Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplementary Information

Table S1. Rietveld refined atomic positions in the $LiCo_{1-y}Fe_yPO_4$ samples (S.G. *Pnma*).

Atom	Wyckoff position	*x*	*y*	*z*	Occ.
$LiCoPO_4$: *a*=10.1742(3) Å, *b*=5.9140(2) Å, *c*=4.6915(2) Å, *V*=282.29(3) Å^3 R_{wp} = 3.36 %, χ^2 = 1.504					
Li	4*a*	0.5	0.5	1.0	1.0
Co	4*c*	0.7195(3)	0.25	0.521(1)	1.0
P	4*c*	0.5979(7)	0.75	0.575(2)	1.0
O (1)	4*c*	0.458(2)	0.75	0.724(2)	1.0
O (2)	4*c*	0.595(1)	0.75	0.258(3)	1.0
O (3)	8*d*	0.660(1)	0.543(1)	0.728(2)	1.0
$LiCo_{0.95}Fe_{0.05}PO_4$: *a*=10.1788(3) Å, *b*=5.9126(2) Å, *c*=4.6910(2) Å, *V*=282.32(2) Å^3 R_{wp} = 3.56 %, χ^2 = 1.626					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7216(2)	0.25	0.5193(8)	0.95
Fe	4*c*	0.7216(2)	0.25	0.5193(8)	0.05
P	4*c*	0.5958(6)	0.75	0.578(1)	1.0
O (1)	4*c*	0.452(1)	0.75	0.721(2)	1.0
O (2)	4*c*	0.591(1)	0.75	0.255(2)	1.0
O (3)	8*d*	0.6633(9)	0.541(1)	0.721(1)	1.0
$LiCo_{0.9}Fe_{0.1}PO_4$: *a*=10.1901(3) Å, *b*=5.9207(2) Å, *c*=4.6905(2) Å, *V*=282.99(2) Å^3 R_{wp} = 3.88 %, χ^2 = 1.896					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7212(3)	0.25	0.5202(8)	0.9
Fe	4*c*	0.7212(3)	0.25	0.5202(8)	0.1
P	4*c*	0.5952(6)	0.75	0.579(1)	1.0
O (1)	4*c*	0.452(1)	0.75	0.721(2)	1.0
O (2)	4*c*	0.595(1)	0.75	0.258(2)	1.0
O (3)	8*d*	0.6621(9)	0.540(1)	0.723(1)	1.0
$LiCo_{0.75}Fe_{0.25}PO_4$: *a*=10.2071(3) Å, *b*=5.9328(2) Å, *c*=4.6899(2) Å, *V*=283.97(2) Å^3 R_{wp} = 4.44 %, χ^2 = 2.165					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7204(2)	0.25	0.5225(8)	0.75
Fe	4*c*	0.7204(2)	0.25	0.5225(8)	0.25
P	4*c*	0.5949(6)	0.75	0.581(1)	1.0
O (1)	4*c*	0.452(1)	0.75	0.722(2)	1.0
O (2)	4*c*	0.593(1)	0.75	0.256(2)	1.0

O (3)	8*d*	0.6628(9)	0.542(1)	0.720(1)	1.0
$LiCo_{0.5}Fe_{0.5}PO_4$: *a*=10.2381(2) Å, *b*=5.9556(1) Å, *c*=4.6878(1) Å, *V*=285.83(2) Å^3 R_{wp} = 5.81 %, χ^2 = 1.559					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7204(2)	0.25	0.5233(7)	0.5
Fe	4*c*	0.7204(2)	0.25	0.5233(7)	0.5
P	4*c*	0.5948(4)	0.75	0.579(1)	1.0
O (1)	4*c*	0.451(1)	0.75	0.721(2)	1.0
O (2)	4*c*	0.5919(9)	0.75	0.253(2)	1.0
O (3)	8*d*	0.6633(7)	0.544(1)	0.719(1)	1.0
$LiCo_{0.25}Fe_{0.75}PO_4$: *a*=10.2721(2) Å, *b*=5.9750(1) Å, *c*=4.6853(1) Å, *V*=287.56(2) Å^3 R_{wp} = 7.33 %, χ^2 = 1.843					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7189(2)	0.25	0.5236(6)	0.25
Fe	4*c*	0.7189(2)	0.25	0.5236(6)	0.75
P	4*c*	0.5945(4)	0.75	0.580(1)	1.0
O (1)	4*c*	0.452(1)	0.75	0.719(1)	1.0
O (2)	4*c*	0.5939(9)	0.75	0.251(2)	1.0
O (3)	8*d*	0.6629(7)	0.544(1)	0.718(1)	1.0
$LiCo_{0.10}Fe_{0.90}PO_4$: *a*=10.2915(2) Å, *b*=5.9865(1) Å, *c*=4.6836(1) Å, *V*=288.55(2) Å^3 R_{wp} = 8.46 %, χ^2 = 1.983					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7182(2)	0.25	0.5240(5)	0.10
Fe	4*c*	0.7182(2)	0.25	0.5240(5)	0.90
P	4*c*	0.5952(4)	0.75	0.5781(9)	1.0
O (1)	4*c*	0.451(1)	0.75	0.722(1)	1.0
O (2)	4*c*	0.5917(9)	0.75	0.251(2)	1.0
O (3)	8*d*	0.6619(6)	0.545(1)	0.719(1)	1.0
$LiCo_{0.05}Fe_{0.95}PO_4$: *a*=10.3058(5) Å, *b*=5.9943(3) Å, *c*=4.6823(3) Å, *V*=289.44(4) Å^3 R_{wp} = 12.52 %, χ^2 = 3.873					
Li	4*c*	0.5	0.5	1.0	1.0
Co	4*c*	0.7189(3)	0.25	0.5233(9)	0.05
Fe	4*c*	0.7189(3)	0.25	0.5233(9)	0.95
P	4*c*	0.5950(7)	0.75	0.583(2)	1.0
O (1)	4*c*	0.453(2)	0.75	0.735(2)	1.0
O (2)	4*c*	0.591(2)	0.75	0.267(3)	1.0
O (3)	8*d*	0.661(1)	0.544(2)	0.721(2)	1.0

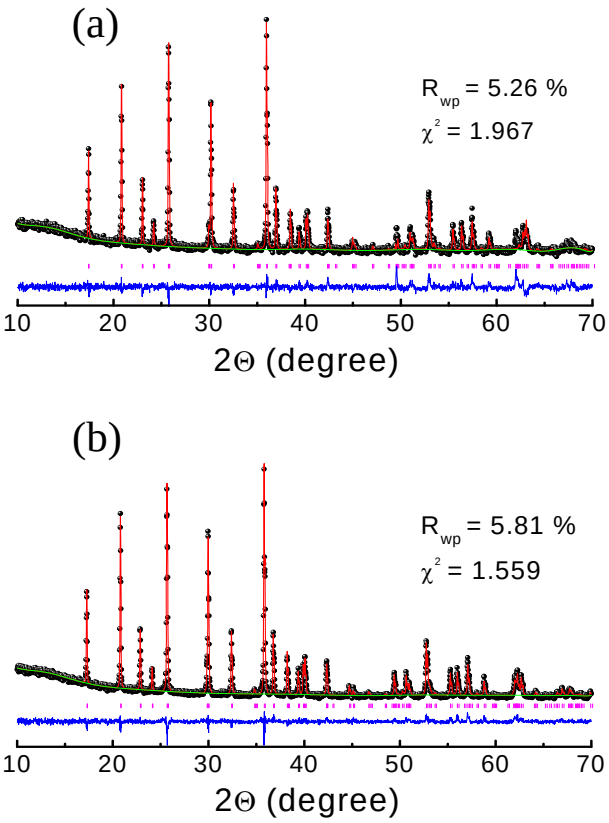

Figure S1. Rietveld refined XRD patterns of $LiCoPO_4$ (a) and $LiCo_{0.5}Fe_{0.5}PO_4$ (b) based on the orthorhombic structure with *Pnma* space group.

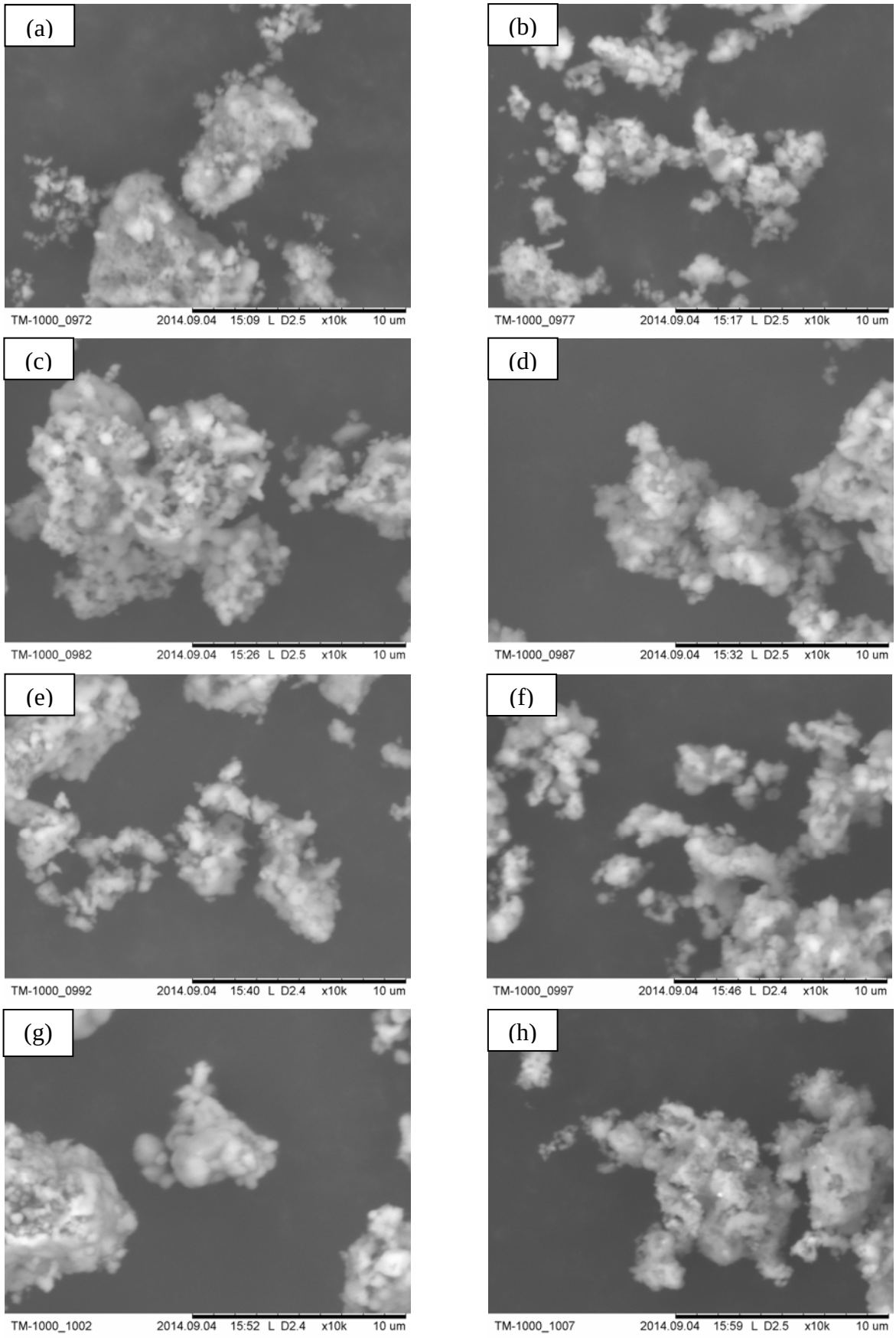

Figure S2. SEM images of $LiCo_{1-y}Fe_yPO_4$ samples: y = 0 (a); 0.05 (b); 0.10 (c); 0.25 (d); 0.50 (e); 0.75 (f); 0.90 (g); 0.95 (h).

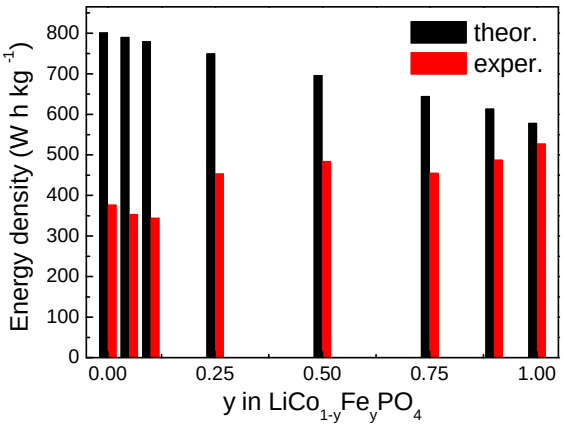

Figure S3. Comparison of theoretical and practical energy densities of the $LiCo_{1-y}Fe_yPO_4$ samples.