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Structural Changes of LiXCo2O4 (1 ≤ x ≤ 2) Nanoporous Cathode Materials upon Lithiation

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Spinel cathode material LiCo2O4 exhibit good electrochemical performance when used in energy storage applications. This is attributed to its high surface-to-volume ratios and shortened Li+ diffusion lengths during cycling. However, some possible flaws have constrained the good electrochemical performance. These flaws include structural changes that carry the risk of structural collapse and crack formation during cycling.
Herein, large-scale simulations using molecular dynamics methods were performed to investigate the structural changes of LixCo2O4 (1 ≤ x ≤ 2) nanoporous materials at different lithium concentrations and cell dimensions of 67, 69 and 75 Å. The structures amorphised and recrystallised efficiently under the NST ensemble producing grain boundaries at Li1.75Co2O4 concentration. Furthermore, the increase in lithium concentration in the structures resulted in pore size reduction. Finally, the structures showed great resilience to volume expansion with increasing lithium concentration. This implies that the LixCo2O4 nanoporous materials have the potential to curb the formation of cracks which cause damage to the battery since they are able to expand freely during lithiation.

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

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