MSE-2: Fluorination of α-MnO₂ for Energy Storage Devices Geoffrey Xiao, Mohammad Hassan, Sam Kulesa

Problem Statement:

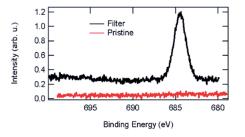
 α -MnO₂ has superior specific capacity for use as a cathode in lithium-ion batteries, but suffers from large decreases in capacity upon charge/discharge cycling. Can fluorination of α -MnO₂ improve capacity retention?

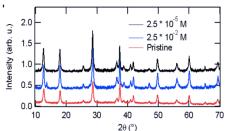
Approach:

Developed fluorination techniques and compared fluorinated α -MnO₂ with pristine α -MnO₂ for energy storage:

- Optimized parameters for multiple fluorination techniques.
- Characterized samples using XRD & XPS to verify structure was maintained and fluorine was present with no contaminants.
- Tested and compared electrochemical performance and magnetic properties of fluorinated and pristine α -MnO₂.

Results:





XPS showed a strong Mn-F bond (684 eV) and no C-F bond (690 eV) in fluorinated MnO₂ (black)

XRD showed structural preservation after solution treatment at two concentrations

- XRD α structure was maintained after fluorination.
- XPS Mn-F bonds with no C-F bonds indicated no contaminants.
- Electrochemical Fluorination improved electrochemical performance.

Discussion & Conclusions:

- Two successful techniques were polymer degradation, in which a fluoropolymer was heated to release fluorine-containing byproducts that reacted with α -MnO $_2$, and a solution technique where fluorine salts were dissolved in a solution and stirred with α -MnO $_2$.
- XRD and XPS showed that the "α" structure was only maintained and fluorine was only incorporated under certain parameters, indicating fluorination process is sensitive.
- Capacity retention improvement in fluorinated α -MnO $_2$ was theorized to be due to stronger Mn-F bonds compared to Mn-O bonds.

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