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Investigating sodium incorporated Li2MnO3 nanostructured cathodes for lithium-ion batteries

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Capacity degradation and voltage fade of Li2MnO3 during cycling are the limiting factors for its practical use as a high capacity lithium-ion battery cathode. The incorporation of sodium ions in the lithium sites can mitigate voltage decay by limiting transition metal migration, impeding the oxygen loss and also improving lithium diffusion of Li-rich layered host materials. In this work, nanostructured Li2MnO3 models have been generated via the simulated amorphisation and recrystallisation (A+R) technique employing the DL_POLY code. Accordingly, sodium was partially introduced into the Li2MnO3 lattice resulting in a series of Li2-xNaxMnO3 (0≤x≤2) models of different lithium and sodium content. The generated models were subjected to various temperatures to determine the temperatures at which amorphisation and recrystallisation materialised. All the molecular dynamics calculations were carried out at temperatures between 1600-1800 K. Lithium-ion diffusion has been significantly increased in models with low sodium content. Particularly, Li1.975Na0.025MnO3 consisting of the lowest sodium content displayed a high diffusion rate. Characterisation of the x-ray diffraction 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. 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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