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Stress-Induced Structural Changes of Lithiated Li1+xMn2O4 (0 ≤ x ≤ 1) Nanoporous Electrode Materials

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Optimising the performance potential in terms of voltage and capacity of Li-ion batteries requires understanding of both electrochemical and mechanical properties of a material. Molecular dynamics (MD) methods are capable of informing the time dependent properties such as amorphisation and recrystallisation (A+R) which can provide understanding of microstructural evolution. As such, MD simulations employing the DL_POLY code were carried out to investigate the effect of lithiation on the Li-Mn-O nanoporous materials under the NST ensemble. The Li-Mn-O nanoporous structures were obtained from spontaneous recrystallisation, during which various lithiated structures yielded to single or multigrained crystals. Furthermore, microstructural analysis depicted evolution of composites of spinel-layered components with defects. The XRDs analysis also confirmed the co-existence of spinel with layered structures owing to the characteristic/signature peaks of both polymorphs. Furthermore, the increment of Li content resulted in volume change in the nanoporous structures resulting in inward expansion within their pores. This may be ascribed to the flexible nature of nanoporous materials attributed to the hollow channels.

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Yes

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MSc

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