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Investigation of structural, electronic, elastic and dynamical properties of Li2Mn0.5Ru0.5O3 cathode material for Li-ion batteries: A first-principles study

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Li₂MnO₃ has been considered as one of the promising cathode materials for lithium-ion batteries due to its high theoretical capacity, nontoxicity, and natural abundance of Mn. However, it has not been commercialized due to poor structural stability and low conductivity during cycling. To ameliorate the electrochemical performance of Li₂MnO₃, we propose doping with Ru, which can stabilize the structure and improve its electronic conductivity. In this study, the cluster expansion technique was used to generate new phases of Li₂Mn_{1-x}Ru_xO₃ (0≤x≤1) with varying concentrations and symmetries. The binary phase diagram predicted Li₂Mn_{0.5}Ru<sub>0.5 as the most stable phase with the lowest negative heats of formation, suggesting thermodynamic stability. In addition, the elastic constants for Li₂Mn_{0.5}Ru_{0.5}O₃ satisfied the required stability criterion for triclinic structures, indicating mechanical stability. The phonon dispersion curves showed no negative vibrations along high symmetry directions of the Brillouin zone, suggesting that the doped phase is dynamically stable. Moreover, the density of states shows a decrease in the band gap of Ru-doped Li₂MnO₃ from 1.506 eV to 0.417 eV, which leads to higher electrical conductivity of the material. Finally, based on these results Li₂Mn_{0.5}Ru_{0.5}O₃ can be proposed as potential cathode materials for use in lithium-ion batteries, which may lead to improved cycling performance.

Apply to be considered for a student ; award (Yes / No)?

yes

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

MSc

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