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Simulated Synthesis of Layered Li_{.2}MnO₃ Nanostructured Cathode Materials

Lithium-ion batteries have been broadly used in various portable electronic devices and the application targets are currently moving from small-sized mobile devices to large-scale electric vehicles and grid energy storage. As such, high-energy cathodes particularly Li2MnO3–LiMnO2 layered–layered materials are of significant interest due to their high specific capacities over wide operating potentials. In this work the Li-rich layered Li2MnO3–LiMnO2 nanostructures, with 4014 atoms are synthesized using DL_POLY code [1] under the micro-canonical ensemble (NVE) at 1800K during the amorphization and recrystallization process. The nanoparticles are deintercalated to mimic the charging process and monitor new phases that form in the stoichiometry from Li2MnO3 nanocluster of 4014 atoms. Characterization of XRDs for intermediate structures exhibit the main characteristics peaks of Li2MnO3 as well as other peaks that emerge and indicate a change in structure. This is in accordance with microstructural snapshots that depict formation of intermediate structures and extraction of Li from Li2MnO3. The resulted structures suggest the better cycle performance of Li-excess materials with Li2MnO3–LiMnO2.

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