Molybdenum modifed on $0.5Li_2MnO_3$-$0.5LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ cathode for high-voltage lithium-ion battery

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The purpose of this study was to develop a high capacity, high voltage and high stability cathode material in the lithium-ion batteries. In this study, Sol-Gel synthesis was applied to synthesize the pristine layered $0.5Li_2MnO_3$-$0.5LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ (LNMC). In order to decrease structural defects, LNMC was doped with Molybdenum. X-ray photoelectron spectroscopy (XPS) was used to characterize the valence states of Mn and Mo in LNMC. X-ray absorption spectroscopy (XAS) was applied to probe the valence states and coordination environment of Mn and Mo at various charge-discharge stages. The results of XPS showed the valence states of Mn in LNMC were all Mn^{4+}, but the valence states of Mn in Mo-doped LNMC were 2.17% Mn^{3+} and 97.83% Mn^{4+}. On the other hand, the XAS results indicated the valence states of Mn and Mo increased slightly and the coordination environment of Mn and Mo had been changed at high voltage. This study found that coordination environment of Mo-doped LNMC changed fewer than pristine LNMC, implying Mo-doped LNMC had more stable electrochemical properties at high voltage. Electrochemical measurements demonstrated that Mo-doped LNMC had a better rate capability and cycling stability in the voltage range of 2V-4.8V than those of pristine LNMC. Similarly, Mo-doped LNMC exhibited higher discharge capacity and capacity-retention than pristine LNMC after 30 cycles (269mAh/g and 83.3% vs. 276mAh/g and 61.2%).