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First-principles investigation of the structural changes in Li-rich cathode composites HEMANT DIXIT, WU ZHOU, JAGJIT NANDA, JUAN-CARLOS IDROBO, VALENTINO COOPER, Oak Ridge National Lab, Oak Ridge, TN, MATERIALS SCIENCE AND TECHNOLOGY DIVISION COLLABORATION — Lithium ion batteries have high energy densities and are widely used in consumer electronics. However, it is essential to improve their power rate and cycle life for long-term usage. Cathode materials containing Li-excess layered oxide compounds, $x\text{Li}_2\text{MnO}_3(1-x)\text{LiMO}_2$, (where $\text{M}=\text{Mn}, \text{Co}, \text{Ni}$ and $x= 0.2-0.7$) have two times higher capacities than the conventional cathode material but during cycling a decrease in energy density and a concomitant development of a low voltage plateau are often observed. Furthermore, recent experimental studies have observed the formation and clustering of the anti-site defects near the surface. Thus a detailed understanding of the structural changes at the atomic scale of these Li-rich composites is essential to establish the correlation between the structural and electrochemical property. We present first-principles density functional theory study of the structural and electronic properties in Li-rich cathode composites. These cathode composites are modelled as solid solutions of the LiMnO_2 ($\text{R}\bar{3}\text{m}$) and Li_2MnO_3 (C_2m) phases. We discuss the stability of the proposed model, the diffusion energy barriers of Li^+ ions calculated using nudged-elastic band method and the formation energies of the antisite defects.

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