First Principle Study of Doping Effects (Ti, Cu, and Zn) on Electrochemical Performance of Li_2MnO_3 for Lithium-ion Batteries

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Abstract

Li-rich layered Mn-based oxides (LMOs) have attracted much attention due to their potential in various applications as cathode materials with high energy density. However, these cathode materials still suffer from drawbacks such as poor rate capability and voltage decay which makes further investigation vital and rational. Herein, the doping strategy is employed to investigate the effect of TM = Ti, Cu, and Zn on $Li_2Mn_{0.5}TM_{0.5}O_3$ for improving electrochemical performances of Li_2MnO_3. The electrochemical properties such as voltage, electrical conductivity, safety, structural stability, and kinetics and mechanism of Li-ion diffusion are evaluated and compared. All doped cathodes decrease the voltage reduction and improve the electrical conductivity coefficient in comparison with LMO. Ti dopants exhibit the potential to increase the maximum voltage of LMO and structural stability. Doping Zn and Cu elements can delay the oxygen loss which leads to a higher life cycle and safety. Also, the substitution of Zn dopants decreases the energy barrier against Li-ion diffusion and consequently, the lower Li-ion diffusion coefficient is expected. Using Ti, Cu, and Zn with $\alpha = 0.5$ in $Li_2Mn_{0.5}TM_{\alpha}O_3$ may furthermore open a door for the synthesis of lithium-rich materials with enhanced performance.

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