

Supporting Information

Towards Enhanced Sodium Storage by Investigation on Li Ions Doping and Rearrangement Mechanism in $\text{Na}_3\text{V}_2(\text{PO}_4)_3$ for Sodium Ion Batteries

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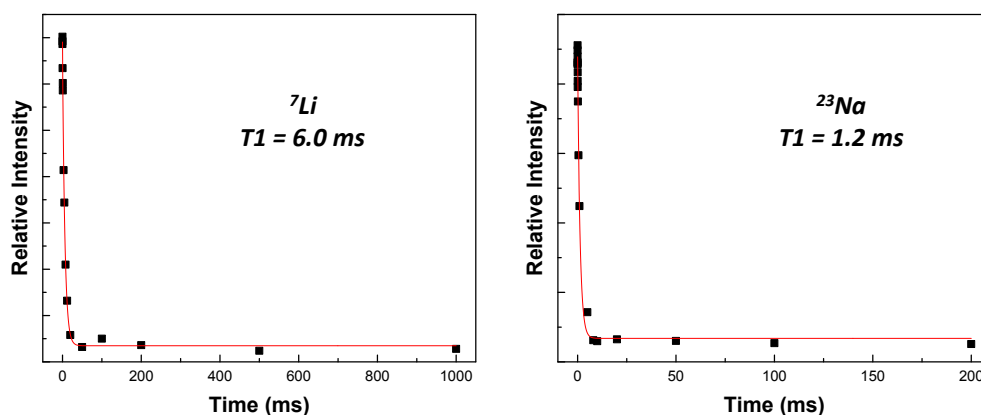


Figure S1. Plot of the longitudinal relaxation time (T_1) measurements for ^7Li in $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ and ^{23}Na in $\text{Na}_3\text{V}_2(\text{PO}_4)_3$.

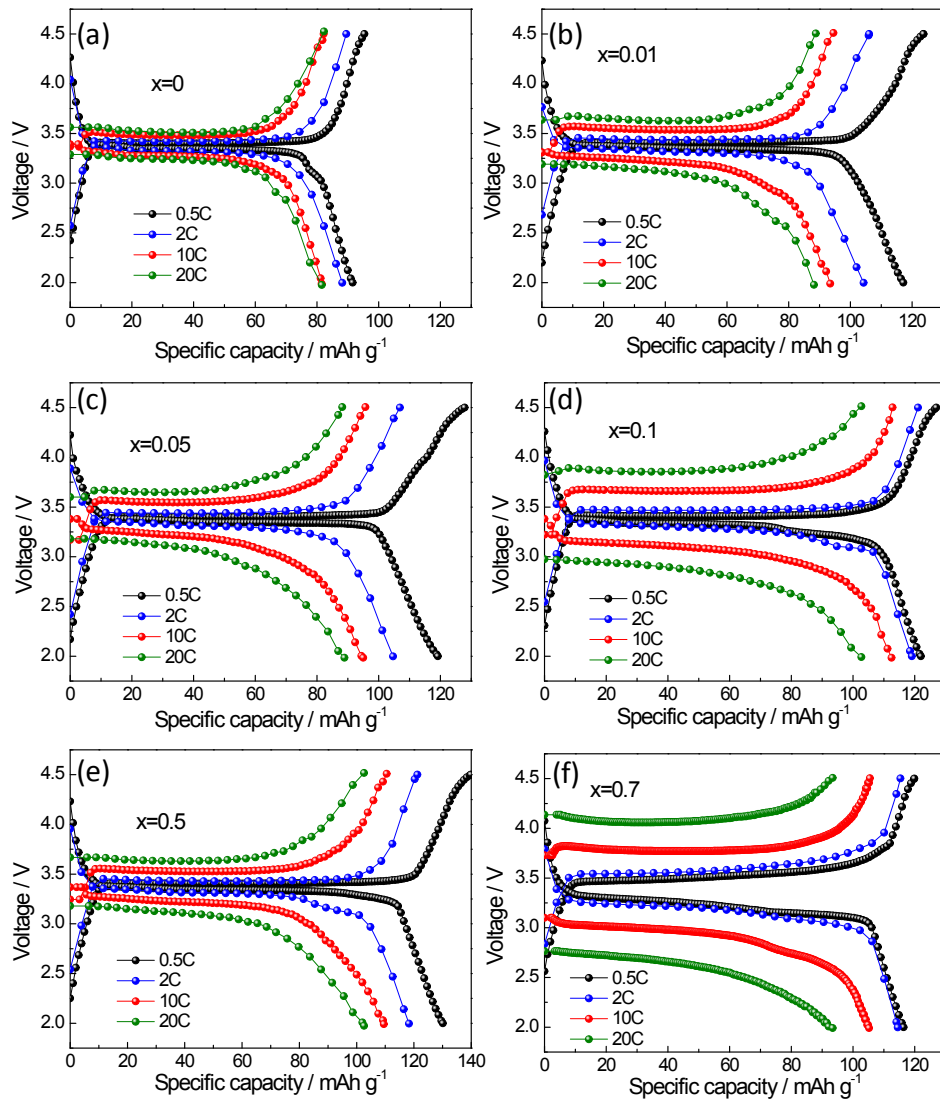


Figure S2. Charge-discharge profiles at different rates (0.5C, 2C, 10C and 20C) for the Na_{3-x}Li_xV₂(PO₄)₃/C samples (a) x = 0, (b) x = 0.01, (c) x = 0.05, (d) x = 0.1, (e) x = 0.5 and (f) x = 0.7.

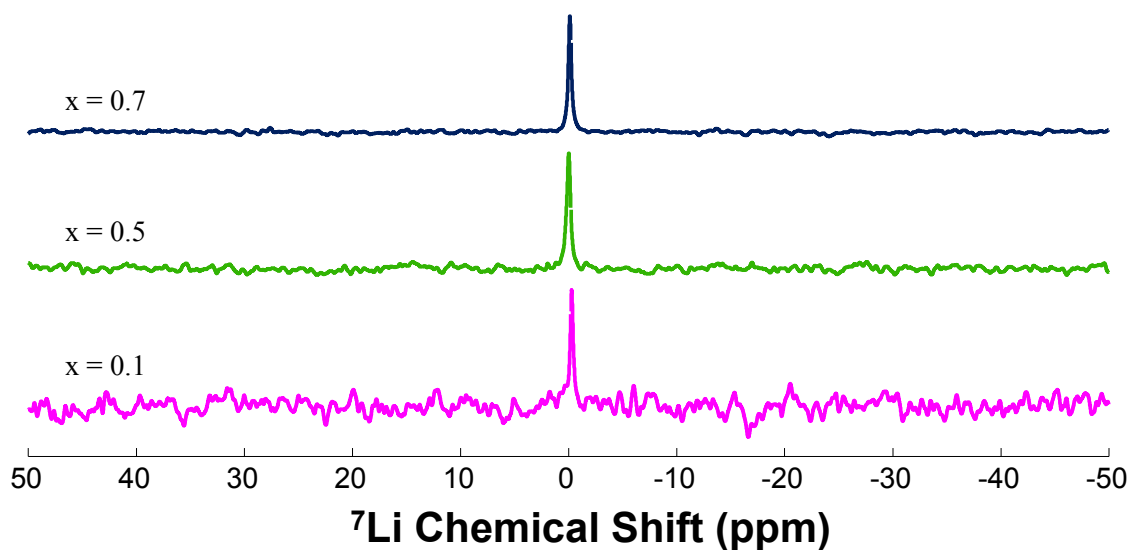


Figure S3. ^7Li liquid NMR spectra of the electrolyte solvent after immersing $\text{Na}_{3-x}\text{Li}_x\text{V}_2(\text{PO}_4)_3$ cathode materials.

Table S1. Theoretical weight ratio and ICP results for the elements in the $\text{Na}_{3-x}\text{Li}_x\text{V}_2(\text{PO}_4)_3/\text{C}$ ($x = 0, 0.01, 0.05, 0.1, 0.5$ and 0.7) samples.

Samples	Na	Li	P	V	C
	Thr./Exp.(%)	Thr./ Exp.(%)	Thr./ Exp.(%)	Thr./ Exp.(%)	Exp.(%)
$x = 0$	13.80/13.80	0.00/0.00	18.60/18.11	20.35/19.09	8.84
$x = 0.01$	13.70/13.65	0.01/0.01	18.53/17.64	20.28/18.41	9.22
$x = 0.05$	13.62/13.60	0.07/0.05	18.67/17.78	20.42/19.73	8.69
$x = 0.1$	13.45/13.13	0.14/0.09	18.75/17.43	20.51/18.96	8.45
$x = 0.5$	11.65/11.51	0.71/0.68	18.84/18.10	20.61/19.74	9.31
$x = 0.7$	10.85/10.94	1.00/0.93	19.07/18.20	20.87/19.14	8.82

Table S2. Relative integral of Na2 and Na1 sites in the ^{23}Na ssNMR spectra of $\text{Na}_{3-x}\text{Li}_x\text{V}_2(\text{PO}_4)_3$ samples.

	Relative Intensity					
	$x = 0$	$x = 0.01$	$x = 0.05$	$x = 0.1$	$x = 0.5$	$x = 0.7$
Na2(M2)	0.66	0.65	0.63	0.53	0.58	0.71
Na1(M1)	0.34	0.35	0.37	0.47	0.42	0.29
Ratio (Na2: Na1)	1.94	1.86	1.70	1.13	1.38	2.45

Table S3. Ions occupancy in the $\text{Na}_3\text{V}_2(\text{PO}_4)_3$, $\text{Na}_{2.9}\text{Li}_{0.1}\text{V}_2(\text{PO}_4)_3$, $\text{Na}_{2.5}\text{Li}_{0.5}\text{V}_2(\text{PO}_4)_3$ and $\text{Na}_{2.3}\text{Li}_{0.7}\text{V}_2(\text{PO}_4)_3$ samples.

Samples	Na1	Na2	V	P	O1	O2	Ratio (Na2/Na1)
$x = 0$	0.7894	0.7466	1	1	1	1	1.8916
$x = 0.1$	0.7959	0.7401	1	1	1	1	1.8598
$x = 0.5$	0.7408	0.7952	1	1	1	1	2.1469
$x = 0.7$	0.6969	0.8391	1	1	1	1	2.4081