Enhancement of the electrochemical performance of the cathode material $NaNi_{0.5}Mn_{0.5-x}Zr_xO_2$

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The development of the cathode material for beyond lithium-ion batteries plays a critical role in advancing technical progress and ensuring the long-term viability of our society. However, because of the poor performance of SIBs, many novel technical solutions are delayed or hindered. Our research work enhanced electrochemical parameters such as capacity retention and structural stability by proposing Zr ion doping because of the larger ionic radius compared to Mn and Ni (r_Mn^(4+)=53 pm, r_Ni^(2+)=69 pm, and r_Zr^(4+)=79 pm), which can enhance the bond of TM and oxygen atoms. The substitution of transition metals by Zr inactive metal ions leads to enlarged interlayer spacing for Na+ and superior micro-nano level cathode structure with a high ion diffusion rate and unblocked diffusion paths for redox agents. Compared to non-substituted NaNi0.5Mn0.5O2, the Zr substituted material exhibits more continuous phase transitions and lattice parameter changes and no substantial contraction of interslab spacing in the layered structure. Zr improves the reversibility of structural changes and structural stability, resulting in superior sodium battery performance. The highest capacity retention illustrates 3% doped material upon the charge, and discharge cycling tests 0.1C rate in the cut-off voltage of 2.0 to 4.5 V. The capacity retention of 3%-Zr doped material demonstrates a 10% improvement in capacity retention after 100 cycles.

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