

Battery Cathode Interface-Readiness Build-Ready Screening with FluxMateria

A complete local battery workflow in 26.8 seconds showed that bulk ranking, interface readiness, battery-native scoring, and build handoff produce four different engineering answers.

Core finding: Bulk winner LiNiO₂ would have been the wrong conclusion. Interface analysis reopened LiMnPO₄. Battery-native scoring elevated LiMnO₂. Prototype handoff selected Li₄Ti₅O₁₂ as the best immediate build candidate.

26.8s

Local runtime
complete workflow

10

Curated cathode
materials

4

Distinct decision
winners

1

Prototype handoff
package

Bulk-only screening buries the engineering answer under one metric.

The Problem

If this workflow had stopped at bulk ranking, it would have told a simplified nickel-rich story. LiNiO₂ would have won because it scores highest on raw specific energy.

Interface behavior, transport, degradation, cycle life, and manufacturability would have been invisible. The engineering conclusion would have been incomplete and potentially misleading.

FluxMateria's Approach

Run all decision layers in one pass: bulk screening, interface analysis against current-collector surfaces, battery-native electrochemistry scoring, and prototype handoff with uncertainty and validation planning.

Separate highest upside, best interface match, and best immediate prototype in one coherent workflow. The answer changes when the question changes.

Would the same cathode remain the winner once bulk performance, interface readiness, battery-native tradeoffs, and immediate build risk were considered together? The answer was no.

Four decision layers. Four different winners.

01

Bulk Screening

Curated lithium-cathode pool ranking on raw properties.

WINNER
LiNiO₂

02

Interface Analysis

Re-rank against aluminum current-collector surfaces.

WINNER
LiMnPO₄

03

Battery-Native

Voltage, transport, degradation, cycle-life, coating co-design.

WINNER
LiMnO₂

04

Prototype Handoff

Uncertainty, validation plan, and build-readiness scoring.

WINNER
Li₄Ti₅O₁₂

Key insight: The workflow did not collapse into one obvious answer. It showed that the answer changes when the question changes. That is the actual value of the battery module.

The Complete Battery Decision Workflow

Curated Candidate Pool

- 10 lithium cathodes
- Engineering-relevant pool
- Not random chemistry

Interface Analysis

- Aluminum current-collector
- Interface readiness scoring
- Surface contact behavior

Battery-Native Scoring

- Voltage-profile interpretation
- Topology-aware Li transport
- CEI / electrolyte / coating

Prototype Handoff

- Degradation + cycle-life engine
- Uncertainty + active learning
- Build-readiness + disclosure

Calibrated holdout summary. The battery-native layer was benchmarked before publication.



Interpretation: The calibrated stack is now strong enough to support public battery case-study publication. The module preserved the correct family separation and energy-ranking order on the calibrated holdout set.

Each layer produced a different winner. That is the core finding.

BULK RESULT



Conventional high-energy layered-oxide story if the study stopped here.

INTERFACE RESULT



Interface analysis reopened a manganese/phosphate direction. Rank 9 to rank 1.

BATTERY-NATIVE



285.49 mAh/g, 3.95 V. Highest upside. Risks: cracking, dissolution, voltage stress.

BUILD HANDOFF



233.52 mAh/g, 1.55 V. Strongest build package. Handoff priority: 88.3.

Material	Role	Capacity	Voltage	Coating	Electrolyte
LiMnO2	Battery-native winner	285.49 mAh/g	3.95 V	Li3PO4	Std carbonate
Li4Ti5O12	Immediate build winner	233.52 mAh/g	1.55 V	TiO2	Std carbonate
LiMnPO4	Interface-corrected	170.87 mAh/g	4.10 V	Li3PO4	Std carbonate
LiMn2O4	Hybrid winner	148.22 mAh/g	4.12 V	AlPO4	Std carbonate
LiNiO2	Bulk-only winner	274.51 mAh/g	3.85 V	LiNbO3	Std carbonate
LiCoO2	High-energy comparator	273.84 mAh/g	3.95 V	LiNbO3	Std carbonate

All values are computational predictions from the calibrated FluxMateria battery-native stack. Recommended electrolyte for all candidates: standard carbonate. Dominant risks and next validation steps detailed in the full case study.

Li₄Ti₅O₁₂ is the best immediate build candidate.

233.52 mAh/g

Specific Capacity

1.55 V

Voltage Surrogate

88.3

Handoff Priority

Build Specifications

Anode family:	Graphite
Electrolyte:	Standard carbonate
Surface coating:	TiO ₂
Readiness score:	75.5
Audit verdict:	Strong

Dominant Risk Modes

- Chemo-mechanical cracking
- Impedance growth
- Manageable interphase risk

Recommended Next Work

Half-cell voltage profile | Pulse-power screening | Rate-capability screen | Post-cycle structural checks

One local workflow now does all of the following coherently — and outputs a prototype package plus validation plan.

Changes the bulk-only conclusion

Interface evidence showed that the bulk winner (LiNiO₂) was not the best overall answer. LiMnPO₄ moved from rank 9 to rank 1.

Changes the interface-only conclusion

Battery-native scoring added voltage, transport, degradation, and cycle life — and elevated LiMnO₂ above the pure interface winner.

Changes the battery-native conclusion

Build-readiness evidence separated highest-upside chemistry from the strongest immediate prototype package.

Outputs a first prototype package

The workflow ends at a build decision — not a generic shortlist. That is why Li₄Ti₅O₁₂ became the best immediate build package.

Key claim: FluxMateria showed that bulk-only screening would have pushed the wrong engineering conclusion. It separated highest-upside chemistry from best immediate build candidate in under half a minute on local hardware.

Complete multi-stage decision workflow on a local machine.

26.8 seconds

Full integrated battery-cathode decision workflow

10 materials | 4 decision layers | 5 winners | prototype handoff included

Traditional Approach

- DFT surface relaxations: ~24 hours each
- Multi-configuration searches: days to weeks
- Battery lifetime testing: months to years
- Results fragmented across separate tools

FluxMateria Integrated Path

- Bulk + interface + battery-native: one run
- Build-readiness scoring included
- Full confirmation in under 30 seconds
- Prototype handoff with validation plan

FluxMateria compressed the computational decision layer, not the lab step. The remaining step is experimental validation.

VALIDATION & LIMITATIONS

- ✓ Calibrated holdout benchmark passed before the study was used as a public case-study decision engine.
- ✓ Family accuracy was 1.0 and energy-rank Spearman was 0.943 on the holdout set.
- ✓ Four decision layers produced four different winners, confirming that each layer adds independent signal.
- ✗ All values in this study are computational predictions, not experimental assays.
- ✗ The study does not replace lab validation. It compresses the decision layer before experimental work.

Research Use Notice

This document describes computational predictions and materials-screening workflows only. FluxMateria outputs are not intended as substitutes for experimental characterization, electrochemical testing, or independent battery cell validation. All shortlisted materials require standard laboratory and prototype-cell confirmation before any engineering or manufacturing commitment.

The remaining step is experimental validation in a lab.

FluxMateria already did the screening, ranking, interface analysis, battery-native scoring, and prototype handoff.
The obvious next step is not more computation. It is cell-level characterization.

Bulk-only ranking chose LiNiO2 → Interface reopened LiMnPO4 → Battery-native elevated LiMnO2 → Handoff
selected Li4Ti5O12

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