Supplementary Information

$Li_3Fe_2(HPO_3)_3Cl$: An Electroactive Iron Phosphite As a New Polyanionic Cathode Material for Li-ion Battery

Hooman Yaghoobnejad Asl,[a] Kartik Ghosh,[b] Melissa P. Vidal Meza[c] and Amitava Choudhury[a,*]

[a]Department of Chemistry, Missouri University of Science and Technology, Rolla, MO 65409, USA

[b]Department of Physics, Astronomy and Materials Science and Center for Applied Science and Engineering, Missouri State University, Springfield, Missouri 65897, USA.

[c]Department of Chemical and Biological Engineering, Missouri University of Science and Technology, Rolla, MO 65409, USA

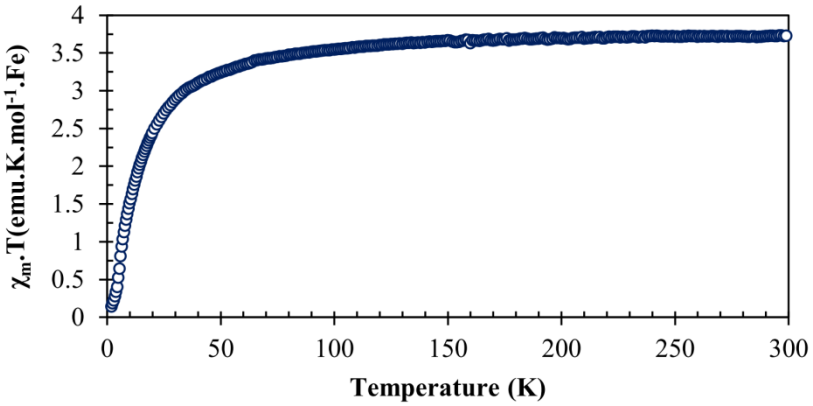

Figure S1. $\chi_m T$ versus T plot indicating the antiferromagnetic behavior of $Li_3Fe_2(HPO_3)_3Cl$ phase at low temperatures.

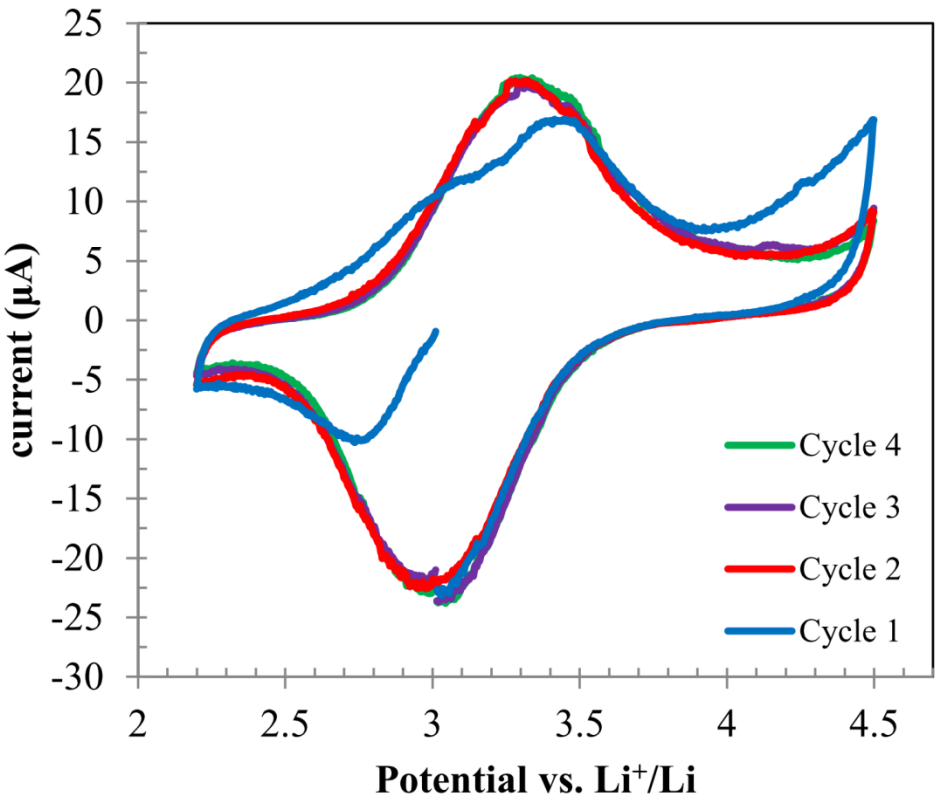

Figure S2. Cyclic voltammograms of $Li_3Fe_2(HPO_3)_3Cl$ cathode with scanning to the lower vertex potential initially.

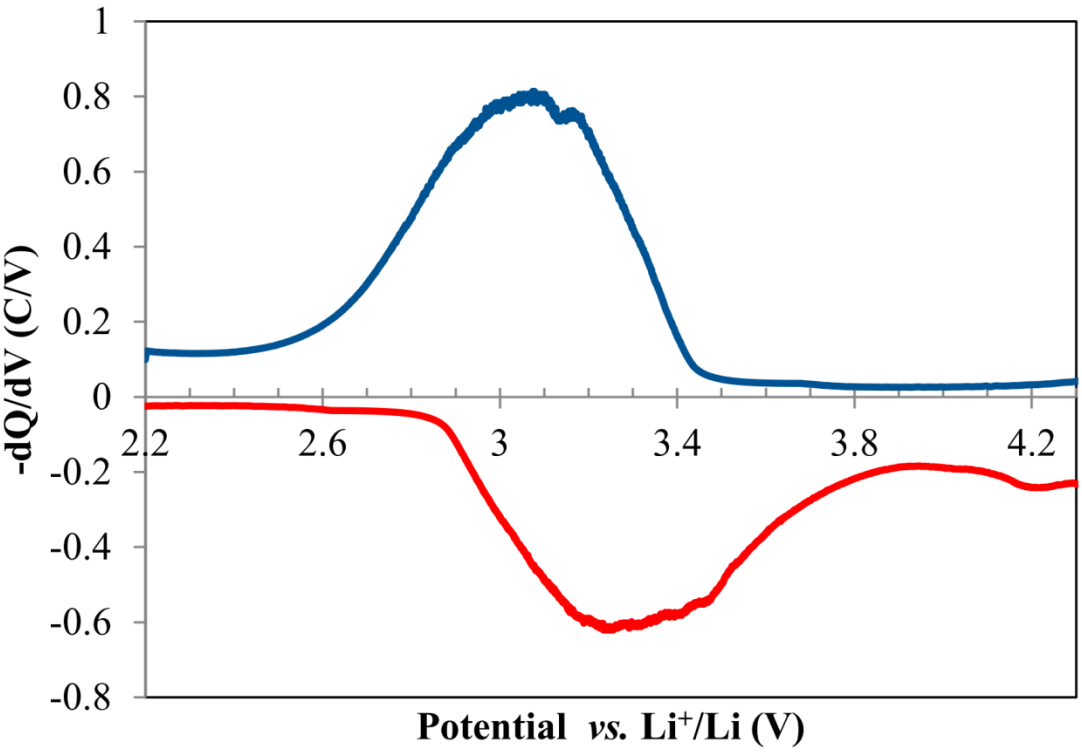

Figure S3 Voltage-charge derivative curve versus potential for discharge (blue) and charge (red) steps of $Li_3Fe_2(HPO_3)_3Cl$ cathode material.

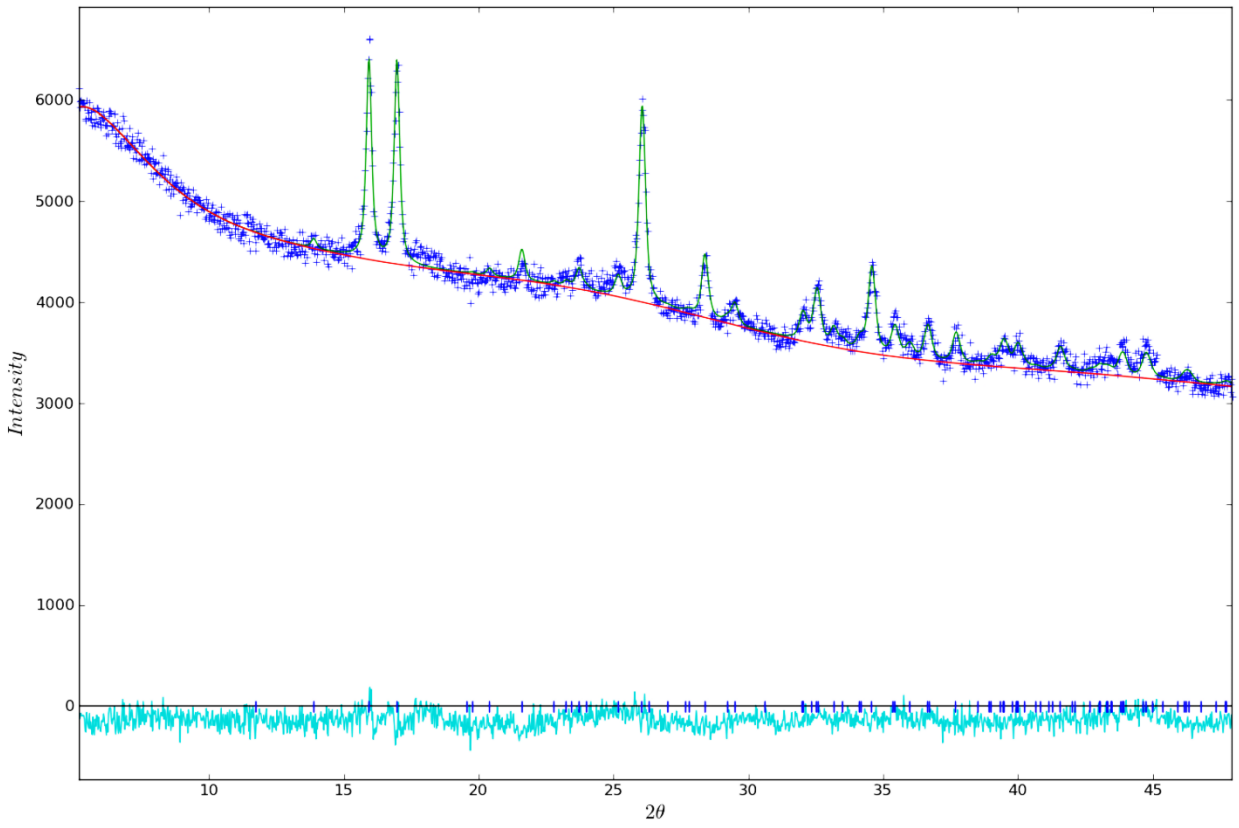

Figure S4 PXRD Rietveld refinement of $Li_3Fe_2(HPO_3)_3Cl$ phase after subjected to charge to 4.5 V *vs.* Li^+/Li.

Table S1 Impedance Fit Parameters for the equivalent circuit shown in Figure 12.

Temperature (°C)	L1 (H)	R1 (Ω)	R2 (Ω)	CPE1-T (F)	CPE1-P	W1-R (Ω)	W1-τ (s)	W1-P
23	4.1×10^{-6}	11.8	341.5	5.35×10^{-5}	0.64	6039	204.4	0.70
29	8.8×10^{-6}	9.9	303.3	1.09×10^{-4}	0.55	5295	206.5	0.71
33	7.8×10^{-6}	8.2	259.5	7.44×10^{-5}	0.62	4707	206.3	0.70
36	7.1×10^{-6}	7.5	254.4	7.43×10^{-5}	0.62	4634	205.2	0.70
40	6.5×10^{-6}	6.3	236.1	8.64×10^{-5}	0.61	4234	202.8	0.70
45	4.9×10^{-6}	5.4	215.6	1.18×10^{-4}	0.59	3733	202.6	0.70
50	6.3×10^{-6}	4.7	206.5	1.43×10^{-4}	0.58	3337	198.2	0.70

$Z_{ws} = \frac{R_W \times tanh(j\omega\tau)^P}{(j\omega\tau)^P}$ where $\tau = {L^2}/{D}$ and L and D are effective diffusion length and diffusion coefficients, respectively.