# Electronic Supplementary Information (ESI)

## Non-stoichiometric carbon-coated $LiFe_xPO_4$ as cathode materials for high-performance Li-ion batteries

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**Table S1**. Element analysis results of $LiFe_xPO_4/C$.

| Samples | Weight ratio% | | | Atomic ratio% |
|---|---|---|---|---|
| | Li | Fe | P | Li/Fe/P |
| $LiFe_{0.96}PO_4/C$ | 3.89 | 30.20 | 17.4 | 0.998:0.962:1 |
| $LiFe_{0.98}PO_4/C$ | 3.82 | 30.20 | 17.2 | 0.991:0.980:1 |
| $LiFe_{1.0}PO_4/C$ | 3.86 | 31.00 | 17.0 | 1.013:1.011:1 |
| $LiFe_{1.02}PO_4/C$ | 3.84 | 31.45 | 17.0 | 1.008:1.026:1 |
| $LiFe_{1.04}PO_4/C$ | 3.90 | 32.56 | 17.4 | 1.000:1.038:1 |

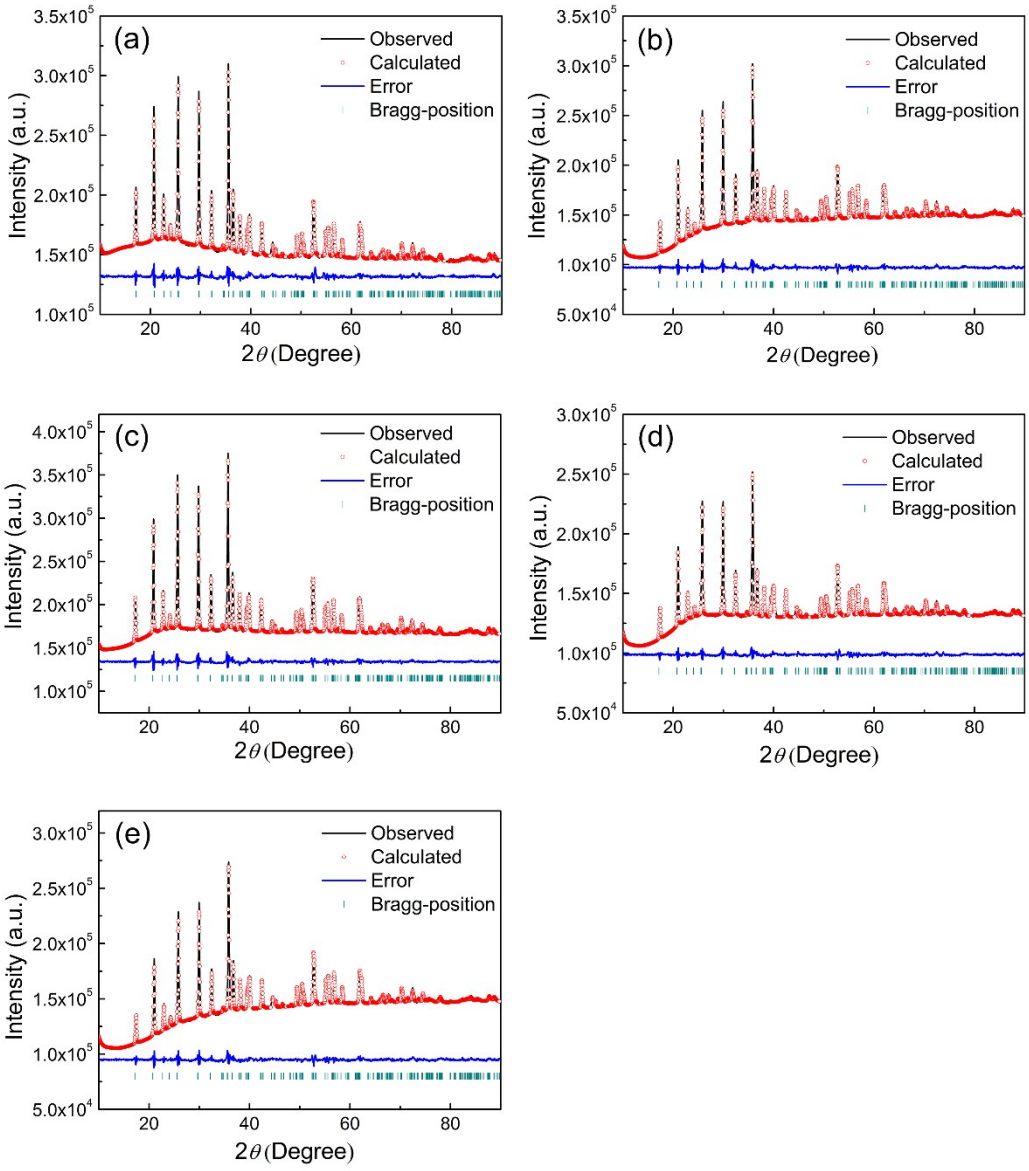


**Fig. S1.** Rietveld refinement results of (a) $LiFe_{0.96}PO_4/C$, (b) $LiFe_{0.98}PO_4/C$, (c) $LiFe_{1.0}PO_4/C$, (d) $LiFe_{1.02}PO_4/C$, and (e) $LiFe_{1.04}PO_4/C$.

**Table S2.** Refined structural parameters of $LiFe_xPO_4/C$ (x = 0.96, 0.98, 1.0, 1.02, 1.04) obtained from Rietveld refinement using X-ray powder diffraction data at room temperature. The symbols *g* and $U_{iso}$ represent the occupation and isotropic thermal parameters, respectively. The numbers within parentheses are the estimated standard deviations of the last significant figure.

(1) $LiFe_{0.96}PO_4/C$

| Atom | Site | *x* | *y* | *z* | *g* | $100*U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Li | 4a | 0.0 | 0.0 | 0.0 | 1.0 | 4.5(4) |
| Fe | 4c | 0.2817(16) | 0.2500(0) | 0.9706(5) | 1.0 | 4.5(4) |
| P | 4c | 0.0953(4) | 0.2500(0) | 0.4170(9) | 1.0 | 4.5(4) |
| O(1) | 4c | 0.0955(9) | 0.2500(0) | 0.7368(15) | 1.0 | 4.5(4) |
| O(2) | 4c | 0.4501(11) | 0.2500(0) | 0.2018(13) | 1.0 | 4.5(4) |
| O(3) | 8d | 0.1617(6) | 0.0496(10) | 0.2818(9) | 1.0 | 4.5(4) |

a = 10.3392(33) Å  b = 6.0150(20) Å  c = 4.7004(19) Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$

R-factors and weight fraction
$R_{wp} = 0.0080$  $R_p = 0.0052$  $\chi^2 = 10.15$

(2) $LiFe_{0.98}PO_4/C$

| Atom | Site | *x* | *y* | *z* | *g* | $100*U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Li | 4a | 0.0 | 0.0 | 0.0 | 1.0 | 7.73(16) |
| Fe | 4c | 0.2819(14) | 0.2500(0) | 0.9704(5) | 1.0 | 7.73(16) |
| P | 4c | 0.0950(31) | 0.2500(0) | 0.4174(8) | 1.0 | 7.73(16) |
| O(1) | 4c | 0.0957(8) | 0.2500(0) | 0.7398(13) | 1.0 | 7.73(16) |
| O(2) | 4c | 0.4495(9) | 0.2500(0) | 0.2096(12) | 1.0 | 7.73(16) |
| O(3) | 8d | 0.1600(6) | 0.0508(9) | 0.2810(8) | 1.0 | 7.73(16) |

a = 10.3393(29) Å  b = 6.0154(17) Å  c = 4.7004(16) Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$

R-factors and weight fraction
$R_{wp} = 0.0076$  $R_p = 0.0051$  $\chi^2 = 8.483$

(3) $LiFe_{1.0}PO_4/C$

| Atom | Site | *x* | *y* | *z* | *g* | $100*U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Li | 4a | 0.0 | 0.0 | 0.0 | 1.0 | 5.25(25) |
| Fe | 4c | 0.2820(13) | 0.2500(0) | 0.9711(4) | 1.0 | 5.25(25) |
| P | 4c | 0.0954(30) | 0.2500(0) | 0.4186(7) | 1.0 | 5.25(25) |
| O(1) | 4c | 0.0941(7) | 0.2500(0) | 0.7427(12) | 1.0 | 5.25(25) |
| O(2) | 4c | 0.4505(9) | 0.2500(0) | 0.2078(11) | 1.0 | 5.25(25) |
| O(3) | 8d | 0.1594(5) | 0.0503(8) | 0.2813(7) | 1.0 | 5.25(25) |

a = 10.3368(28) Å  b = 6.0141(16) Å  c = 4.7006(15) Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$

R-factors and weight fraction
$R_{wp} = 0.0078$  $R_p = 0.0049$  $\chi^2 = 10.53$

(4) $LiFe_{1.02}PO_4/C$

| Atom | Site | *x* | *y* | *z* | *g* | $100*U_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|
| Li | 4a | 0.0 | 0.0 | 0.0 | 1.0 | 7.04(18) |
| Fe | 4c | 0.2819(13) | 0.2500(0) | 0.9704(4) | 1.0 | 7.04(18) |
| P | 4c | 0.0955(31) | 0.2500(0) | 0.4179(7) | 1.0 | 7.04(18) |
| O(1) | 4c | 0.0945(7) | 0.2500(0) | 0.7419(12) | 1.0 | 7.04(18) |
| O(2) | 4c | 0.4495(9) | 0.2500(0) | 0.2090(12) | 1.0 | 7.04(18) |
| O(3) | 8d | 0.1598(5) | 0.0507(8) | 0.2795(7) | 1.0 | 7.04(18) |

a = 10.3365(31) Å  b = 6.0142(18) Å  c = 4.7006(17) Å
$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$

R-factors and weight fraction
$R_{wp} = 0.0066$  $R_p = 0.0046$  $\chi^2 = 5.866$

| (5) $LiFe_{1.04}PO_4/C$ | | | | | | |
|---|---|---|---|---|---|---|
| Atom | Site | *x* | *y* | *z* | *g* | $100*U_{iso}$ (Å$^2$) |
| Li | 4a | 0.0 | 0.0 | 0.0 | 1.0 | 7.98(16) |
| Fe | 4c | 0.2818(15) | 0.2500(0) | 0.9706(5) | 1.0 | 7.98(16) |
| P | 4c | 0.0953(33) | 0.2500(0) | 0.4171(8) | 1.0 | 7.98(16) |
| O(1) | 4c | 0.0961(8) | 0.2500(0) | 0.7397(13) | 1.0 | 7.98(16) |
| O(2) | 4c | 0.4488(10) | 0.2500(0) | 0.2084(13) | 1.0 | 7.98(16) |
| O(3) | 8d | 0.1601(6) | 0.0501(9) | 0.2812(8) | 1.0 | 7.98(16) |
| a = 10.3372(33) Å b = 6.0141(20) Å c = 4.7005(18) Å<br>$\alpha = 90°$ $\beta = 90°$ $\gamma = 90°$ | | | | | | |
| R-factors and weight fraction<br>$R_{wp} = 0.0073$ $R_p = 0.0049$ $\chi^2 = 7.681$ | | | | | | |

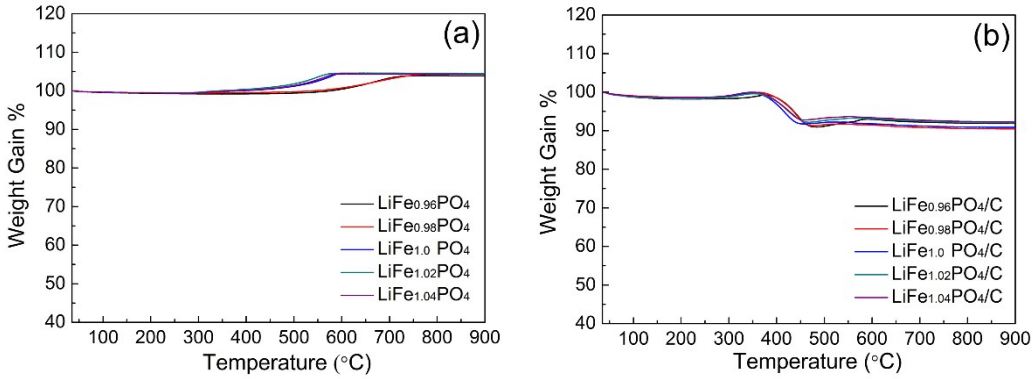


**Fig. S2** TG curves of (a) $LiFe_xPO_4$ and (b) $LiFe_xPO_4/C$.

**Table S3** Carbon content of $LiFe_xPO_4/C$.

| Samples | Carbon content (wt%) |
|---|---|
| $LiFe_{0.96}PO_4/C$ | 13.22 |
| $LiFe_{0.98}PO_4/C$ | 14.59 |
| $LiFe_{1.0}PO_4/C$ | 14.18 |
| $LiFe_{1.02}PO_4/C$ | 12.99 |
| $LiFe_{1.04}PO_4/C$ | 12.78 |