Supplementary Information for

Three-Dimensional Phase Evolution and Stress-Induced Non-Uniform Li Intercalation Behavior in Lithium Iron Phosphate

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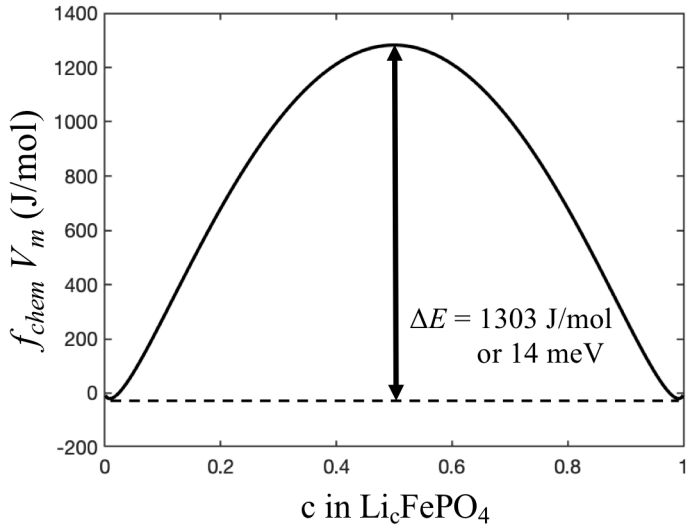
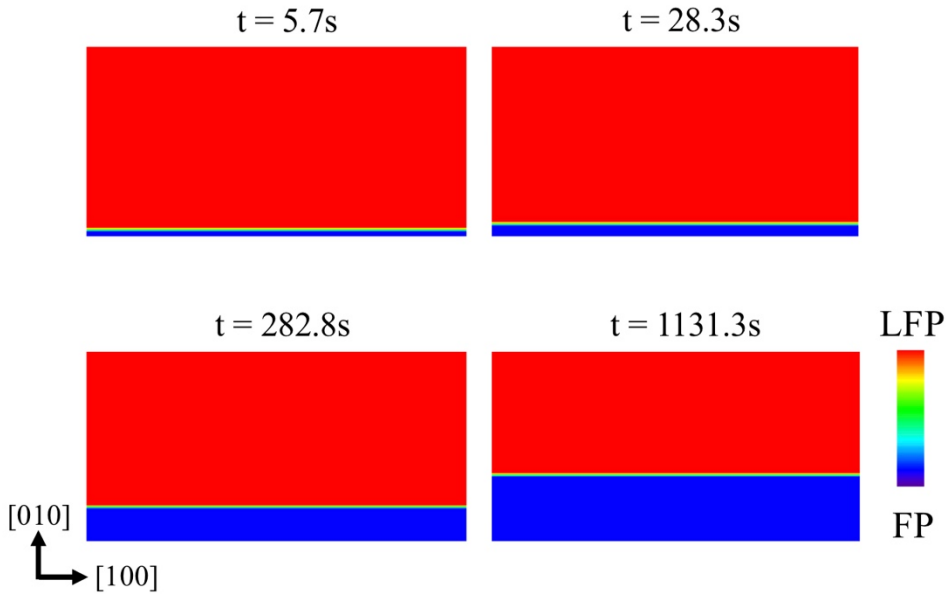


Supplementary Figure S1. Molar chemical free energy density of Li_cFePO_4 as given by Eq. 2 in the main text.



Supplementary Figure S2. Phase-field simulation of FP phase growth under 100 mV overpotential in the absence of coherency stress by assuming zero misfit strain between LFP and FP phases. Simulation domain size is $L_{[100]} \times L_{[001]} \times L_{[010]} = 256 \times 128 \times 256$ nm. The (001) cross section of Li concentration distribution is shown.

Supplementary Movie 1. Phase-field simulation of FP phase growth in a $LiFePO_4$ single crystal upon delithiation at a constant overpotential $\Delta\phi$ = 100 mV. Li is removed from the bottom surface of the computation domain. The animation on the top visualizes the evolution of the region with Li concentration $c < 0.5$. The animation at the bottom shows the (001) cross section of the Li concentration field, the position of which is indicated by the shaded plane in Figure 1a.