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Combustion Synthesis of Mn-Rich Disordered Rocksalt (DRX) Oxyfluoride Cathodes for Li-ion Batteries

Lithium-excess disordered rocksalt (DRX) materials are a promising class of Co- and Ni-free lithium-ion battery cathodes that offer high specific energy density (up to 1000 Wh kg^{-1}) and reversible capacity (up to 300 mAh g^{-1}). Compared to traditional Li-ion cathodes (e.g., $LiNi_xMn_yCo_{1-x-y}O_2$), DRX oxides/oxyfluorides are compatible with a wider range of earth abundant transition metals, such as Ti and Mn. DRX cathodes are traditionally synthesized via solid-state or mechanochemical reactions, which are difficult to scale and provide little control over particle morphology. Furthermore, recent development of DRX compositions show Mn-rich concentrations substantially improve performance by increasing Mn-redox and inhibiting irreversible O-redox. To address this issue, the present study reports a scalable, two-step reaction route to prepare Mn/Ti-based DRX oxyfluoride cathodes with the nominal composition $Li_{1.1}Mn_{0.8}Ti_{0.1}O_{1.9}F_{0.1}$ (LMTF1811). The first step utilizes a glycine-nitrate combustion reaction to produce an orthorhombic $Mn_{0.8}Ti_{0.1}O_{1.4}$ (MTO814) precursor, which is subsequently lithiated and fluorinated by reacting with Li_2CO_3 and LiF. The effects of annealing temperature (900℃-1100℃) and cooling rate (5-120℃ min^{-1}) on the product's structure and DRX phase conversion are explored. Interestingly, heating at 1000℃ and quenching between 5 and 120℃ min^{-1} shows varying phase purities between 80 and 95%, respectively. However, heating to 1100℃ produces Mn-rich phase-pure DRX regardless of quench rate. Phase-pure DRX prepared through this novel synthesis platform exhibit promising electrochemical performance, attaining reversible capacities ~200 mAh g^{-1} with 86% capacity retention after 100 cycles in Li metal half-cells.

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Topical Area

Hard matter: energy materials

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