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Exploration of intermediate phases that form during lithium and oxygen extraction from the Li2MnO3 nanoporous cathode material

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Li2MnO3 has been classified as an active intercalation host material for lithium ion batteries (LIBs) due to its large specific capacity. However, its degradation nature reported to be due to oxygen loss and phase transformation during cycling hinders its practical application. Furthermore, the mechanism behind the degradation has not been fully understood. As such, studying the crystal growth process of these intermediate phases during charging is of great significance. In this work the simultaneous removal of oxygen and lithium from the nano-Li2MnO3 will be studied in a quest to explore the formation of different intermediate structures. Molecular dynamics simulations was used to carry out the spontaneous crystal growth of the nanoporous structures. The NVE ensemble was used in amorphisation and NVT for recrystallisation during the crystal growth. Our results reveal highly defective structures which are vacancy driven, and the atomic substitutions are noted in the layers. Furthermore, the XRDs and microstructures reveal the formation of layered and spinel-type structures as the lithium and oxygen content decreased.

Apply to be
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yes

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

MSc

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