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Impact of Nickel (Ni) doping on Li1.2Mn0.8O2 Cathode Material

Several studies have been conducted to overcome the poor cycling stability, voltage fade, and low coulombic efficiency barriers in practical applications of Lithium manganese oxides. Transition metal doping (Ni) has been considered a suitable technique to enhance the stability of these materials. In this study, we employ a genetic algorithm to generate and identify new phases of Ni-doped Li1.2Mn0.8O2, starting from a 1x1x1 supercell structure of Li2MnO3. Li2MnO3 has garnered interest as a potential cathode material for lithium-ion batteries due to its high energy density and specific capacity. In this work, the genetic algorithm produced 12 phases of Ni-doped Li1.2Mn0.8O2 with negative formation enthalpies, suggesting thermodynamic stability. The generated phases Li1.2Mn0.6Ni0.2O2 and Li1.2Mn0.3Ni0.5O2 are regarded to be the most favorable stable phases because of their lowest energy of formation. Furthermore, first principles calculations were performed to study the thermodynamic, mechanical, and electronic properties of these materials. The study shows that the materials are thermodynamically stable with negative heats of formation. The materials were all found to be mechanically stable under a strain of 0.001 with the Pugh ratio predicting the materials to be brittle. The density of states of Li1.2Mn0.8O2 shows the presence of a band gap of (0.266eV) at Fermi level indicating that the material is a semiconductor. Conversely, Li1.2Mn0.6Ni0.2O2 exhibits half-metallic ferromagnetic behavior with an indirect band gap of 0.00 eV, while Li1.2Mn0.3Ni0.5O2 is a magnetic metal with no band gap. These findings open a path further evaluation on stable phases of lithium manganese cathode materials. The calculations were performed at the CHPC Lengau cluster using 48 cores.

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