NRC·CNRC

Mississauga Advanced Materials Research Facility

Autonomous Laboratory: Self-Driving Labs to accelerate battery cathode material discovery

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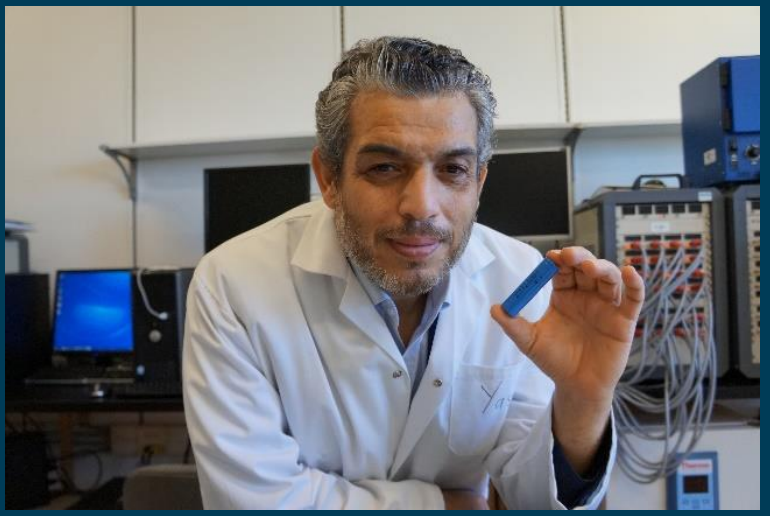
Critical Battery Materials Initiative | CBMI

Our Mission:

To develop automated, AI-enabled platforms that can discover critical battery materials and processes in a third of the time it takes today, enabling the growth of the critical minerals and battery supply chain and helping Canada reach net zero by 2050.

- 4-year program (2023-27)
- $10M in Capital Investments
- $20M in Operating Budget
- $10M in Grant & Contribution funding for collaborative projects

NRC Advanced Materials Research Facility, Mississauga

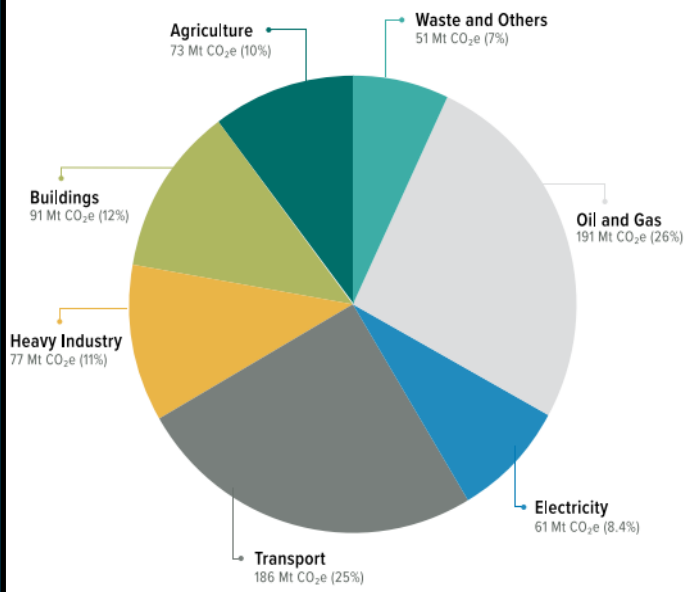


Dr. Yaser Abu-Lebdeh, Battery Materials Innovation Lead

The Critical Battery Materials Gap Accelerating Midstream Development

The Drive

Path to Net Zero

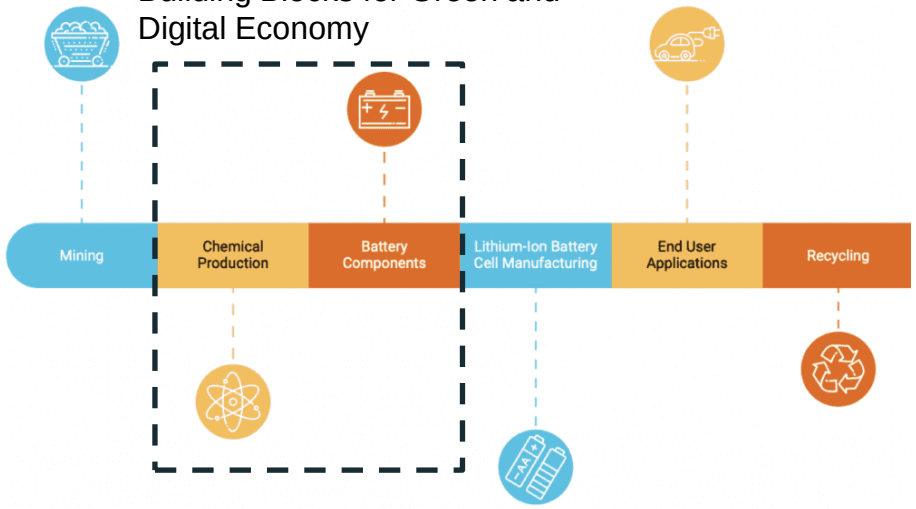


2030 Emissions Reduction Plan – Sector-by-sector overview - Canada.ca

The Gap

Midstream Battery Materials Innovation

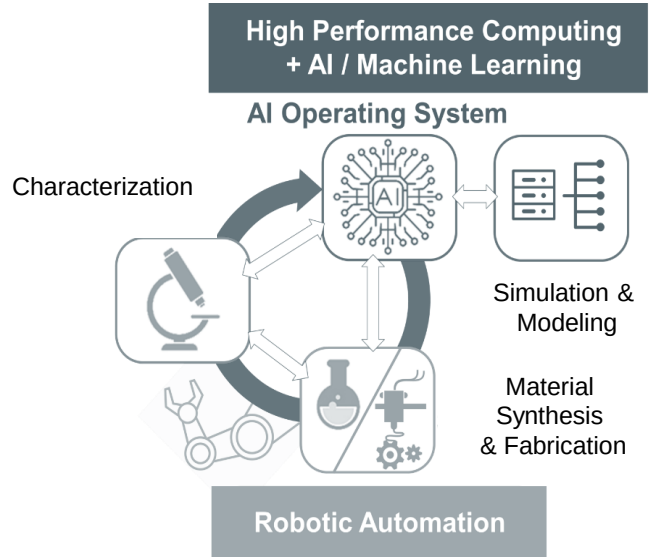
Critical Minerals are the Building Blocks for Green and Digital Economy



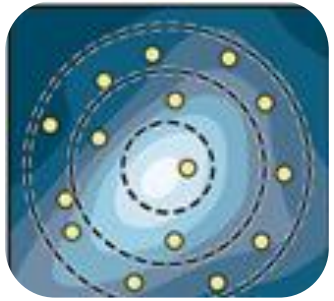
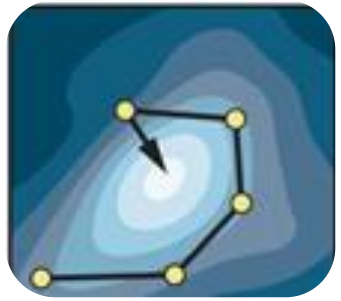
The Canadian Critical Minerals Strategy - Canada.ca
BMAC | Battery Metals Association of Canada (bmacanada.org)

The Response

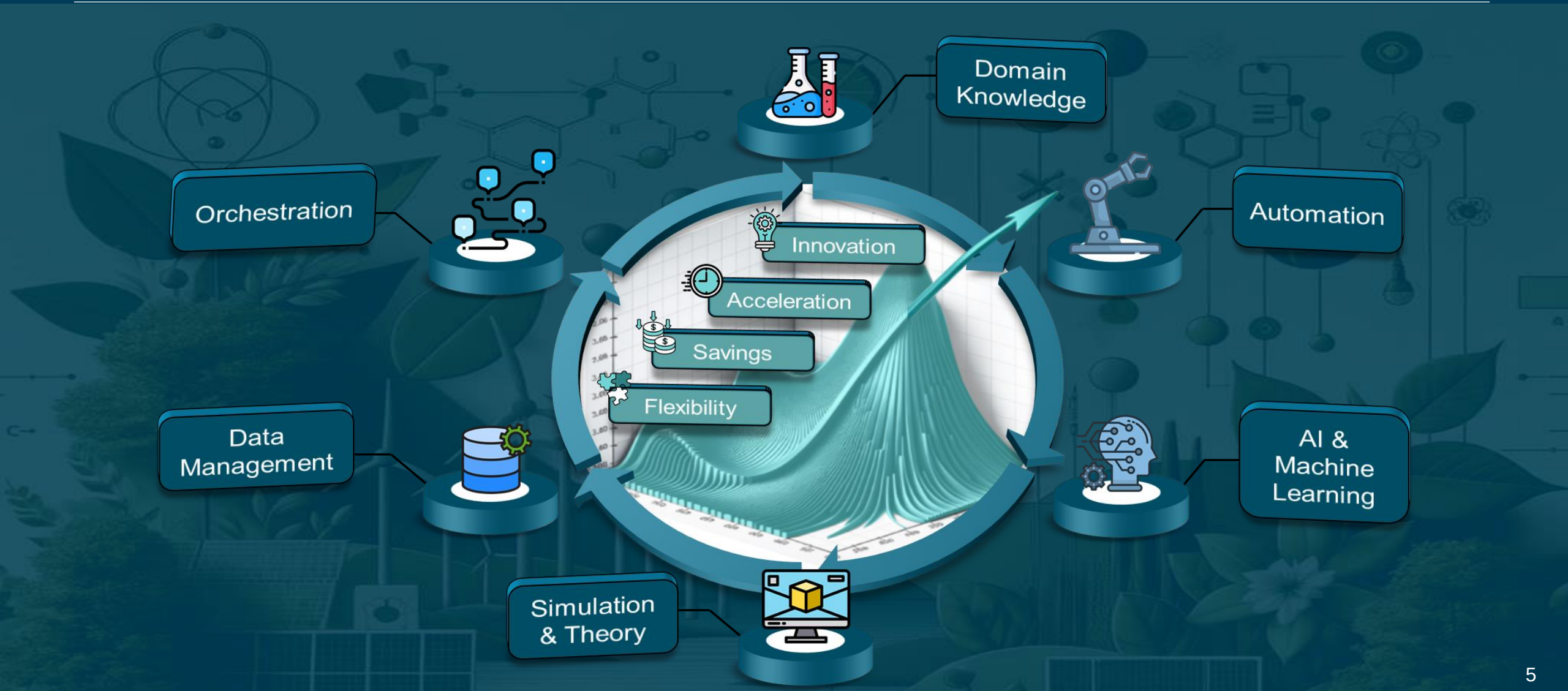
Midstream Accelerated Growth



An Evolution in Laboratory Investigation

	Human-centric	High-throughput Experimentation	Self Driving Laboratory (SDL)
Strategy			
Parameter space			

Material Acceleration Platforms (MAPs)



Team Competencies

Mechatronics & Automated Experimentation

- Standardized approach to implementing a mechatronics systems & subsystems (incl. CAD design)
- Development of bespoke automated platforms for high throughput experimentation

AI & Machine Learning, Data Science

- ML & AI development across various material domains, through a focus on 'universal' algorithm development and demonstration
- Up-to-date on this quickly advancing fields and how to apply this for materials research

Simulation & Theory

- Simulation framework to address a variety of classes of materials, towards a specific application, with a significant role in data ontology
- HPC and computing pipeline directly integrated into self-driving laboratory

MAPs Expert

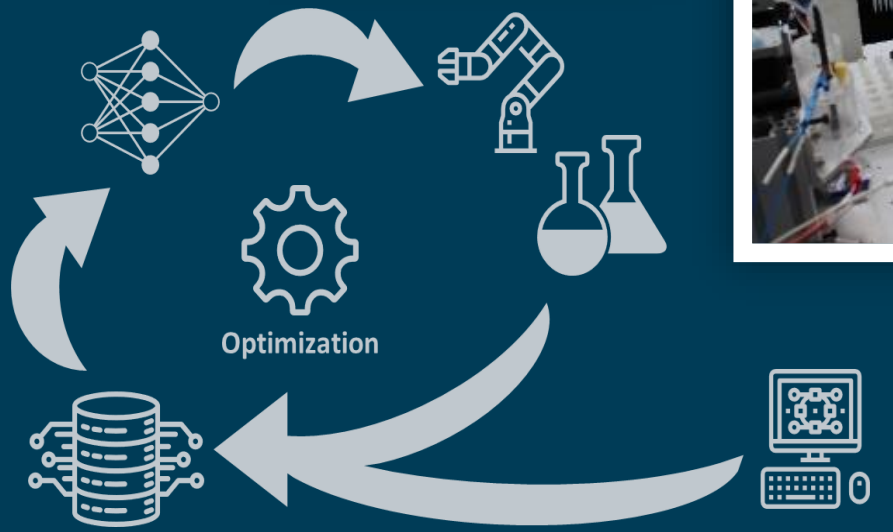
- Developed know-how/expertise in MAP workflow development, deployment, and implementation to obtain scientifically-valid results
- Data science and 'chemical intuition' into development of MAP

The Why of AI-Enabled Self-Driving Labs (SDLs) for Batteries

- We aspire to create new tools that combine the power of robotic automation, in-situ characterization and artificial intelligence/machine learning to accelerate the pace of clean energy research for materials discovery and process optimization

- Force multipliers measure how efficient exploration of material and process space (goal: 3x to 10x, or more for cathode materials candidates)

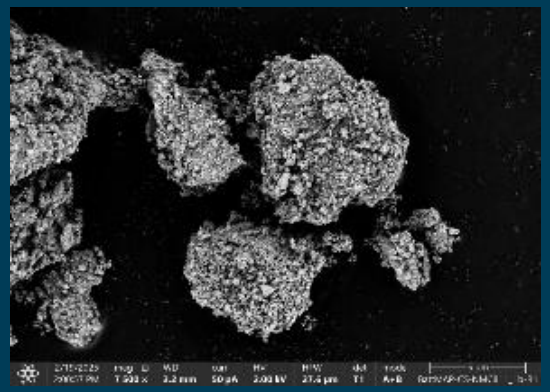
- <u>Rapid identification of candidates for scale-up with partners</u>

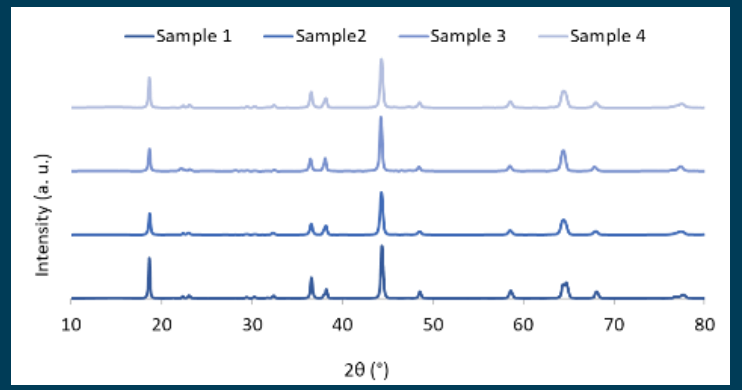


*SDLs also referred to as Material/Process Acceleration Platforms (MAPs/PAPs)

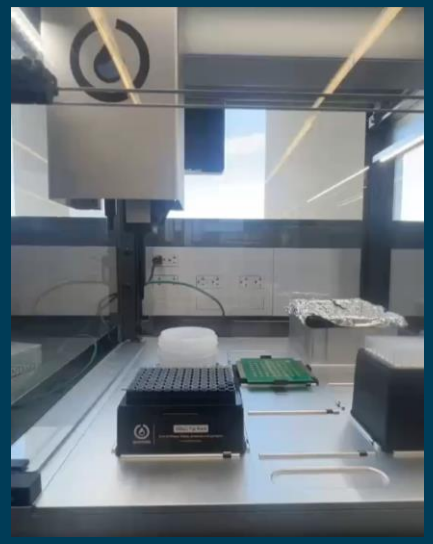
Critical Battery Materials Initiative (CBMI): Battery Materials Acceleration Platform (BattMAP)

- Automated high-throughput Cathode Active Material (CAM) Synthesis:

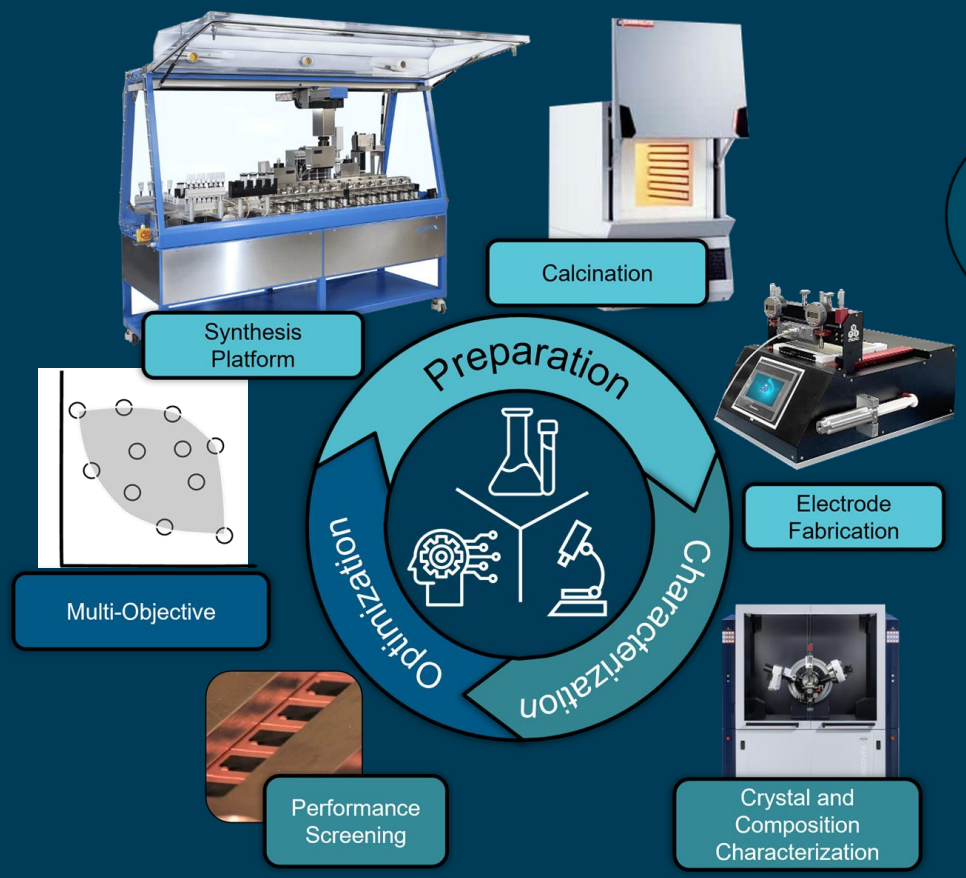




- Automated material deposition and robotic electrode assembly:
  - Array of 64 electrodes for high-throughput screening of electrochemical properties

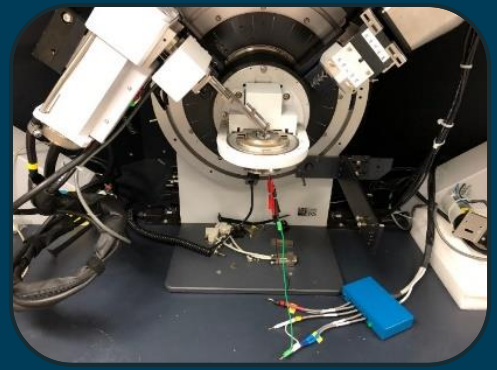


High Energy Density Li-ion Battery Cathode Materials

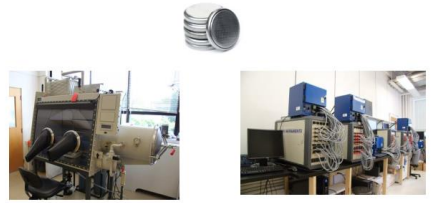


Extensive material characterization suite post-optimization

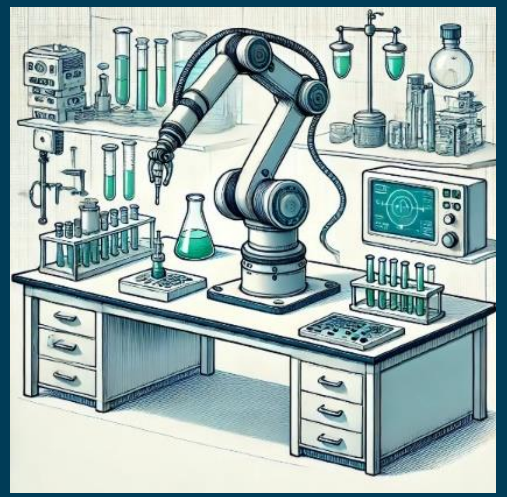
Lab-Scale XAS



In-Situ XRD

1. Battery Material Development	2. Small-scale Battery Testing and diagnostics	3. Lab-scale Battery Prototyping
		
Small scale synthesis of battery electrodes in g-scale to Kg-scale .	*Coin cell (<3mAh) assembly and testing Electrochemical analysis Post-mortem analysis*	*Lab-scale but industry relevant pouch cell (<1000 mAh) assembly and testing*

Tool Development:
Automated Materials Optimization Orchestrator



Data

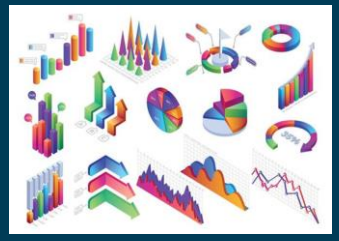
ML Algorithms
(Bayesian ML, Active Learning, …)

AutoMat∞r

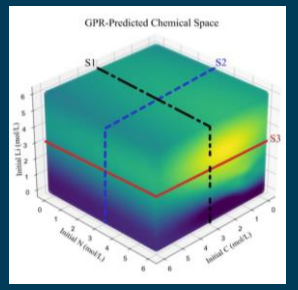
LLMs Agents

Publications/ Instructions

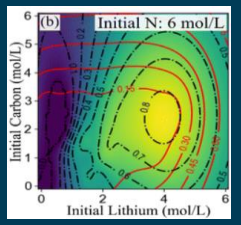
Knowledge & Insight



Models & Digital Twins



Optimization (Design of Experiment)



AI-Powered MAPs

LabSynchD

HPC

Monitor

Make and Experiment

Data Digitization and Storage

SOKEGraph

AI

Control

Analyze and Optimize

Spectra 2 Structure

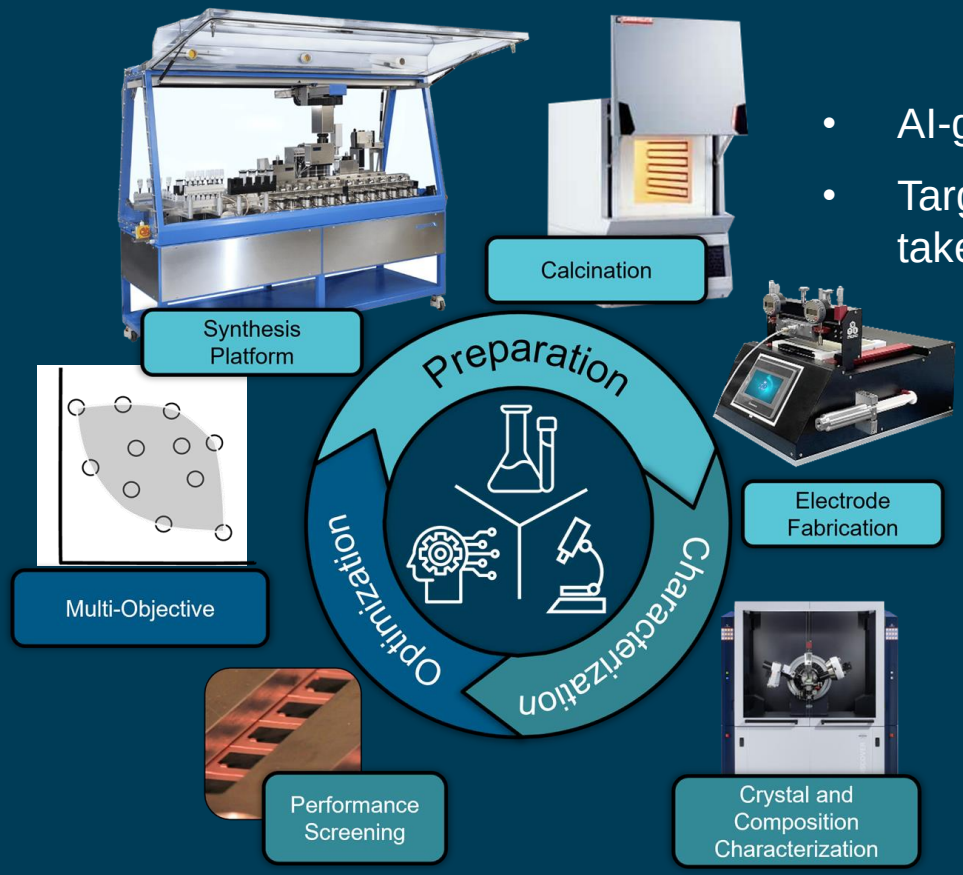
Design and Discover

MatLLM

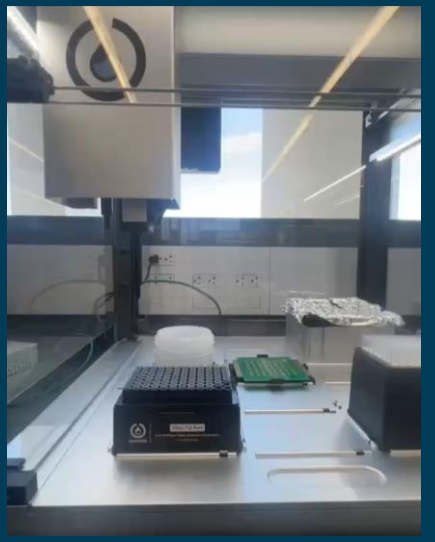
AutoMat∞r

Accelerating Discovery and Productivity

- Semi-closed loop MAP (human-in-the-loop)
- Robotic Automation: Material synthesis: 24x acceleration (demonstrated)
  Characterization screening: 64x acceleration (in-progress)
- AI-guided discovery: Predicted 12x acceleration
- Target: Find a optimized candidate material from a design space that would normally take 100 years of traditional research in only 1 month of MAP research time



Synthesis platform



Electrode fabrication

Materials Acceleration Demonstration Ecosystem (MADE)

What is MADE:

- Joint NRC-NRCan program dedicated to developing accelerated materials discovery tools (including MAPs) for clean energy applications

Team of 20+ research and technical staff from both NRC and NRCan

Vision:

- Enable the widespread use of sustainable energy technologies to improve the quality of life for all Canadians.

Mission:

- Accelerate materials from discovery to demonstration in an agile and responsive manner. Collaborate strategically to develop capacity and expertise for next generation talent.

Integrated MAPs Pipeline
Acceleration Towards New Battery Materials

Critical Mineral Processing MAP

Primary Sources & Recycled Batteries to Precursors

Battery Materials Discovery MAP

Precursors to Cathode Materials

Scale-up to Prototype

Scale Production - Materials

Scale Production - Precursors

To end application/ adopters

Critical Minerals for Energy Storage

Material Discovery

Feedstock Processing

Li-Brine

Li_2CO_3 crystallization
AI-guided optimization of Li_2CO_3 yield and purity

Recycled Battery Materials

Leaching & Impurity Removal
Cathode Precursors

1

Synthesis Techniques:
Sol-Gel & Co-Precipitation *(cathode materials)*
Calcination

Characterization Techniques:
Elemental Composition
Structure Characterization (XRD)

Cathode Material Synthesis

2

Performance Optimization

Electrode Preparation & Performance Screening

Material Preparation:
Inkjet and/or slot die coating

Electrochemical Characterization:
Capacity & Stability

3

AI-Battery RUL Prediction

Small – cell battery testing
AI-assisted performance and lifetime prediction

NRC NRCan

Acknowledgments

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CEI - Ottawa

Jennifer Littlejohns
Lawrence Charlebois
Yaser
Ben Yu
Andriy Plugatyr
Adam Bernicky

External Partners

Link to the CBMI website

CBMI general inquiries email:
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Thank you
Merci
Arigatō