

SCALING UP OF HIGH-PERFORMANCE SINGLE CRYSTAL NI-RICH CATHODE MATERIALS WITH ADVANCED LITHIUM SALTS | AMMTO

Jie Xiao, Pacific Northwest National Laboratory

Industry partner: Albemarle

Contract Number:DE-LC-000L080 | Project Period: 2020-2023

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Project Overview

- **Innovation**
 - Develop an innovative and cost-efficient drop-in approach for scaling up single crystal Ni-rich cathode such as $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ (NMC811) and $\text{LiNi}_{0.9}\text{Mn}_{0.05}\text{Co}_{0.05}\text{O}_2$ (NMC90) with advanced lithium salts
 - Validate scaled single crystal cathode materials at industry-relevant conditions
- **Barriers addressed:**
 - Reduce manufacturing cost
 - Simplify manufacturing process
- **Impact**
 - Bridge the gap between disruptive single crystal cathode manufacturing and historical IP foundation of polycrystal NMC cathode
 - Address the scientific challenges in scaling up single crystal Ni-rich NMC and close the knowledge gap between lab-level synthesis and industry-scale manufacturing
 - Accelerate technology translation from lab innovations to industry manufacturing

Project Outline

Innovation: Address scientific challenges in scaling up high-performance single crystal nickel-rich cathode materials with reduced manufacturing cost

Project Lead: Jie Xiao, Pacific Northwest National Laboratory

Project Partners: Subramanian Venkatachalam, Albemarle

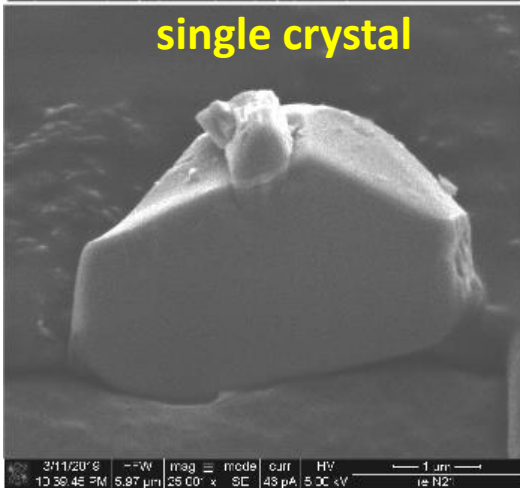
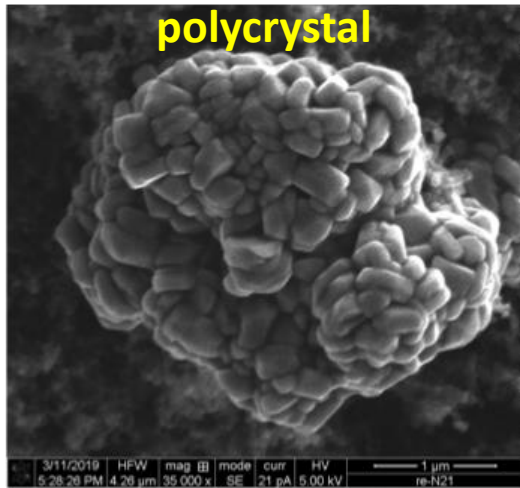
Timeline: 1/2021(delayed start) - 4/2023, 70% completed

Budget:

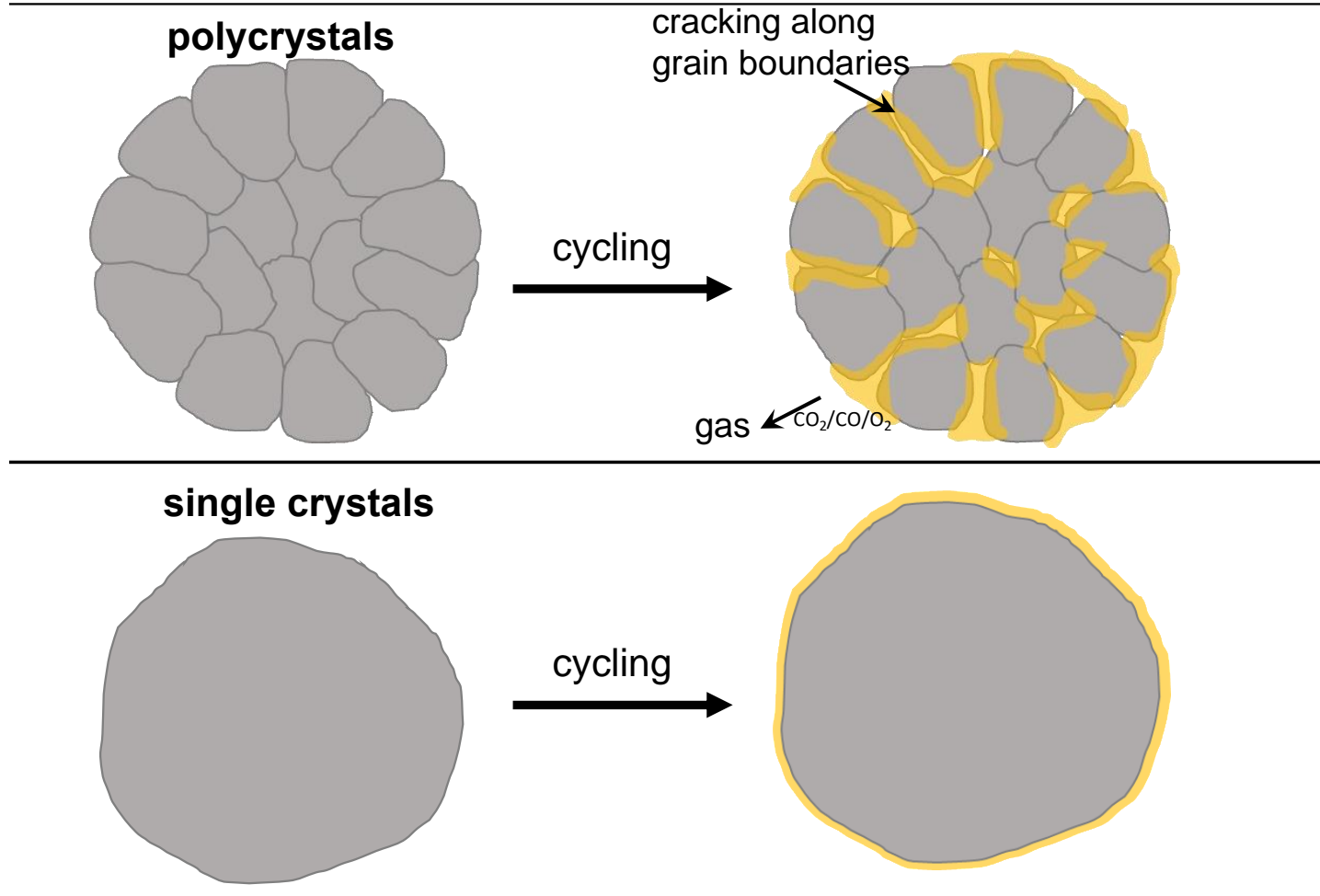
	FY21 Costs	FY22 Costs	FY23 Costs	Total Planned Funding
DOE Funded	\$350,000	\$350,000	\$300,000	\$1,000,000
Project Cost Share	\$447,341	\$284,399	\$268,260	\$1,000,000
In-kind	\$283,397	\$284,399	\$268,260	
Cash	\$163,944			

End Project Goal: Prove the feasibility of the proposed technology and demonstrate up to 1 kg/batch synthesis of NMC811 and NMC90 single crystals which are validated in realistic 2Ah pouch cells tested

Background: Why Ni-rich Cathode and Why Single Crystals?



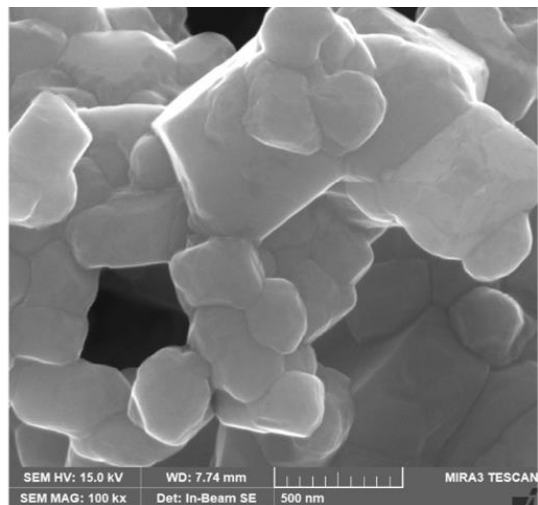
2019 DOE AMR review, bat407_Xiao_p



- Conventional polycrystal NMC811 has >200 mAh/g capacity but suffers from cracking, gas generation and moisture sensitivity, all of which are associated with grain boundaries in polycrystals.
- Single crystal without grain boundaries may potentially mitigate the problems of polycrystal NMC811.

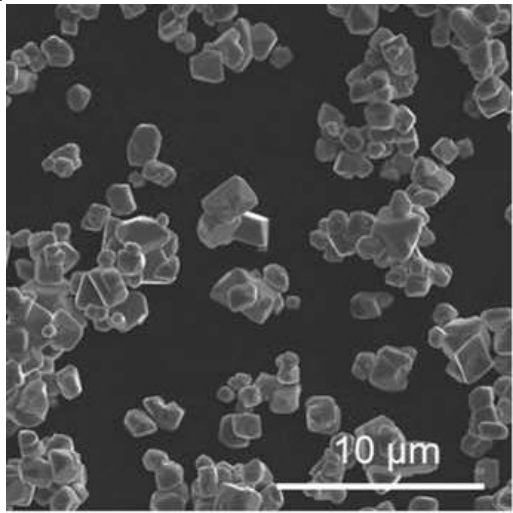
Background: Five Common Approaches for Single Crystal Synthesis

Hydrothermal-Assisted



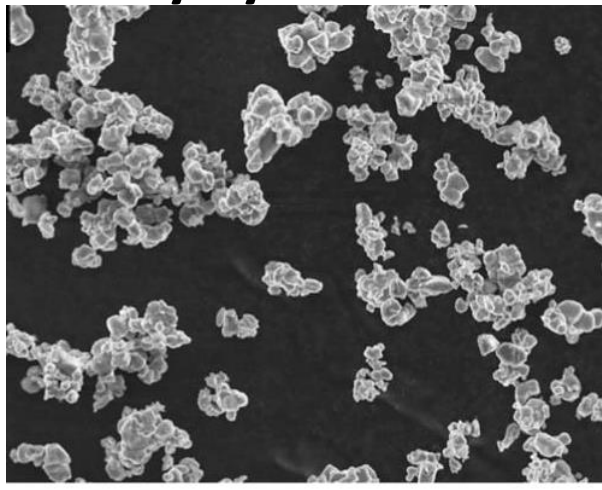
J. Power Sources, 2020, 477, 228701.

Molten Salts



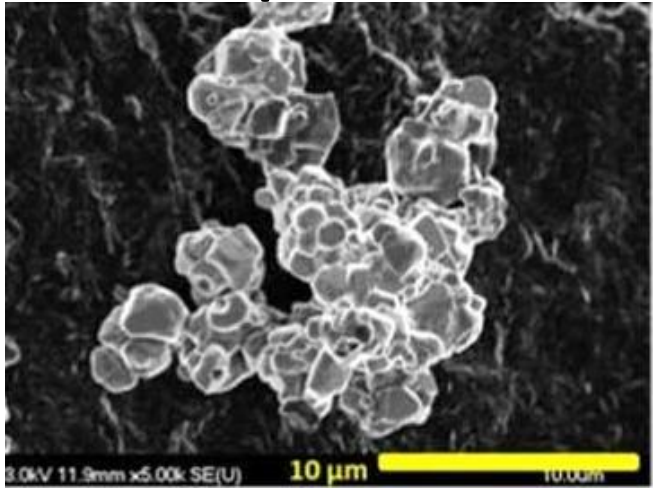
Science, 2020, 370, 1313.

Dry Synthesis

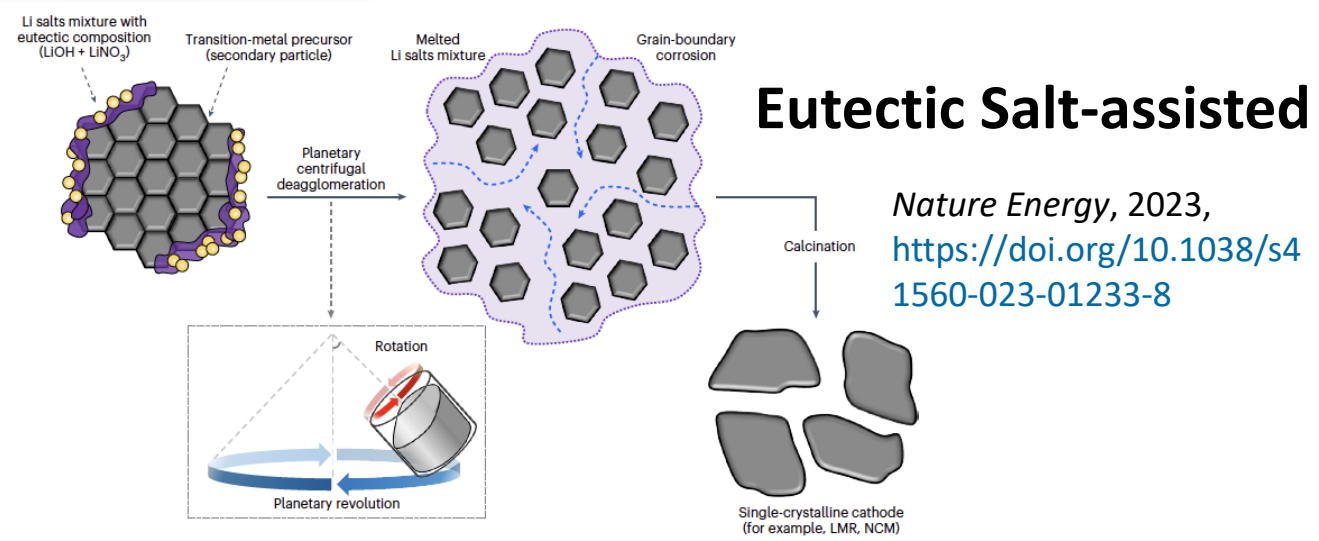


J. Electrochem. Soc., 2020, 167, 130536

Two-Step Lithiation

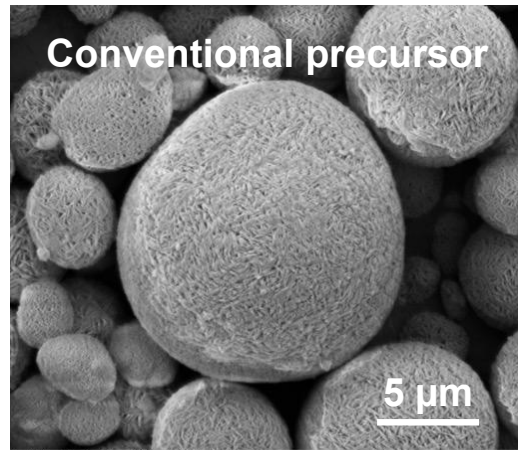


J. Electrochem. Soc., 2021, 168, 040531

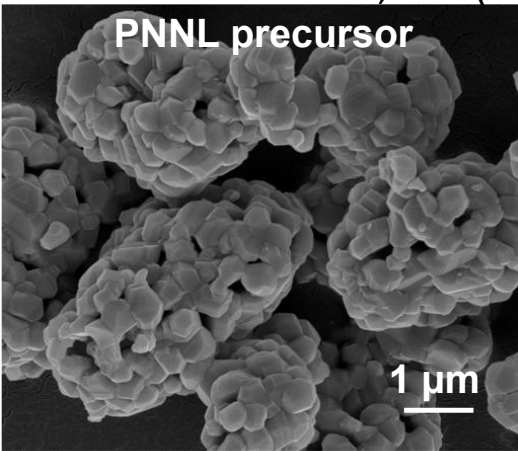


- For fundamental research: single crystals developed from molten salts or hydrothermal method have well defined facets and are good model materials
- For manufacturing: Both raw materials and processing need to be cost efficient.

Strategic Approach: An Innovative Drop-In Approach to Scale up Deagglomerated Single Crystal NMC811 and NMC90

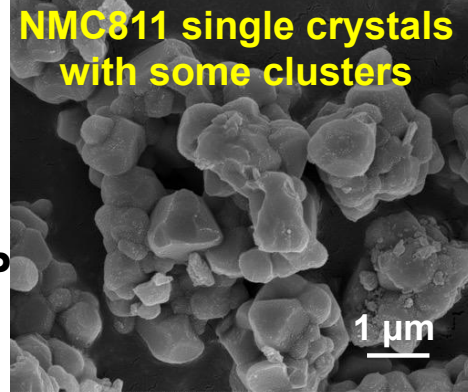
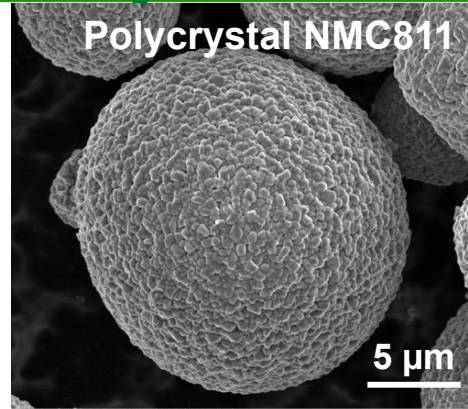


J. Power Sources **283**, 211 (2015)



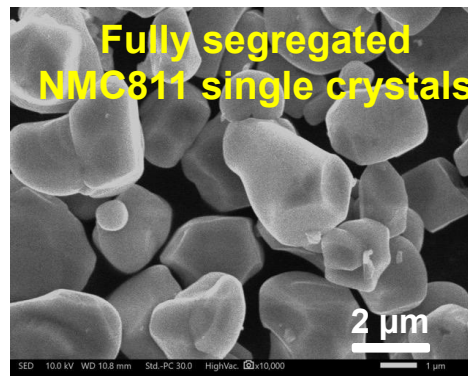
* Manuscript under review

+ LiOH →



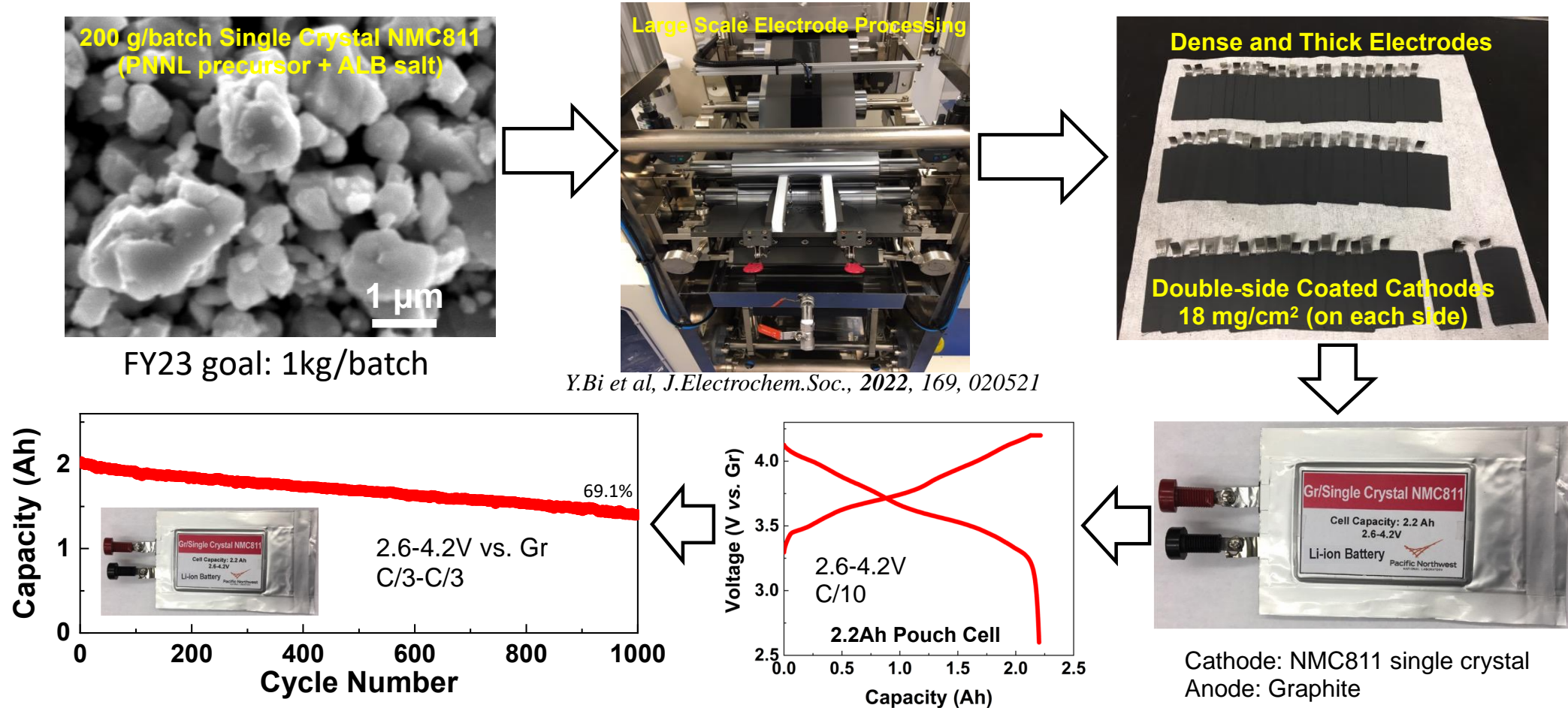
+ LiOH
background IP →

+ New Li Salt
New IP →



- Conventional NMC manufacturing approach produces polycrystals.
- PNNL's precursors form single crystals without significant agglomerations
 - The same polycrystal NMC manufacturing facility can be used.
 - Background IP developed under VTO/Advanced Battery Research program
- Since 2021 AMO and VTO have jointly supported this project to scale up single crystal Ni-rich NMC based on the background IP
- A new PNNL-Albemarle joint IP was filed :
 - Enabled by the combination of Albemarle's Li salt and PNNL's precursor
 - Fully segregated single crystals
 - Simplified manufacturing process
 - No corrosive water during calcination

Achievements: Identify and Address Scientific Challenges at Different Stages during Materials Scaleup



- 200g/batch synthesis of single crystal NMC811 (and NMC90) has been demonstrated after addressing quite **different scientific challenges**: raw materials selection, crystal homogeneity during large-scale synthesis, heat distribution etc.
- The scaled NMC811 single crystals have been validated in 2Ah Li-ion pouch cell which demonstrates 1,000 stable cycling.

Future Work, Technology Transfer, & Impact

Future Work:

- Apply knowledge gathered from materials scaleup to complete 1kg/batch synthesis of NMC811 and NMC90 single crystals with consistent quality
- Investigate the roles of the recently discovered new lithium salt and understand its impact on cathode manufacturing cost

Technology Transfer:

- PNNL will work with commercial partners to license and commercialize the technologies.
- Albemarle's lithium business will support the licensing activity of the joint development and help transfer the program knowhow to their future customers.

Impact:

- Address the scientific challenges in developing and manufacturing high-performance single crystal Ni-rich NMC cathode materials.
- Develop new IP to support domestic companies to quickly establish cathode manufacturing capabilities and leapfrog other countries in battery manufacturing

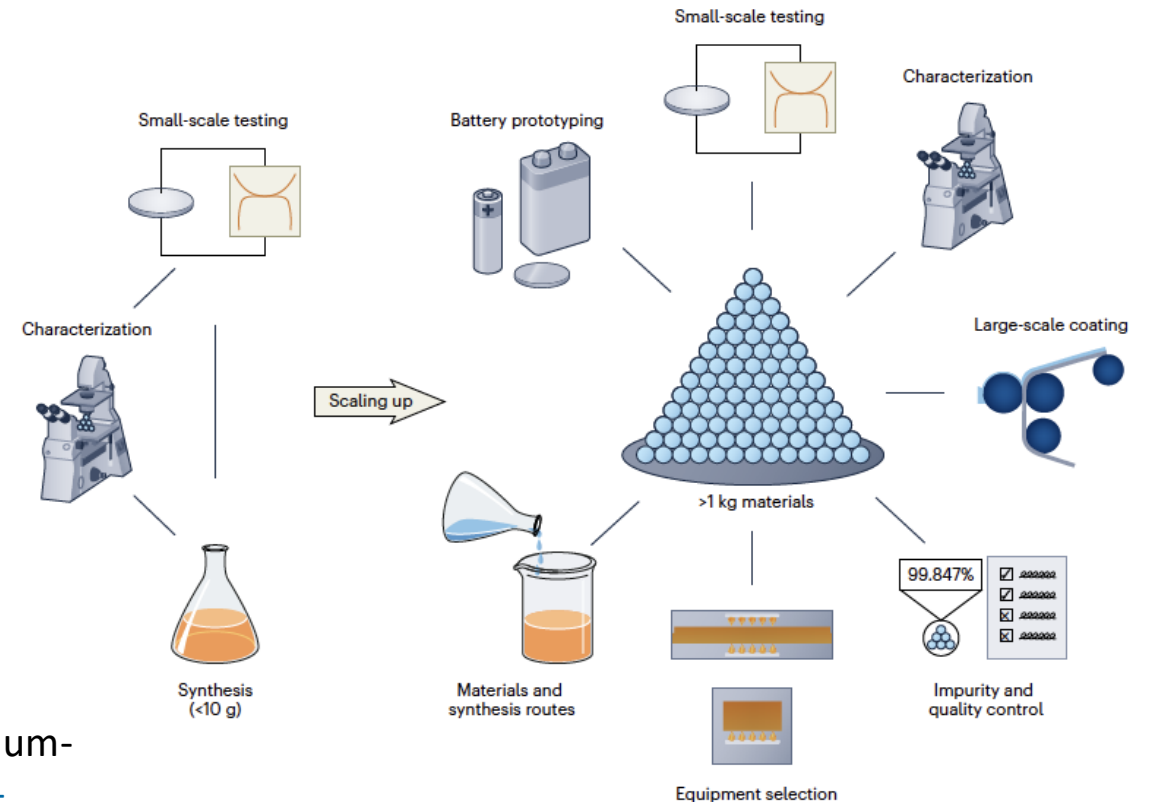
Questions?

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J. Xiao et al., From Lab Innovations to Materials Manufacturing for Lithium-based Batteries, Nature Energy, 2023, <https://doi.org/10.1038/s41560->