Introducing large-radius elements into layered perovskite for low-voltage lithium storage

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Table S1 Parameters of $LiSmTiO_4$.

	a (Å)	*b* (Å)	*c* (Å)	*α/β/γ*
$LiSmTiO_4$	11.557961	5.350223	5.345824	90 °

Table S2 Fractional atomic parameters of $LiSmTiO_4$ with *Pbcm* space group.

atom	site	*x*	*y*	*z*	occupancy
Li	4*d*	0.522327	0.522327	0.000000	1
Sm	4*d*	0.877723	0.012580	0.250000	1
Ti	4*d*	0.298715	0.005600	0.250000	1
O1	4*c*	0.260215	0.250000	0.000000	1
O2	4*c*	0.734028	0.250000	0.000000	1
O3	4*d*	0.099685	0.922669	0.250000	1
O4	4*d*	0.475755	0.080721	0.250000	1

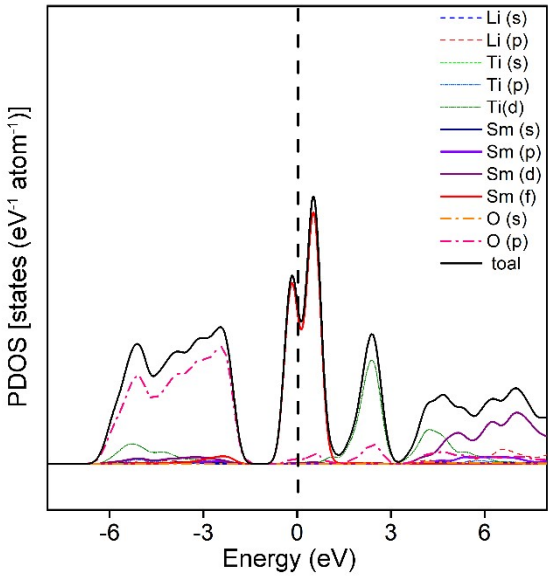

Figure S1. Projected density of states (PDOS) for pristine LSTO.

The Vienna Ab-initio Simulation Package (VASP) package with density functional theory (DFT) was used for the calculations. The electronic exchange-correlation energy was determined using the Perdew–Burke–Ernzerhof functional within the generalized gradient approximation. The cutoff energy was set to 400 eV, and the convergence criteria were 1.0×10^{-3} eV for energy and 0.01 eV $Å^{-1}$ for stress. The projected density of states (PDOS) of LSTO was calculated using a Monkhorst−Pack grid of 4 × 8 × 8 k-points. The crystal structure of LSTO was optimized using a bulk structure consisting of four LSTO units ($[LSTO]_4$).

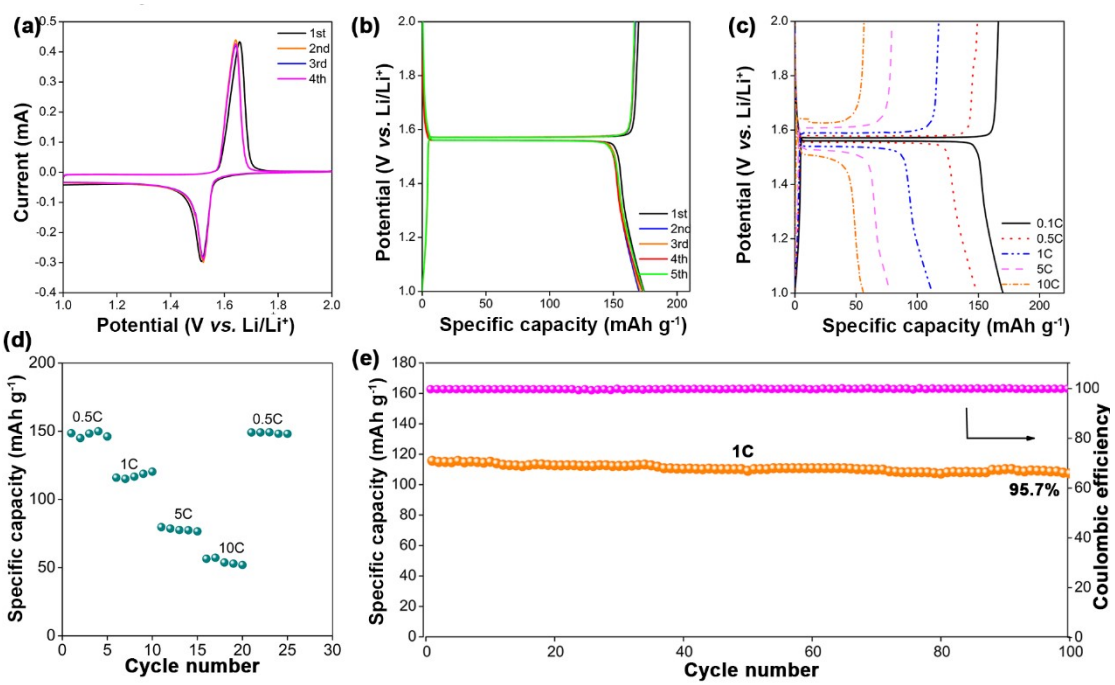

Figure S2. Electrochemical performance of $Li_4Ti_5O_{12}$/Li half cell. (a) CV curves measured at a sweep rate of 0.2 mV s^{-1}. (b) the first five galvanostatic discharge and charge curves of the $Li_4Ti_5O_{12}$ in a half-cel configuration. (c,d) Galvanostatic discharge and charge curves from 0.1C up to 10C and corresponding rate performance summary based on galvanostatic capacity. (e) The cycle performance of $Li_4Ti_5O_{12}$ at 1C.

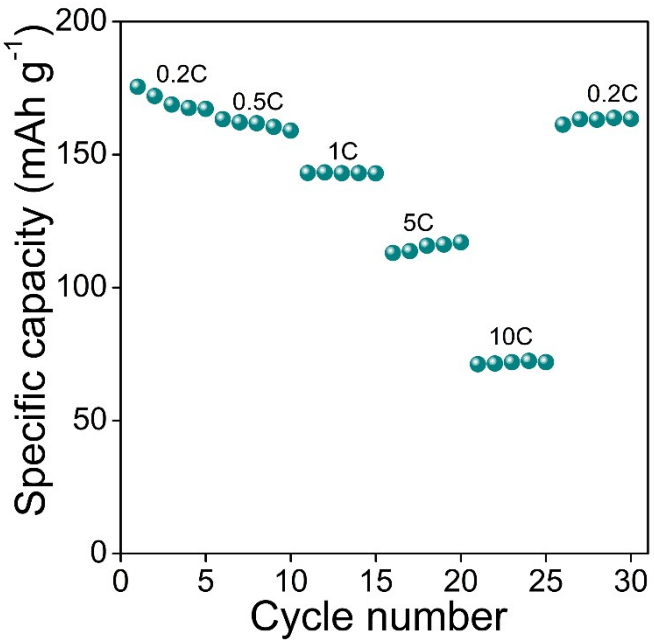

Figure S3. The corresponding rate performance summary based on galvanostatic capacity.

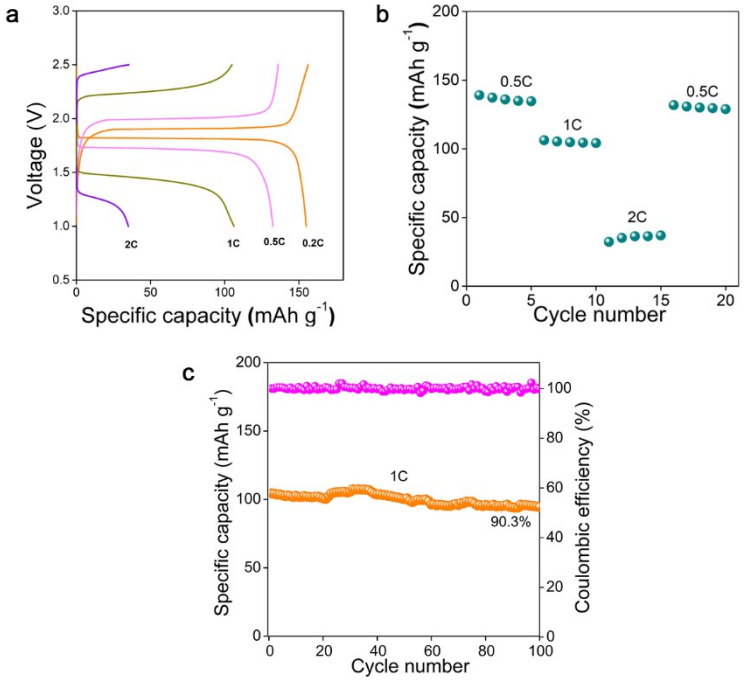

Figure S4. Electrochemical performance of the $LiFePO_4$|| $Li_4Ti_5O_{12}$ full cell. (a) Charge-discharge curves at various current rates from 0.2C to 2C from 1.0 V to 2.5 V. (b) The corresponding rate performance summary based on galvanostatic capacity. (c) The cycling stability at 1C over 100 cycles and corresponding Coulombic efficiency of the $LiFePO_4$|| $Li_4Ti_5O_{12}$ full cell.

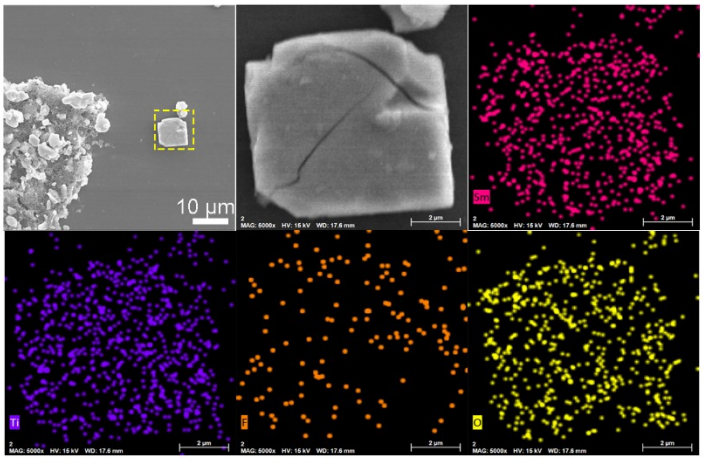

Figure S5. EDS mapping of the electrode after 10 cycles.

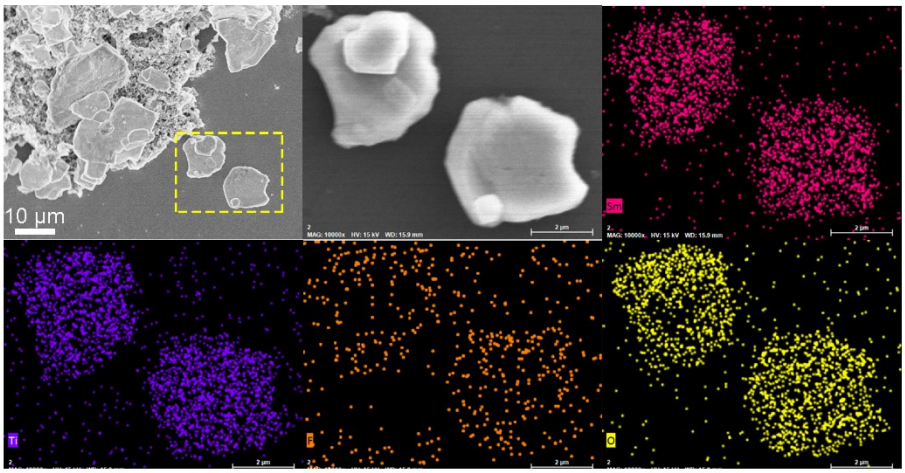

Figure S6. EDS mapping of the electrode after 100 cycles.