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Simulated synthesis of Li-intercalated layered (Li2MnO3)-spinel (LiMn2O4) composite nanoarchitectures.

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The layered-spinel composites are amongst the utmost propitious cathode materials with potential to advance lithium ion batteries, to date. They demonstrate tremendous improvement on structural stability, cycling performance and higher specific capacity, > 250 mAh/g. Recent studies have focused mainly on enhancing the specific capacity of these layered-spinel composites. However, there is limited knowledge on how incorporating such layered-spinel composite electrodes affects the working voltage of lithium ion batteries. In this study, molecular dynamics (MD) method was employed to generate nanospherical layered (Li2MnO3) - spinel (LiMn2O4) composite, with different lithium concentrations. The simulations yielded crystalline nanospheres with grain-boundaries except that of Li1.6Mn2O4. RDF graphs were plotted for all systems and confirmed complete crystallisation of all structures. XRDs indicated the existence of layered Li2MnO3, spinel LiMn2O4 and spinel Mn3O4. Increases in Li-content resulted in a decrease in Mn3O4 concentration. Frenkel defects and grain boundaries were observed. The simulated layered-spinel components exist in all lithiated structures.

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yes

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

MSc

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