Supporting Information

Lithium deintercalation behavior in Li-rich vanadium phosphate as a potential cathode for Li-ion batteries

Quan Kuang,[a] Zhiping Lin,[a,b] Yanming Zhao,*[a,c] Xiaolong Chen,[d] and Liquan Chen[d]

[a] *School of Materials, South China University of Technology, Guangzhou 510640, P. R. China*
[b] *School of Physics, Guangdong University of Technology, Guangzhou 510090, P. R. China*
[c] *Department of Physics, South China University of Technology, Guangzhou 510640, P. R. China*
[d] *Institute of Physics, Chinese Academy Science, Beijing 100080, P. R. China*

Table S1. Structure parameters of $Li_9V_3(P_2O_7)_3(PO_4)_2$ determined from Rietveld refinement of high power X-ray diffraction at 300 K and first-principles density functional calculations (enclosed in parentheses).

Atoms	*Wyckoff Sites*	*x*	*y*	*z*	*Occupancy*
P(1)	4d	2/3 (0.6667)	1/3 (0.3333)	0.6245 (0.6228)	1.00
P(2)	12g	0.3157 (0.3146)	0.0883 (0.0877)	0.8454 (0.8462)	1.00
V	6f	0.5679 (0.5692)	0 (0)	3/4 (0.75)	1.00
Li(1)	2b	0 (0)	0 (0)	0 (0)	1.00
Li(2)	4d	2/3 (0.6667)	1/3 (0.3334)	0.8846 (0.8752)	1.00
Li(3)	12g	0.3364 (0.3377)	0.1016 (0.0997)	0.0622 (0.0615)	1.00
O(1)	4d	2/3 (0.6667)	1/3 (0.3333)	0.5131 (0.5108)	1.00
O(2)	6f	0.2105 (0.2089)	0 (0)	3/4 (0.75)	1.00
O(3)	12g	0.6763 (0.6795)	0.1878 (0.1893)	0.6638 (0.6633)	1.00
O(4)	12g	0.4798 (0.4814)	0.1052 (0.1069)	0.8355 (0.8348)	1.00
O(5)	12g	0.3292 (0.3284)	0.2536 (0.2523)	0.8451 (0.8476)	1.00
O(6)	12g	0.2229 (0.2222)	0.9937 (0.9918)	0.9356 (0.9364)	1.00

Space group: $P\bar{3}c1$ (trigonal), unit cell parameters: a=b=9.737 (9.6761) Å, c=13.615 (13.4806) Å, α=β=90°, γ=120°. Cell volume: 1117.89 (1093.31) Å^3. Reliability factors—R_p: 7.5%, R_{wp}: 11.8%.