Opportunities for Computing

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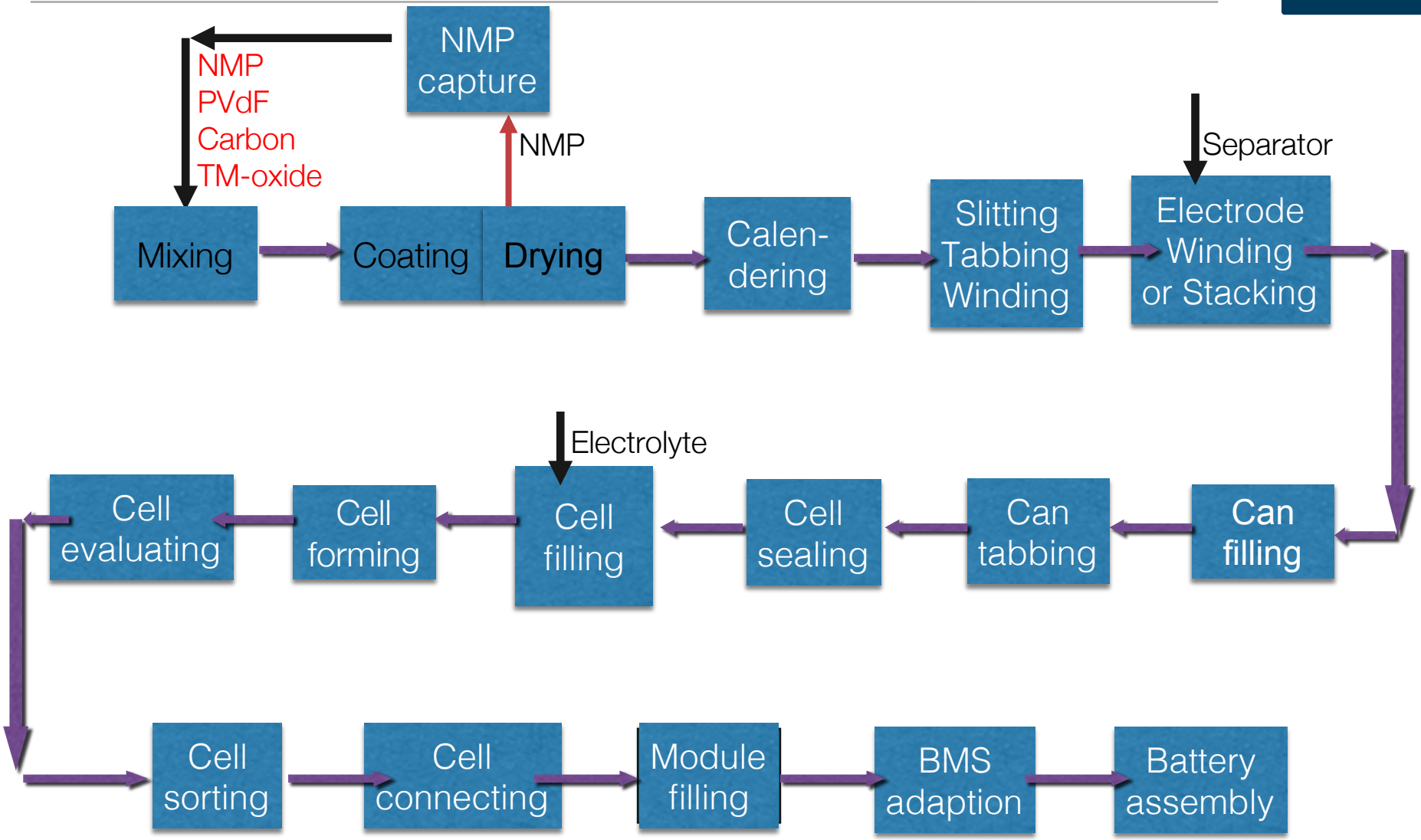
1. Integrating new materials into existing R2R process can be slow
2. Computing can aid this process
3. Developments over the last 5 years give us new avenues

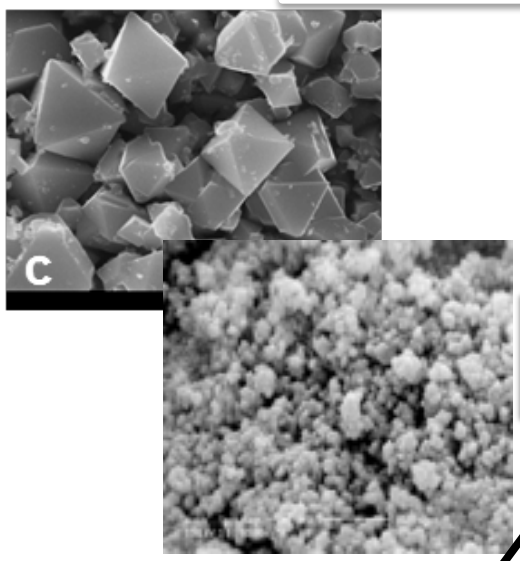
Li-ion batteries as an example



Intuition-based approach makes improvements time consuming

The challenge: Bringing science to intuition

Water based, composite particles, new materials, solid state

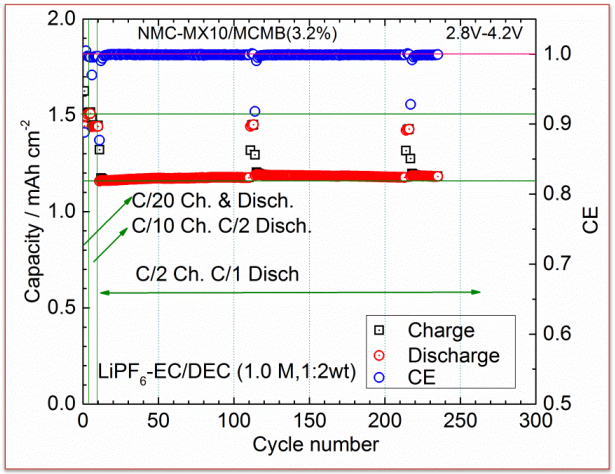


NMP
PVdF
Carbon
TM-oxide

NMP capture

NMP

Mixing → Coating | Drying → Calen-dering



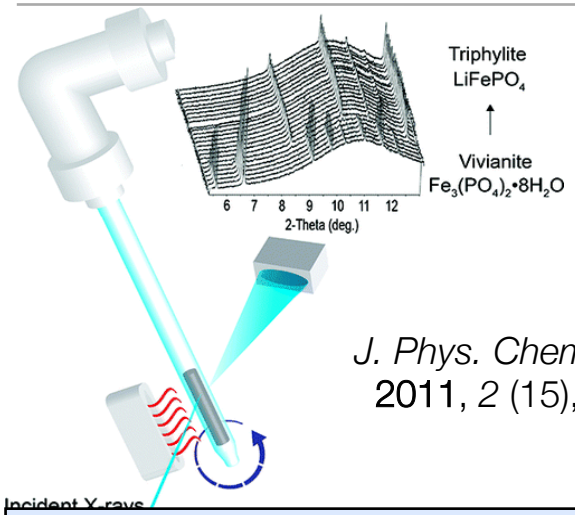
Viscosity, stability, ratios, solvent

Speed, cracking, uniformity, thickness

Contact resistance, cracking, porosity

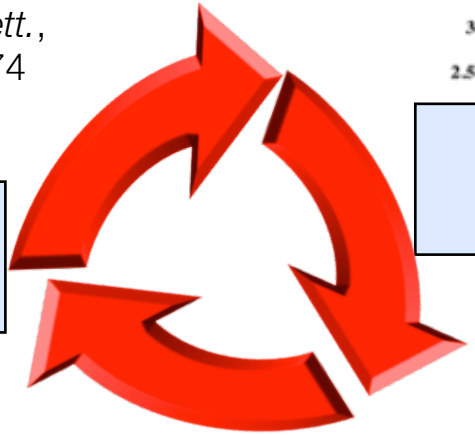
1. Can we bring scientific understanding?
2. How do we link material discovery to device fabrication?

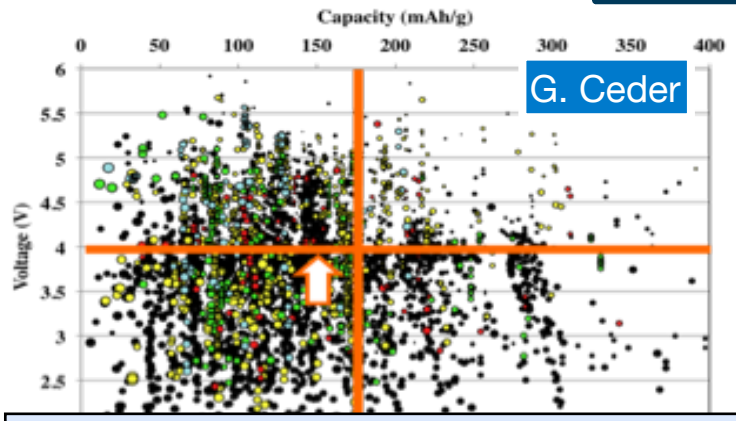
Innovations in the last 5 years open new avenues



J. Phys. Chem. Lett., **2011**, *2* (15), 1874

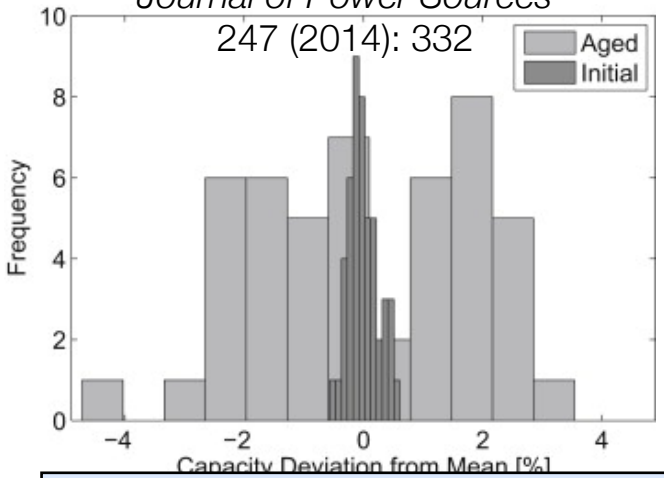
"Watching" materials and structures grow



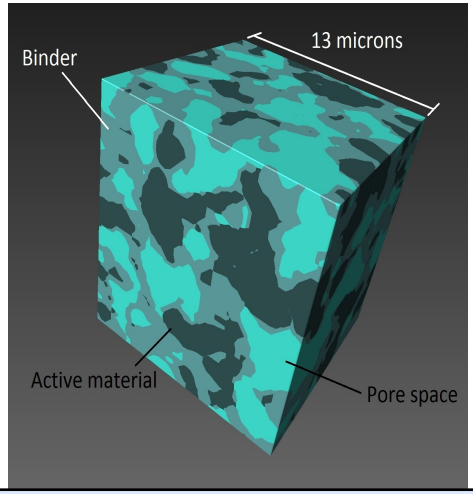


MGI: From discovery to synthesis

Journal of Power Sources
247 (2014): 332



Date mining



From materials to structures

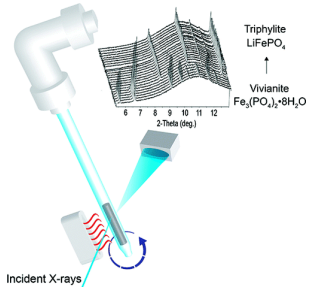
Bridging the materials-process-performance continuum

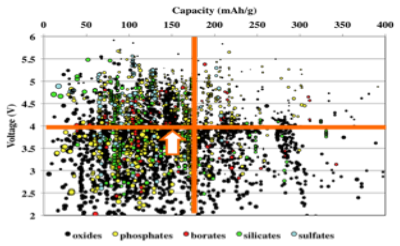
"Applied" Materials Genome

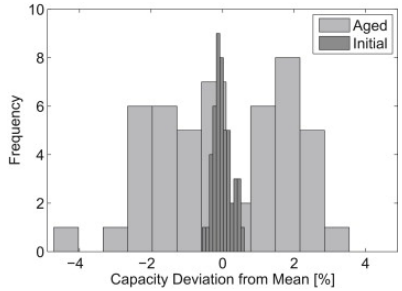
Science of processing

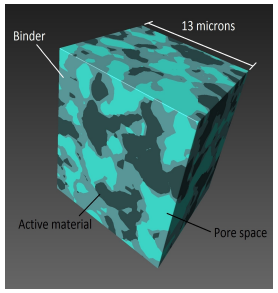
Today: Property prediction of ideal materials

Today: Continuum prediction of performance and life









Goal: Predicting device-relevant properties of materials

Goal: Predicting device behavior from process conditions