Electronic Supplementary Material

Highly selective and green recovery of lithium ions from lithium iron phosphate powders with ozone

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Table S1. $\Delta_f G^\circ$(kJ·mol^{-1}) of different species at 25 ℃ (298.15 *K*)

Species	$\Delta_f G^\circ$ $(kJ \cdot mol^{-1})$	Species	$\Delta_f G^\circ$ $(kJ \cdot mol^{-1})$	Species	$\Delta_f G^\circ$ $(kJ \cdot mol^{-1})$
Fe^{2+}	-78.87	Fe^{3+}	-4.61	H_3PO_4	-1118.9
$Fe(OH)_2$	-492.1	$Fe(OH)_3$	-705.6	Li^+	-293.7
$LiFePO_4$	-1481.0	$FePO_4$	-1184.36	Li_3PO_4	-1965.9
H_2O	-237.1				

Table S2. Equilibrium equations relative to the *E*-pH diagram of Li-Fe-P-H_2O system at 25 ℃ (298.15 *K*)

No.	Reactions	E vs pH equations
a	$2H^+ + 2e^- = H_2$	E=-0.05916pH
b	$O_2 + 4e^- + 4H^+ = 2H_2O$	E=1.2288-0.05916pH
1	$Fe^{3+} + e^- = Fe^{2+}$	E=0.7679-0.05916lg[Fe^{2+}]/[Fe^{3+}]
2	$FePO_4 + 3H^+ = Fe^{3+} + H_3PO_4$	pH=-3.486-1/3lg[Fe^{3+}][H_3PO_4]
3	$FePO_4 + 3H^+ + e^- = Fe^{2+} + H_3PO_4$	E=0.1508-0.05916lg[Fe^{2+}] [H_3PO_4] − 0.1775pH
4	$LiFePO_4 + 3H^+ = Fe^{2+} + Li^+ + H_3PO_4$	pH=0.6137-1/3lg[Li^+][Fe^{2+}] [H_3PO_4]
5	$FePO_4 + Li^+ + e^- = LiFePO_4$	E=0.04145+0.05916lg[Li^+]
6	$Li_3PO_4 + Fe(OH)_3 + 3H^+ = FePO_4 + 3Li^+ + 3H_2O$	pH=6.0831-lg[Li^+]
7	$Li_3PO_4 + Fe(OH)_3 + 3H^+ + e^- = LiFePO_4 + 2Li^+ + 3H_2O$	E=1.1226-0.1183 lg[Li^+] − 1.775pH
8	$Fe(OH)_3 + H^+ + e^- = Fe(OH)_2 + H_2O$	E=0.2452-0.05916pH
9	$Fe(OH)_2 + Li_3PO_4 + 2H^+ = LiFePO_4 + 2Li^+ + 2H_2O + 2H_2O$	pH=7.4253-lg[Li^+]

Fig. S1. Image of Li_2CO_3 product.

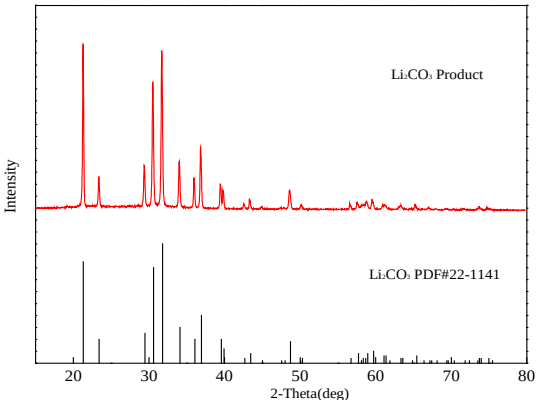

Fig. S2. XRD pattern of Li_2CO_3 product.

Fig. S3. Image of recycled leaching residue.

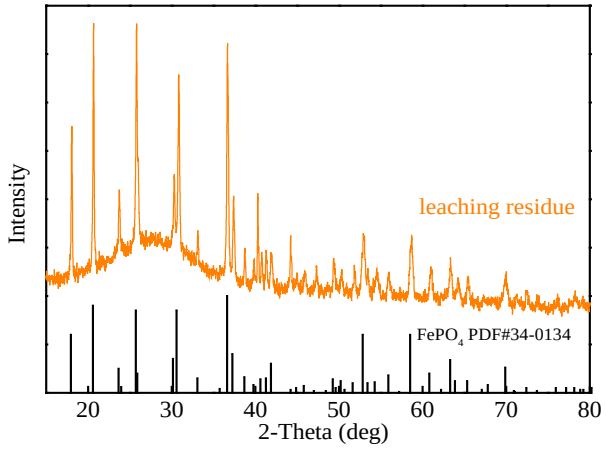

Fig. S4. XRD pattern of recycled leaching residue.

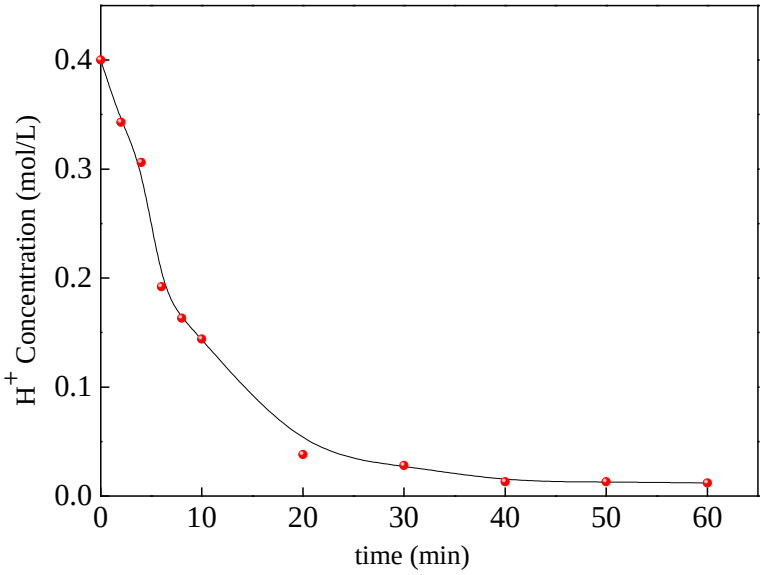

Fig. S5. Acid concentration in leaching solution at different reaction times.

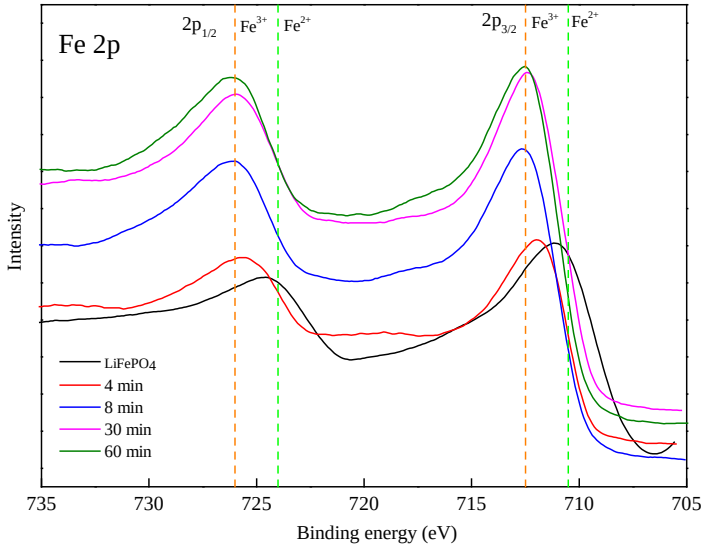

Fig. S6. XPS analyses of various solids.

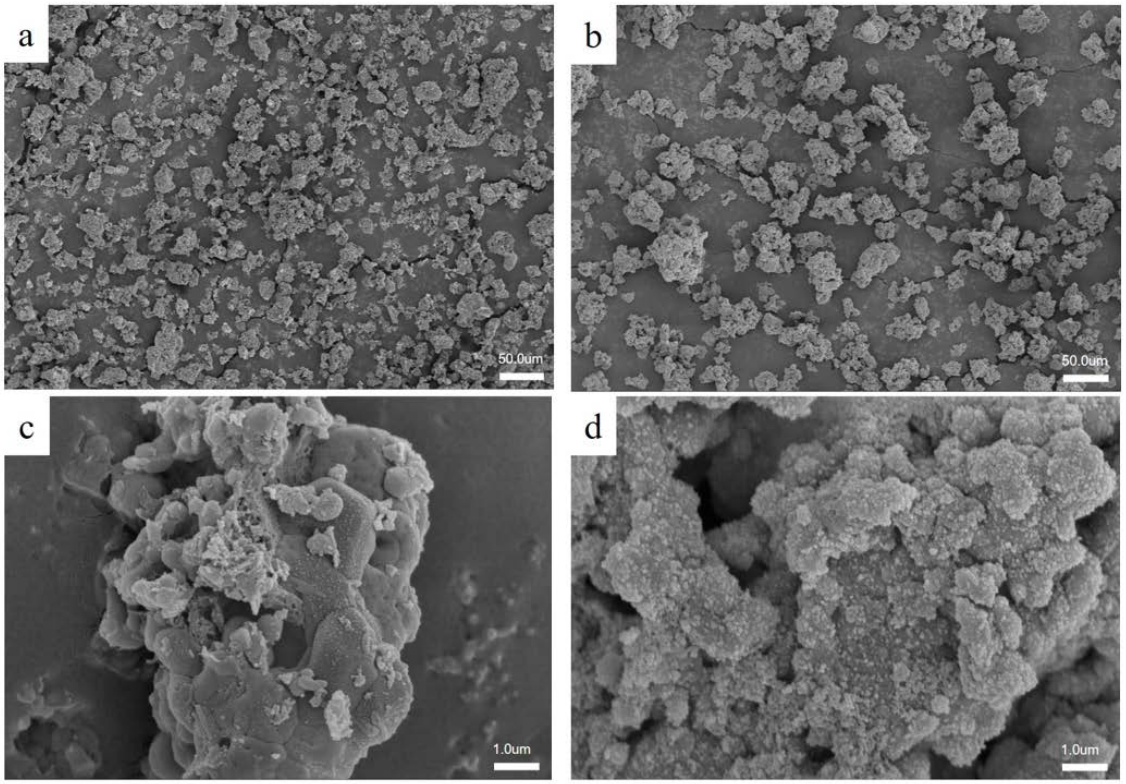

Fig. S7 SEM images of $LiFePO_4$ (a) (c)and leaching residue (b) (d).

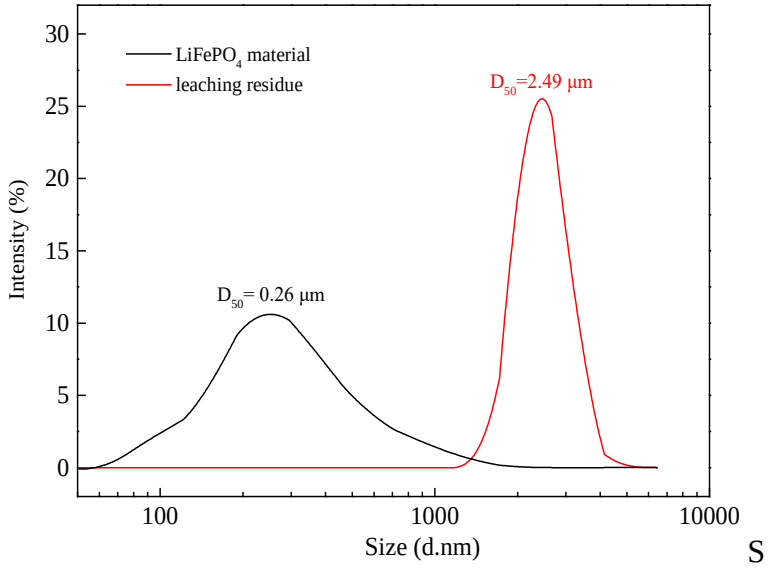

Fig. S8 Particle size distributions of LFP materials before and after leaching.