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Supporting information for article:

In operando quantitation of Li concentration for a commercial Li-ion rechargeable battery using high-energy X-ray Compton scattering

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S1. **Determination of the boundary for *S*-parameter analysis**

In order to determine the parameters of d and r in S-parameter analysis, energy spectra of positive electrode in SOC0 and SOC100 were measured. Figure S1 shows difference energy spectrum, ΔI. Here, ΔI is defined as $\Delta I = I_{SOC0} - I_{SCO100}$. The I_{SOC0} and I_{SOC100} are energy spectra for full charged state and full discharged state, respectively. In order to reveal the boundary of low momentum and high momentum regions, Gaussian model fitting was performed to difference energy spectrum. In the Fig. S1, we observed small peak which correspond to increment of Li ions around $p_z = 0$ a.u. It is confirmed that the contribution of Li ions appears at low region previously (Suzuki et al., 2016). There is Li contribution from $p_z = -1$ a.u. to $p_z = 1$ a.u. At $p_z = \pm 1.5$ a.u., negative part appears. This negative part indicates the change of electronic structure by Li insertion as it has been found from previous study of $Li_xMn_2O_4$ (Suzuki et al., 2015). At $p_z > 5$ a.u. and $p_z < -5$ a.u., the variation between I_{SOC0} and I_{SOC100} is almost zero. Hence, we use $d = 1$ a.u. as the low momentum region and $r = 5$ a.u. as high momentum region. This boundary was applied to analysis of negative electrode since same trend shows in Li_xAl.
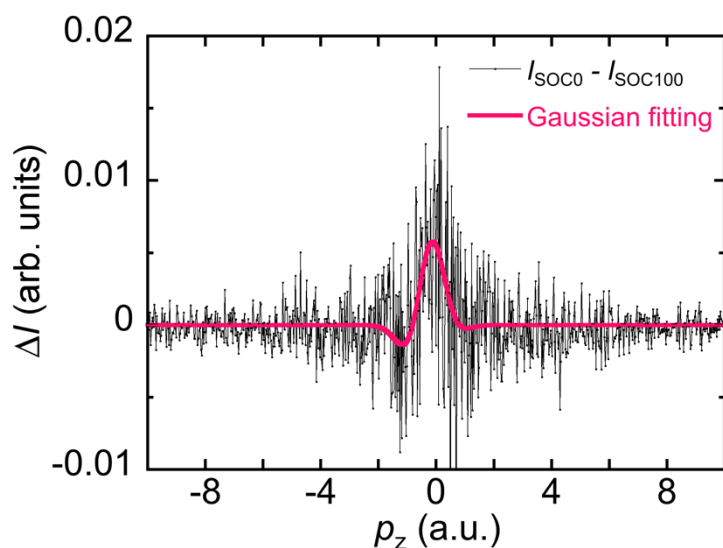

Figure S1 Difference energy spectrum (black solid line) between the energy spectra of SOC0 and SOC100 in positive electrode materials. Red solid line shows the result of Gaussian model fitting.