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Crystal Growth and Agglomeration of Heterostructured Layered-Spinel Li-Mn-O Primary Particles

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Layered-spinel Li-Mn-O nanostructured materials have ignited significant interest as cathode materials in lithium-ion batteries due to their simultaneously great reversible capacity (302 mAh/g), amongst other exceptional properties. However, their high electrode surface area has lead to side reactions with the electrolyte resulting in capacity fade. As such, we employ molecular dynamics methods to simulate spontaneous growth, crystallization and aggregation of primary particles under the NVE, NPT and NVT ensembles, prior to their surface modification. Characterization of the recrystallized particles depicted the presence of heterostructured layered-spinel components and microstructural features such as microtwinning and intrinsic defects, which are essential for achieving high storage capacity. The vacancies and substitutions help facilitate faster mobility of Li through the lattice and additional pathways. The primary nanoparticles were agglomerated with periodic neighbours to formulate secondary particles. Agglomeration yielded different morphologies of particles with various simulation cells, such as spherical and rod-like structures. Efficient agglomeration of such primary particles will add valuable insights to the attainment of highly conformal coating strategies and subsequently, the design of high-capacity batteries with enhanced storage capacity and performance.

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