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Investigating the effect of sodium partial substitution on nanostructured Li2MnO3 cathodes during the simulated charge process

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The exploration of new electrode materials exhibiting improved electrochemical performance and low cost for high-density lithium-ion batteries (LIBs) applicable in electric vehicles is one of today's most challenging issues in material research. Li2MnO3, as a prospective high-capacity (459 mAh.g-1) cathode, suffers from capacity degradation and voltage decay during the cycling process. Incorporating sodium ions in the lithium sites can mitigate voltage decay by limiting transition metal migration, impeding oxygen loss, and improving lithium diffusion of Li-rich layered host materials. In this work, the structural stability of the spherical Li2MnO3, generated through the simulated amorphisation and recrystallisation (A+R) technique was improved by introducing a certain amount of sodium into its lattice structure. The molecular dynamics (MD) calculations were carried out at temperatures between 1600-1800 K, employing the DL –POLY code. Characterisation of the x-ray diffraction (XRD) patterns revealed peak broadening along with the shifting of peaks at 2Θ˜38 to the right due to the enlarged lithium layers occupied by sodium ions to facilitate lithium diffusion. Moreover, the undesired phase transformation from layered to spinel was observed at a later stage of charge for the sodium-doped systems, suggesting that the presence of sodium stabilizes the structure and minimizes the migration of manganese into lithium layers. These findings shed insights on the role of sodium substitution on the nanostructured Li2MnO3 cathodes and will help guide the enhancement of high-capacity energy storage.

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

Yes

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

PhD

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