Electronic Supplementary Information

Kinetics in conventional carbon coated-$Li_3V_2(PO_4)_3$ and nanocomposites $Li_3V_2(PO_4)_3$/graphene as cathode materials for power lithium ion batteries

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Graphene Oxide (GO) making

Graphite oxide (GiO) was prepared by a modified Hummers method (ref.30 in main text). 100 ml of concentrated H_2SO_4 (98 %) were added slowly into the mixture of 2.0 g of $NaNO_3$ and 4.0 g of natural graphite (300 mesh) below 0 ºC. The mixture was stirred for 30 minutes before slow addition of 15 g $KMnO_4$ in an hour. Then, the mixture was heated to 35±3 ºC and stirred for 2 hours. Subsequently, 180 ml of water was dropwise added under vigorous stirring, causing a quick rise in temperature to near 100 ºC. The slurry was stirred at this temperature for another 30 minutes. Afterwards, 14 ml of H_2O_2 solution (30 wt%) and 120 ml of water were added sequentially to dissolve insoluble manganese species. The resulting graphite oxide suspension was filtrated and washed using 300 ml dilute HCl (3%) solution. After dispersing the collected precipitate into 1200 ml water, the solution was centrifuged and washed twice with water. The colloidal G_iO was obtained and dried under vacuum at 80 ºC for two days. The resulting product was ground into powder (100 mesh).

50 mg G_iO powder was dispersed into 500 ml H_2O, and a brown homogeneous suspension was obtained after ultrasonicated for 4 hours.

Supplementary Tables and Figures

Table S1 Atomic sites and fractional coordinates of LVP, LVP/C and LVP/G.

Atom [a]	*x*			*y*			*z*		
	LVP [b]	LVP/C [c]	LVP/G [d]	LVP	LVP/C	LVP/G	LVP	LVP/C	LVP/G
Li1(4e)	0.3024(7)	0.3249(3)	0.2083(3)	0.4325(3)	0.3214(2)	0.3025(5)	0.2710(4)	0.2763(2)	0.2534
Li2(4e)	0.5949(2)	0.4934(3)	0.7553(6)	0.4325(3)	0.2083(2)	0.1474(7)	0.4029(8)	0.4007(2)	0.4554(0)
Li3(4e)	0.9213(2)	0.9285(3)	0.9906(2)	0.4325(3)	0.2283(2)	0.2668(2)	0.3156(3)	0.2940(2)	0.3692(2)
V1(4e)	0.2485(5)	0.2484(8)	0.2457(1)	0.1088(6)	0.1098(8)	0.1080(2)	0.4620(4)	0.4631(3)	0.4613(0)
V2(4e)	0.7513(8)	0.7541(4)	0.7580(1)	0.3889(6)	0.3880(9)	0.3859(8)	0.4714(6)	0.4699(0)	0.4688(9)
P1(4e)	0.1046(4)	0.1105(5)	0.1217(3)	0.1474(7)	0.1404(0)	0.1438(8)	0.1020(7)	0.0963(5)	0.0993(5)
P2(4e)	0.6064(1)	0.5974(4)	0.6022(7)	0.3542(0)	0.3510(3)	0.3508(8)	0.1129(6)	0.1176(4)	0.1163(9)
P3(4e)	0.0397(9)	0.0398(6)	0.0387(3)	0.4930(9)	0.4895(0)	0.4930(7)	0.2569(0)	0.2493(6)	0.2550(1)
O1(4e)	0.4257(8)	0.4456(8)	0.4698(4)	0.3299(7)	0.3197(5)	0.3169(5)	0.0843(9)	0.1060(8)	0.1007(8)
O2(4e)	0.9317(2)	0.9324(7)	0.9122(8)	0.1567(0)	0.1441(5)	0.1447(0)	0.1147(4)	0.1148(7)	0.1001(5)
O3(4e)	0.3471(0)	0.3478(7)	0.3335(4)	0.2651(4)	0.2682(4)	0.2672(5)	0.4802(2)	0.4853(8)	0.4714(8)
O4(4e)	0.8049(6)	0.8002(7)	0.7955(9)	0.2158(2)	0.2226(5)	0.2256(4)	0.4903(7)	0.5043(7)	0.4917(9)
O5(4e)	0.1763(3)	0.1739(8)	0.1727(4)	0.0383(0)	0.0390(5)	0.0406(2)	0.0574(4)	0.0367(7)	0.0330(1)
O6(4e)	0.6489(1)	0.6378(8)	0.6447(8)	0.4742(5)	0.4753(4)	0.4633(0)	0.0800(7)	0.1102(7)	0.1047(5)
O7(4e)	0.4596(5)	0.4433(7)	0.4374(6)	0.0710(8)	0.0674(4)	0.0605(8)	0.3678(7)	0.3836(7)	0.3744(2)
O8(4e)	0.9297(5)	0.9111(7)	0.9177(5)	0.4086(0)	0.4085(4)	0.4173(1)	0.3274(7)	0.3230(7)	0.3251(5)
O9(4e)	0.1640(3)	0.1831(7)	0.1924(8)	0.4325(3)	0.4213(5)	0.4377(7)	0.1687(1)	0.1634(6)	0.1727(4)
O10(4e)	0.6193(1)	0.6127(5)	0.6113(7)	0.4325(3)	0.0689(2)	0.0666(2)	0.1365(9)	0.1380(5)	0.1390(3)
O11(4e)	0.1659(5)	0.1613(7)	0.1608(6)	0.4325(3)	0.1816(5)	0.1806(3)	0.2602(2)	0.2550(7)	0.2595(2)
O12(4e)	0.6451(9)	0.6348(1)	0.6030(9)	0.4325(3)	0.3228(8)	0.3146(8)	0.2823(5)	0.2894(1)	0.2855(1)

[a.] The atomic number is shown in Fig. S4

[b.] For pure LVP, lattice constants a=8.6115(3) Å, b=12.0461(9) Å, c=8.5993(0) Å, and γ = 90.554(0)°, V = 892.02 Å^3. The reliable factors are wRp% = 4.62%, Rp = 3.29%, χ^2 = 1.007, and R_f = 1.43%.

[c.] For LVP/C, lattice constants a=8.6393(4) Å, b=12.0979(5) Å, c=8.6347(2) Å, and γ = 90.522(1)°, V = 902.45 Å^3. The reliable factors are wRp% = 4.03%, Rp = 3.20%, χ^2 = 0.6237, and R_f = 1.51%.

[d.] For LVP/graphene, lattice constants a=8.6445(9) Å, b=12.0889(9) Å, c=8.6284(9) Å, and γ = 90.573(1)°, V = 901.67 Å^3. The reliable factors are wRp% = 5.57%, Rp = 4.21%, χ^2 = 1.006, and R_f = 2.77%.

Table S2 Calculated bond lengths (Å) of the samples LVP, LVP/C and LVP/G.

Bond	LVP	LVP/C	LVP/G	CP75012h*
Li1-O1	1.9282(0)	1.8032(2)	2.6208(3)	2.114(5)
Li1-O3	1.9524(3)	1.9272(1)	2.2138(6)	1.843(5)
Li2-O2	2.78485(4)	2.645(24)	-	2.092(1)
Li2-O4	2.03145(4)	2.801(24)	-	2.120(8)
Li3-O2	1.92522(3)	1.853(19)	2.829(20)	1.967(9)
Li3-O4	1.81023(3)	2.128(20)	2.047(19)	1.882(4)
V1-O3	2.06345(5)	2.101(6)	2.06408(5)	2.008(9)
P1-O2	1.49834(3)	1.548(7)	1.81078(4)	1.556(1)

*: The data are referred from the reference [11] in main text.

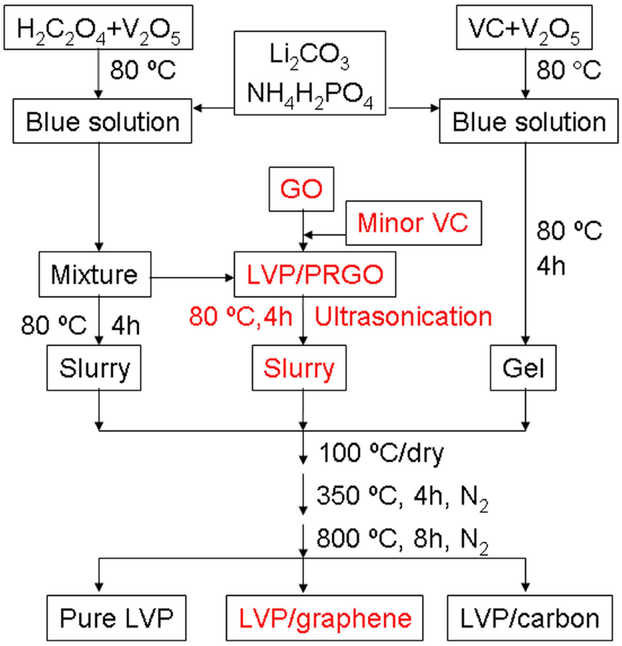

Fig. S1 Schematic preparation routes for the samples LVP, LVP/C and LVP/G.

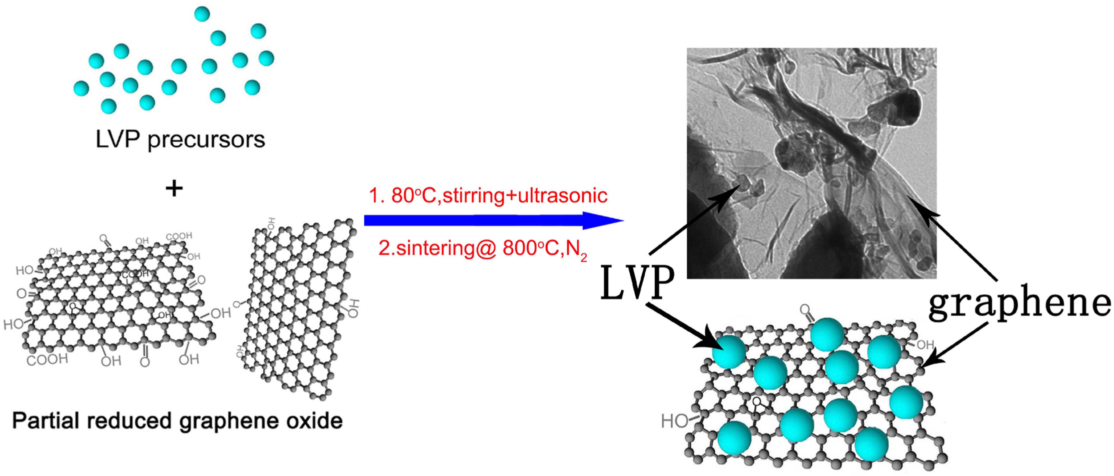

Fig. S2 Schematic diagram of the synthesis and the structure of LVP/G composite.

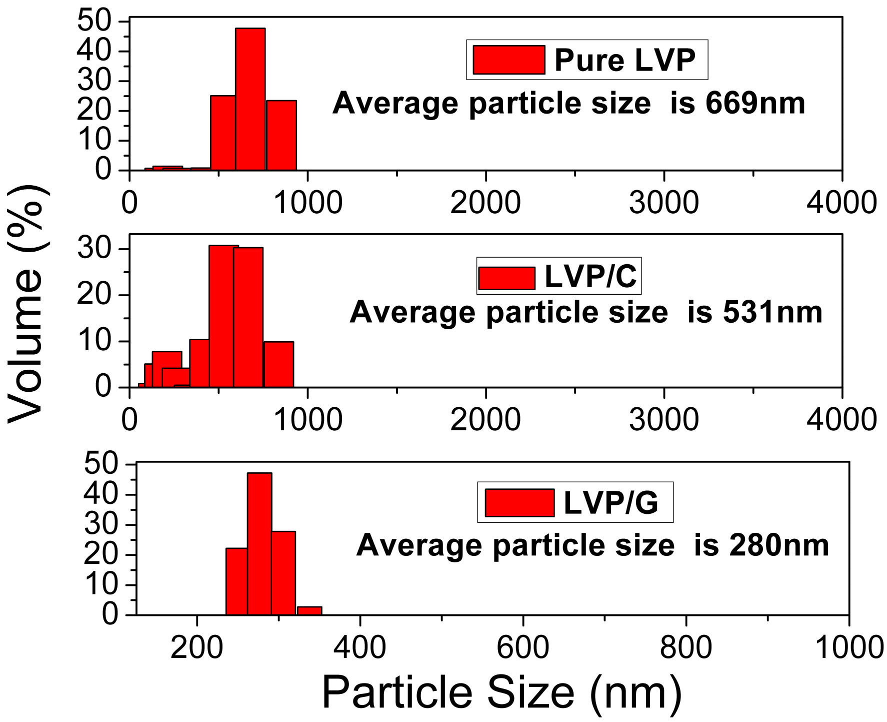

Fig. S3 Particle size distributions of pure LVP, LVP/C and LVP/graphene materials

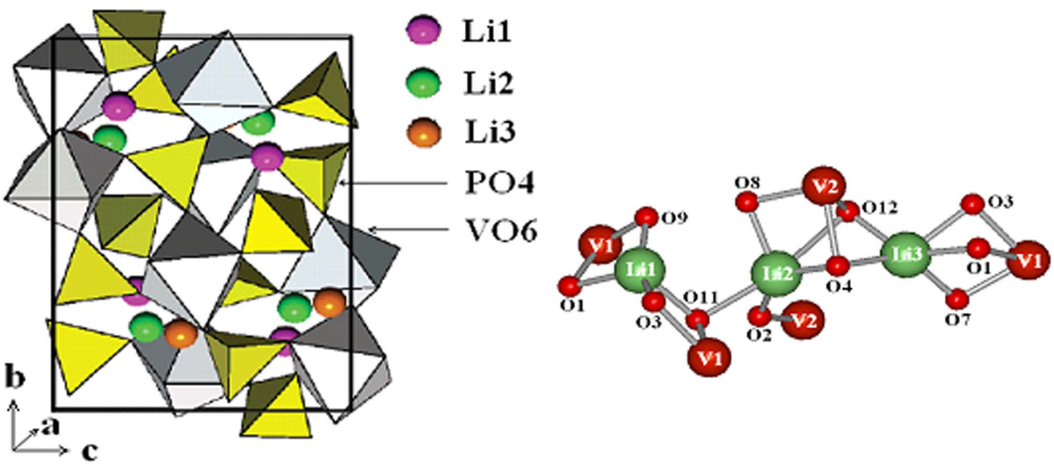

Fig. S4 (a) Lattice structure and (b) Li atomic coordination environments of $Li_3V_2(PO_4)_3$.

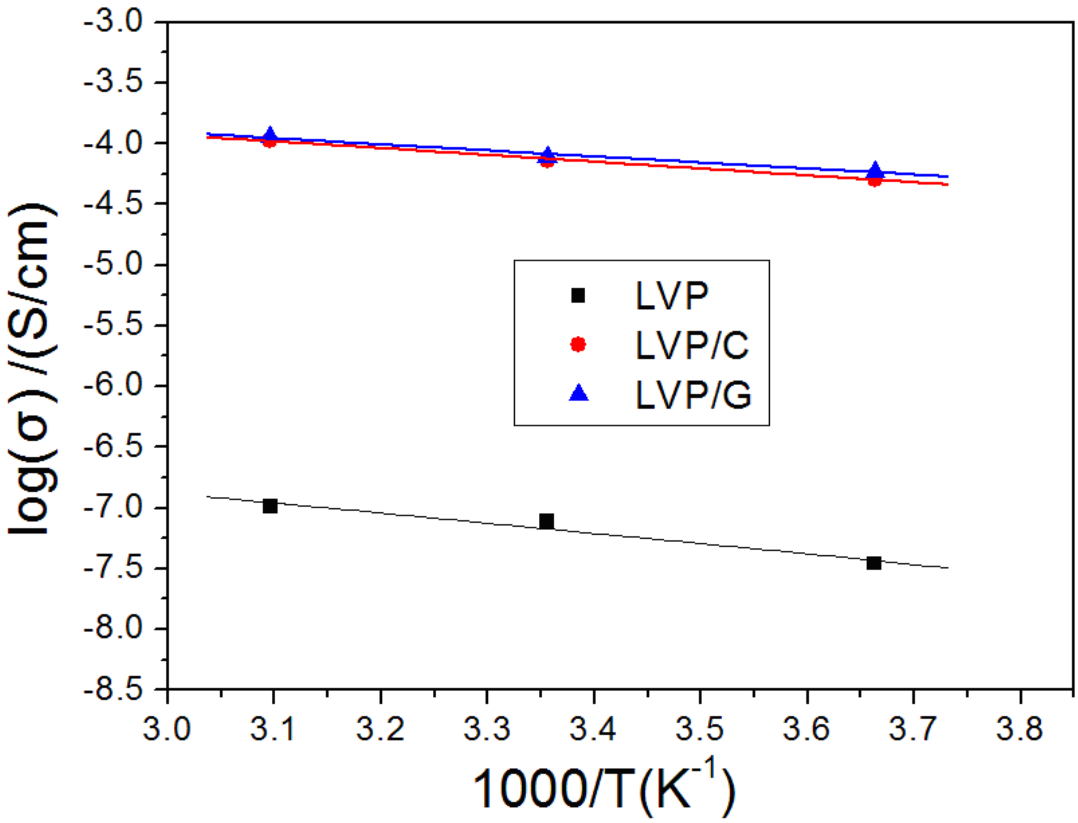

Fig. S5 Grain interior DC conductivity vs. reciprocal temperature of the samples LVP, LVP/C and LVP/G.

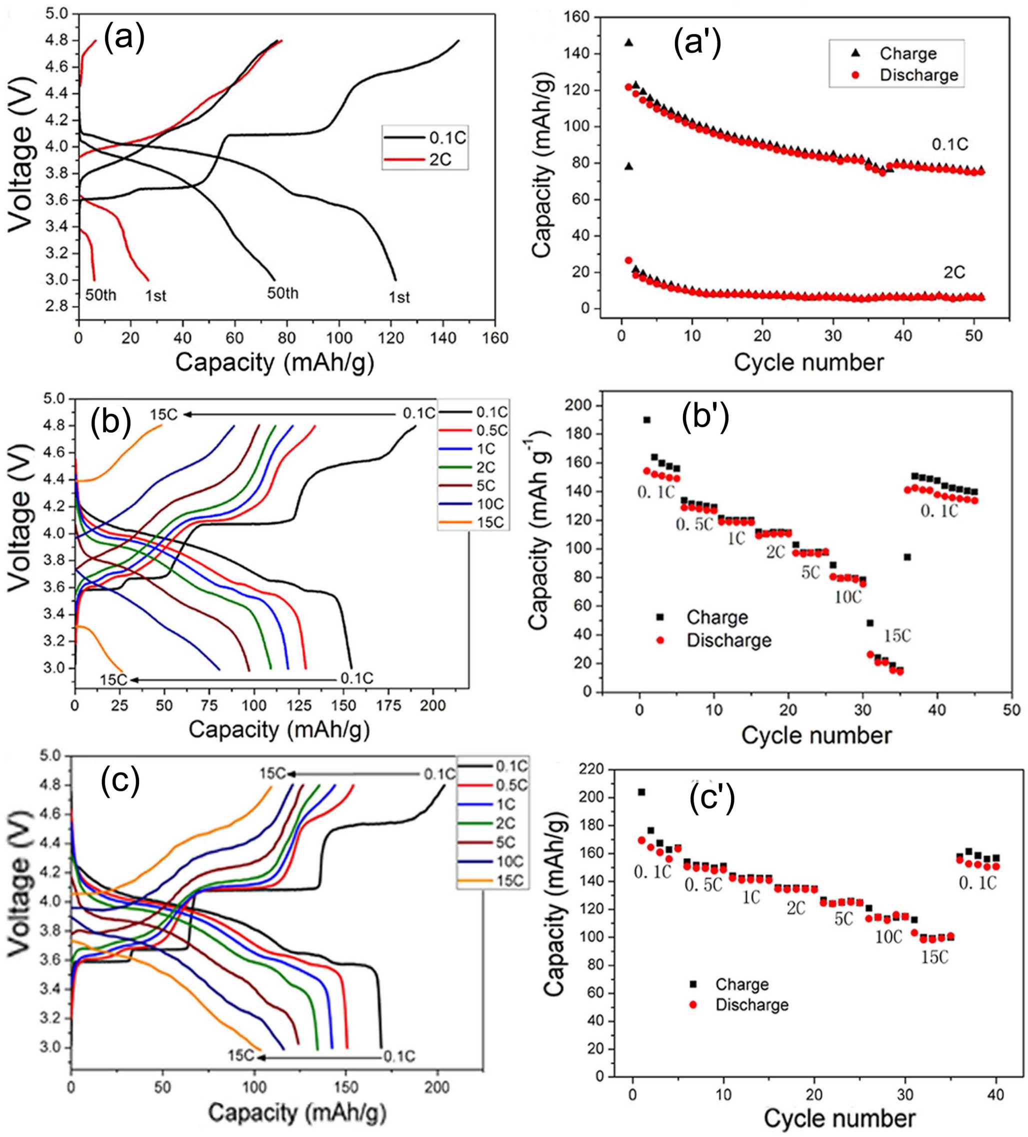

Fig. S6 The charge/discharge profiles and cycle performance at various constant charge-discharge current rates for the samples (a) pure LVP, (b) LVP/C and (c) LVP/G. The cut-off voltage is between 3 and 4.8V.