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COMPUTATIONAL AND EXPERIMENTAL STUDIES ON NMC BATTERY PRECURSORS

Abstract:

Nickel manganese cobalt batteries, also known as lithium-ion batteries, because of their higher energy capacity and high power, extended cycle life, improved rate stability, superior safety efficiency density, and low cost of nickel and manganese raw materials, have the potential to ensure energy storage. Li-ion batteries are rechargeable batteries that have shown to be one of the most efficient and handy ways of storing energy while being environmentally friendly and renewable. The major challenge or disadvantage of rechargeable batteries is their inability to maintain energy and supply enough for the longest period to meet human demand. In this research project, we investigated the stability of manganese nickel carbonate (Mn1.5Ni0.5CO3) using Vienna Ab initio Simulation Package (VASP) code through the generalised gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof (PBE) exchange-correlation. Computational and experimental data were in agreement to the results of lattice parameters, heats of formation, elastic properties, density of states (DOS), and x-ray diffraction (XRD). Phonon dispersion curves show no negative frequencies along the gamma region thus, the structures are stable and in agreement with the calculated elastic constants.The temperature has been shown to have a substantial effect on battery performance, safety, and cycle life. Then the Cluster expansion and Monte-Carlo simulations were employed to determine phase changes and high-temperature properties.

Keywords: Lithium-ion batteries, NMC, Mn1.5Ni0.5CO3,

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