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## Structural analysis of cation mixing in NCA-type battery cathodes

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Lithium-ion batteries with high-nickel content  $\text{Li}_x\text{Ni}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$  (NCA) cathodes and high-performance graphite are emerging as key components in electric vehicles, offering high energy and power densities at low costs [1, 2]. However, the efficiency of these batteries is hindered by the diffusivity of Li-ions, particularly in nickel-rich cathodes where  $\text{Li}^+/\text{Ni}^{2+}$  cation mixing can block the 2D diffusion pathways, reducing the cell capacity and structural stability [3]. This study presents a systematic ex situ neutron powder diffraction analysis of NCA cathodes from real 18650-type cells, showing decreasing lithium concentration with higher charge states and the absence of cation mixing within the NCA structure during the electrochemical cycle, as revealed by Rietveld refinement.

[1] Zhao, G., et al., iScience, 25(2), 2022 (DOI: 10.1016/j.isci.2022.103744).

[2] Purwanto, A., et al., Materials Research Express, 5(12), 2018 (DOI: 10.1088/2053-1591/aae167)

[3] Dolotko, O., et al., Journal of Power Sources, 255, 2014 (DOI: 10.1016/j.jpowsour.2014.01.010)

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