

**Supporting Information for:**  
**Regenerating Spent LiFePO<sub>4</sub> with Tailored Molecular  
Groups: From Bulk Lattice Repair to Surface  
Conductive Coating for Enhanced Cycling Stability**

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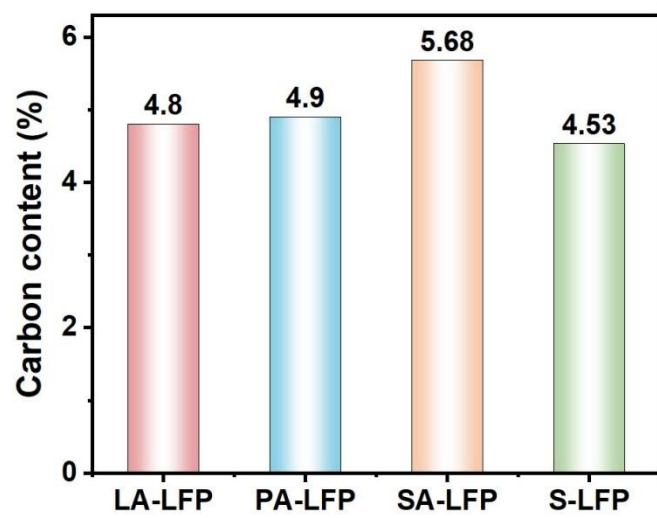


Fig.S1 The carbon content of as-prepared samples

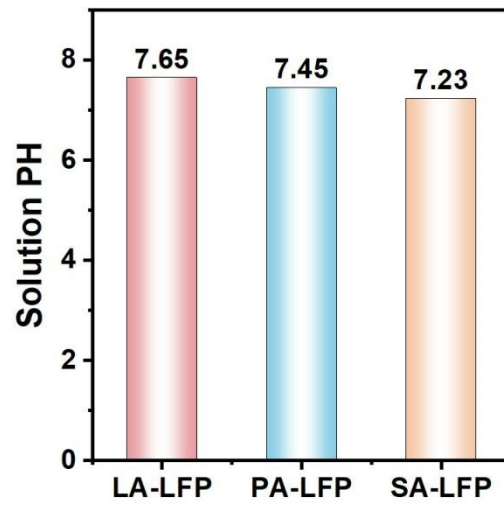


Fig.S2 pH value for different amino acid solutions of as-regenerated samples

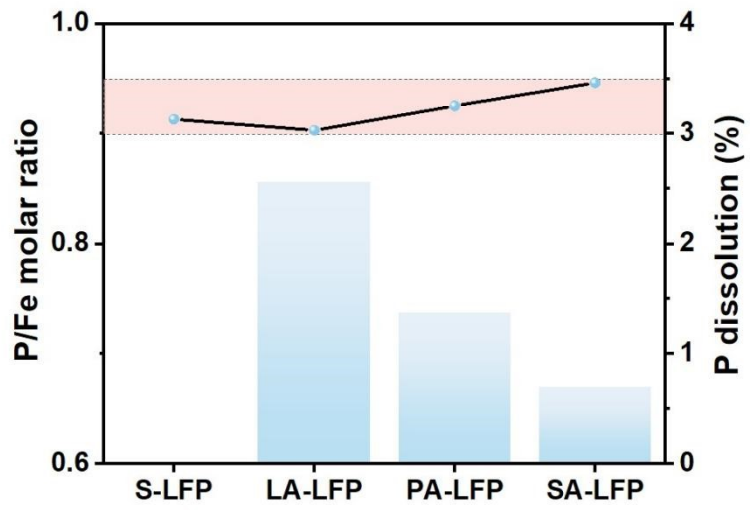


Fig.S3 The ICP results of P/Fe in the samples and P element in the hydrothermal solution

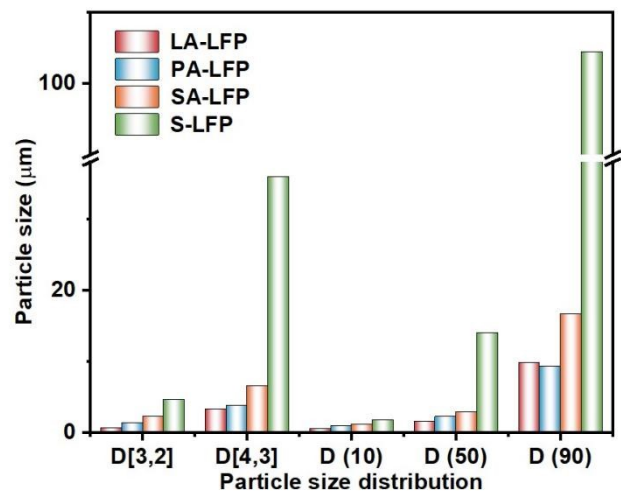


Fig.S4 The particle size parameters of the samples

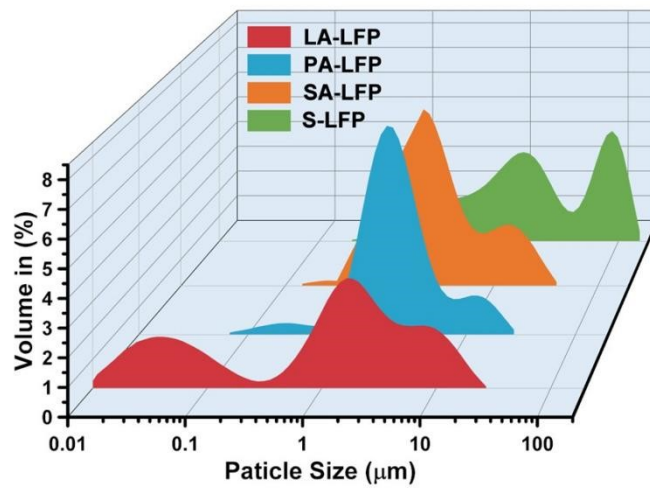


Fig.S5 The particle size distribution of the samples

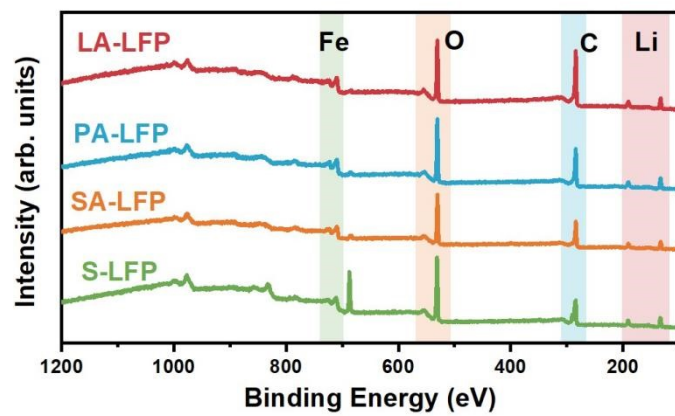


Fig.S6 The full XPS spectrum of the samples

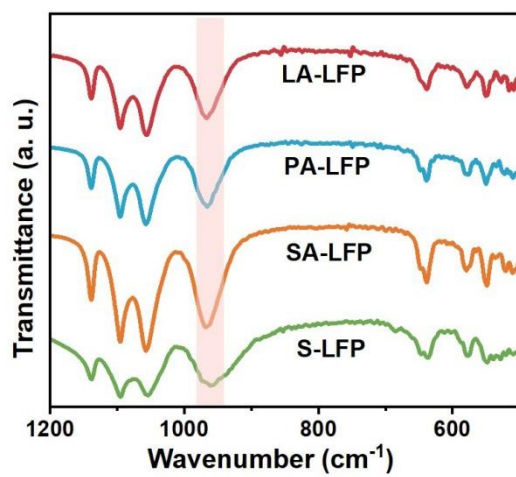


Fig.S7 The FTIR spectrum of the samples

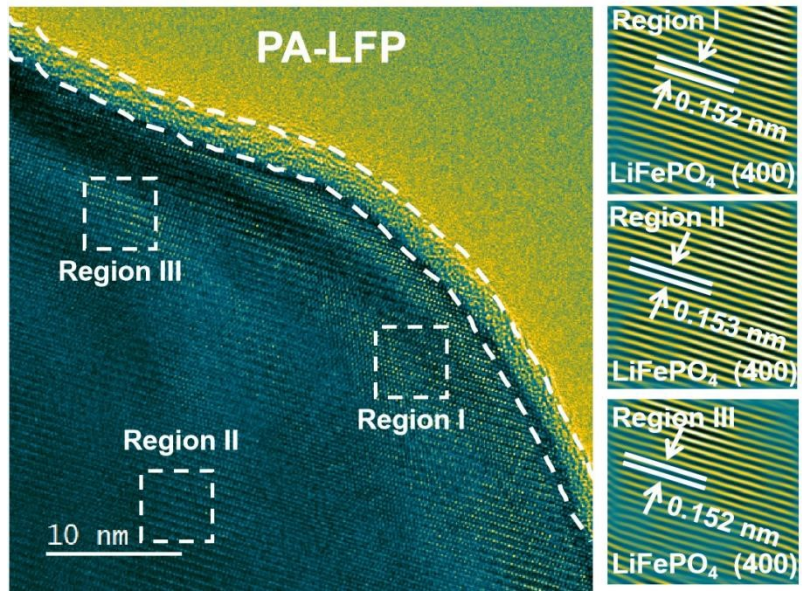


Fig.S8 TEM images of PA-LFP

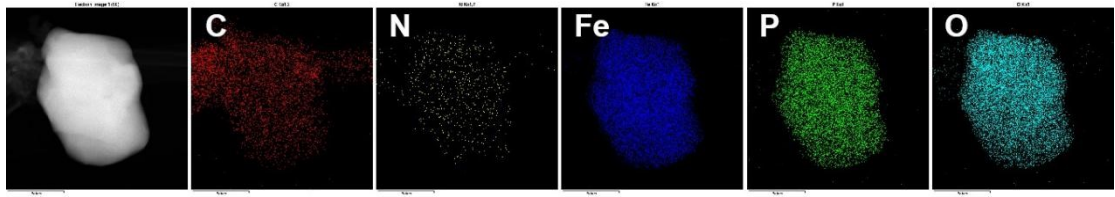


Fig.S9 Mapping images of PA-LFP

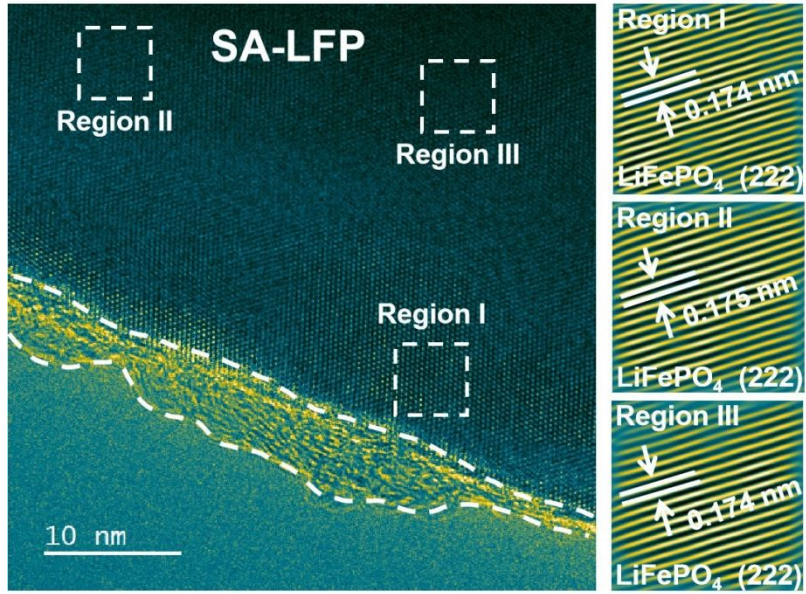


Fig.S10 TEM images of SA-LFP

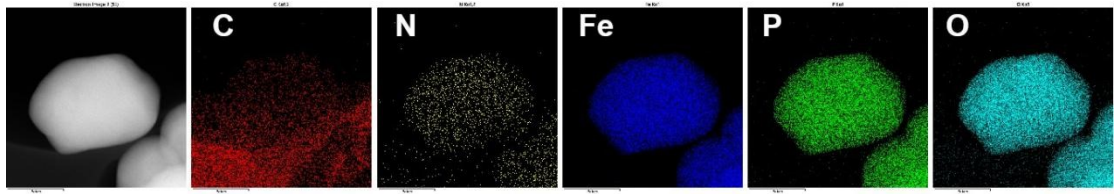


Fig.S11 Mapping images of SA-LFP

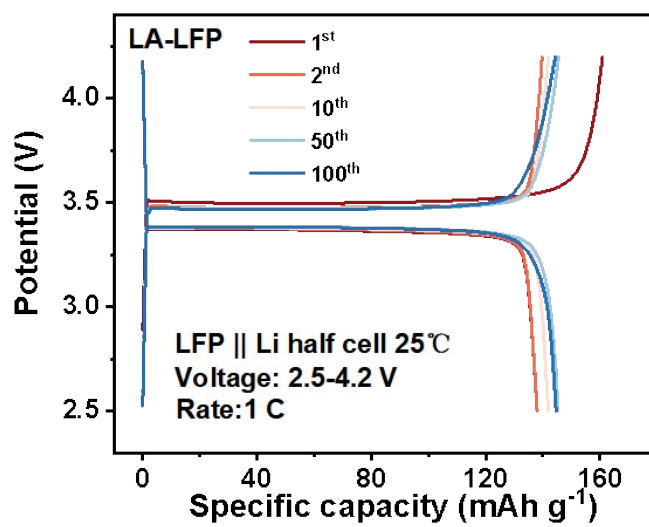


Fig.S12 The charge-discharge platforms of LA-LFP from 1st to 100th cycle and their rate properties

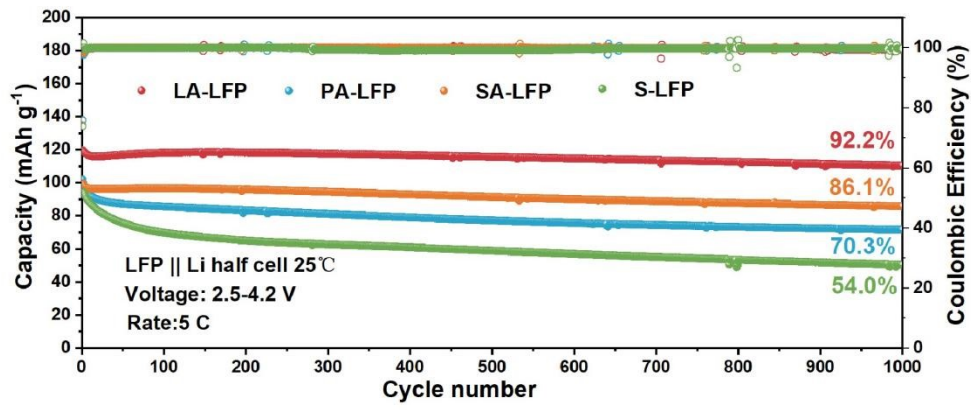


Fig.S13 Cycling performance of samples at 5.0 C

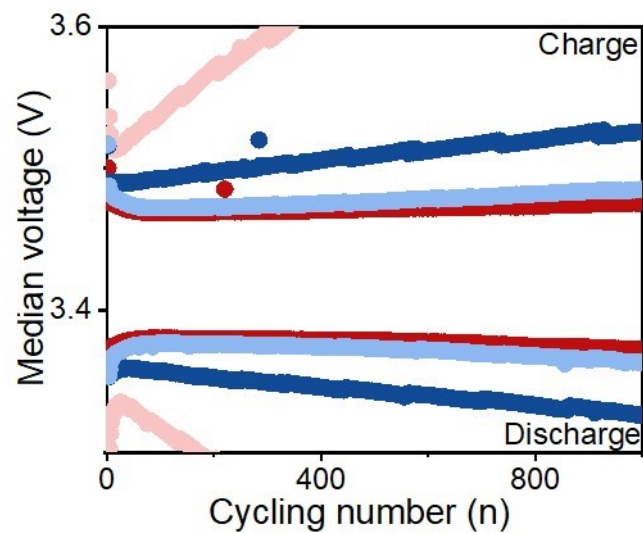


Fig.S14 The charge/discharge median voltages of samples at 1.0 C

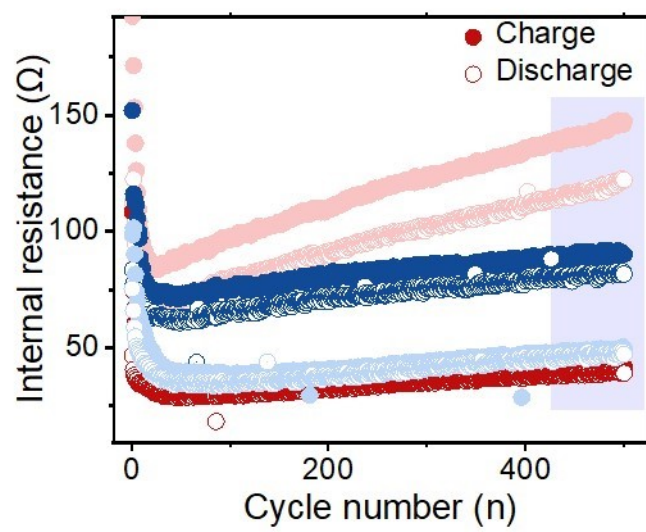


Fig.S15 The internal resistance of samples at 1.0 C

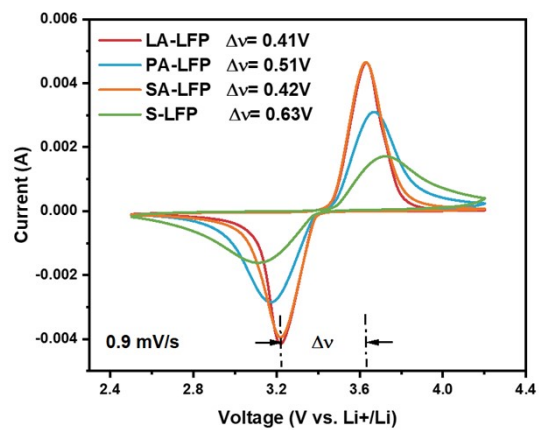


Fig.S16 Voltage difference of as-regenerated samples at 0.9 mV s<sup>-1</sup>

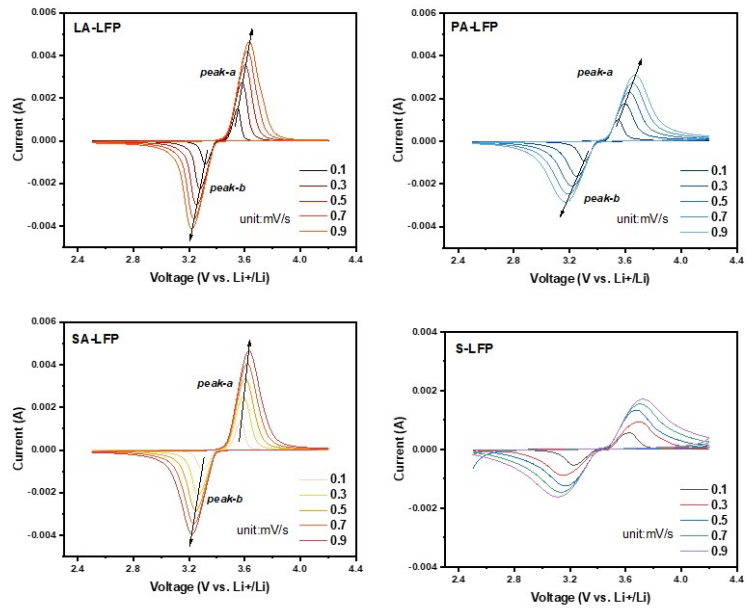


Fig.S17 CV curves of as-regenerated samples

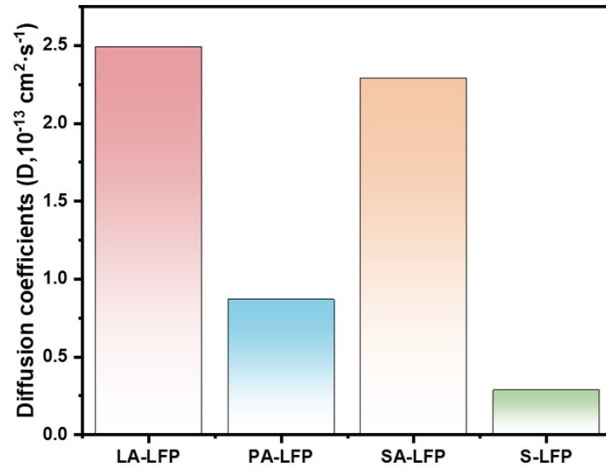


Fig.S18 The calculated results of diffusion coefficient about as-regenerated samples

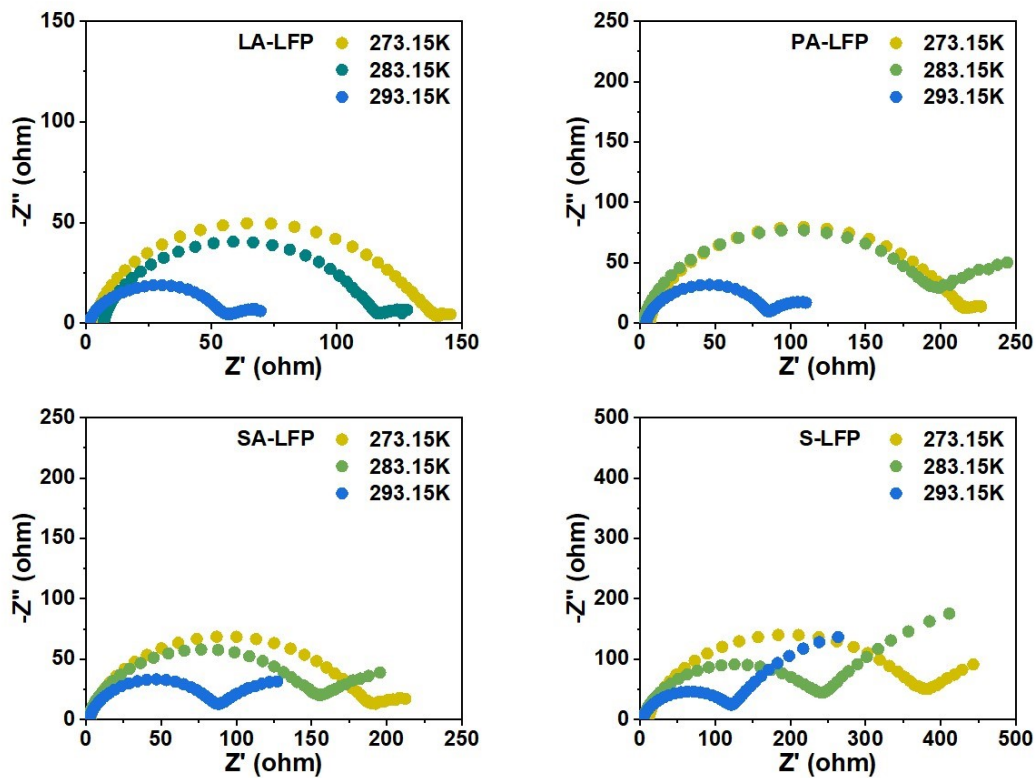


Fig.S19 Nyquist plots of samples at different temperatures

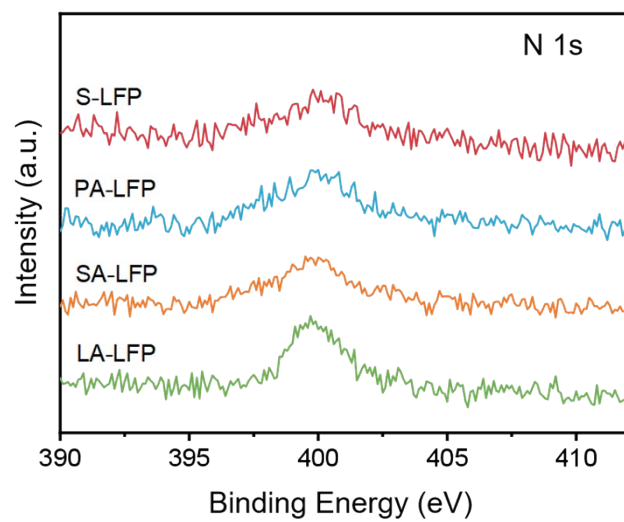


Fig.S20 The N1s XPS spectrum of the samples

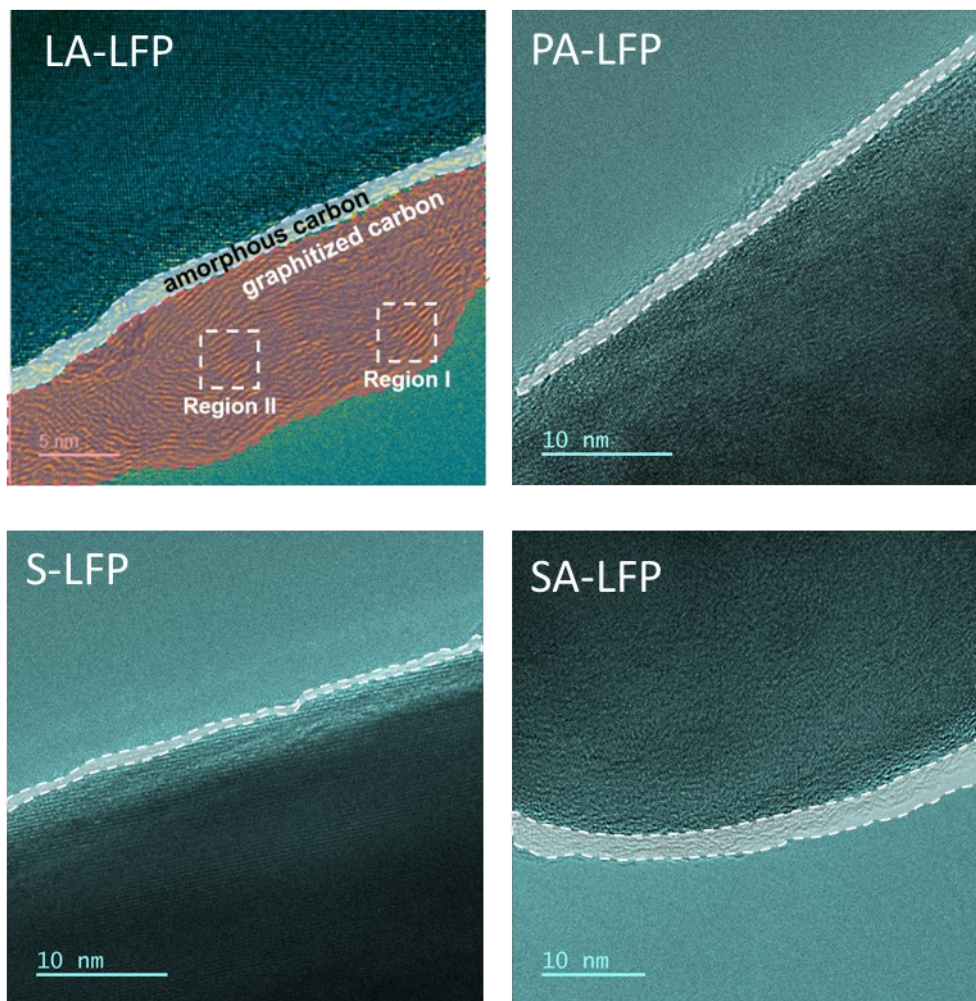


Fig.S21 The comparison of samples carbon layer

Table S1 Rietveld refinement results of high-resolution powder XRD of S-LFP sample

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 83.72%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.3273	6.0066	4.6909
<b>Li-Fe Anti-sites</b>	2.00%			
<b>FePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 16.28%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
	5.8090	9.8390	4.7760	272.97
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 3.07%</b>	<b>R<sub>p</sub> 3.15%</b>	<b>R<sub>wp</sub> 4.04%</b>	<b>R<sub>exp</sub> 2.30%</b>	

Table S2 Rietveld refinement results of high-resolution powder XRD of LA-LFP sample

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 100.00%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.3344	6.0104	4.6939
<b>Li-Fe Anti-sites</b>	0.60%			
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 4.07%</b>	<b>R<sub>p</sub> 3.44%</b>	<b>R<sub>wp</sub> 4.46%</b>	<b>R<sub>exp</sub> 2.21%</b>	

Table S3 Rietveld refinement results of high-resolution powder XRD of PA-LFP sample

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 100.00%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.3351	6.0110	4.6943
<b>Li-Fe Anti-sites</b>	1.20%			
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 4.70%</b>	<b>R<sub>p</sub> 3.75%</b>	<b>R<sub>wp</sub> 5.00%</b>	<b>R<sub>exp</sub> 2.30%</b>	

Table S4 Rietveld refinement results of high-resolution powder XRD of SA-LFP sample

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 100.00%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.3293	6.0073	4.6915
<b>Li-Fe Anti-sites</b>	1.70%			
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 4.56%</b>	<b>R<sub>p</sub> 3.53%</b>	<b>R<sub>wp</sub> 4.65%</b>	<b>R<sub>exp</sub> 2.18%</b>	

Table S5 Rietveld refinement results of XRD of LA-LFP sample after cycles

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 100.00%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.2911	5.9809	4.6728
<b>Li-Fe Anti-sites</b>	1.30%			
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 5.03%</b>	<b>R<sub>p</sub> 4.59%</b>	<b>R<sub>wp</sub> 5.86%</b>	<b>R<sub>exp</sub> 2.61%</b>	

Table S6 Rietveld refinement results of XRD of SA-LFP sample after cycles

<b>LiFePO<sub>4</sub> (Space Group Pnma) Phase Ratio: 100.00%</b>				
<b>Lattice Parameters</b>	<b><i>a</i> / Å</b>	<b><i>b</i> / Å</b>	<b><i>c</i> / Å</b>	<b><i>V</i> / Å<sup>3</sup></b>
		10.2775	5.9779	4.6643
<b>Li-Fe Anti-sites</b>	3.30%			
<b>Agreement Factors</b>				
<b><math>\chi^2</math> 3.79%</b>	<b>R<sub>p</sub> 3.94%</b>	<b>R<sub>wp</sub> 5.06%</b>	<b>R<sub>exp</sub> 2.6%</b>	