

Enhanced electrochemical performance of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ by niobium doping for pseudocapacitive applications

Jinka Chandrasekhar ¹, Merum Dhananjaya ¹, Obili M. Hussain ^{1,*}, Alain Mauger ², and Christian M. Julien ^{2,*}

¹ Thin film Laboratory, Department of Physics, Sri Venkateswara University, Tirupati 517502, India

² Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, CNRS UMR 7590, 4 place Jussieu, 75005 Paris, France

* Correspondence: hussainsvu@gmail.com (O.M.H.); christian.julien@sorbonne-universite.fr (C.M.J.)

Table S1. The lattice parameters of the $\text{Li}_4\text{Ti}_{5-x}\text{Nb}_x\text{O}_{12}$ samples synthesized by solid-state reaction at 900 °C.

Doping (mol%)	Lattice parameter (Å)	Unit volume (Å ³)	Dislocation density (10 ⁻¹⁰ cm ⁻²)	Crystallite size (nm)
0	8.349(1)	582.00	4.72	46.0
2	8.361(3)	584.48	5.60	42.2
4	8.368(4)	585.95	5.79	41.5
6	8.374(5)	587.39	5.83	41.3
8	8.377(1)	587.87	5.90	41.1
10	8.361(4)	584.58	5.45	42.1

Table S2. Results of the Rietveld refinement for pristine LTO and 8%Nb-doped LTO.

Composition	$x=0.00$	$x=0.08$
Lattice parameter (Å)	8.349(1)	8.377(1)
Site occupancy		
8a		
Li1	0.999(2)	0.999(1)
Ti1	0.001(1)	0.001(2)
16d		
Ti2	0.833(4)	0.765(3)
Li2	0.167(1)	0.166(3)
Nb	-	0.079(1)
32e		
O	1(-)	1(-)
R_{wp}	0.112	0.103
R_p	0.073	0.066
χ^2	2.01	1.81

R_{wp} : weighted profile residual, R_p : profile residual, and χ^2 : goodness of fit.

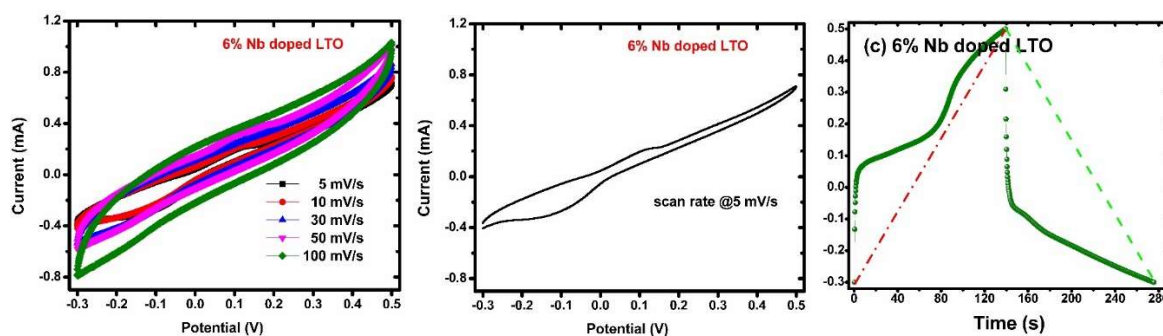


Figure S1. Electrochemical performance of the $\text{Li}_4\text{Ti}_{4.94}\text{Nb}_{0.06}\text{O}_{12}$ sample: (a) CV curves of at various scan rates (5 – 100 mV s⁻¹), (b) CV curve recorded at scan rate of 5 mV s⁻¹ showing the faradaic contribution, (c) GCD curves recorded at current density of 2 A g⁻¹ showing the faradaic voltage plateau.

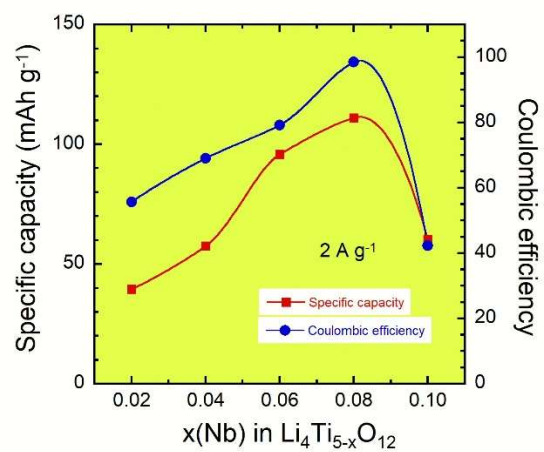


Figure S2. Composition dependence of the specific capacity and coulombic efficiency of $\text{Li}_4\text{Ti}_{5-x}\text{Nb}_x\text{O}_{12}$ samples measured at current density of 2 A g^{-1} .