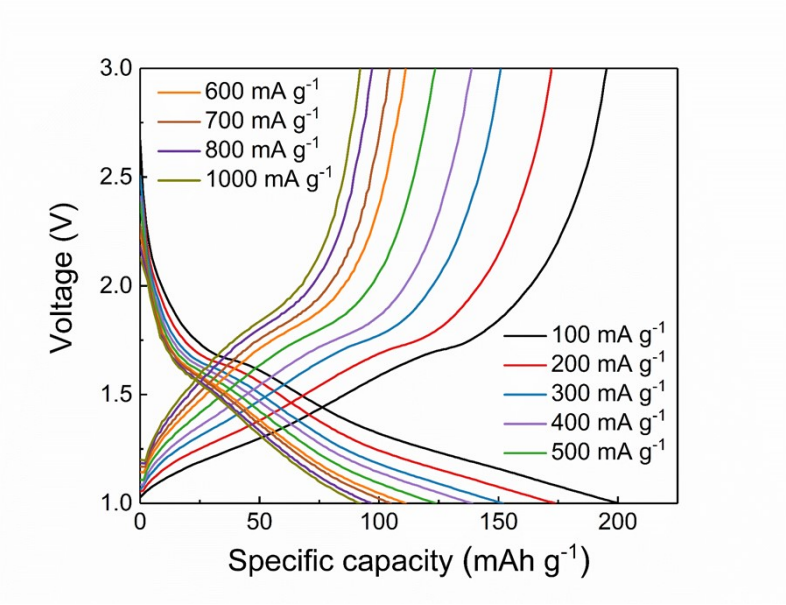

Fig. S6. Charge-discharge profiles of $SrNb_6O_{16}$ at 100-1000 mA g^{-1}.

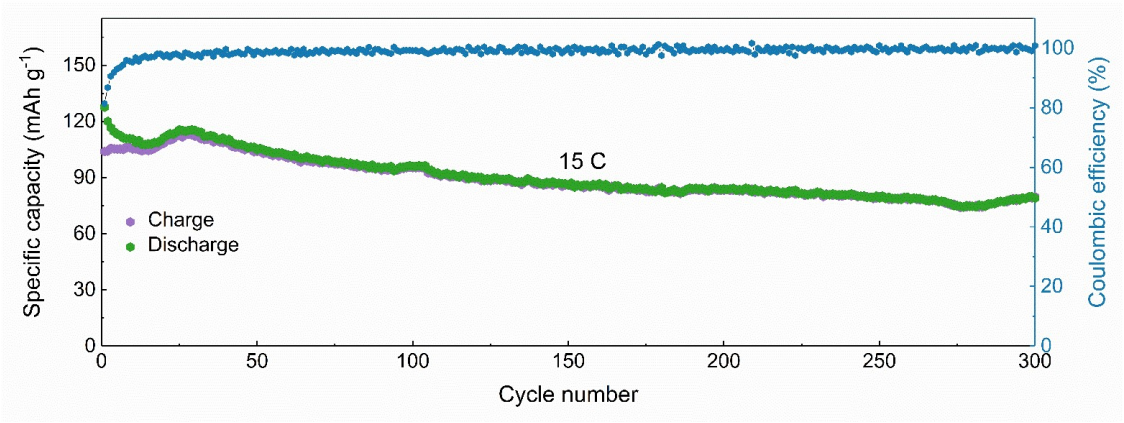

Fig. S7. Long-term cycling stability of $SrNb_6O_{16}$ at a current rate of 15 C.

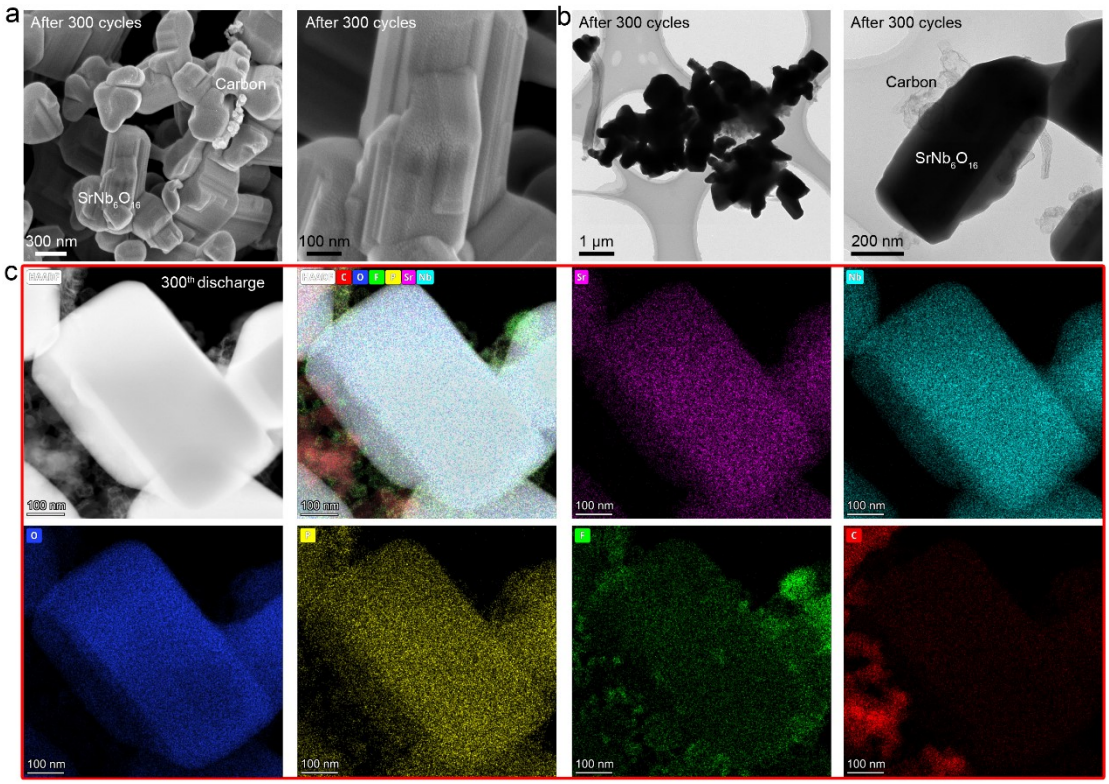

Fig. S8. (a) SEM images of the $SrNb_6O_{16}$ after 300 cycles, and (b) TEM images of the $SrNb_6O_{16}$ after 300 cycles, and corresponding elemental mapping images of the $SrNb_6O_{16}$ at 300^{th} discharge state.

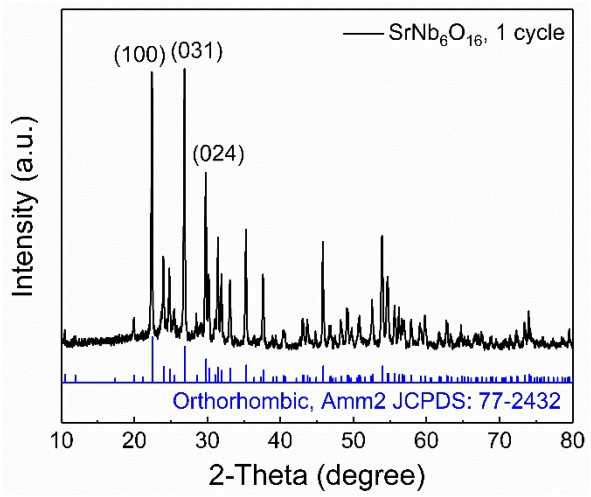

Fig. S9. XRD pattern of $SrNb_6O_{16}$ after a cycle.

Table S1. Rietveld refinement data obtained for $SrNb_6O_{16}$.

No.	Atom	u	v	w	Occupancy
a=3.9540 Å, b=10.1874 Å, c=14.7861 Å, Rp=7.26%, Rwp=9.34%					
1	Sr(1)	0.50000	0.00000	0.40400	0.61709
2	O(1)	0.50000	0.00000	0.00000	0.52117
3	O(2)	0.50000	0.00000	0.22600	0.88178
4	Nb(1)	0.00000	0.00000	0.00000	0.66867
5	Nb(2)	0.00000	0.00000	0.21420	0.65830
6	O(10)	0.00000	0.00000	0.51900	0.47955
7	Nb(3)	0.00000	0.31860	0.06200	0.70024
8	Nb(4)	0.00000	0.31530	0.31540	0.64065
9	O(5)	0.00000	0.11900	0.10500	0.76741
10	O(6)	0.00000	0.13300	0.31100	0.54308
11	O(7)	0.00000	0.30500	0.44700	0.59390
12	O(8)	0.00000	0.35100	0.17800	0.80958
13	O(3)	0.50000	0.32400	0.05000	1.00000
14	O(4)	0.50000	0.32300	0.30700	0.97976
15	O(9)	0.00000	0.50000	0.35600	0.68709

Table S2. SEM EDS mapping. Semi-quantitative analysis of the main elements in $SrNb_6O_{16}$.

Element	(weight, %)	(atomic, %)
Sr	15.23	7.15
Nb	58.77	26.02
O	26.00	66.83

Table S3. The comparison of electrochemical performance between this work and previous reported anode materials.

Samples	Rate	Initial Coulombic efficiency (%)	Reversible capacity (mAh g^{-1})	Discharge plateau (V)	Polarization (V)	Reference
$SrNb_6O_{16}$	0.3 C	88	223	1.65	0.07	This work
$TiNb_2O_7$	0.4 C	85	255	1.57	0.16	Ref. 1
$FeNbO_4$	0.2 C	63	307	0.57	0.37	Ref. 2
$WNb_{12}O_{33}$	1 C	81	184	1.67	0.13	Ref. 3
KNb_5O_{13}	0.3 C	79	130	1.59	0.18	Ref. 4
VNb_9O_{25}	0.3 C	60	207	1.46	0.32	Ref. 5
$Pb_3Nb_4O_{13}$	0.1 C	56	265	1.91	0.34	Ref. 6
Nb_2O_5	1 C	98	160	1.55	0.27	Ref. 7
$Nb_{12}O_{29}$	0.6 C	76	79	1.6	0.26	Ref. 8
$Li_4Ti_5O_{12}$	0.5 C	95	165	1.55	0.08	Ref. 9
$LiCrTiO_4$	0.5 C	87	144	1.50	0.43	Ref. 10
$SrLi_2Ti_6O_{14}$	0.1 C	74	168	1.37	0.05	Ref. 11

Reference:

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