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Supporting information for

Atomic-Scale Insight into the Lattice Volume Plunge of Li_xCoO₂ at Deep Delithiation

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(b)



(c)



Figure S1. The layered $LiCoO_2$ structure with the R3m space group used for DFT calculations (a); the measured lattice volume variation of Li_xCoO_2 using in-situ XRD (b); the lattice c (c), lattice a (d) variation of Li_xCoO_2 during delithiation.



(a)



Figure S2. The 3D (a) and 2D (b) electron localization function in Li_xCoO₂ during delithiation



(a)



(b)



(c)



(d)



(e)



(f)

Figure S3. The total density of state of Li_xCoO_2 during delithiation (a); the atomic environment of $O_{number 30}$, $O_{number 76}$, $Co_{number 20}$, and $Co_{number 38}$ (b); the PDOS of $O_{number 30}$ with surrounded Li extracted (c), the PDOS of $O_{number 76}$ without surrounded Li extracted (d), the PDOS of $Co_{number 20}$ (e), and the PDOS of $Co_{number 38}$ (f) during delithiation.