Supporting Information

A New Layered Titanate Na₂Li₂Ti₅O₁₂ as High Performance Intercalation Anode for Sodium-Ion Batteries

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Figure S1. X-ray diffraction pattern of as-prepared KLT sample.

FORMULA K2LI2TI5O12, SPACE GROUP CMCM					
$A_{\rm OR} = 3.8123$ (Å), $B_{\rm OR} = 15.5912$ (Å), $C_{\rm OR} = 2.9734$ (Å)					
ATOM	site	x	У	Z	осс
TI	4c	0	0.2	0.25	1
K	4b	0	0.5	0	0.3333
LI	4b	0	0.5	0	0.3333
01	4c	0	0.9	0.25	1
02	4c	0	0.7	0.25	1

Table S1. Structural parameters of KLT.



Figure S2. HR-TEM image of NLT (inset: corresponding intensity profile for the line

scan across the lattice fringes and the FFT).



Figure S3. TG curves of as-obtained KLT and NLT sample heated in air at a heating rate of 10 °C min⁻¹.



Figure S4. (a) The charge/discharge profiles of NLT in different cycles at current density of 50 mAg⁻¹ in the voltage range of 0.01 - 2 V. (b) Rate performance of KLT in different current densities. (c) Long-term cycling performance at a current density of 50 mAg⁻¹.



Figure S5. The first discharge/charge curves of NLT.



Figure S6. The charge-discharge profiles with different rate of NLT.



Figure S7. (a) Cycling stability and (b) Coulombic efficiency for sodium cells of NLT electrode prepared with NaCMC or PVDF binders, discharged/charged at 0.1 Ag^{-1} in the voltage range of 0.01 - 2 V.



Figure S8. (a, b) GITT profiles of NLT for 1st and 4th at a current density of 20 mA g^{-1} , respectively. Diffusion coefficient calculated from the GITT profiles for the electrode at (c) first and (d) fourth cycle, respectively.



Figure S9. Current step diagram of desodiation process of the NLT electrode for SIBs.

Figure S8a and b show the GITT curves of NLT electrode at the first and fourth cycles in a voltage range of 0.01 - 2.0 V. During the GITT measurements, the cell is

working with a pulse current at 20 mA g⁻¹ for an interval of 10 min followed by an open circuit relaxation of 40 min to obtain the steady-state voltage (E_s). A single titration profile is illustrated in Figure S9c with schematic labelling parameters, ΔE_{τ} , ΔE_s , etc. The diffusion efficient of an electrode can be estimated by Fick's second law of diffusion with the following equation:

$$D = \frac{4}{\pi} \left(\frac{m_B V_M}{M_B S} \right)^2 \left(\frac{\Delta E_s}{\tau \left(dE_\tau / d\sqrt{\tau} \right)} \right)^2 \ (\tau \ll L^2 / D) \tag{1}$$

Where $m_{\rm B}$ is electrode active mass, $M_{\rm B}$ is the molar mass of material, $V_{\rm M}$ is the molar volume of the material, *S* is the overall contract area of the electrode and electrolyte, *L* is the electrode thickness and τ is the pulse duration. Linear behavior of the potential *vs.* $t^{1/2}$ relationship shown in Figure S9a and b makes it possible for us to simplify equation (1) to the following form:

$$D = \frac{4L^2}{\pi\tau} \left(\frac{\Delta E_s}{\Delta E_\tau}\right)^2 (\tau \ll L^2/D) \qquad (2)$$

Based on equation (2), the diffusion coefficients of Na⁺ calculated from the GITT curves as a function of the cell voltage in the first and fourth sodiation/desodiation processes are shown in Figure S8c and d.



Figure S10. The CV curves of NLT at a scan rate of 0.1 mV s^{-1} .