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## Simulated Synthesis of Layered $\text{Li}_{0.2}\text{MnO}_3$ 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  $\text{Li}_2\text{MnO}_3$ – $\text{LiMnO}_2$  layered–layered materials are of significant interest due to their high specific capacities over wide operating potentials. In this work the Li-rich layered  $\text{Li}_2\text{MnO}_3$ – $\text{LiMnO}_2$  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  $\text{Li}_2\text{MnO}_3$  nanocluster of 4014 atoms. Characterization of XRDs for intermediate structures exhibit the main characteristics peaks of  $\text{Li}_2\text{MnO}_3$  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  $\text{Li}_2\text{MnO}_3$ . The resulted structures suggest the better cycle performance of Li-excess materials with  $\text{Li}_2\text{MnO}_3$ – $\text{LiMnO}_2$ .

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