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First principles study of layered xLi₂MnO₃•(1-x)LiMO₂ (M = Mn, Ni, Co, etc.) cathode materials

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Abstract content
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The demand for higher energy density lithium ion batteries makes Li-rich layered xLi₂MnO₃•(1-x)LiMO₂ (M = Mn, Ni, Co, etc.) among the most attractive candidates for future cathode materials. It drawn much attention recently as alternative cathode materials because of its high specific capacities > 280 mAh/g [1] when charged to over 4.6V. Unfortunately, xLi₂MnO₃•(1-x)LiMO₂ suffers some practical problems for commercial application, including 1) first cycle irreversible capacity loss associated with the elimination of oxide ion vacancies from the layered lattice, 2) limited performance at high rates associated with the insulating Li₂MnO₃ component and thick solid electrolyte interfacial (SEI) layer, 3) capacity fade after moderate cycling caused by interfacial stability, electrolyte oxidation, surface film formation and transition metal dissolution and 4) voltage fade during long cycling caused by structural instability and phase changes. To overcome these limitations, efforts, such as surface modification [2] and elemental doping [3] have been investigated by experimental and theoretical approaches. First principles density functional theory calculations have been used on Li-rich layered cathode materials [4] to elucidate and exemplify the relationship between structures, electronic, phase stability and electrochemical properties and play an important role in developing and optimizing new energy storage and conversion materials. In this study we are going to investigate structural, electrical and thermal properties of xLi₂MnO₃•(1-x)LiMO₂ using density functional theory (DFT) in the first principles calculations. Based on atomic scale understanding of those mechanisms, we will reveal some helpful methods to overcome the performance degradation problems in these cathode materials.

[1] H. Yu etal., J. Phys. Chem. Lett. 2013, 4, 1268−1280
[2] S-T. Myung etal., J. Phys. Chem. C, 2007, 111, 4061-4067
[3] M. Iftekhar, etal., J. Electrochem. Soc., 2014, 161(14), A2109-A2116
[4] T. Tamura etal., Modelling and Simulation in MSE, 2012, 20(4), 045006-1-045006-9

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