Development of Model Metal Oxide Electrode Interfaces for Electrochemical Energy Investigations

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Typical Li-Ion Battery Cathode Structure*

(Heterogeneous/disordered)

Mixed Mechanism Lithiation+

Atomic Layer Deposition (ALD)

TiO$_2$/C Electrode by ALD

Goal: Develop and evaluate model material systems using ALD that facilitate high resolution analysis of interfacial charge transfer processes.


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**Newly Available Analysis Techniques:**
- *in situ* Spectrophotometry
- Spectroscopic Ellipsometry
- Thickness-scale correlated mechanism deconvolution
- High resolution, spatially resolved chemical analysis – TOF SIMS

- All can be adopted for different ALD-based material systems

**Surprising ToF SIMS Results**
- F\(^{-}\) detected throughout the TiO\(_2\) layer
- Likely related to HF formation (from LiPF\(_6\) + H\(_2\)O)
- Contrary to accepted Ti\(^{4+}\) reduction scheme

**CV of Li-TiO\(_2\) Electrode**

**Secondary Ion Mass Spec: Reversible F\(^{-}\) anion co-intercalation**

*CV of Li-TiO\(_2\) Electrode*

*1M (LiPF\(_6\)) in 1:1 EC:DEC*

*Li-ion Battery*

*Surprising ToF SIMS Results*

*After Lithium Insertion*

*After Lithium Extraction*