

Supplementary Materials

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Text S1

The solubility of Li₂CO₃ is 1.33 g at room temperature. The calculation process of Li⁺ concentration in saturated Li₂CO₃ solution is as follows:

$$\text{Moles of Li}_2\text{CO}_3 = \frac{\text{Mass of Li}_2\text{CO}_3}{\text{Molar mass of Li}_2\text{CO}_3} = \frac{1.33 \text{ g}}{73.89 \text{ g/mol}} \approx 0.0180 \text{ mol}$$

$$\text{Moles of Li}^+ = 2 \times \text{Moles of Li}_2\text{CO}_3 = 2 \times 0.0180 \text{ mol} = 0.0360 \text{ mol}$$

The solubility of LiF is 0.13 g at room temperature. The calculation process of Li⁺ concentration in saturated LiF solution is as follows:

$$\text{Moles of LiF} = \frac{\text{Mass of LiF}}{\text{Molar mass of LiF}} = \frac{0.13 \text{ g}}{25.94 \text{ g/mol}} \approx 0.00501 \text{ mol}$$

$$\text{Moles of Li}^+ = \text{Moles of LiF} = 0.00501 \text{ mol}$$

Therefore, the concentration of Li⁺ in saturated Li₂CO₃ solution is much higher than that in saturated LiF solution. In other words, the utilization rate of Li⁺ in the preparation of LiF is higher than that in the preparation of Li₂CO₃.

Text S2

The price of Li₂CO₃ per ton of battery grade is CNY 76350, while the price of LiF per ton of battery grade is CNY 143500 (<https://new-energy.smm.cn/> accessed January 2025).

Take 1 ton product as an example:

$$\text{Moles of Li}_2\text{CO}_3 = \frac{\text{Mass of Li}_2\text{CO}_3}{\text{Molar mass of Li}_2\text{CO}_3} = \frac{1000000 \text{ g}}{73.89 \text{ g/mol}} \approx 13466 \text{ mol}$$

$$\text{Price of non-molar of Li} = \frac{\text{Price per tonne of battery-grade Li}_2\text{CO}_3}{2 \times \text{Moles of Li}_2\text{CO}_3} = \frac{76350}{2 \times 13466} = 2.38$$

$$\text{Moles of LiF} = \frac{\text{Mass of LiF}}{\text{Molar mass of LiF}} = \frac{1000000 \text{ g}}{25.94 \text{ g/mol}} \approx 38358 \text{ mol}$$

$$\text{Price of non-molar of Li} = \frac{\text{Price per tonne of battery-grade LiF}}{\text{Moles of LiF}} = \frac{143500}{38358} = 3.74$$

LiF had good economic benefits because of its high purity, high yield, simple process, low production cost and high added value. However, the recovery process of Li₂CO₃ was complex, the energy consumption was high, and the purity and yield were relatively low, resulting in high production costs and relatively poor economic benefits. Therefore, the profit of preparing LiF is higher than that of preparing Li₂CO₃.

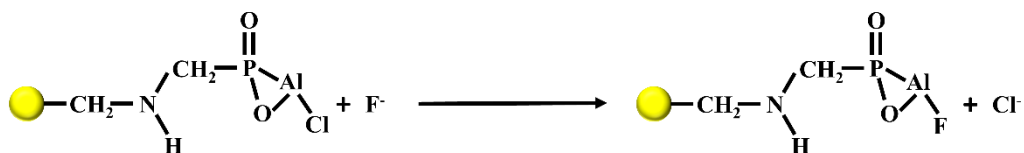


Figure S1. Defluorination mechanism of Cl-functional resin.

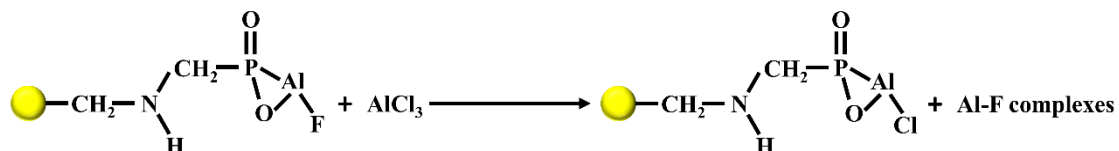


Figure S2. Regeneration mechanism of Cl-functional resin.

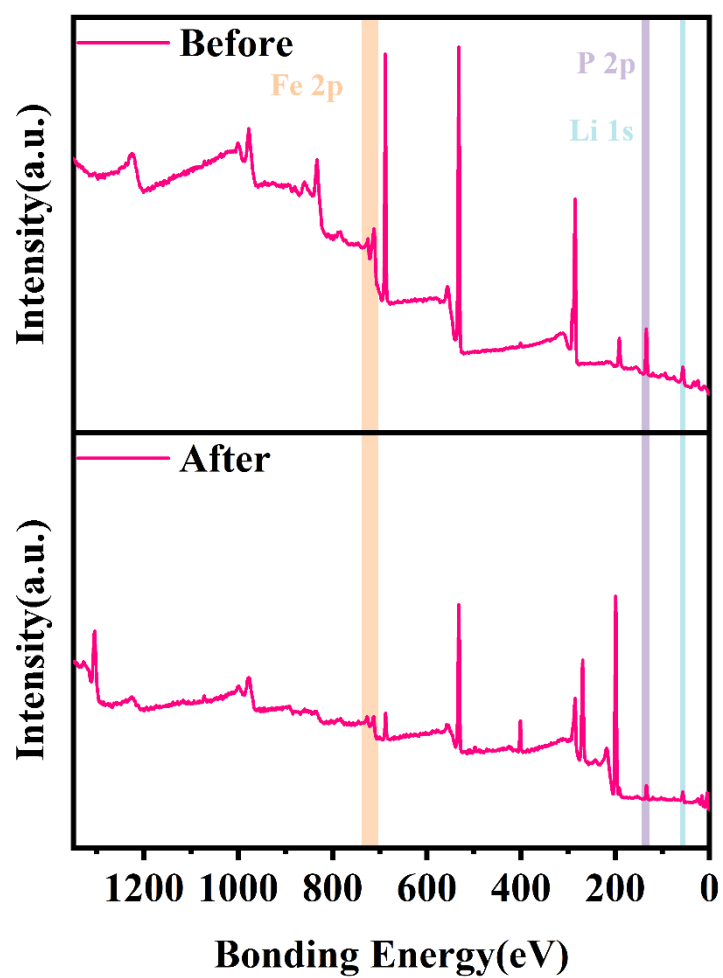


Figure S3. XPS spectra of LFP samples before and after $\text{H}_2\text{O}_2\text{-NH}_4\text{Cl}$ mechanical chlorination.

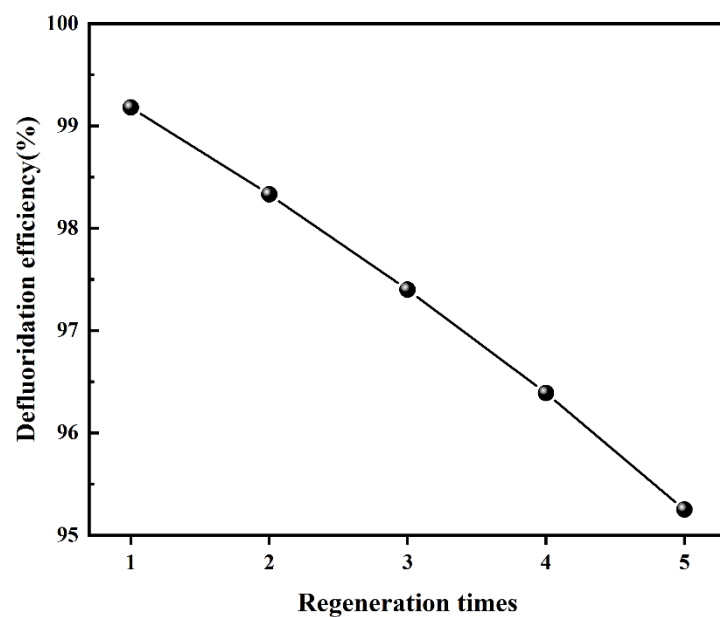


Figure S4. Defluorination efficiency of resin under regeneration times.

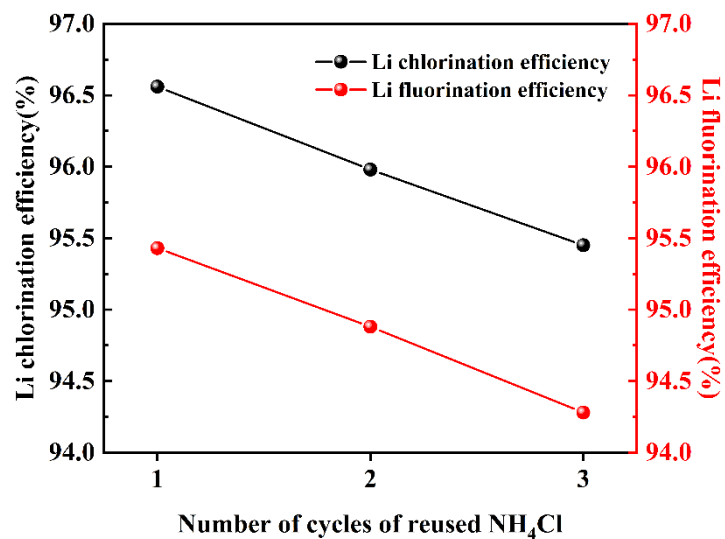


Figure S5. Chlorination efficiency and fluorination efficiency of Li under number of cycles of reused NH_4Cl .