Li-rich Li$_5$FeO$_4$ (LFO) cathode material as pre-lithiation additive for enabling high-energy Si•C/NMC batteries

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Silicon containing anodes employed in Li-ion cells are known to drastically boost the energy density of a full LIB battery by providing a high intrinsic capacity via Li$_x$Si intermetallic alloy formation/utilization compared to capacity-limited graphite anodes. However because a >300% volume change occurs between (de)lithiated Li$_x$Si states, a irreversible trapping of cyclable Li in the full cell negatively impacts performance, potentially by lowering cycle life. In this new approach, we enable new high-energy Si-containing Li-ion full cell systems with NMC cathodes by supplementing the lithium content in the cell from the cathode side via co-blending NMC powder with the anti-fluorite compound, Li$_5$FeO$_4$ (LFO) that contains a tremendously high gravimetric capacity. For example, in a Li/LFO half cell, we observe a huge gravimetric capacity on the first charge (Figure 1 and Ref. 1). The LFO can release upwards of 750 mAh/g usable capacity on this sacrificial first charge. Note the LFO on discharge is electrochemically inactive above 3.0 V (vs Li$^+$), and thus will not contribute reversible capacity in a typical Si•C/NMC(LFO) cell cycled in a voltage range above about 2.5 V. The Li in LFO also provides small aliquots of Li during long-term cycling in Si cells that spares NMC from overcharge. This presentation will highlight the features of LFO, an effective lithium-source additive material.

Figure 1. First charge and discharge voltage profile of Li/Li$_5$FeO$_4$ cell between 4.7 and 1.0 V; C rate is C/40; black curve: standard LFO material, and cyan curve: optimized LFO material.


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