Electronic Supplementary Material (ESI) for Materials Advances.

Electronic Supporting Information

Shear-structure $MoNb_6O_{18}$ as New Anode for Lithium Ion Batteries

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Experimental

The $MoNb_6O_{18}$ sample was prepared with a conventional solid-state reaction method. In brief, MoO_3(99.5 %) and Nb_2O_5 (99.99 %) were mixed with molar ratio of 3:2 in an agate mortar with pestle in absolute ethanol for two hours. The mix-oxides was pressed into a pellet with a diameter of 25 mm at 2 MPa, and preheated in a crucible on platinum sheet at 600 ^oC for 6 h with a heating rate of 5 ^oC/min. After cooling down to room temperature, the pellet was re-grounded for one hour in absolute ethanol, and then pressed into a pellet (~ 0.6 g) with a diameter of 10 mm at 6 MPa, followed by heating in a crucible with platinum sheet in air at 1000 ^oC for 6 h a rate of 5 ^oC/min.

The X-ray diffraction (XRD) patterns were collected on a PANalytical Empyrean X-ray diffractometer equipped with Cu-Kα radiation. The morphology and microstructure of the samples were recorded by using GeminiSEM 300 field emission scanning electron microscope (FESEM) and an JEM2010-HR transmission electron microscope (TEM). The content of elements was analyzed on PerkinElmer Optima 8000 inductively coupled plasma (ICP) optical emission spectrometer.

The electrochemical performance was carried out in CR2032 coin-type cells. The working electrode was prepared mixing 80 wt% active material, 10 wt% conductive carbon, 10 wt% polyvinylidene difluoride binder in N-methyl pyrrolidone. The obtained slurry was pasted on Al foil and dried under vacuum at 100 ^oC for 12 h. The mass loading of active materials ($MoNb_6O_{18}$) in the composite electrode was 2~3 mg/cm^2. CR2032-type coin cells were assembled in a glove box filled with argon. Li foil was used as the counter and reference electrode. A polypropylene microporous film (Celgard 2400) was used as the separator. 1 M $LiPF_6$ solution in a mixture solvent of ethylene carbonate and dimethyl carbonate (1:1, v/v) was used as electrolyte. The galvanostatic charge-discharge (GCD) measurements were measured by using a Neware CT-3008-5V5mA battery testing system. Cyclic voltammetry (CV) and electrochemical impedance spectra (EIS) were performed by using a Chenhua CHI760E Electrochemical Workstation. The full cell was fabricated with $MoNb_6O_{18}$ as the anode and commercial $LiMn_2O_4$ (MTI-Shenzhen Kejing Star) as the cathode, denoted for LMO//MNO. The galvanostatic charge-discharge (GCD) measurements of

the LMO//MNO full cells were measured in the voltage range of 1.0-3.2 V at 0.2 C. The capacity of LMO//MNO full cell was calculated based on the mass of MNO anode.

Based on two-electron transfer per transition metal ion, the theoretical capacity (C_0) of $MoNb_6O_{18}$ was 399 mAh/g and calculated by:

$$C_0 = \frac{nF}{3.6M} = \frac{14 \times 96485}{3.6 \times 941} \approx 399\ mAh/g$$

Where n is the number of electrons transferred per formula unit, F is Faraday constant (96485 C/mol), 3.6 is a conversion factor between coulombs and the conventional milliampere-hour, and M is the molar mass in per formula unit. So, 1 C is defined as 399 mA/g in this work.

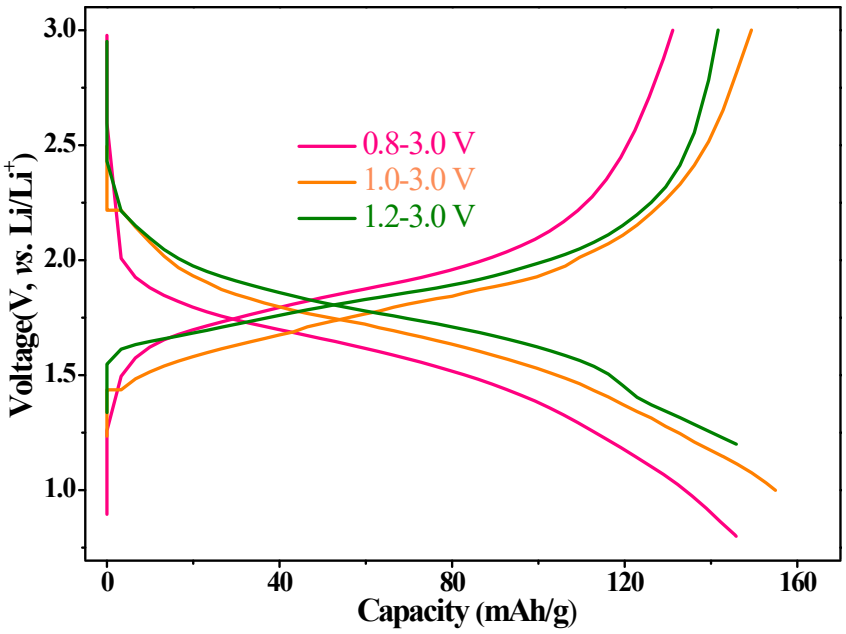

Fig. S1. Initial discharge-charge voltage profiles of $MoNb_6O_{18}$ at 1 C.

Table S1. Comparison of the MNO electrode with reported Nb-based and other anode electrodes in previous literature in terms of capacity and rate capability.

Composition	Morphology	Current density	Initial discharge/charge capacity (mAh/g), initial CE	Discharge capacity (mAh/g)	Ref.
$MoNb_{12}O_{33}$	porous microspheres	0.1C	351/321, 91.5%	275, 1C 100 cycles	24
$MoNb_{12}O_{33}$	micron-sized particles	0.1C	349/294, 84.2%,	210, 1C 100 cycles	24
$Mo_3Nb_{14}O_{44}$	nanowires	0.1 C	321/288.9, 90%	140, 10C 1000 cycles	26
$Mo_3Nb_{14}O_{44}$	micron-sized particles	0.1 C	323/2987.8, 92.2%	95, 10C 1000 cycles	26
$SiO/Ti_3C_2T_x$	nanocomposite	200 mA/g	1986.7/1378.8, 69.4%	750, 1A/g 120 cycles	5
Nb_2O_5	nanorods	50 mA/g	305/294, 97.3%	160, 100mA/g 270 cycles	20
SnO_2//CC	Nano-sized	0.15 mA/cm^2	4.38/3.1 mAh/cm^2, 70.8%	1.69 mAh/cm^2 1.5 mA/cm^2, 500 cycles	34
$MoNb_6O_{18}$	micron-sized particles	0.2 C	219.3/212.4, 96.8%	142.3, 1 C 60 cycles	This work

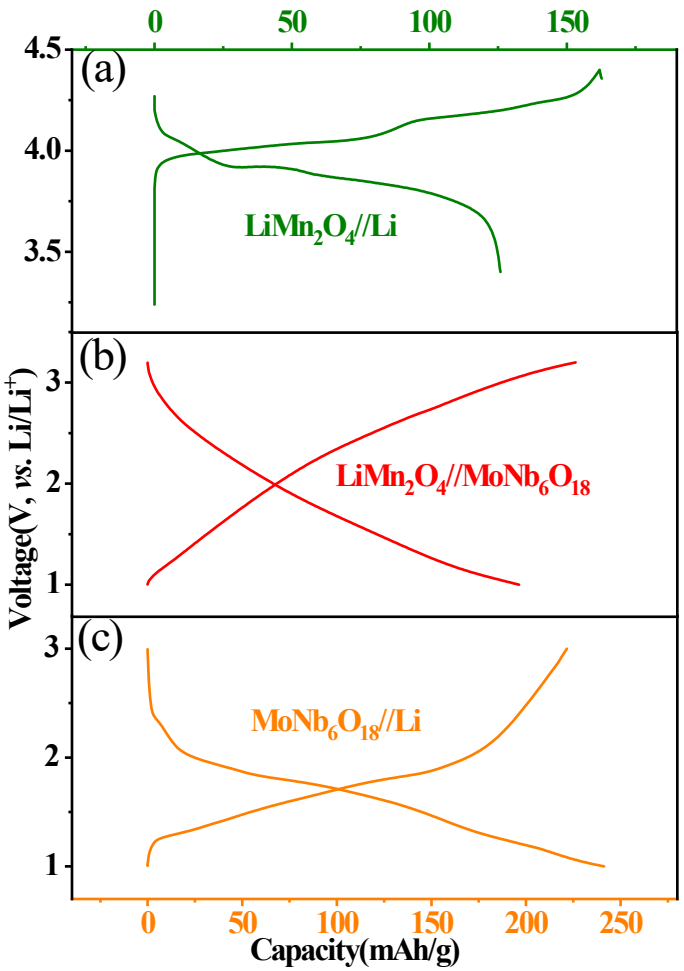

Fig. S2. Charge-discharge profiles of (a) $LiMn_2O_4$//Li half cell, (b) $LiMn_2O_4$//$MoNb_6O_{18}$ full cell, (c) $MoNb_6O_{18}$//Li half cell at 0.2 C.

Based on the charge capacity of LMO cathode and the discharge capacity of MNO anode, the mass ratio was 1.5 : 1 ($mass_{cathode}$: $mass_{anode}$ = 1.5 : 1).