Materials Informatics & Modeling

From Molecules to Market: Multiscale Machine Learning & Informatics for Solid-State Electrolyte Design, Integration and Scale-Up

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03/25/2026

International Battery Seminar: AI for Energy Storage

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Agenda

Multiscale Machine Learning & Informatics for Solid-State Electrolyte Manufacturing

- **Overview:** Role of Artificial Intelligence and Materials Informatics at Solid Power

- **Use Case 1:** Ultra-Early Cell Performance Prediction and Failure Mode Detection: *80%-90% speedup in testing and integration*

High–accuracy Capabilities

<5% error (RMSE) in predicting true time series

85+% accuracy on correct assignment of failure cause

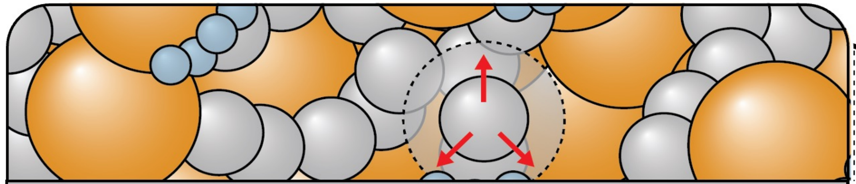
- **Use Case 2:** Intelligent Design of Experiments and Feedback for Knowledge-Informed Electrolyte Manufacturing

- **Conclusion**

Introduction

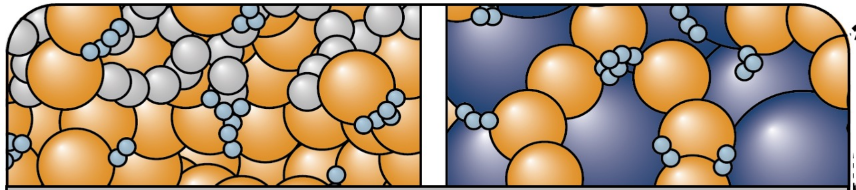
Strong coupling across mechanics, interfaces, and electrochemistry

What are the key challenges?



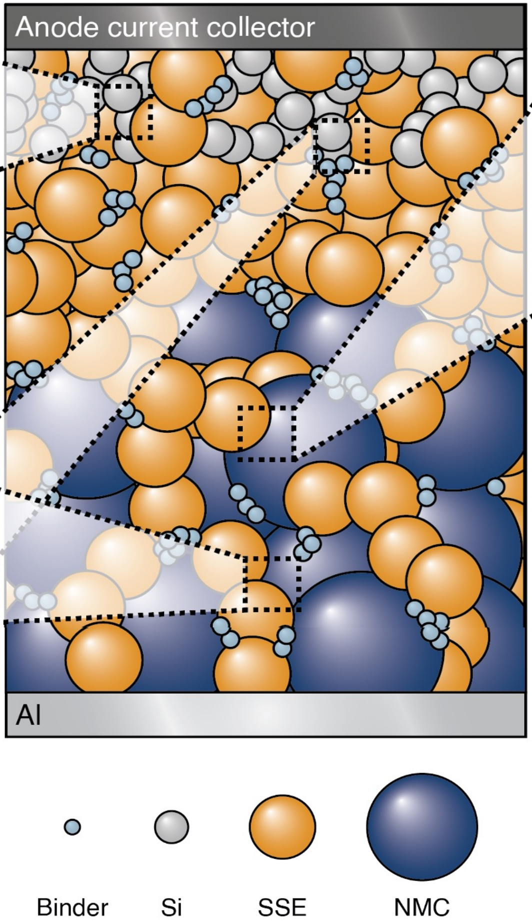
Chemo-Mechanical Coupling

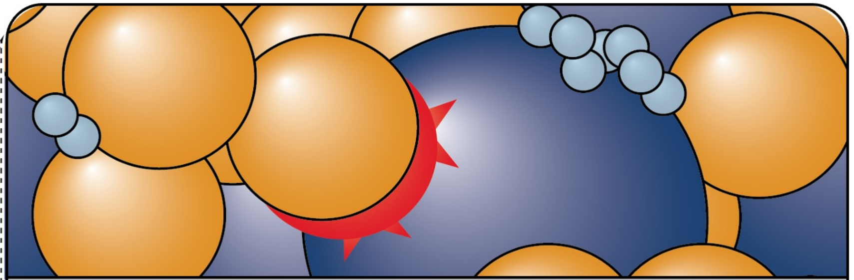
- Intercalation strain alters interfacial contacts and electrochemical potentials.
- Stack pressure dependence



Interfacial Stability

- Contact loss and void formation
- Local current constriction
- Grain-boundary vs bulk conductivity differences





Compatibility

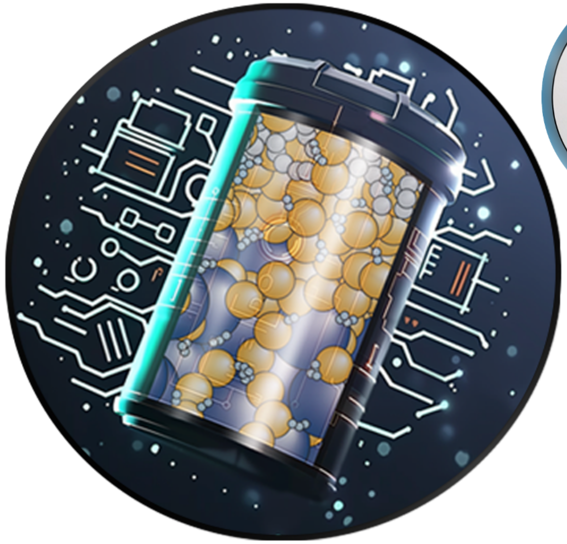
- All solid-state batteries are very sensitive to aggregation of constituents.
- Particle size distributions
- Electronic leakage through electrolyte
- Lithium plating/stripping-induced stress

Solid-state electrolyte (SSE) manufacturing and characterization require a multiscale understanding, because electrolyte properties, interfacial behavior, and cell-level performance are tightly coupled.

Overview of Materials Informatics & Modeling at Solid Power

Multiscale Machine Learning & Informatics for Solid-State Electrolyte Manufacturing

The Materials Informatics & Modeling (MIM) division at Solid Power deploys ML and AI across three ways to domains: (1) Progress Multipliers (acceleration), (2) Value Enhancers (optimization), & (3) Breakthrough Discovery & Innovation (new materials and architectures).



Materials Informatics & Modeling

Dr. Forrest Laskowski
Director of MIM

Dr. Amir Taqieddin

Alan Filer

Dr. Donghee Chang

Dr. Roja Esmaeeli

Domain Knowledge & Physics Grounded ML Solutions

Faster

Improved Decisions

Innovative Outcomes

Business Impact?

Tangible Metrics

Actionable Insights

Must both be measurable and move the needle.

Interpretability?

Transparent Algorithms

Physics-informed Algorithms

Results must be relatable to real world knobs.

Sustainable Deployment?

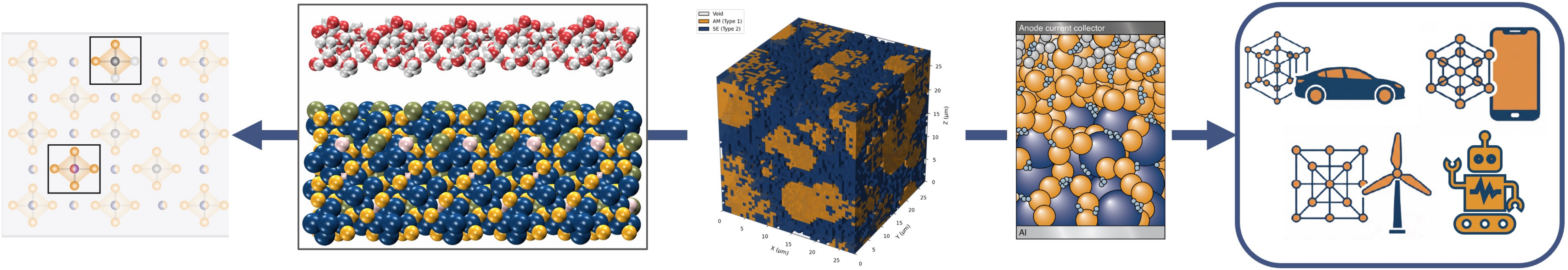
Self-Improving (Active Learning)

Low-Touch Maintenance

Models must not require significant ongoing support.

Role of Machine Learning & Informatics

Where are the ML models integrated at Solid Power?



Scale

Atoms & Molecules ← **Inverse Design** ← Structure-Process-Property ← Performance, Safety & Durability → **Forward Engineering** → Commercialization

Target

Expediting R&D Loops

New Solid-State Electrolytes ← R&D → Streamlining Processes ← Cell & Process Engineering → Early Anomaly & Fault Detection

Improving Data Interpretability ← Production → Strengthen IP and Valuation

- 10+ years of proprietary data, strengthened with open-source datasets: *for improved robustness and transferability.*
- Physics-aware AI tailored to each problem: *physics-driven neural networks, ML interatomic potentials, and Bayesian optimization.*
- Active learning across experiments and production: *continuous improvement in predictions and decisions.*

Impact of Materials Informatics & Modeling at Solid Power

What these tools changed in practice over the last 18 months?

Measurable Impact by MIM at Solid Power

Infrastructure:

(1) ATLAS: centralized data platform for rapid correlation (~50x faster data evaluation)
(2) Custom pipelines: AI for materials discovery & tuning
(3) SPARK-iT: AI/ML prediction platform

Innovation:

(1) 5+ patent disclosures by MIM over 18 months on using AI/ML for ASSB.
(2) 2 journal publications (1 published and 1 under review) + 1 public GitHub repo.

Resources: Awarded large allocation (both CPU and GPU access) for AI/ML and informatics on solid state electrolytes.

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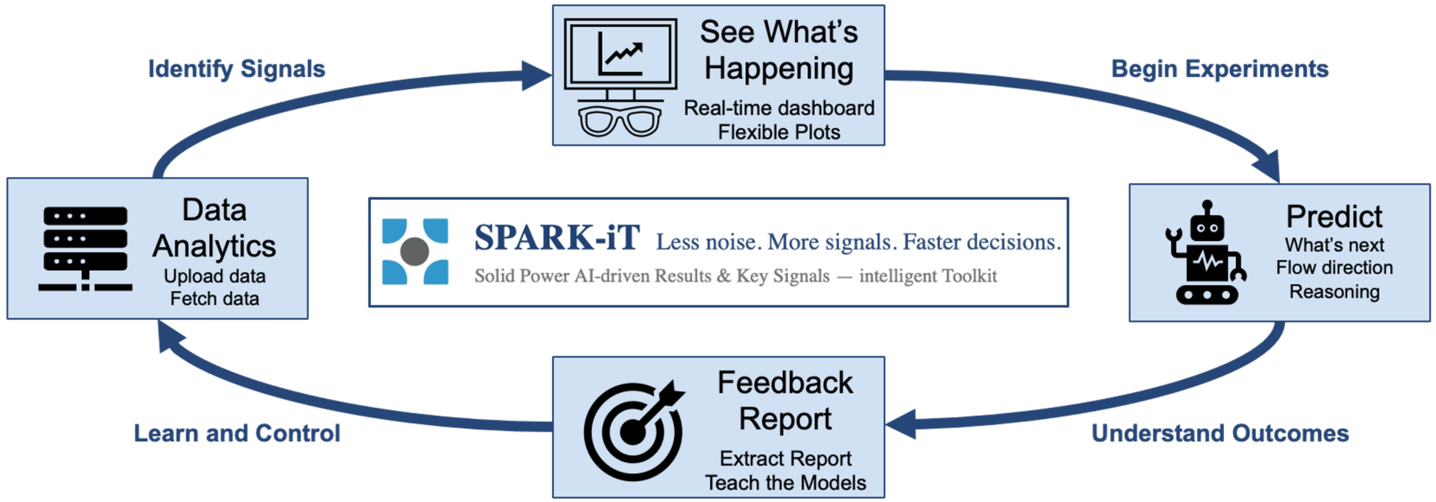
NSF ACCESS

SPARK-iT Less noise. More signals. Faster decisions.
Solid Power AI-driven Results & Key Signals — intelligent Toolkit

AI/ML Prediction Platform



The core capabilities of SPARK-iT

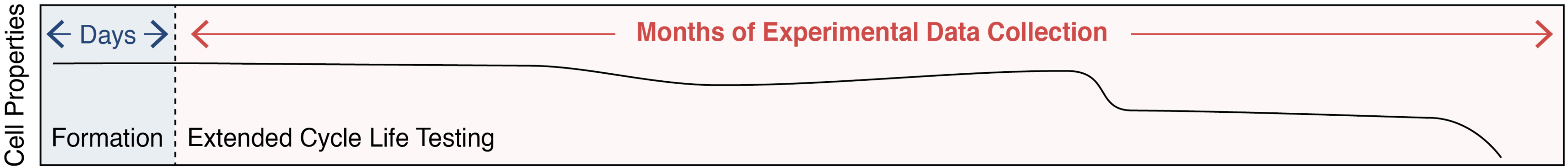
- Automated EIS Fitting & Analysis
- Predictive Cell Analytics Studio ← Use Case 1
- Intelligent Design of Experiments ← Use Case 2

Use Case 1: Ultra-Early Cell Performance Prediction and Failure Mode Detection

Ultra-Early Cell Performance Prediction & Failure Mode Detection

SPARK-IT – An early-warning and decision-support platform for cell testing

Typical Battery Testing Protocol



Problem: *Traditional workflows can take months to understand how material and process decisions influence end-of-life (EOL) performance*

Requirements: *How can we learn earlier and decide faster?*

Ultra-Early Cell Performance Prediction & Failure Mode Detection

SPARK-IT – An early-warning and decision-support platform for cell testing

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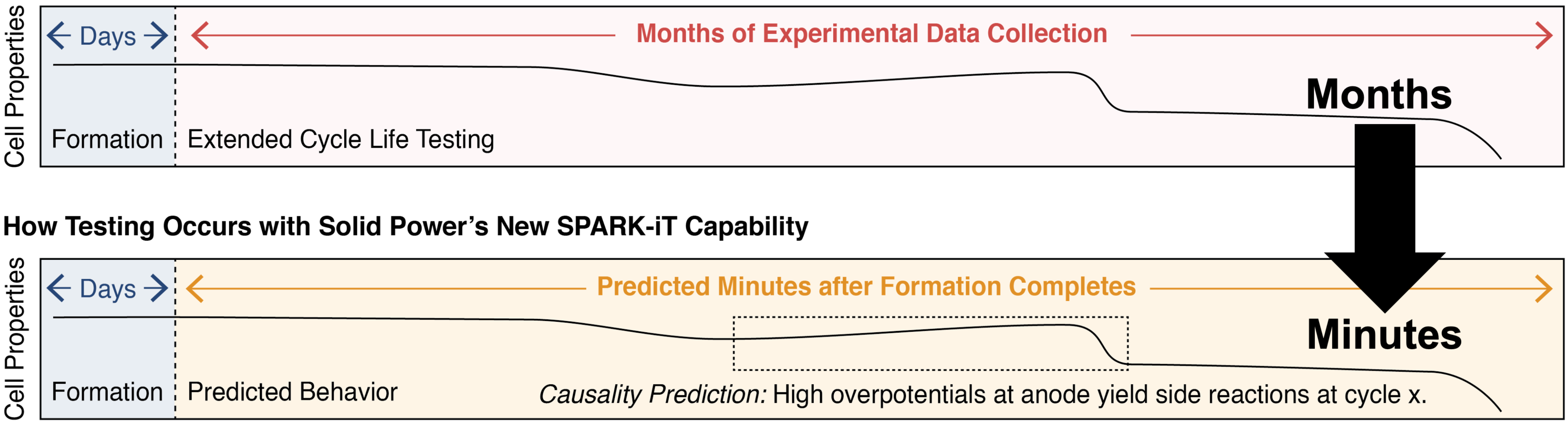


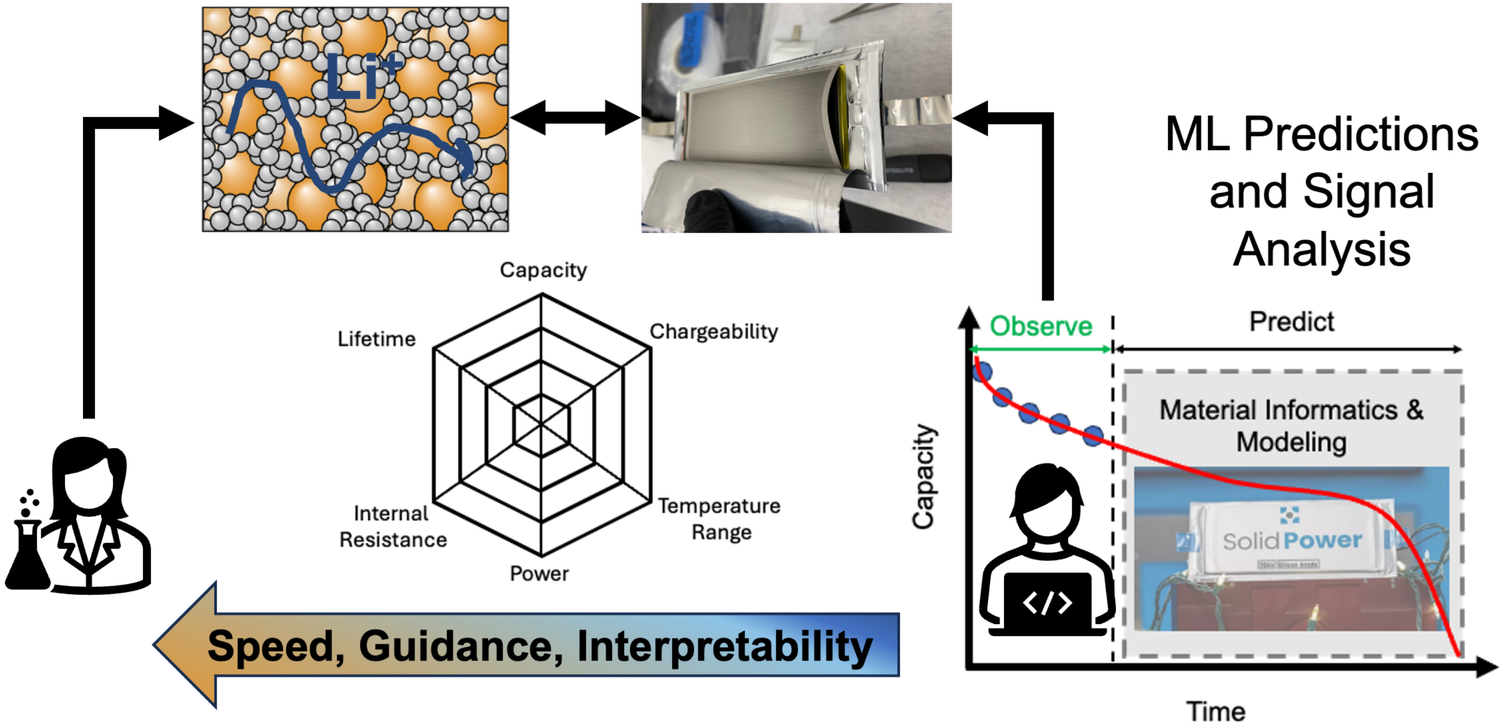
The goal is to **predict ultra-early**, **explain clearly**, and **support the next decision**.

Cell Performance Prediction and Failure Mode Detection

SPARK-iT: cell performance prediction to materials manufacturing

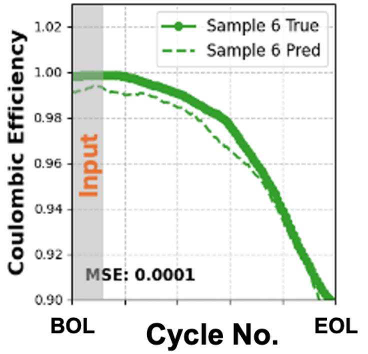
A faster workflow for cell analytics and electrolyte manufacturing

We learn earlier, decide faster, and test more efficiently

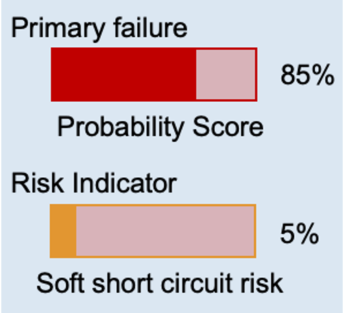


#1 CE Prediction Model + #2 Failure Mechanism

(1) Speed:
Predictions from formation cycles only



(2) Interpretability:
Mechanism-aware diagnostics and feedback



(3) Accuracy: *RMSE < 5% + 85+% accuracy for failure mode (#1 CE prediction model + #2 Failure mode detection model)*

Interpretable Cell Performance Prediction

#1 CE Prediction Model

SPARK-iT: cell performance prediction to materials manufacturing

Combined Neural Networks with Physics

CE model goals:

(1) $X(time\ series\ data) \Rightarrow Y\ (\textbf{CE Profile})$

(2) $X(time\ series\ data) \Rightarrow Y\ (\textbf{EOL Cycle})$

- Historical Data → Data Cleaning: Internal data + open source = transferability
- Extract Features
- Augmentation + Clustering: Robustness & generalization
- Algorithm Training → Prediction + Deployment: Customized for physics interpretability an uncertainty quantification

Part 1: Data Preparation

1) Extract Features

Turning raw cycling data into model-ready signals

a) Time-series Features: data for every timestep within every cycle which are: current, voltage, temperature, capacity, and energy

b) Cycle-based Features: actual cycle-based data and their statistics: mean, min, max, variance, etc + material properties/processing.

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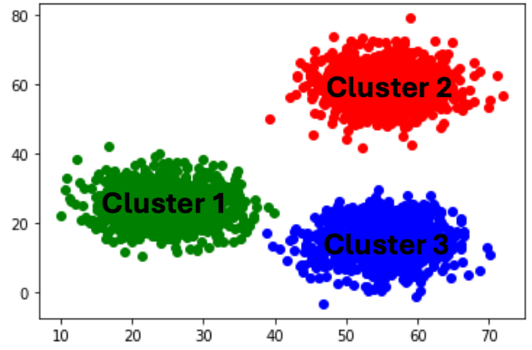
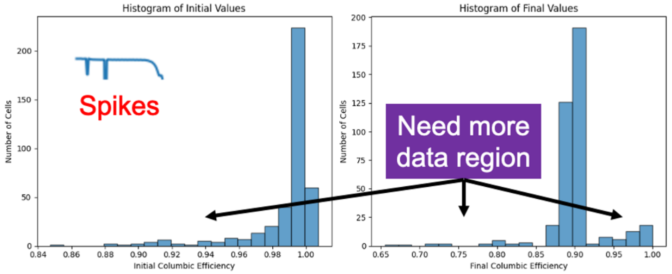
2) Clustering and Augmentation

a) Cross-validation: split data best on their correlations to ensure no overfitting or underfitting for better model generalization

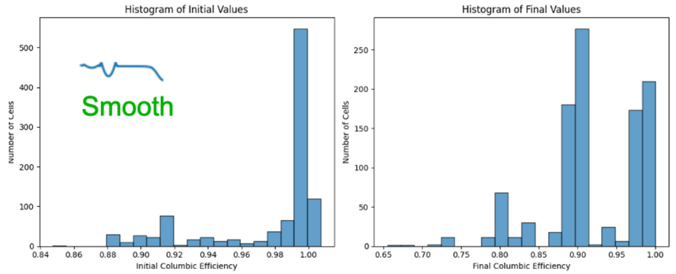


b) Augmentation: apply noise to ensure model has proper data balance and robust for data variations

Before Augmentation



After Augmentation



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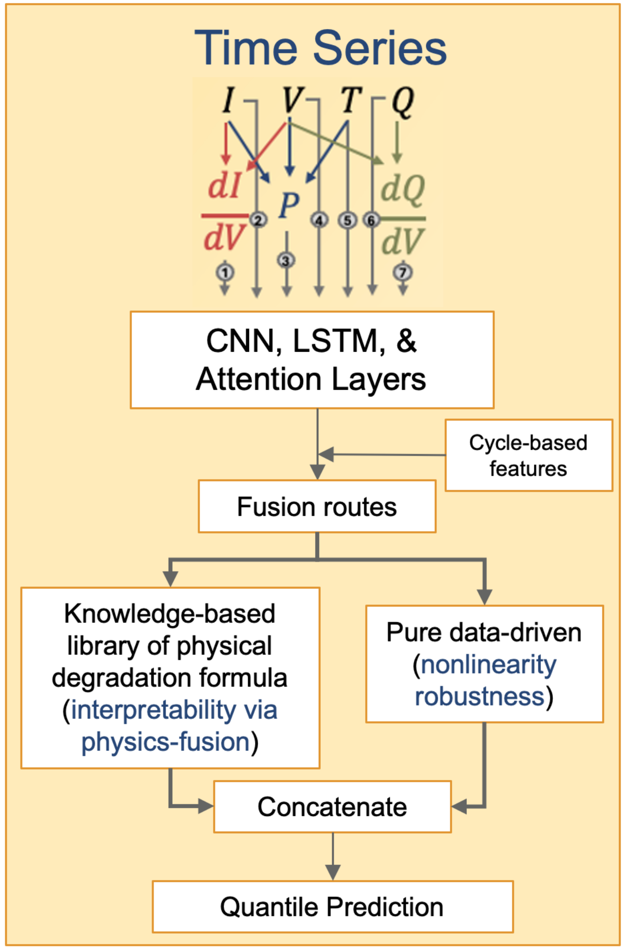
Part 2: Algorithm Training

Neural Network Algorithm



Key Highlights:

- PyTorch based
- RayTune and Optuna are used for hyperparameter optimization
- Tested the algorithm on both internal and open source data
- Tested the algorithm on prediction of CE, discharge capacity, and charge capacity

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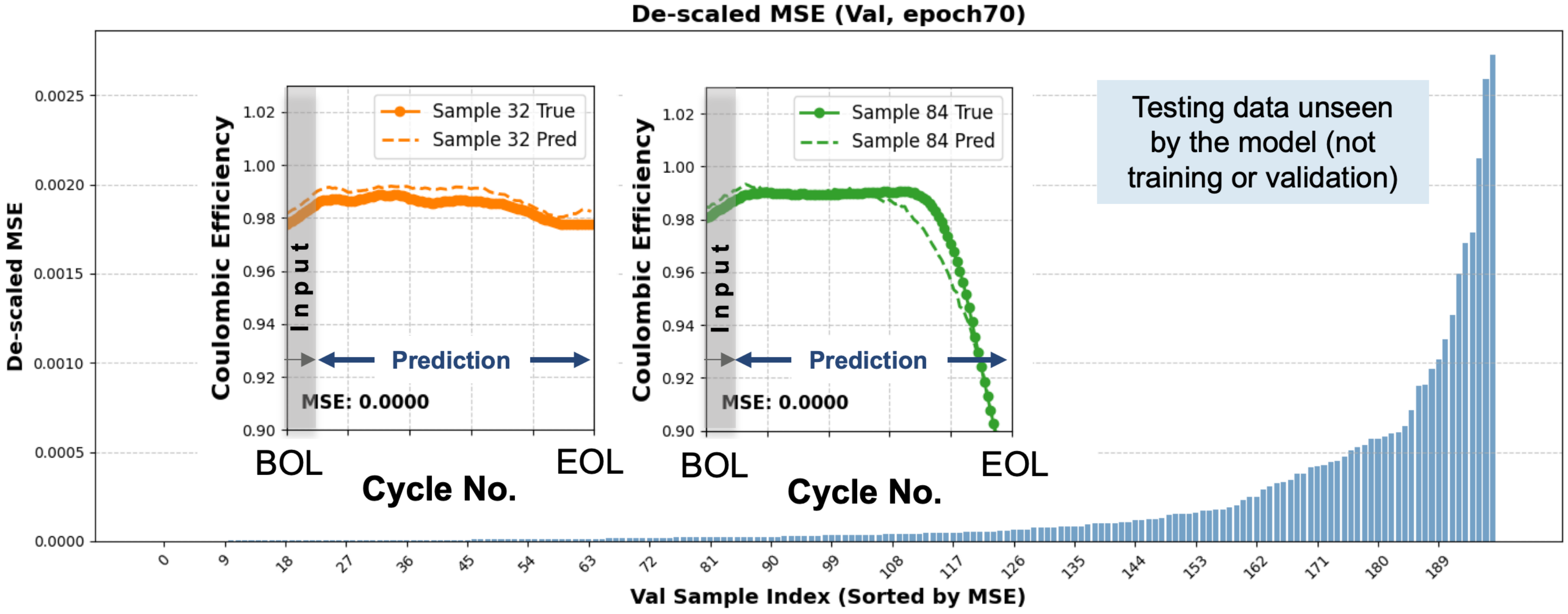
Prediction + Deployment

Customized for physics interpretability an uncertainty quantification

Part 3: Using early-cycle data to predict later behavior



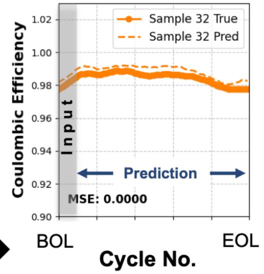
$$\text{Mean square error (MSE)} = \frac{1}{N}\sum\left((true\ value) - (predicted\ value)\right)^2$$

Using 70 epochs, the algorithm is trained to produced errors less than 5% on testing data

Interpretable Cell Performance Prediction

#1 CE Prediction Model

SPARK-iT: cell performance prediction



Part 3: Using early-cycle data to predict later behavior

The model works perfectly on predicted various degradation mechanisms in different cells.

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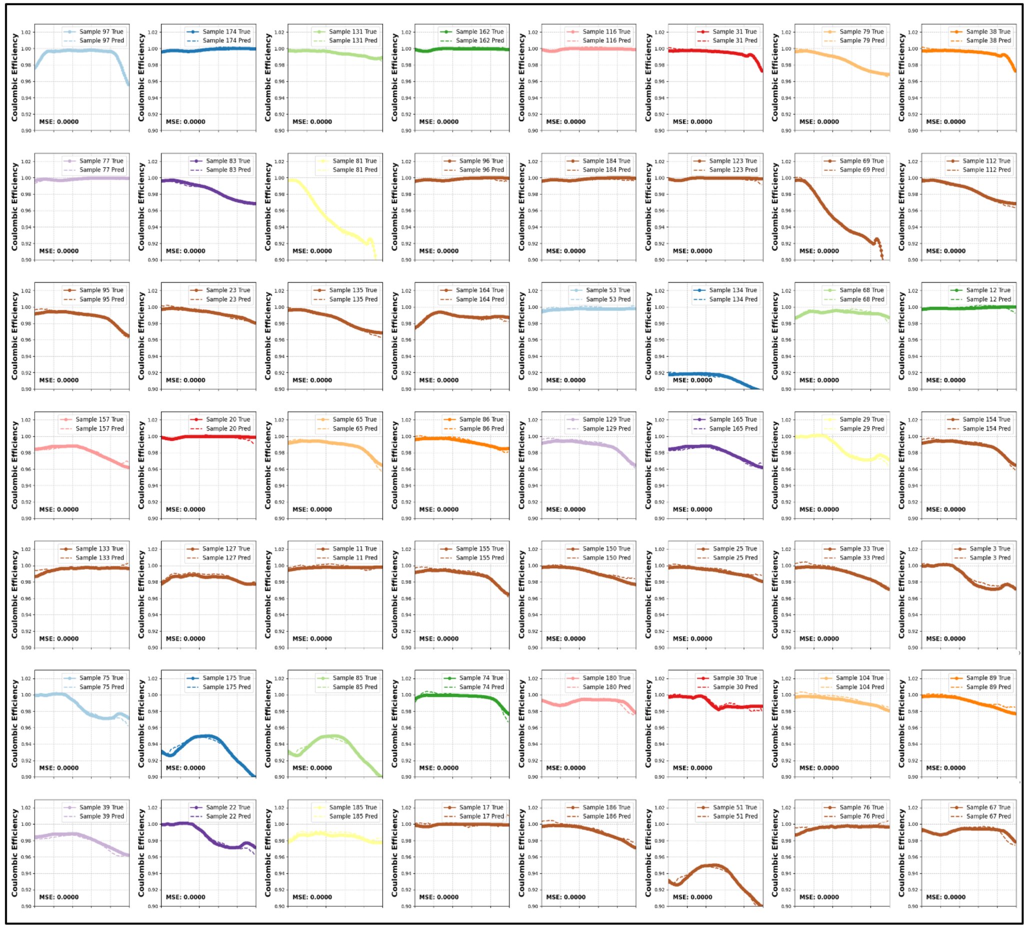

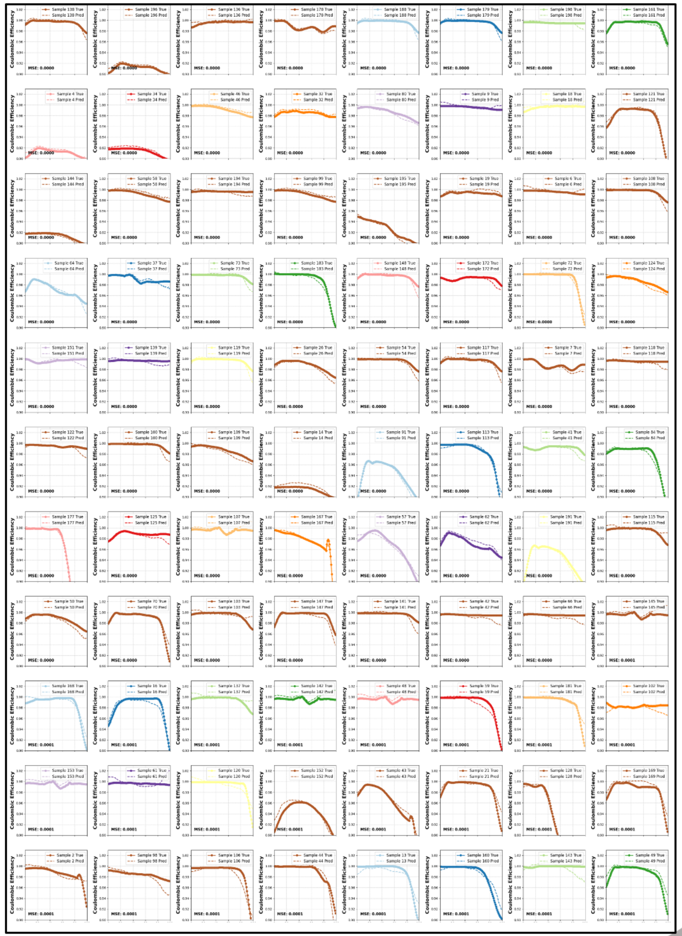

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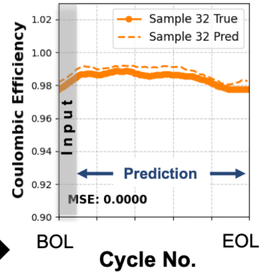

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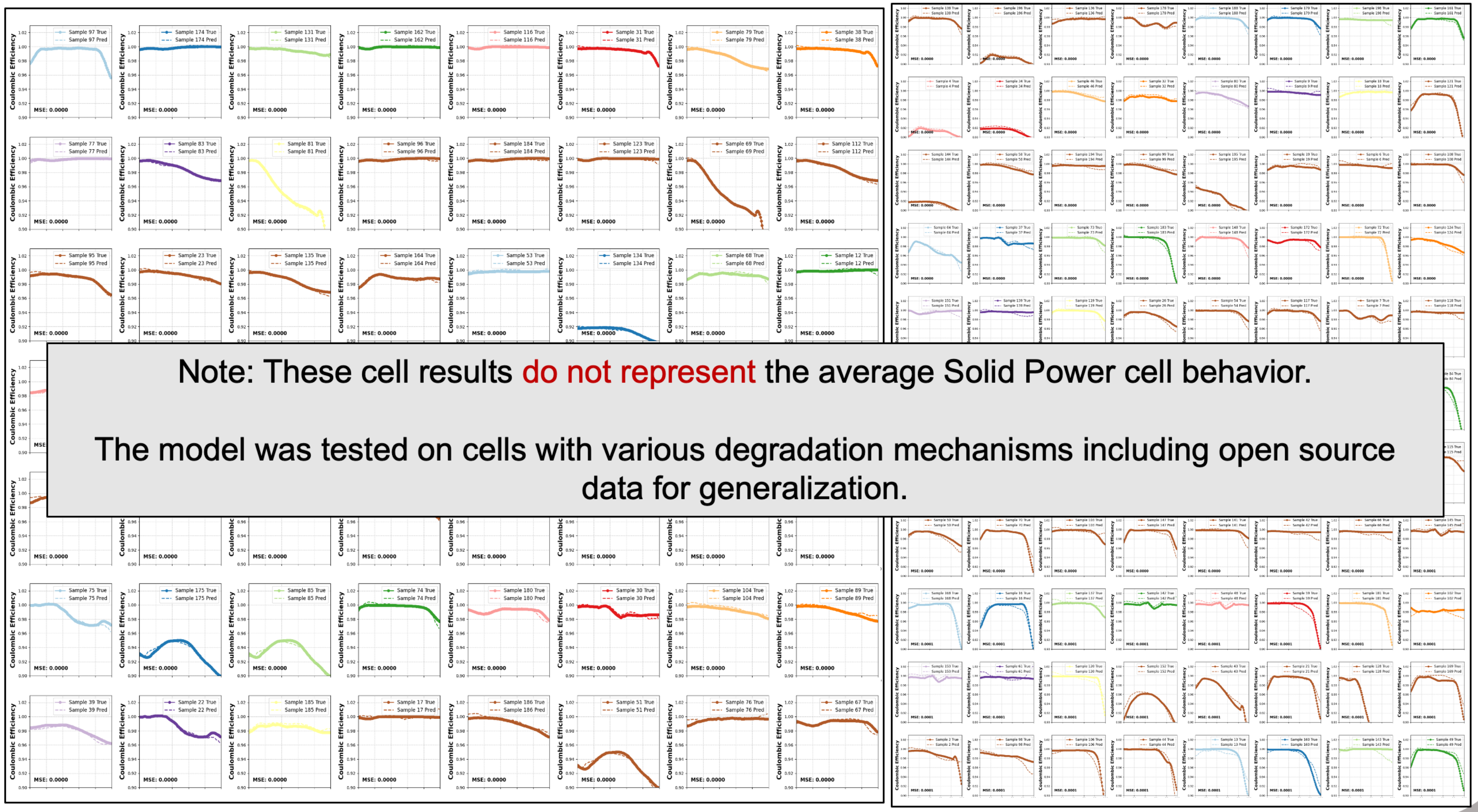

Note: These cell results do not represent the average Solid Power cell behavior.

The model was tested on cells with various degradation mechanisms including open source data for generalization.

Interpretable Cell Performance Prediction

#1 CE Prediction Model

SPARK-iT: cell performance prediction to materials manufacturing

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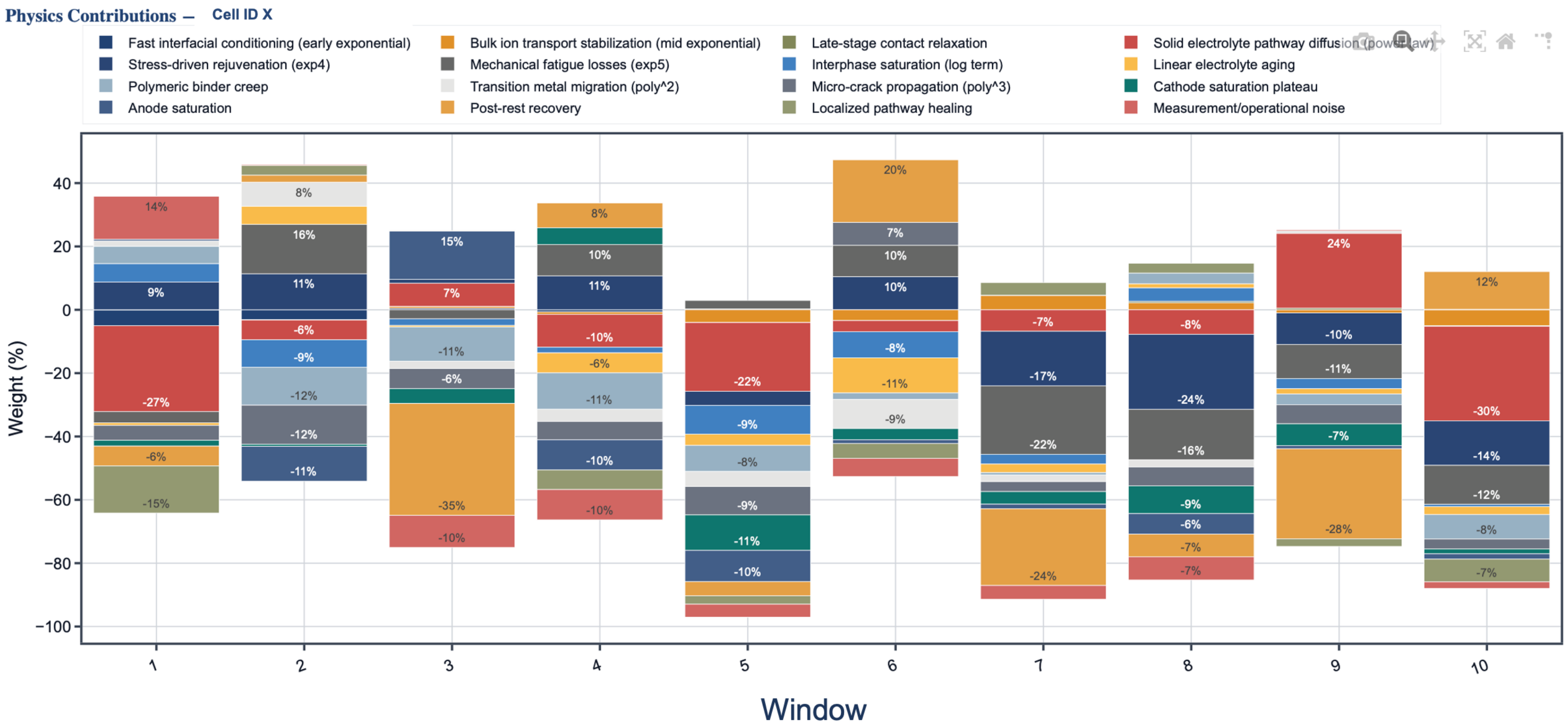


- The EOL range is divided into small windows (above example 10 windows) to enable tracing signals and interpret degradation mechanisms more effectively. For example, a cell with EOL of 900 cycles and 10 windows allows tracing the degradation for every 90 cycles (single window)

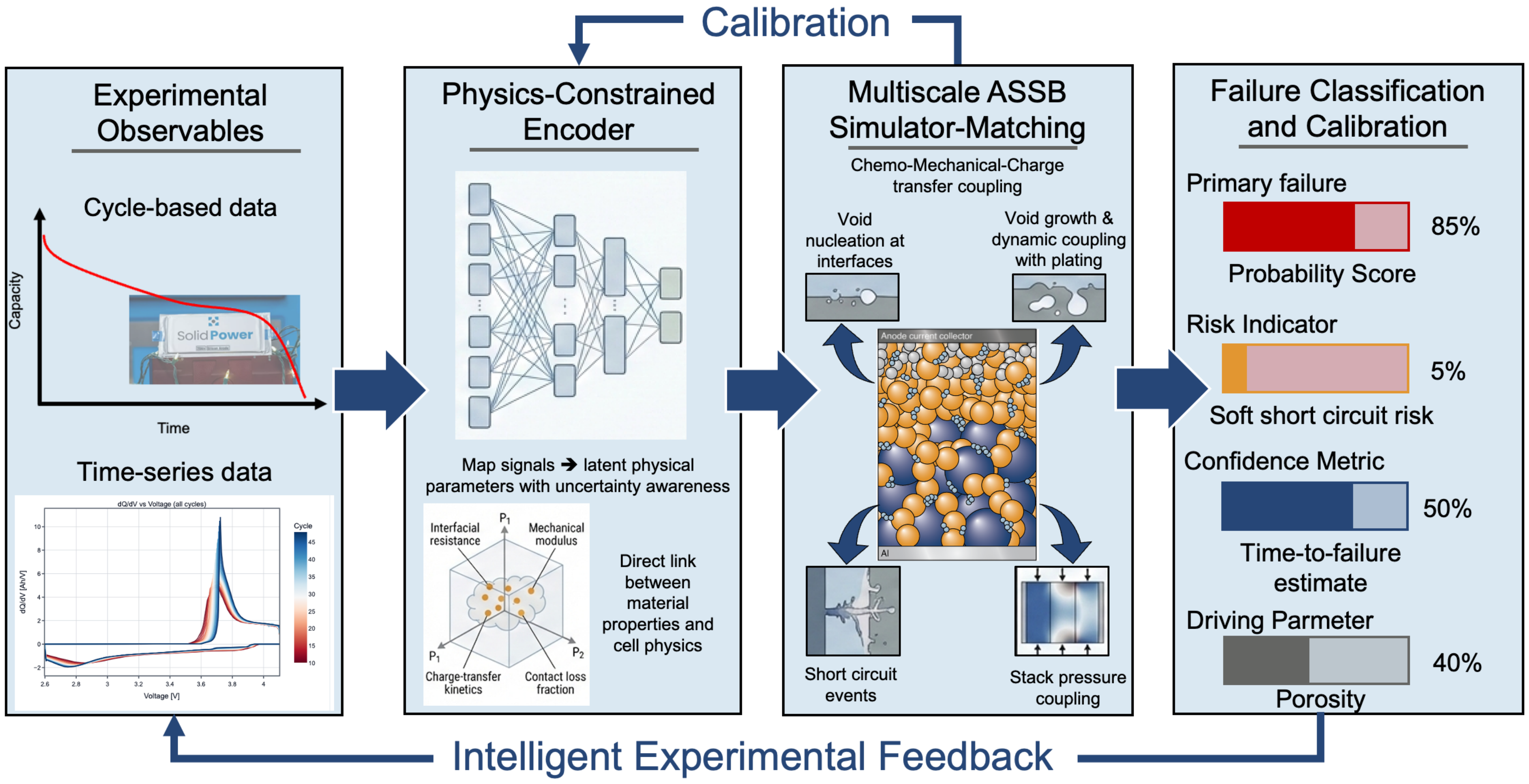
Window-level interpretation of degradation

Interpretable Cell Performance Prediction

#2 Failure Mechanism

SPARK-iT: cell performance prediction to materials manufacturing

- **Goal:** identify and rank primary and secondary failure modes with physics-grounded interpretability.
- **ML Integration:**
  - (1) An encoder maps experimental observables (e.g., time series data) to latent physical parameters,
  - (2) Physics-based simulations act as a differentiable surrogate or structured regularizer
  - (3) Failure modes are classified and ranked in a physically constrained latent space.
- **Outcome**: Predictive failure diagnostics with interpretable, mechanism-aware feedback.



A physics-guided model for classifying likely failure modes

Failure mode model goal:

$X(time\ series\ data)$
$\Rightarrow Y$ (**Failure Modes**)

- Historical Data
- Data Cleaning
- Extract Features
- Augmentation + Clustering
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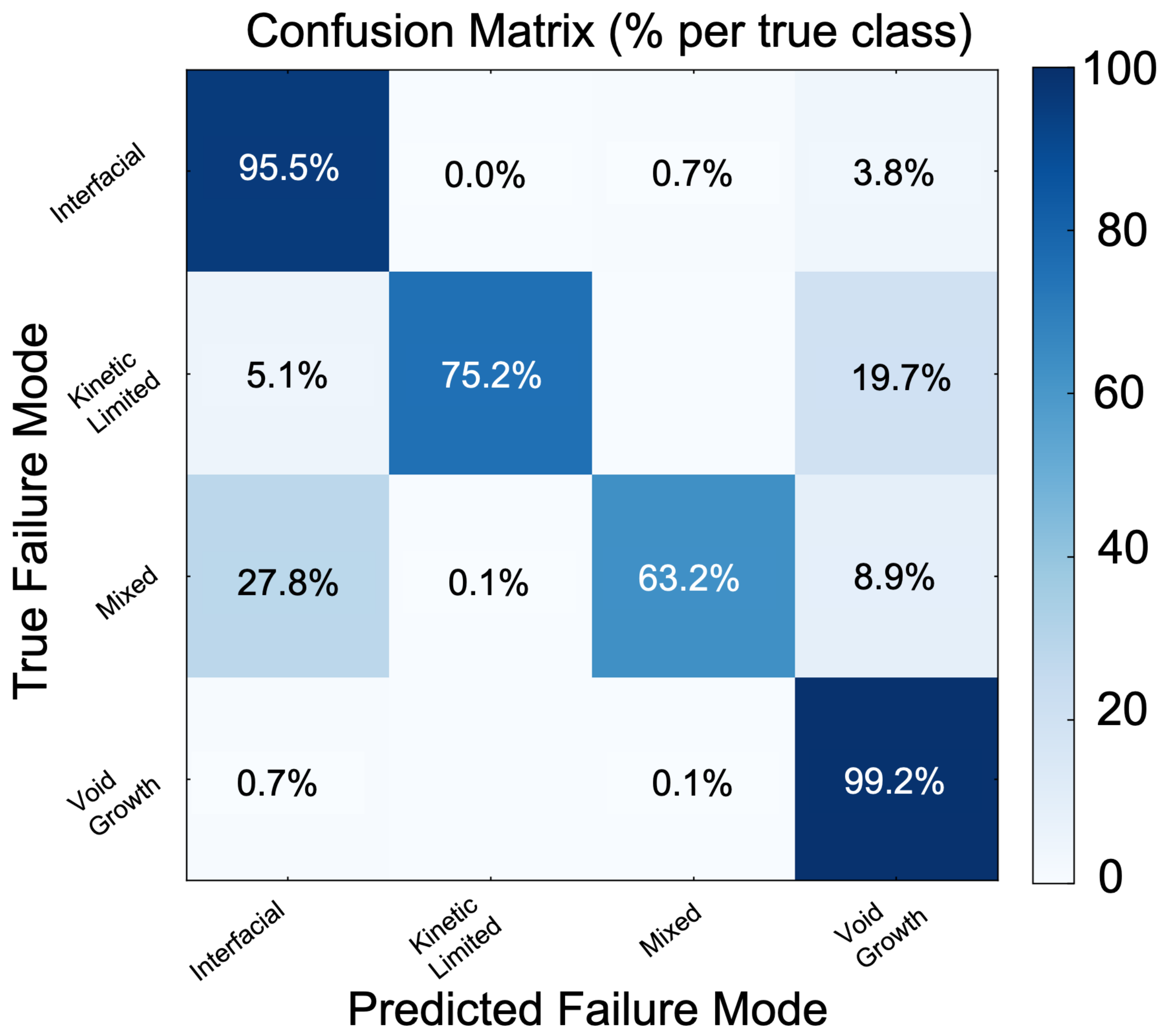
Change from CE model 1

Interpretable Cell Performance Prediction

#2 Failure Mechanism

SPARK-iT: cell performance prediction to materials manufacturing



Example output from SPARK-iT

Key takeaways — Cell ID X

- Mechanism: Void Growth with Kinetics Limited interplay
- QC: low first-cycle CE, early C/3 inefficiency, OCV drift
- Low first-cycle CE indicates initial inefficiency
- CE inefficiency accumulates during early C/3 cycles
- OCV drift suggests side reactions or parasitic losses

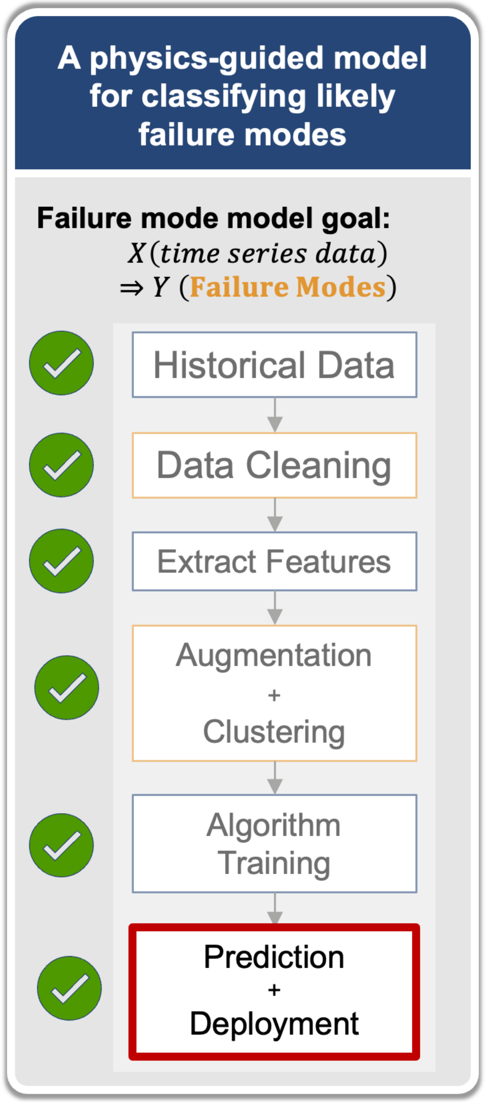
Next recommended steps — Cell ID X

- Gentle step-up formation; limit depth-of-discharge swings
- Stabilize temperature bands; monitor CE oscillations
- RPT+dQ/dV to track impedance and phase changes
- Refine first cycles CC/CV; confirm CE recovery by cycle 4
- Extend rest windows in C/3; check CE stabilization

Performance: *~85% primary classification accuracy of failure modes*

Output: *Ranked, human-readable failure diagnostics*

Impact: *Faster and more consistent expert decisions*

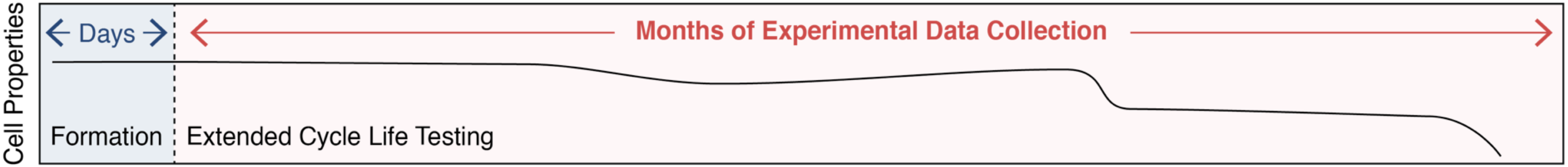


Ultra-Early Cell Performance Prediction & Failure Mode Detection

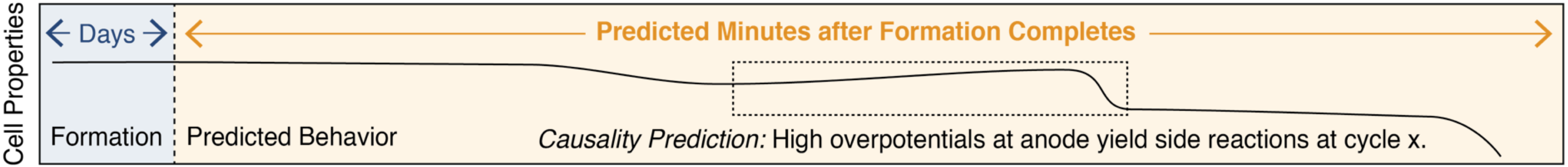
SPARK-iT: cell performance prediction to materials manufacturing

#1 CE prediction model + **#2 Failure Mechanism**

Typical Battery Testing Protocol



How Testing Occurs with Solid Power's New SPARK-iT Capability



High–accuracy Capabilities

<5% error (RMSE) in predicting true time series

85+% accuracy on correct assignment of failure cause

Enabled by our Unique ASSB Data

Takeaway: SPARK-iT compresses multi-month R&D loops into mere days, allowing rapid resolution of blockers for powder customers.

Use Case 2: Intelligent Design of Experiments (DOEs) and Feedback for Knowledge-Informed Electrolyte Manufacturing

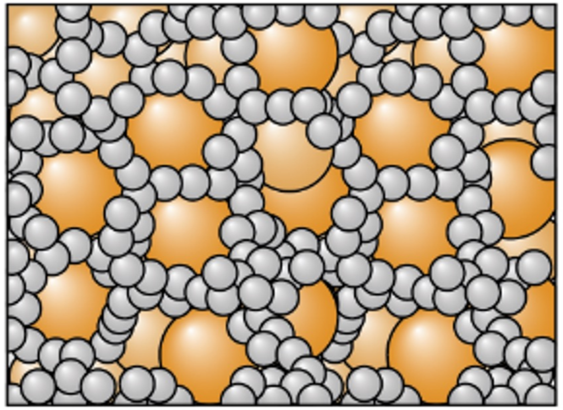
Knowledge-Informed Electrolyte Manufacturing

AI-driven design of experiments platform for control and optimization

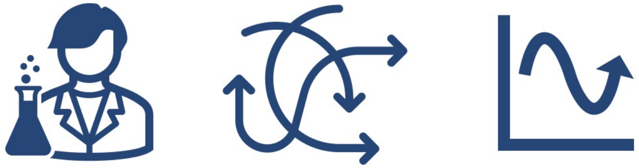
Targets

Q1: How to enable faster, consistent, efficient and systematic exploration of solid-state electrolyte manufacturing?

Q2: Can AI-driven tools accelerate and improve this process?



Current challenges

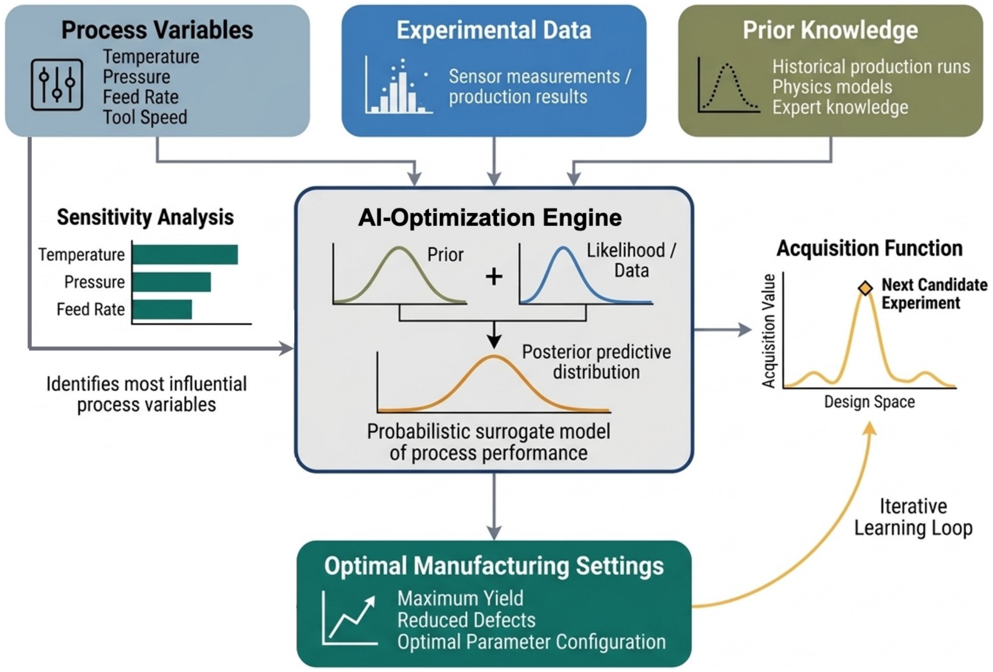


(1) Large Experimental Design Space: Many parameters create thousands of possible experiments

(2) Competing Multiple Goals: Performance, stability, cost, safety, and manufacturability must be optimized together

(3) Complex Multi-Scale Relationships: Processing, structure, and performance interact across atomic to cell scales

Solution: Translate technical goals into optimization targets

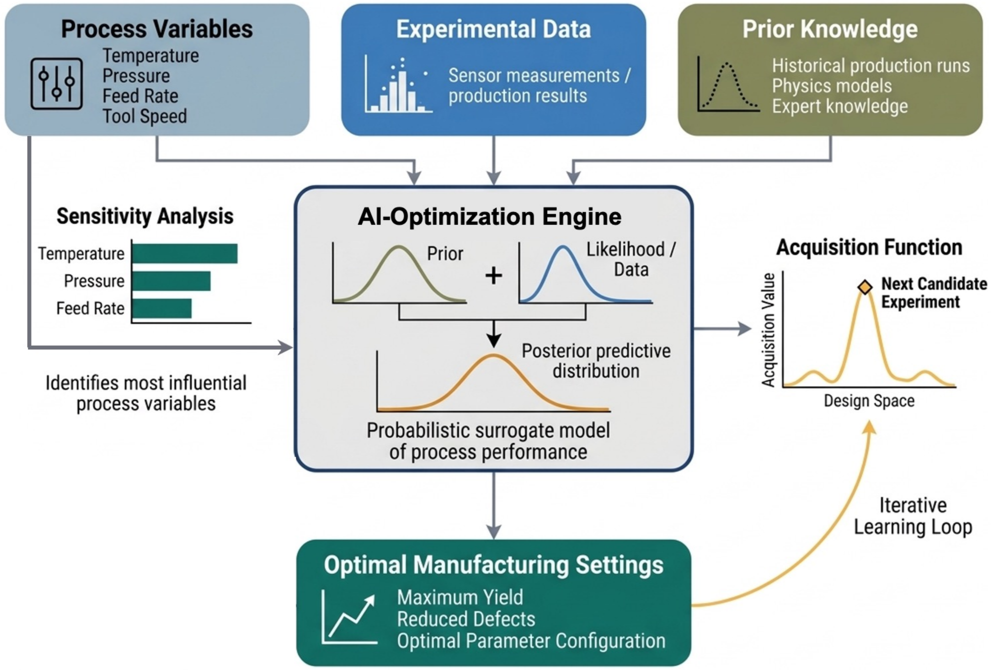


An AI-DOE engine that learns from every experiment

Knowledge-Informed Electrolyte Manufacturing

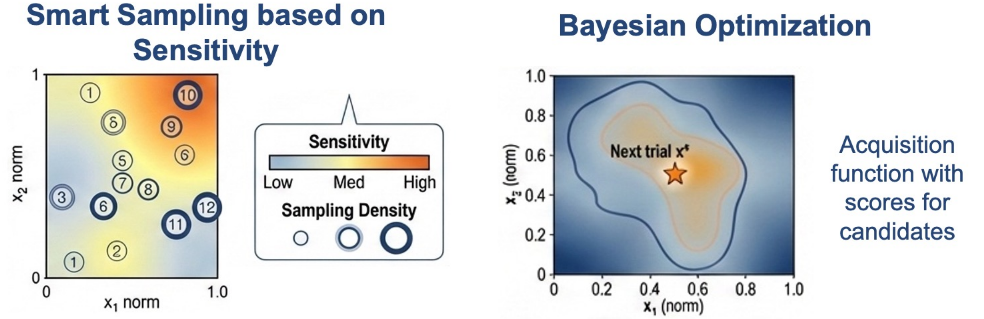
AI-driven design of experiments platform for control and optimization

Solution: Translate technical goals into optimization targets



An AI-DOE engine that learns from every experiment

Capabilities



(1) Smart Experiment Selection: focus on impactful parameters

(2) Learning From Each Experiment: AI recommends the next experiment

(3) Multi-Objective Optimization: Simultaneously optimize competing targets, e.g.: (↑ Ionic conductivity, ↓ Viscosity, ↓ Cost, ↑ Cycle life.)

(4) Balance Exploration vs Exploitation: Unified framework spanning materials → processing → cell-level performance.

Knowledge-Informed Electrolyte Manufacturing

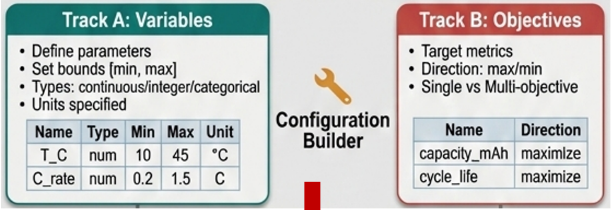
A closed-loop workflow for smarter experiments

SPARK-iT Less noise. More signals. Faster decisions.
Solid Power AI-driven Results & Key Signals — intelligent Toolkit

Knowledge-driven workflow for DOE

Stage 1: Project Setup

Stage 2: Design



Stage 3: Data Quality Check & Suggestions

432 rows | **6 params** | **0 objectives** | 72.0 samples/param

Missing Data

OK No columns with >10% missing data

Constant Columns

1 temperature_formation

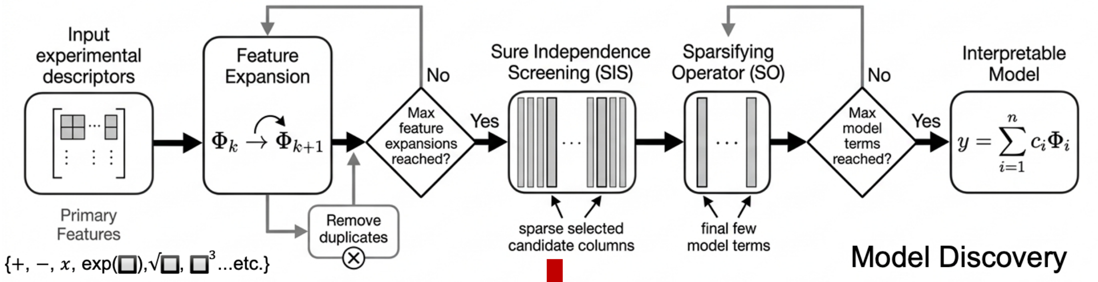
These columns have the same value in every row — they provide no useful information.

Redundant Columns (highly correlated)

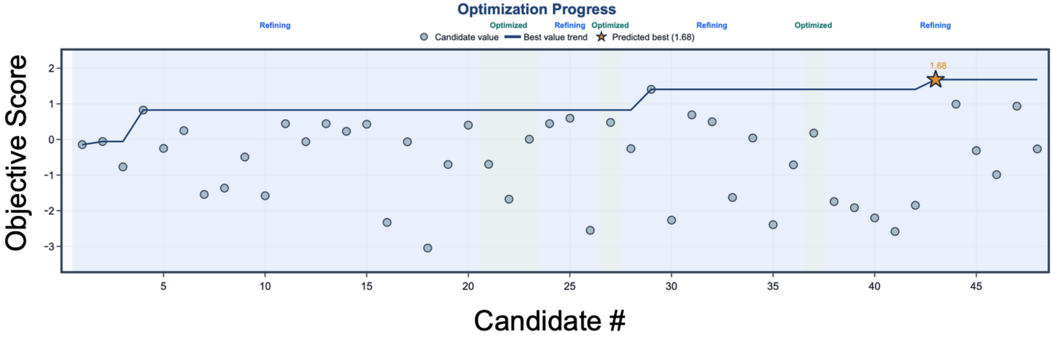
CycleCount ↔ number_of_cycles r=0.96

These columns move together — keeping both adds noise without new information.

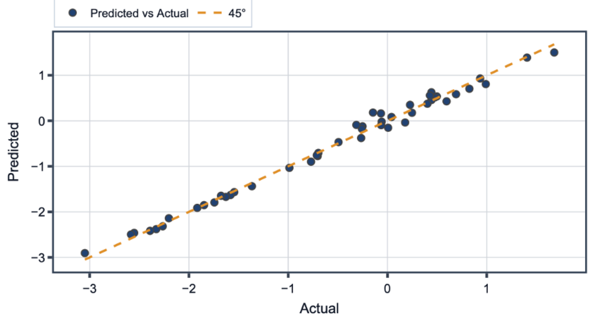
Stage 4: Interpretable Featurization



Stage 5: Optimization



Stage 6: Analysis & Reporting



★ **Top Recommended Candidates So Far**

Best 3 out of 37 experiments, ranked by launch_readiness_score (highest first).

Rank	
#1	I=3, T=25.7, r=4.44
#2	I=2.05, T=31.1, r=0.655
#3	I=2.21, T=29, r=4.61

Stage 7: Expert Review

Further steps/tune? Include advance options?

Generative Data Augmentation

Transfer Learning

Knowledge-Informed Electrolyte Manufacturing

Closed-loop intelligent experimental design framework via SPARK-iT

Example/Tutorial: Bayesian optimization of three process parameters for fast charging*

*This is a hypothetical example intended to illustrate the workflow and is **not based** on actual Solid Power data or experiments

Tutorial Setup

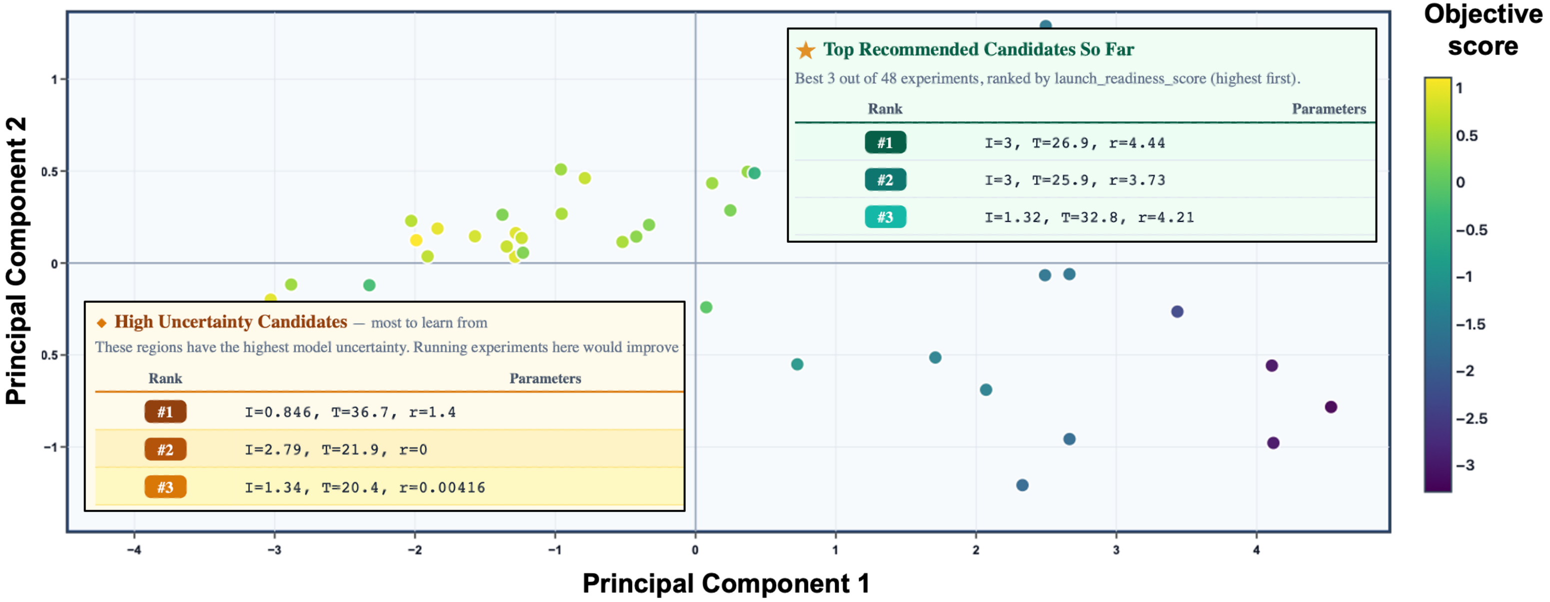
Inputs:
(1) I
(2) T
(3) r

Constraints:
(1) $T + 4.5 \cdot I + 0.25 \cdot r \leq 41.5$
(2) $28/I + r \leq 26$

Optimizer: Custom Intelligent DOE in SPARK-iT

Objective: Maximize fast charging score function: $f(I, T, r)$

Mapping opportunity and uncertainty in the design space



Knowledge-Informed Electrolyte Manufacturing

Closed-loop intelligent experimental design framework via SPARK-iT

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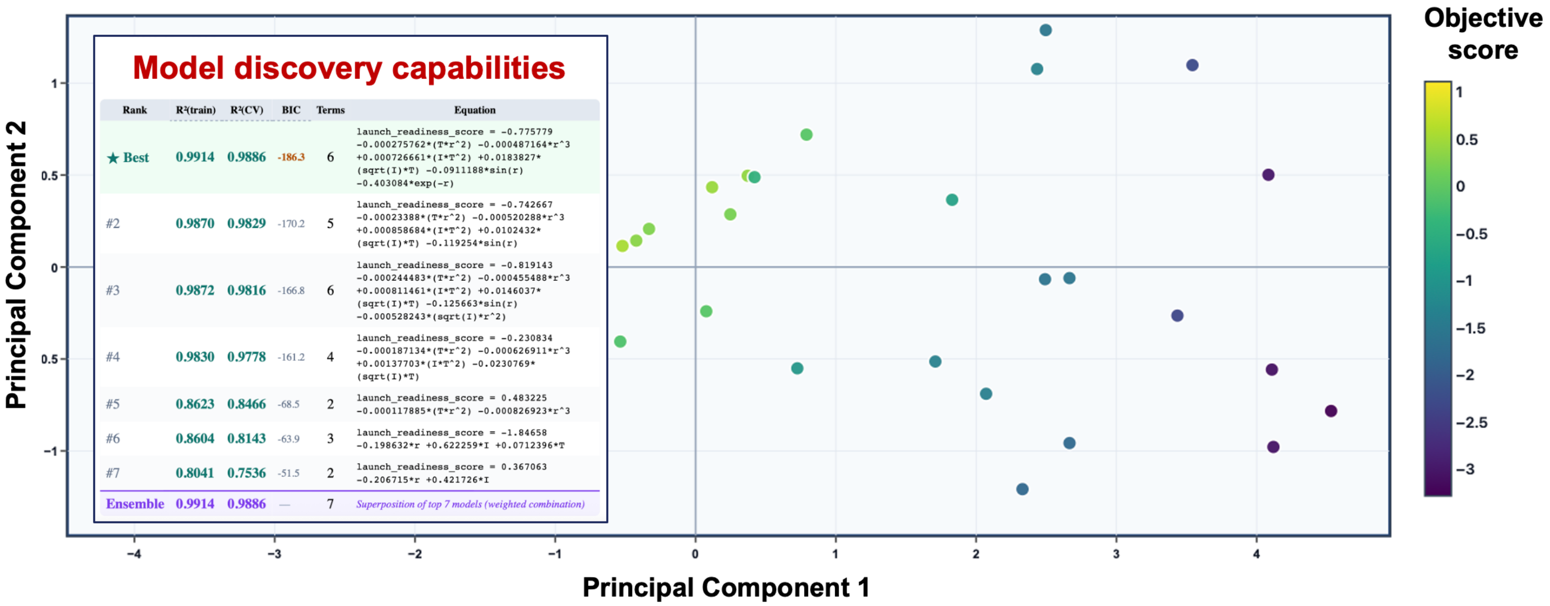


Model discovery capabilities

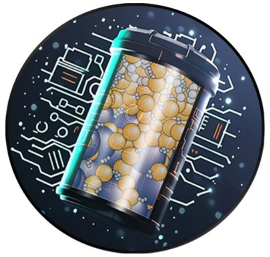
Rank	R²(train)	R²(CV)	BIC	Terms	Equation
★ Best	0.9914	0.9886	-186.3	6	launch_readiness_score = −0.775779 −0.000275762*(T*r^2) −0.000487164*r^3 +0.000726661*(I*T^2) +0.0183827*(sqrt(I)*T) −0.0911188*sin(r) −0.403084*exp(−r)
#2	0.9870	0.9829	-170.2	5	launch_readiness_score = −0.742667 −0.00023388*(T*r^2) −0.000520288*r^3 +0.000858684*(I*T^2) +0.0102432*(sqrt(I)*T) −0.119254*sin(r)
#3	0.9872	0.9816	-166.8	6	launch_readiness_score = −0.819143 −0.000244483*(T*r^2) −0.000455488*r^3 +0.000811461*(I*T^2) +0.0146037*(sqrt(I)*T) −0.125663*sin(r) −0.000528243*(sqrt(I)*r^2)
#4	0.9830	0.9778	-161.2	4	launch_readiness_score = −0.230834 −0.000187134*(T*r^2) −0.000626911*r^3 +0.00137703*(I*T^2) −0.0230769*(sqrt(I)*T)
#5	0.8623	0.8466	-68.5	2	launch_readiness_score = 0.483225 −0.000117885*(T*r^2) −0.000826923*r^3
#6	0.8604	0.8143	-63.9	3	launch_readiness_score = −1.84658 −0.198632*r +0.622259*I +0.0712396*T
#7	0.8041	0.7536	-51.5	2	launch_readiness_score = 0.367063 −0.206715*r +0.421726*I
Ensemble	0.9914	0.9886	—	7	*Superposition of top 7 models (weighted combination)*

Key Highlights:

- Scalable workflow for DOE across R&D, process engineering, and production.
- Specialized domain capabilities developed to support targeted real applications.

Conclusion & Takeaways

Multiscale Machine Learning & Informatics for Solid-State Electrolyte Manufacturing



Materials Informatics & Modeling

Progress Multiplication
Faster learning cycles

Value Enhancement
Performance • Reliability • Manufacturability
Support External Customers

Breakthrough Discovery
New materials & design paradigms

AI/ML must be deployed against real, operational technical bottlenecks to create measurable industrial impact.

SPARK-iT Less noise. More signals. Faster decisions.
Solid Power AI-driven Results & Key Signals — intelligent Toolkit

Towards unified, physics-driven, and accurate signals

(1) **Reduces testing time** by 80–90% for solid-state battery evaluation with prediction error <5%.
(2) **Identifies cell failure modes** with ~80% average accuracy (~85% for primary failure mode).
(3) **Provides mechanistic interpretability**, linking degradation behavior to underlying material and interfacial properties.
(4) **Enables intelligent, closed-loop DOE** for accelerated optimization.

Thank you!

Solid Power is a solid-state battery materials company focused on solid-state electrolyte technology. We leverage/design AI/ML/informatics tools when doing so accelerates materials discovery, process understanding, and data-driven decision making. Our **core value is advancing electrolyte materials,** manufacturing, and integration into next-generation batteries, **with AI-enabled workflows supporting** (not replacing) rigorous electrochemistry, materials science, and engineering.