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Atomistic Simulation Study of Li-rich Li1.2Mn0.8O2 Cathode Materials

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The cathode materials that can exhibits a capacity of >270 mAh/g with little or no capacity fade are the most promising next-generation cathode active materials for Li-ion batteries. Hence, the layered oxides relative to the stoichiometry Li1+yMn1-yO2 can deliver discharge capacities of >250 mAh/g after they have been activated by charging first to a voltage of 4.6–4.9 V in a Li-cell. However, the structural inherent complexity of Li-rich oxides causes deficiencies, and the ways to illuminate them have not yet established. In the present work, we investigate the structures of the pure and Li-rich, LiMnO2 and Li1.2Mn0.8O2 at the nanoscale to shorten the path length of lithium-ion transportation, in an attempt to improve the rate performance of the systems. High-temperature molecular dynamics simulations running a DL_POLY code was utilized to carry out the amorphization and recrystallization technique under a microcanonical ensemble (NVE) and a canonical ensemble (NVT) respectively. The microstructure snapshots confirm the two defective phase composites of Li2MnO3/LiMnO2 with crystallographic defects within the nanostructures; dominated mainly by Li and Mn ions mixing layers and grain boundaries. Furthermore, the calculated XRD patterns confirm the single-phase formation of orthorhombic LiMnO2 in the pure structure and formation of the two-phase together with a spinel-type Li2Mn2O4 in the Li-rich nanoparticles. The findings of the current study will provide a better understanding of the Li-rich structures.

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

Yes

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

MSc

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