Ferrocene based carbon–Iron/lithium fluoride nanocomposite as stable electrode material in lithium batteries

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An incessant increase of mobile electronic devices requires high-energy density Li-ion batteries. The energy density of a battery intimately depends on the properties of electrode materials. The fundamental way to attain high capacity is to utilize all possible oxidation states of the electrode material by reversible conversion reaction. High capacity was observed in nanocomposites with transition metal oxides using such a conversion reaction that involves their reduction to nanosized metal, and lithium oxides. Although transition metal fluorides have higher theoretical energy densities than oxides, only little efforts have been made due to their poor electronic conductivity. Recently, reversible electrochemical activities of metal fluorides nanocomposites (TiF₃, VF₃, FeF₃, CoF₃, BiF₃, etc) have been reported. Some of these exhibited reversible specific capacities as high as 600 mAh/g. However, the application of metal fluoride cathodes is still hampered by their reaction irreversibility, poor cycling stability, and in some cases requires high temperature to attain this value. Incorporation of transition metal/flourides into nanocarbons is considered to be an effective method to improve cycling performance. In this respect, carbon nanotubes, catalytically grown carbon fibers, porous carbon materials, and graphitic carbons have gained much attention.

Herein we present our efforts to obtain iron-confined-nanocarbon/LiF nanocomposite from an appropriate mixture of ferrocene and LiF by thermal treatment at 700 °C in a closed reactor under argon atmosphere. The nanocomposite produced consists of multi-walled carbon nanotubes and onion-type graphite structures in which iron particles are encapsulated, and LiF is dispersed throughout the matrix. The nanocomposite employed as the cathode of a Li battery exhibited a reversible capacity of 280 mAh/g in the potential range 0.5-4.3 V and of 170 mAh/g in the range of 1.3-4.3 V at a current density of 20.83 mA/g. After an initial decrease in the first cycles the nanocomposite cathode showed capacity retention of 97% after 300 cycles, as well as a durable rate capability. However, efforts are in progress to optimize the Fe and carbon contents of the nanocomposite in order to increase the capacity of the system.