Single-phase lithiation and delithiation of simferite compounds $Li(Mg,Mn,Fe)PO_4$

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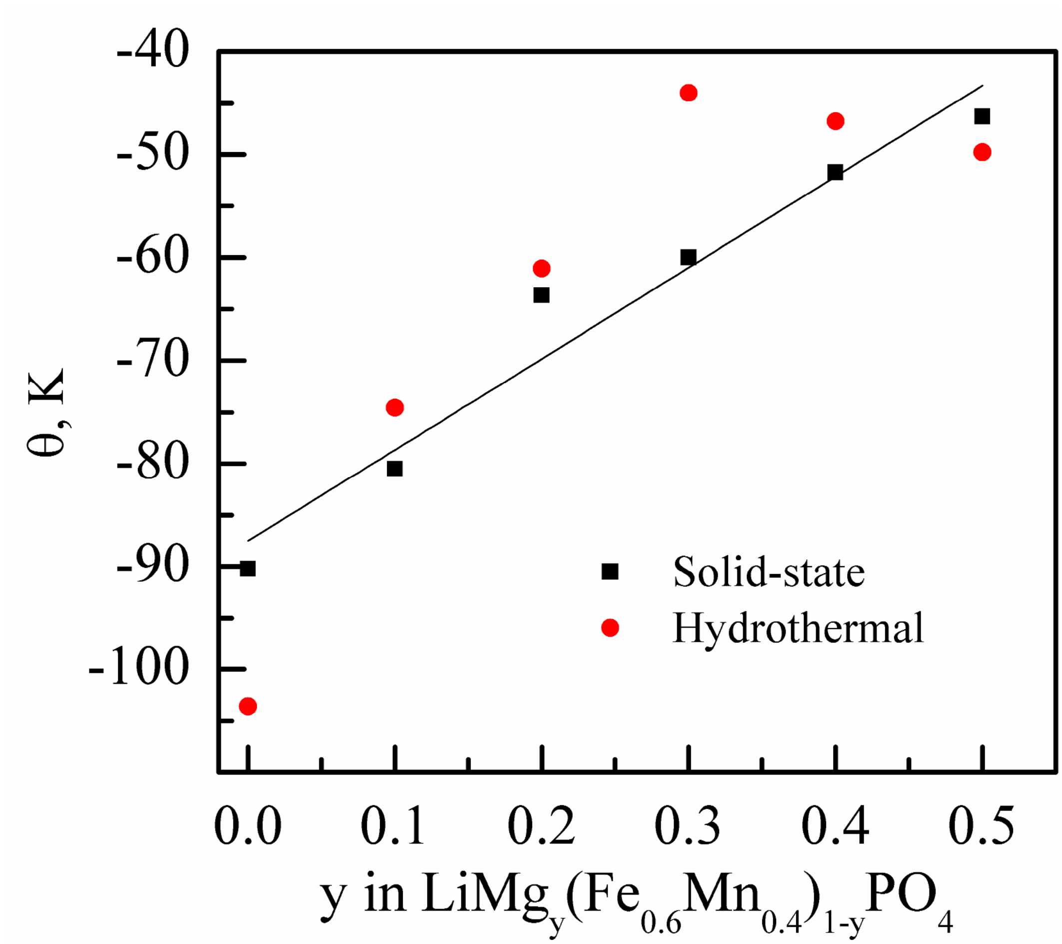

Figure S1: Comparison of the Curie-Weiss temperature as a function of Mg concentration in $Li(Mg_y(Fe_{0.6}Mn_{0.4})_{1-y})PO_4$, $(0 \leq y \leq 0.5)$ for solid-state and hydrothermal synthesized samples.

Table S1: Sample composition and lattice parameters.

Sample Composition	*a* (Å)	*b* (Å)	*c* (Å)	V (Å³)	R_p,%	χ^2
[a]$LiFe_{0.6}Mn_{0.4}PO_4$	10.3697(2)	6.0393(1)	4.7110(1)	295.03(1)	6.7	1.9
[b]$[Li_{0.94}Fe_{0.05}][Fe_{0.6}Mn_{0.4}]PO_4$	10.3856(5)	6.0416(3)	4.7173(2)	295.99(1)	6	1.9
[a]$LiMg_{0.1}Fe_{0.54}Mn_{0.36}PO_4$	10.3491(2)	6.0304(1)	4.7129(1)	294.13(1)	6.2	1.7
[a]$LiMg_{0.2}Fe_{0.48}Mn_{0.32}PO_4$	10.3205(2)	6.0150(1)	4.7096(1)	292.36(1)	6.0	1.7
[b]$[Li_{0.91}Fe_{0.04}][Mg_{0.2}Fe_{0.48}Mn_{0.32}]PO_4$	10.3660(6)	6.0250(3)	4.7207(2)	294.83(2)	5	1.8
[a]$LiMg_{0.3}Fe_{0.42}Mn_{0.28}PO_4$	10.3010(2)	6.0056(1)	4.7104(1)	291.40(1)	5.4	1.5
[a]$LiMg_{0.4}Fe_{0.36}Mn_{0.24}PO_4$	10.2695(2)	5.9884(1)	4.7048(1)	289.34(1)	6.1	1.8
[a]$LiMg_{0.5}Fe_{0.3}Mn_{0.2}PO_4$	10.2505(2)	5.9765(1)	4.7041(1)	288.18(1)	5.6	1.8
[b]$[Li_{0.92}Fe_{0.04}][Mg_{0.5}Fe_{0.3}Mn_{0.2}]PO_4$	10.2652(5)	5.9800(3)	4.7083(2)	289.02(2)	6.0	1.8

[a]Solid-state and [b]hydrothermal synthesized sample

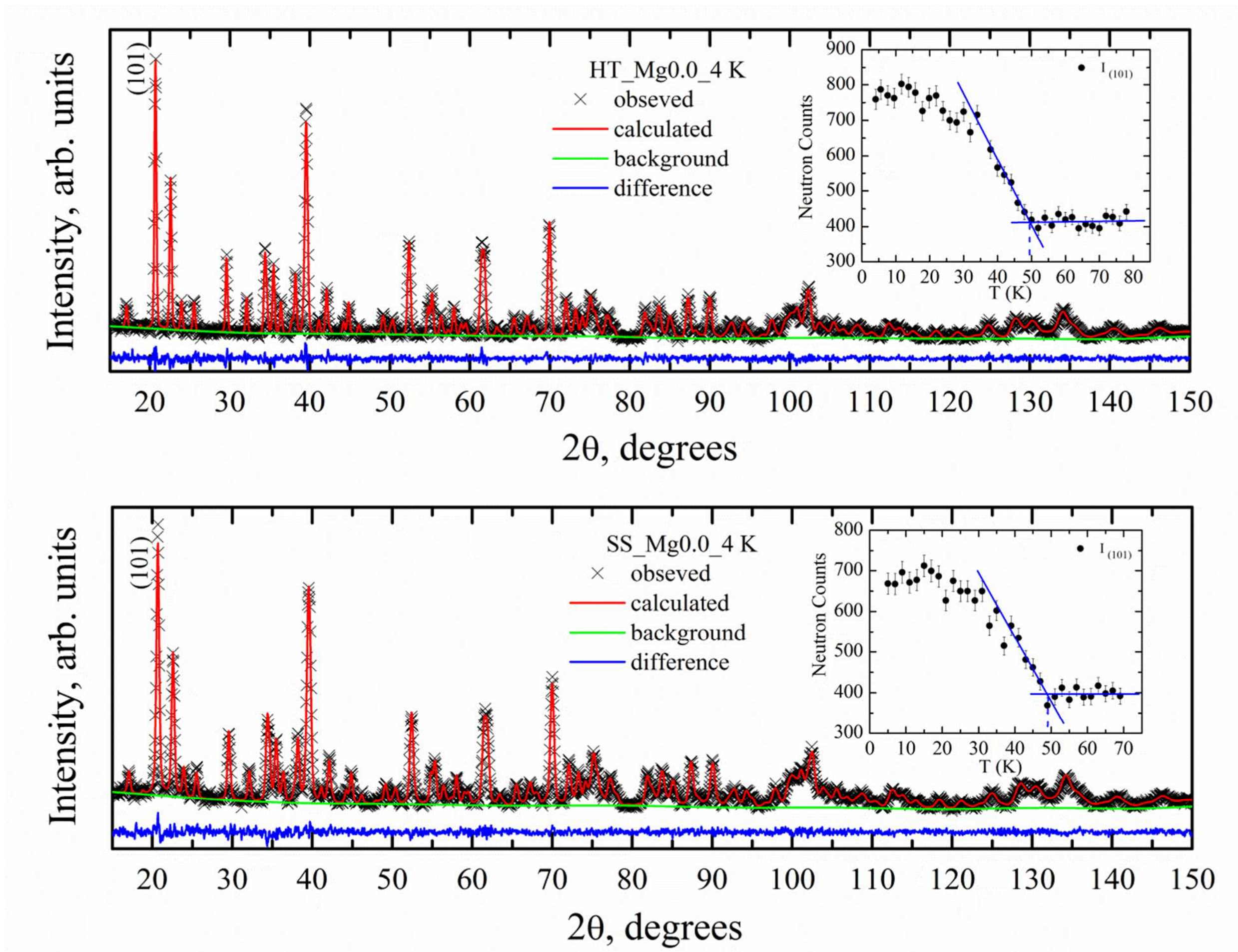

Figure S2. Neutron diffraction patterns at 4 K of hydrothermal (top) and solid-state (bottom) $LiFe_{0.6}Mn_{0.4}PO_4$ and their structural (space group Pnma) and magnetic (Shubnikov group Pnma’) refinements. The insets show intensity of (101) reflection as a function of temperature.

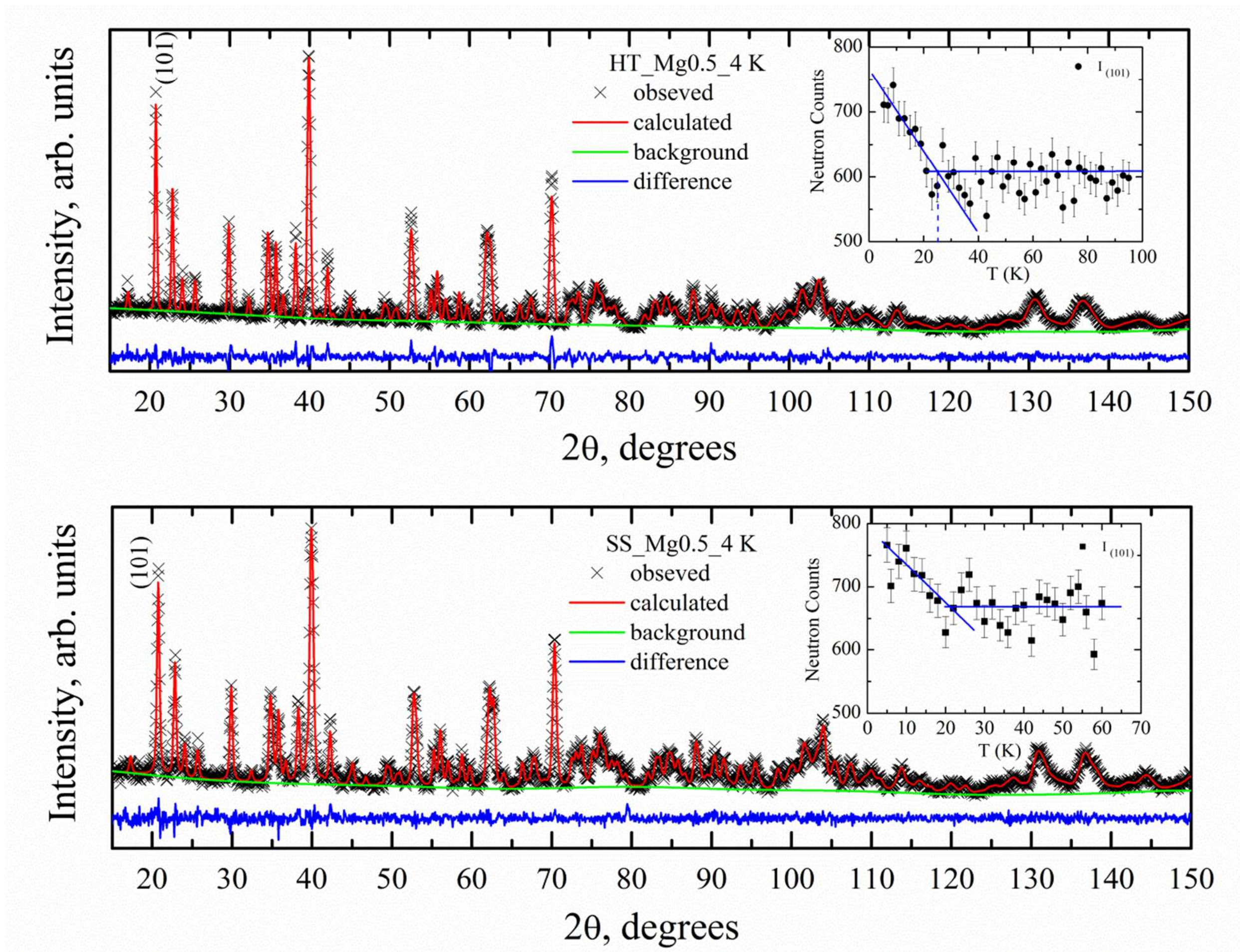

Figure S3. Neutron diffraction patterns at 4 K of hydrothermal (top) and solid-state (bottom) $LiMg_{0.5}Fe_{0.3}Mn_{0.2}PO_4$ and their structural (space group Pnma) and magnetic (Shubnikov group Pnma') refinements. The insets show intensity of (101) reflection as a function of temperature.

Table S2: Lattice parameters and magnetic moments of $LiMg_y(Fe_{0.6}Mg_{0.4})_{1-y}PO_4$ from neutron diffraction data refinements at 4 K.

Sample	*a* (Å)	*b* (Å)	*c* (Å)	V (Å³)	μ, μ_B	R_p,%	χ^2
HT, y = 0	10.3578(6)	6.0293(3)	4.7048(3)	293.82(3)	4.29(4)	4.5	0.9
HT, y = 0.2	10.3423(5)	6.0137(3)	4.7095(2)	292.91(3)	4.48(6)	4.1	1.2
HT, y = 0.5	10.2392(9)	5.9658(5)	4.6960(3)	286.86(6)	4.5(2)	4.7	1.1
SS, y = 0	10.3427(6)	6.0291(4)	4.7019(3)	293.20(4)	4.30(5)	3.9	0.8
SS, y = 0.2	10.2914(9)	6.0025(5)	4.6982(2)	290.23(6)	4.24(9)	4.0	0.8
SS, y = 0.5	10.2211(8)	5.9623(4)	4.6921(3)	285.95(5)	3.5(2)	4.0	0.9