Exploring the effect of proton on Mn-based Li-rich cathode materials for Li-ion batteries

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Li-rich cathode materials have recently attracted much attention as a promising candidate for next-generation Li-ion batteries (LIBs), due to their high specific capacity. In this system, oxygen redox reaction plays an important role, which can make more Li^+ ions to participate in (de)intercalation process [1][2]. Nevertheless, some problems exist in Li-rich materials, such as severe irreversible capacity loss in the first cycle and poor cycling performance, which are closely related to the oxygen redox process. Moreover, the factors affecting reversibility for oxygen redox are also not fully understood [3].

Based on the background, a series of proton-inserted Li_2MnO_3 (LMO) samples have been investigated. Electrochemical test and DFT calculation results demonstrate that the proton insertion can improve the electrochemical performance effectively without affecting the structural integrity. Combining with TGA analysis, it can be proved that a higher discharge capacity can be delivered with more proton insertion. Especially, for the LMO-acid sample, the initial discharge capacity can reach as high as 302 mAh g^{-1} with Coulombic efficiency of 99% at a current density of 10 mA g^{-1}. This study gives an idea on optimizing the oxygen redox reaction to increase the energy density for Mn-based Li-rich materials.

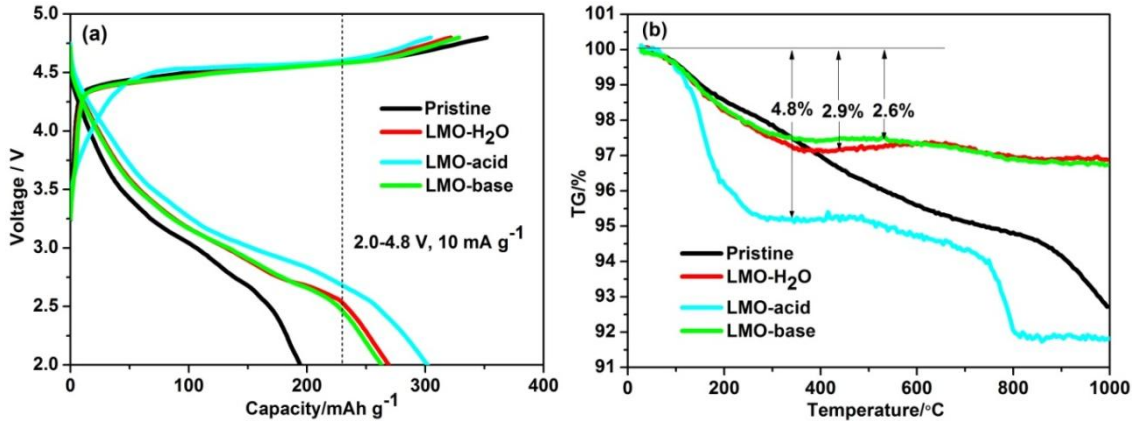

Fig.1 (a) The initial charge-discharge curves of the pristine and proton-inserted LMO samples. (b) The TGA data of the pristine and proton-inserted LMO samples.

References:

[1] McCalla E, Abakumov A M, Saubanère M, et al. Science, 2015, 350(6267): 1516-1521.
[2] Luo K, Roberts M R, Hao R, et al. Nature chemistry, 2016, 8(7): 684-691.
[3] Yabuuchi N, Nakayama M, Takeuchi M, et al. Nature communications, 2016, 7: 13814.