

Table S1. Atomic coordinations, atomic occupancies, bond lengths obtained from Rietveld refinements of sample S, H, G, and their element valences derived from different models

Sample S	Atoms		Sites	x	y	z	B / Å ²	Occupancies
	Li/Fe		4a	0.00000	0.00000	0.00000	2.8300	0.979/0.021
	Fe/Li		4c	0.28220	0.25000	0.97350	0.4860	0.933/0.067
	P		4c	0.09530	0.25000	0.41680	0.8280	1.0
	O		4c	0.09590	0.25000	0.74360	1.1170	1.0
	O		4c	0.45450	0.25000	0.20440	0.4340	1.0
	O		8d	0.16500	0.04600	0.28170	0.6860	1.0
Bond length (Å)								
Li/Fe	-O1	2.1624 (6)	Fe/Li	-O1	2.2050 (1)	P	-O1	1.5346 (6)
	-O1	2.1624 (6)		-O2	2.0824 (9)		-O2	1.5609 (7)
	-O2	2.0961 (2)		-O3	2.2485 (3)		-O3	1.5537 (7)
	-O2	2.0961 (2)		-O3	2.0632 (8)		-O3	1.5537 (7)
	-O3	2.1738 (4)		-O3	2.0632 (8)			
	-O3	2.1738 (4)		-O3	2.2485 (3)			
Atoms	Valences							
	Bond valence sum				Charge distribution model			
Li/Fe	0.984 (2.031)				1.009 (2.018)			
Fe/Li	2.031 (0.984)				1.984 (0.992)			
P	4.886				5.007			
O1	1.869				1.924			
O2	1.952				1.980			
O3	2.016				2.048			

Sample H	Atoms	Sites	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> /Å ²	Occupancies
	Li/Fe	4a	0.00000	0.00000	0.00000	2.9451	0.974/0.026
	Fe/Li	4c	0.28225	0.25000	0.97446	0.5653	0.932/0.068
	P	4c	0.09562	0.25000	0.41726	0.8354	1.0
	O	4c	0.09641	0.25000	0.74228	0.9483	1.0
	O	4c	0.45384	0.25000	0.20794	0.6964	1.0
	O	8d	0.16467	0.04653	0.28392	0.6530	1.0

Bong length (Å)

Li/Fe	-O1 2.1682 (9)	Fe/Li	-O1 2.2047 (5)	P	-O1 1.5254 (2)
	-O1 2.1682 (9)		-O2 2.0814 (6)		-O2 1.5758 (8)
	-O2 2.0869 (4)		-O3 2.2517 (1)		-O3 1.5456 (6)
	-O2 2.0869 (4)		-O3 2.0651 (0)		-O3 1.5456 (6)
	-O3 2.1766 (4)		-O3 2.0651 (0)		
	-O3 2.1766 (4)		-O3 2.2517 (1)		

Atoms	Valences	
	Bond valence sum	Charge distribution
Li/Fe	0.992 (2.035)	1.016 (2.033)
Fe/Li	2.047 (0.986)	1.982 (0.991)
P	4.952	5.001
O1	1.906	1.952
O2	1.925	1.907
O3	2.043	2.071

Sample G	Atoms		Sites	x	y	z	B / Å ²	Occupancies
	Li/Fe		4a	0.00000	0.00000	0.00000	3.689	0.976/0.024
	Fe/Li		4c	0.28240	0.25000	0.97459	0.388	0.936/0.064
	P		4c	0.09480	0.25000	0.41752	0.674	1.0
	O		4c	0.09703	0.25000	0.74488	0.771	1.0
	O		4c	0.45463	0.25000	0.20723	0.440	1.0
	O		8d	0.16483	0.04608	0.28450	0.517	1.0
Bond length (Å)								
Li/Fe	-O1	2.1645 (5)	Fe/Li	-O1	2.1951 (7)	P	-O1	1.5362 (3)
	-O1	2.1645 (5)		-O2	2.0853 (1)		-O2	1.5600 (2)
	-O2	2.0872 (4)		-O3	2.2545 (3)		-O3	1.5520 (0)
	-O2	2.0872 (4)		-O3	2.0611 (2)		-O3	1.5520 (0)
	-O3	2.1794 (5)		-O3	2.0611 (2)			
	-O3	2.1794 (5)		-O3	2.2545 (3)			
Atoms	Valences							
	Bond valence sum				Charge distribution			
Li/Fe	0.991 (2.046)				1.009 (2.018)			
Fe/Li	2.041 (0.989)				1.985 (0.993)			
P	4.917				5.065			
O1	1.879				1.919			
O2	1.973				1.987			
O3	2.028				2.047			

Refs.	Synthesis conditions	Morphology	size of primary particles	Loading material: conductive additive: PVDF
ACS Nano 5637-5646, 7 (6), 2013	Hydrothermal 400°C for 2h	Nanosheets	3.7-4.6 nm thick	80:10:10 Carbon nanotubes
J. Power Source 223, 100-106, 2013	Hydrothermal 150°C for 12h	Nanoparticles	5-20 nm	80:10:10 Carbon black
RCS Advances 3, 3421-3427, 2013	Hydrothermal 160°C for 2h Solvothermal 400°C for 12h	Nanoparticles	66.5 nm	80:15:5 Carbon black
NanoLett. 14, 5632- 5636, 2012	Solvothermal 180 °C for 10h	Nanoplates	30 nm thick	50:35:15 Carbon black
Nature	Solid state reaction	Nanoparticles	50 nm	80: 15: 5 Carbon black
Chem Comm	Impinge jet reaction followed by 350°C for 6 h and 700°C for 10h	Nanoparticles	50 nm	75: 15 :10 Carbon black