Bridging computation and experiment for energy materials discovery

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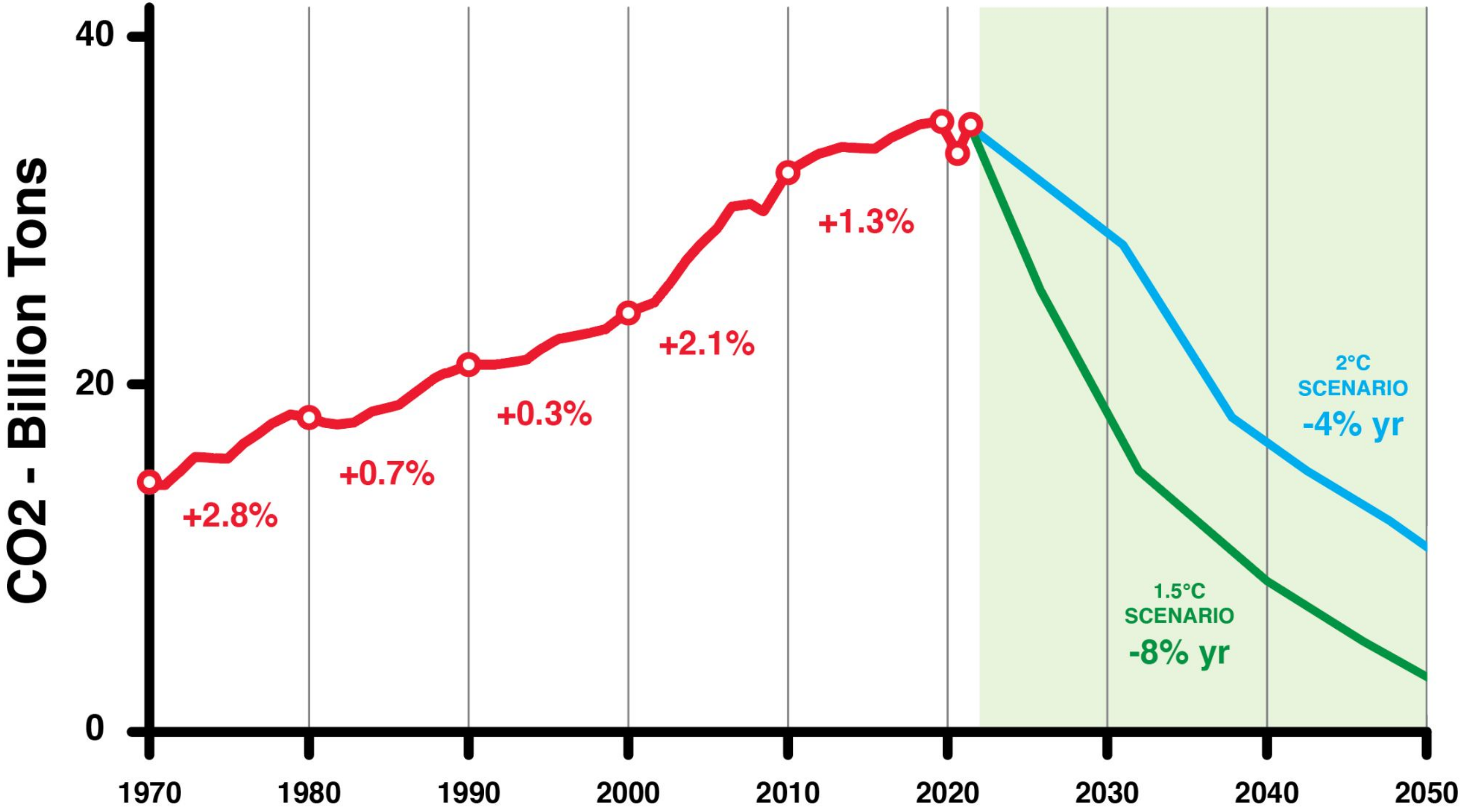
Linda Hung
Manager, Energy & Materials Division, TRI

- TRI overview
- Battery lifetime
- Novel materials

Complex Scientific Workflows at Extreme Computational Scales
IPAM, May 2, 2023

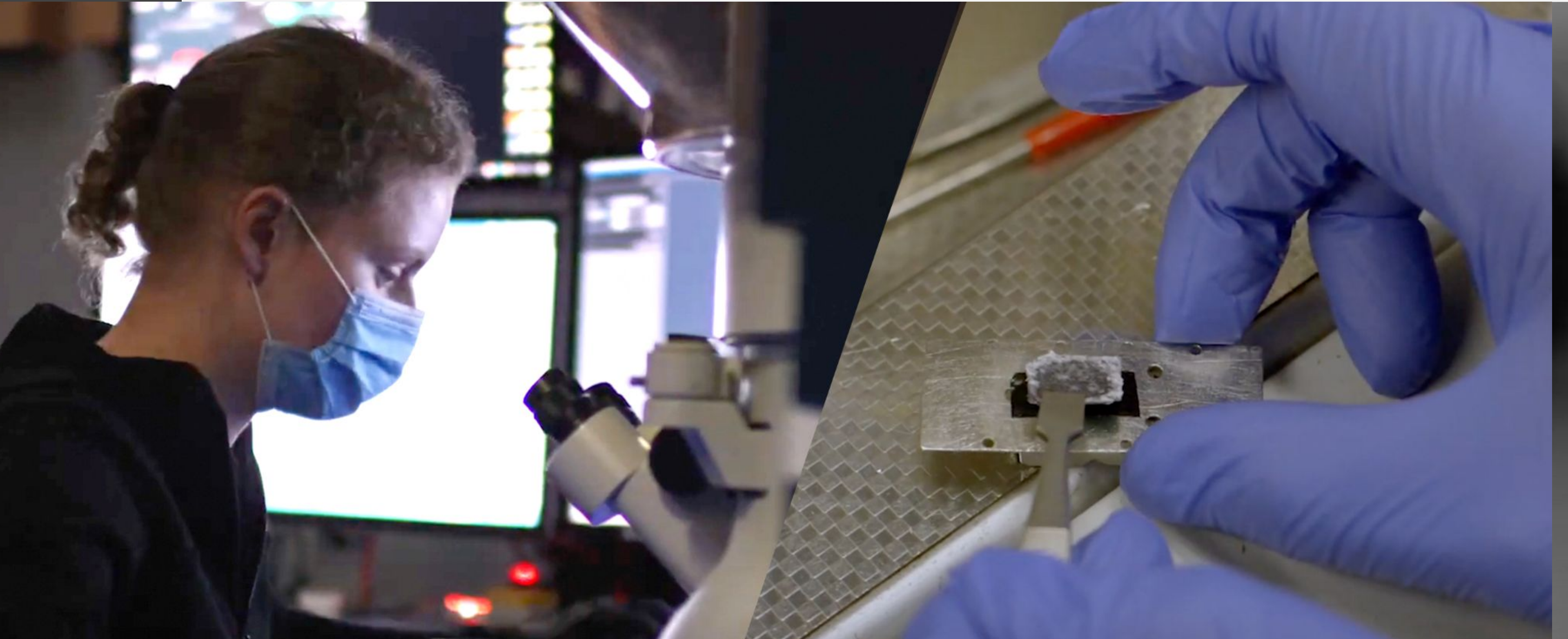
Challenge - Global carbon emissions



Challenge - Resources and sustainability

The world needs:

Better materials



The world needs:

More batteries

The world needs:

Diverse solutions

Energy and Materials Division

Materials Discovery

Better materials are needed for breakthrough performance

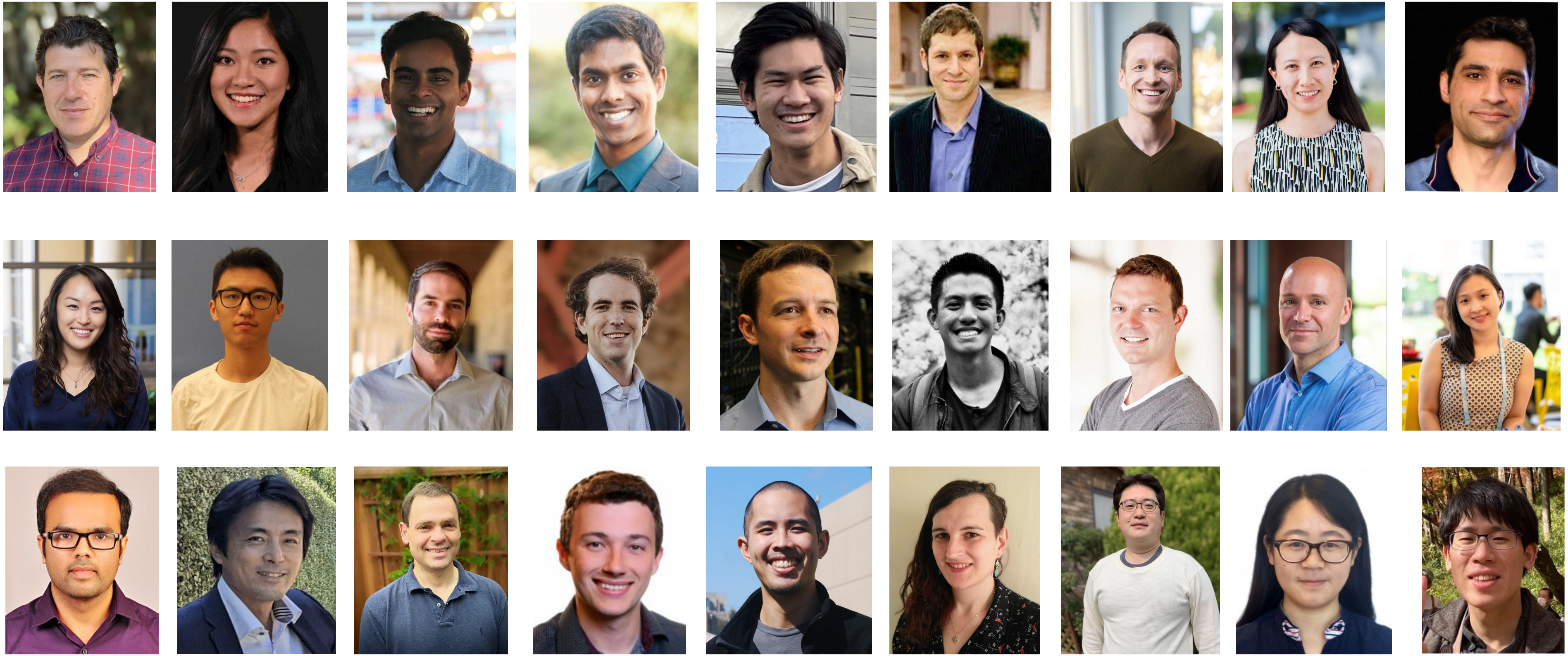
Battery Manufacturing

To make **more batteries**, we must perfect battery manufacturing.

Carbon Neutrality

Which **diverse solutions** are viable depends on economics, society, and policy.

E&M team members



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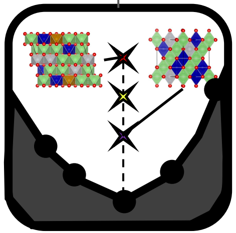
212 Northern Avenue

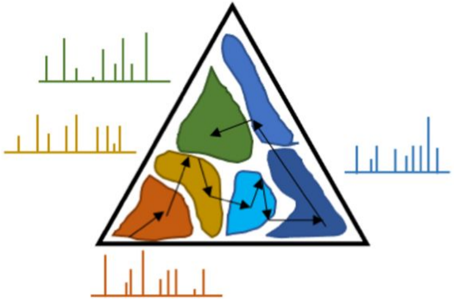
MATERIALS DISCOVERY

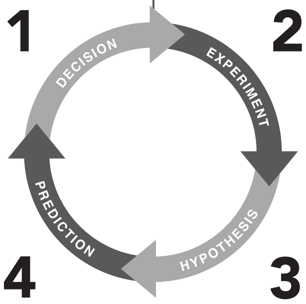
A typical project

Unique	Tailored	AI-powered	
1 *Data Generating Process*	**2** *Data*	**3** *Analysis*	**4** *Feedback*

At universities, national labs, or internal to TRI







Applications: batteries, fuel cells, fundamental materials

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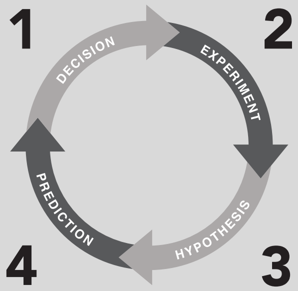
Our tools for compute

Challenges with accelerating materials discovery

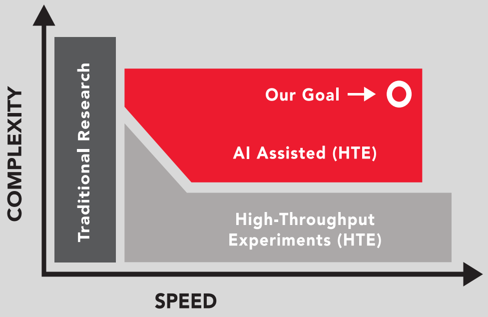
Efficiency is too low

Our approach
Automation & closed loop discovery.



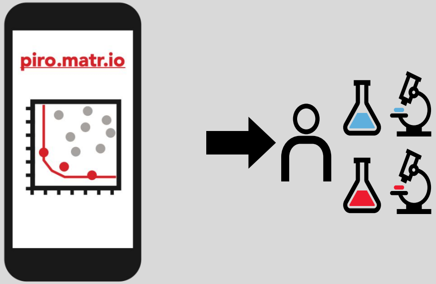
Experimental feedback is very difficult

Our approach
AI powered data analysis.



Lack of theory to enable design

Our approach
Actionable input to experiments



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Challenges with accelerating materials discovery

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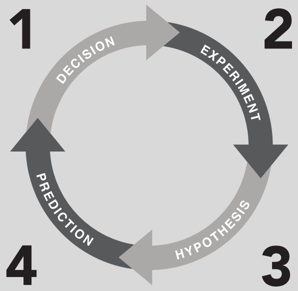

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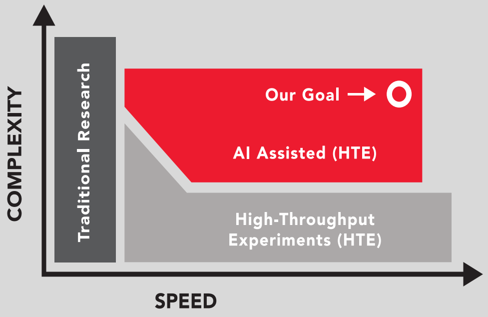
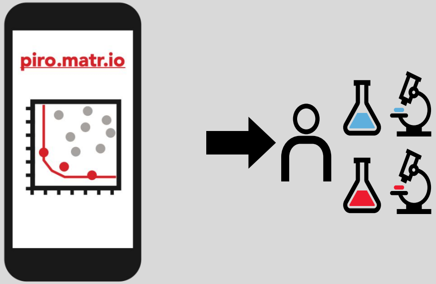


Battery lifetime

Lack of theory to enable design

Our approach
Actionable input to experiments



Novel materials


Shijing Sun


Amalie Trewartha

Battery state of health

Data-driven and physics-driven approaches

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How long do we expect a battery to last?

Chemistry

History

Environment

… infinite ways to charge and discharge (use), leading to **diverse** lifespans

Electrical cycling testing provides insight at all stages of the battery life cycle

Cell R&D → Cell Production → Module & Pack Design → System Integration → Consumer Use → 2nd Life & Recycling

- **Cell R&D:** Rapid capacity tests provide **feedback and guidance** to innovation in new battery chemistry
- **Module & Pack Design:** Tight production standards and **quality control** aim to prevent bad batteries from being used
- **Consumer Use:** BMS aims to **prevent failure** from environment and operator behavior through monitoring
- **2nd Life & Recycling:** Cycling data **diagnoses state of health** of batteries to judge suitability for 2nd life

… traditional multi-factor systems optimization requires testing **until end of life**,
This process takes **years**.

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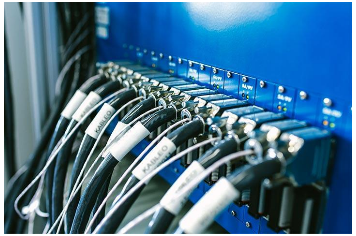
Challenges of battery cycling data

Testing systems are designed for *low-throughput*, *manual* testing

- Each testing system has its own format
- Metadata is vitally important but not stored
- They may not distinguish cycle types - e.g. Diagnostics vs accelerated aging
- Time-series is not necessarily the most helpful format for every problem

- Traditional battery cycling takes **months per battery**
- Feedback and optimization takes **years**

	test_time	date_time	step_time	step_index	cycle_index	current	voltage	charge_capacity	c
1	0.000100	1.494646e+09	-1780.003052	0	0	0.0	3.301788	0.0	
2	9.998300	1.494646e+09	-1770.004883	0	0	0.0	3.301751	0.0	
3	20.002001	1.494646e+09	-1760.001221	0	0	0.0	3.301784	0.0	
4	30.000601	1.494646e+09	-1750.002563	0	0	0.0	3.301805	0.0	
5	30.000700	1.494646e+09	-1750.002441	0	0	0.0	3.301805	0.0	
6	40.001900	1.494646e+09	-1740.001343	0	0	0.0	3.301790	0.0	



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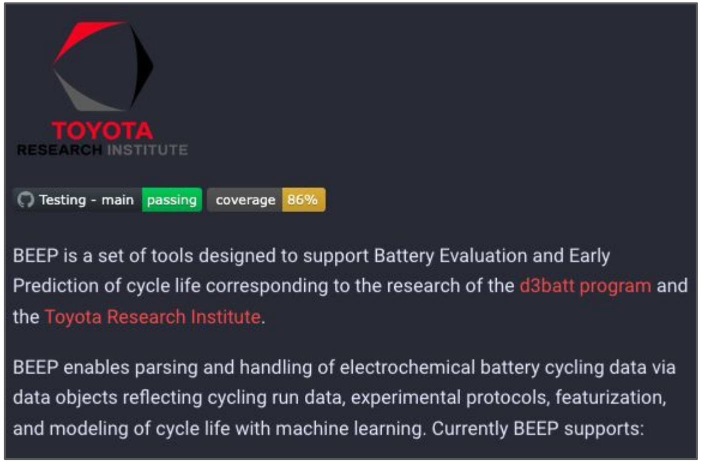
BEEP: Battery Evaluation and Early Prediction

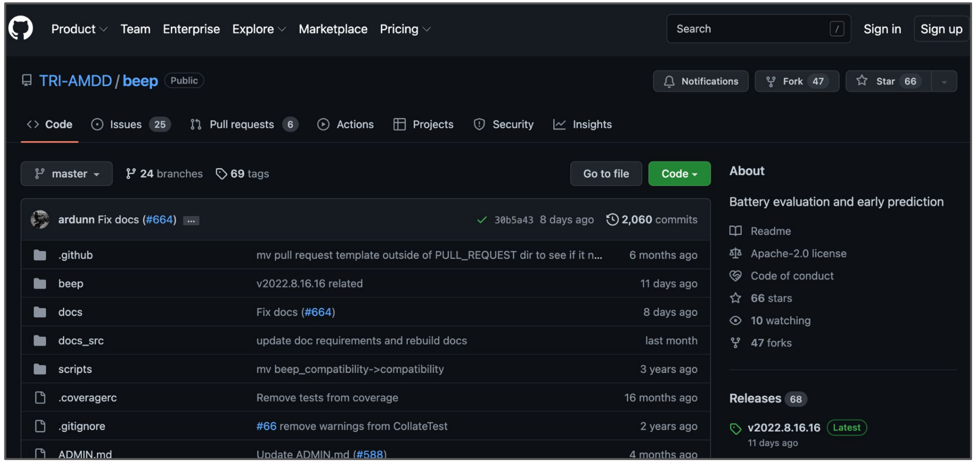
```
pip install beep
```

https://github.com/TRI-AMDD/beep

Support multiple cycler manufacturers including:

- Maccor
- Arbin
- BioLogic
- Neware
- Indigo
- Novonix (**NEW**)

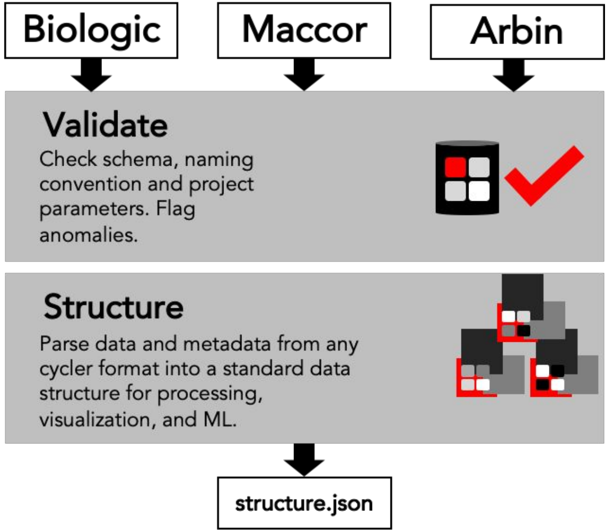


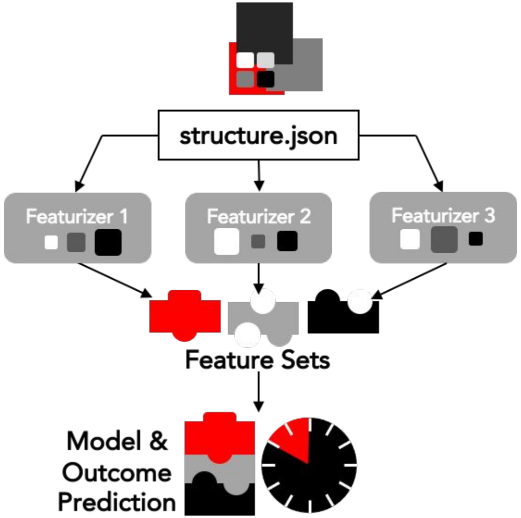


"BEEP: A Python Library for Battery Evaluation and Early Prediction," P.K. Herring *et al.*, SoftwareX **11**, 100506 (2020).

BEEP makes battery cycling data ML ready

Highlight #1 - **structuring**: process data from multiple hardware vendors into one common data structure.





Highlight # 2 – **feature extraction**: transform structured data into ML-ready feature objects, alongside corresponding metadata.

"BEEP: A Python Library for Battery Evaluation and Early Prediction," P.K. Herring *et al.*, SoftwareX **11**, 100506 (2020).

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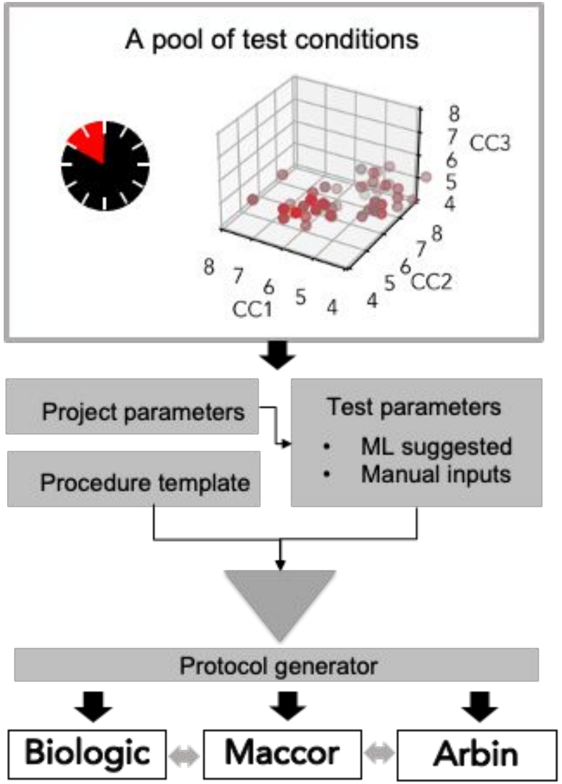
BEEP provides programmatic scheduling of testing



Highlight #3 - **scheduling**:

- Communicate with hardware to launch high-throughput experiments
- Reduce manual errors and expedite scheduling
- Protocols convertible between cyclers

"BEEP: A Python Library for Battery Evaluation and Early Prediction," P.K. Herring *et al.*, SoftwareX **11**, 100506 (2020).

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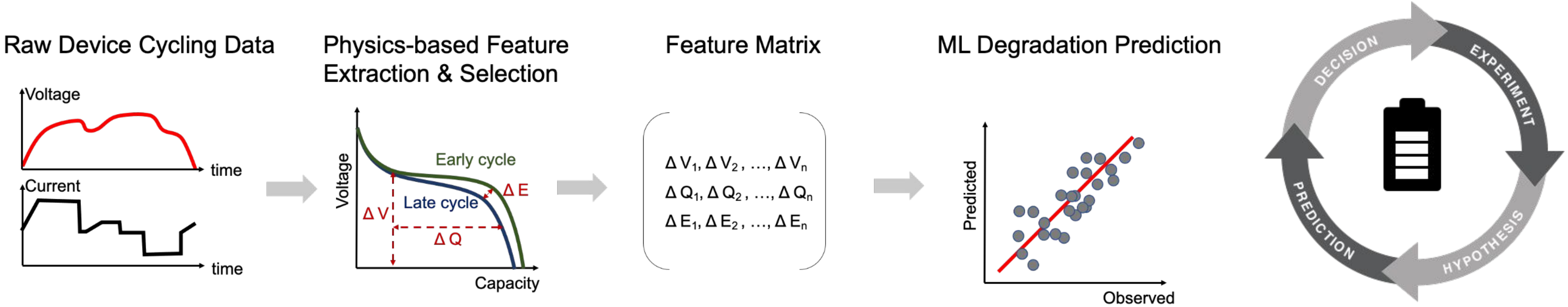
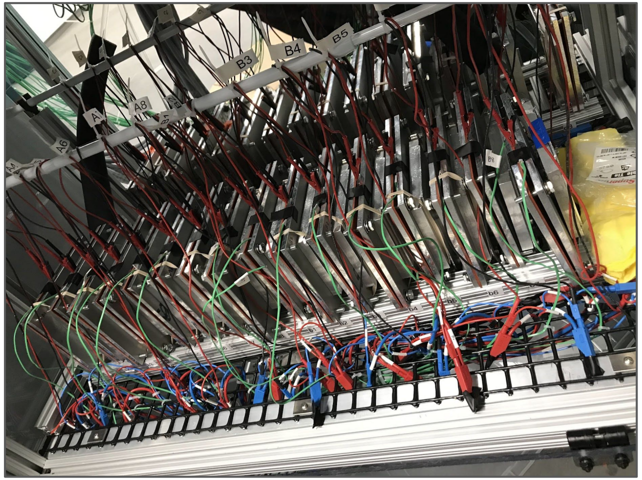
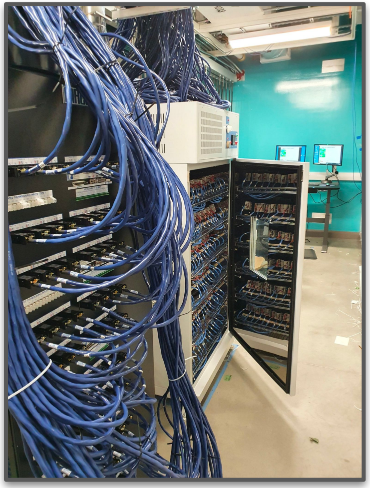
BEEP automation enables data-driven degradation prediction



- Large, diverse cycling dataset collected and processed automatically
- Machine learning based analysis: extracting subtle signals from battery cycling data to offer ***actionable, interpretable*** insights into cell internal state

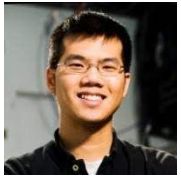
High-throughput testing at SLAC





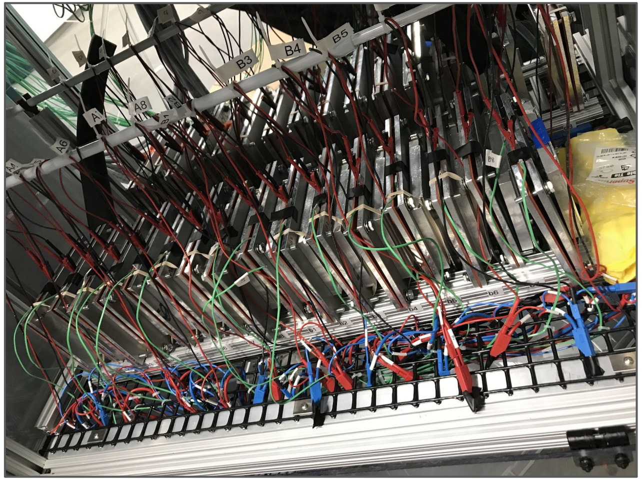
D3BATT

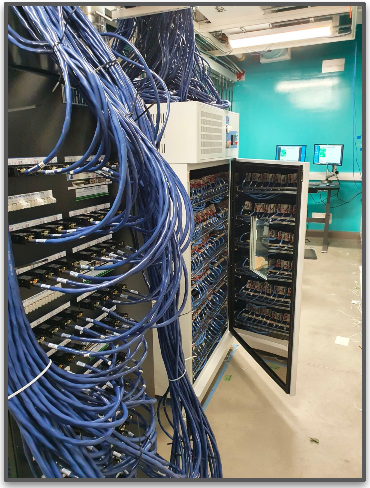
Data-Driven Design of Li-ion Batteries



Professor Will Chueh

High-throughput testing at SLAC





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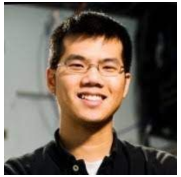
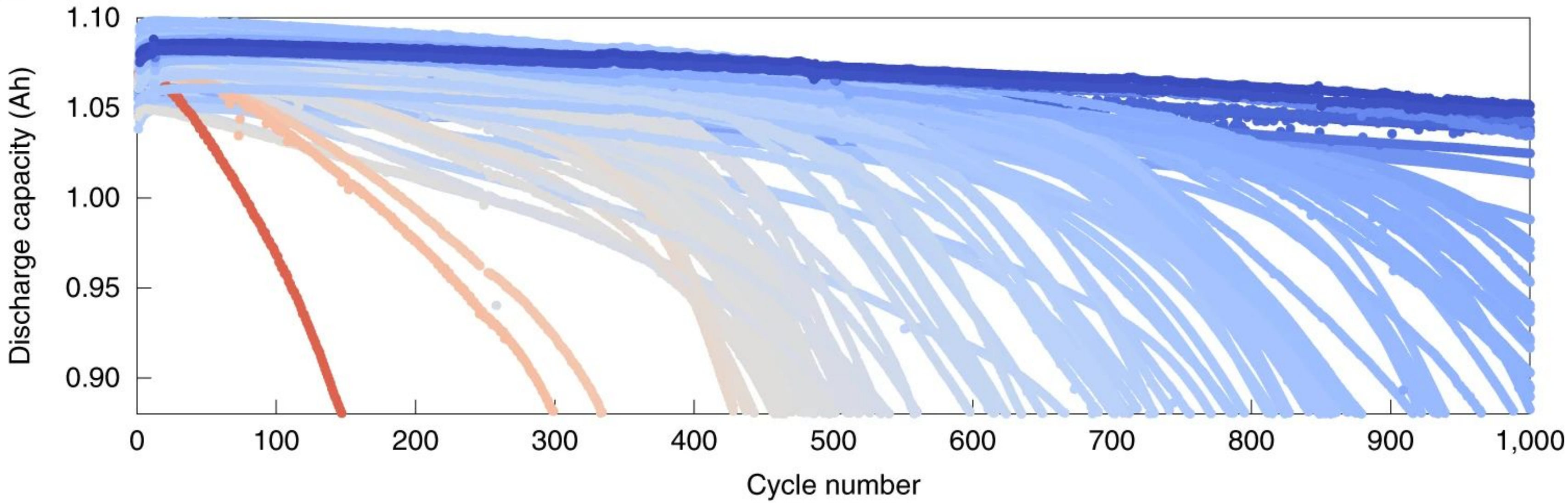


Professor Will Chueh

Airflow S3 Sagemaker

Challenge: full aging tests are time-consuming



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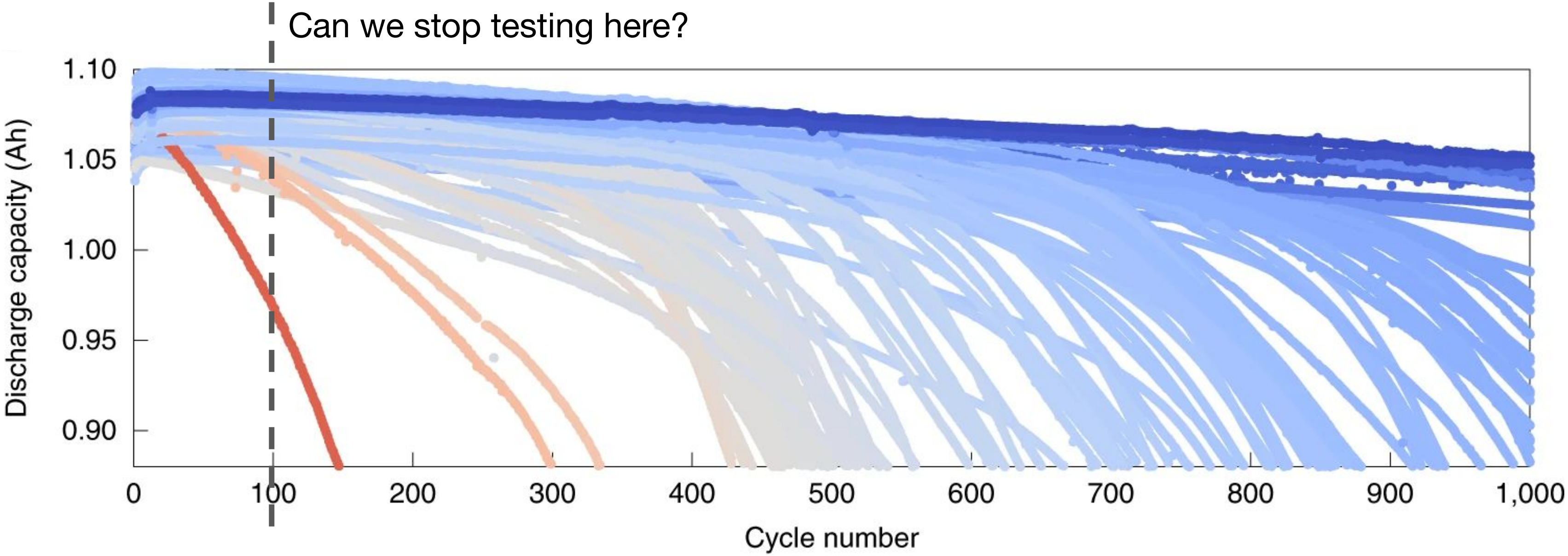
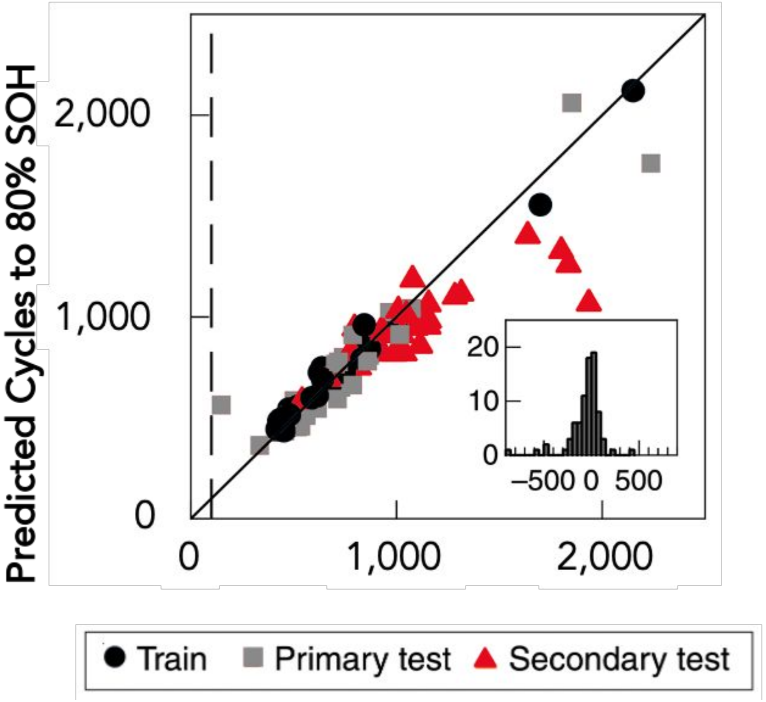
Challenge: full aging tests are time-consuming



"Data-driven prediction of battery cycle life before capacity degradation," K.A. Severson *et al.*, *Nat Energy* **4**, 383 (2019).

Previously at TRI: early-prediction reduces test time by 10x

- Features from early cycle predict cycle life
- ML predictions made before observed decrease in capacity
- > 90% accuracy using first 100 aging cycles on LFP cells



“Data-driven prediction of battery cycle life before capacity degradation,” K.A. Severson *et al.*, *Nat Energy* **4**, 383 (2019).

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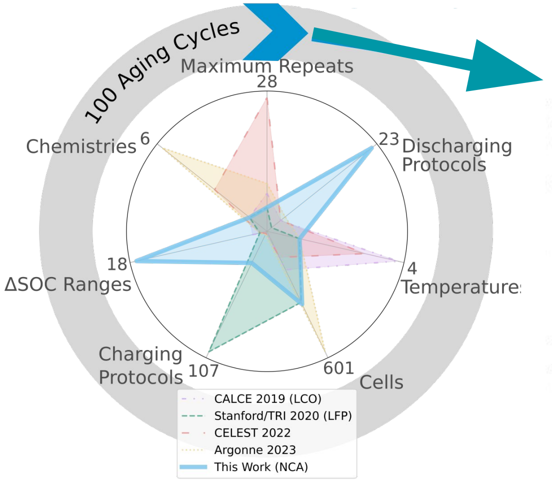
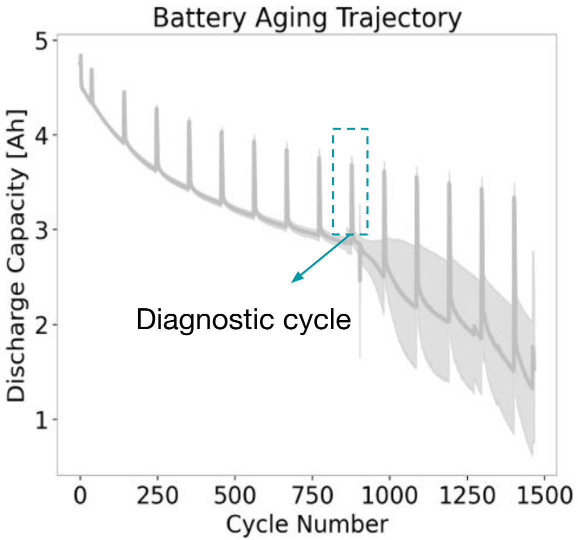
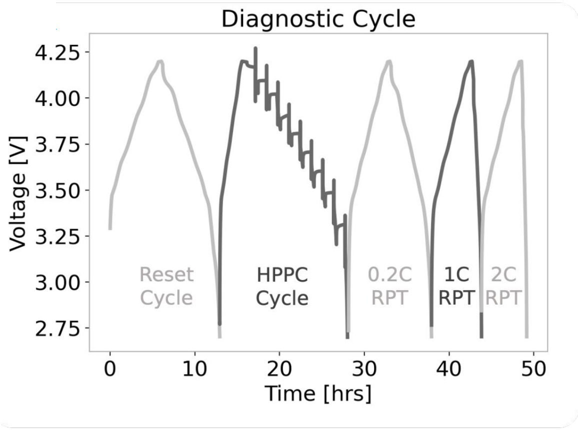
New dataset: diverse usage with standardized diagnostics







- **363 cells** tested until the end of 1st lifetime on NCA/Gr + SiOx cells[1]
- **218 cycling conditions** with diverse discharge profiles unexplored previously
- **Standardized** diagnostics enable comprehensive health evaluation and comparison

"Interpretable Data-Driven Modeling Reveals Complexity of Battery Aging", Bruis van Vlijmen *et al.*, DOI: 10.26434/chemrxiv-2023-zdl2n (2023).

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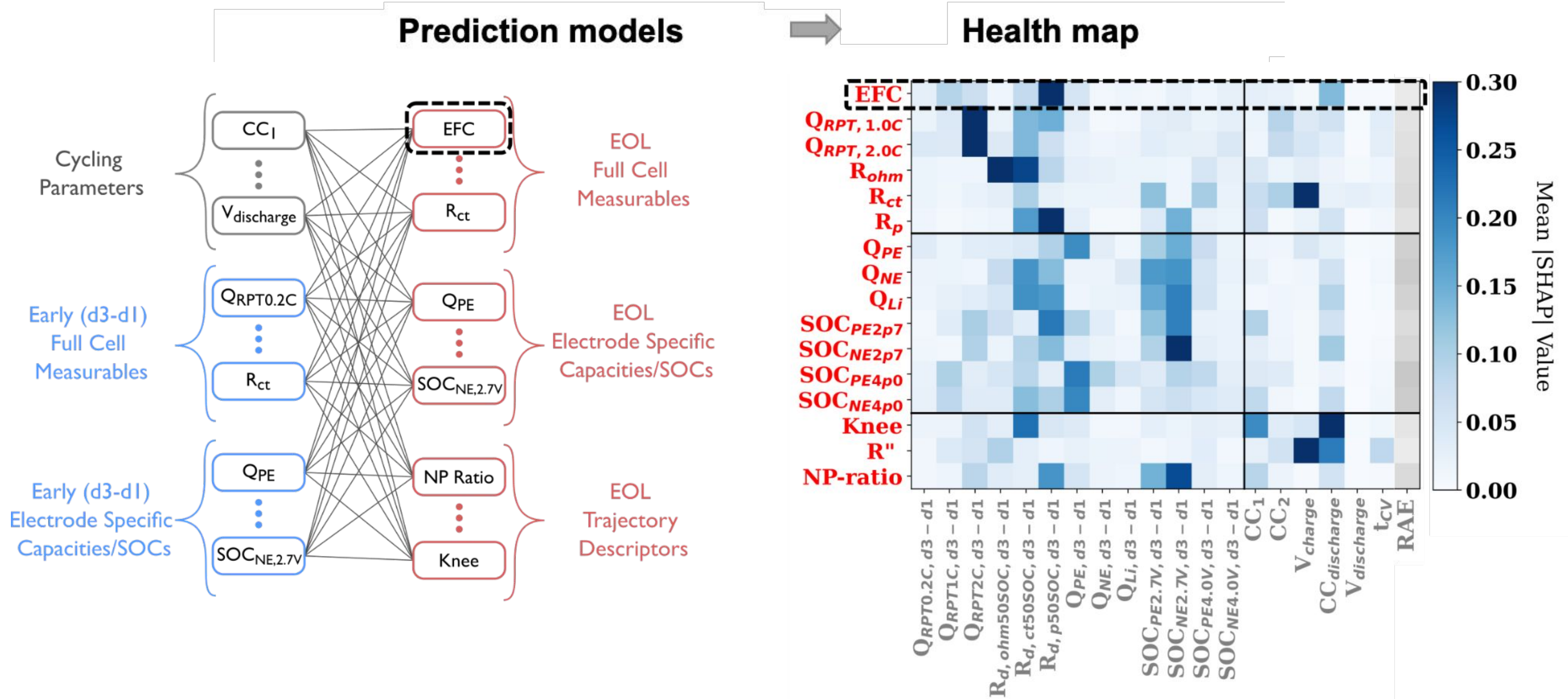
Early-prediction using physically meaningful features



Health map generated from early prediction models provide actionable insights to battery design and optimization

"Interpretable Data-Driven Modeling Reveals Complexity of Battery Aging", Bruis van Vlijmen *et al.*, DOI: 10.26434/chemrxiv-2023-zdl2n (2023).

Battery state of health - continuing challenges

Efficiency is too low

- Early prediction for cycling
- Efficient / fast simulation

Experimental feedback is very difficult

- Datasets: other points of battery lifecycle
- Datasets: diverse battery chemistries
- Characterization

Lack of theory to enable design

- Models that accounting for relevant processes in physics-based models

Joey
Montoya

Materials discovery

From simulation to synthesis

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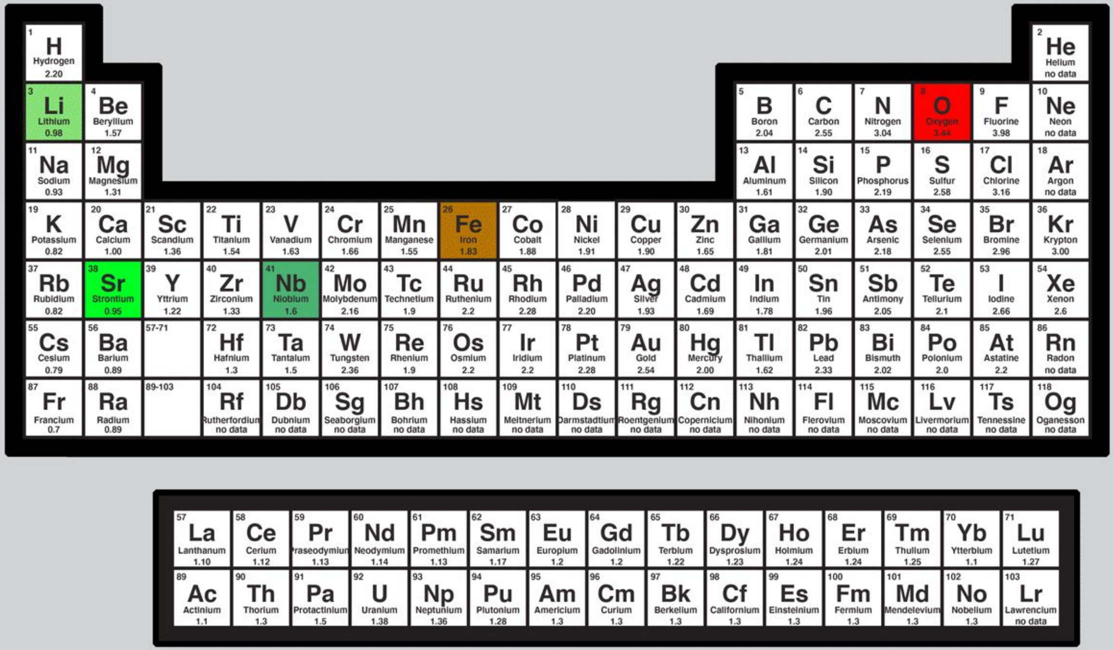
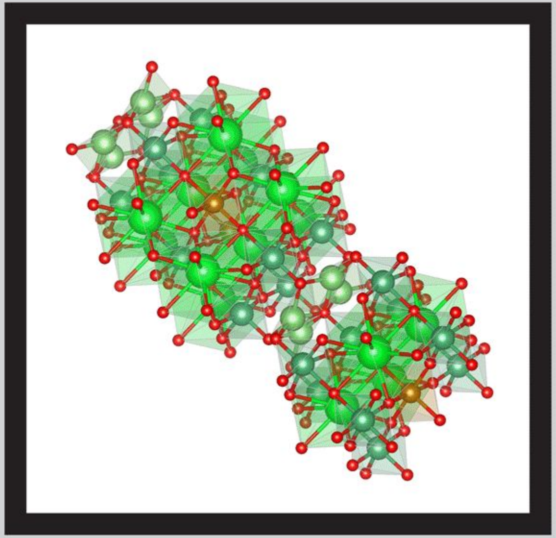
The infinite search space

COMPOSITION

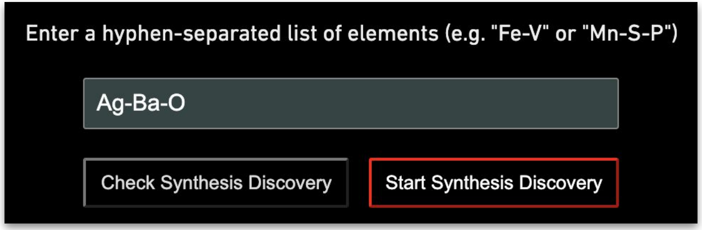


STRUCTURE

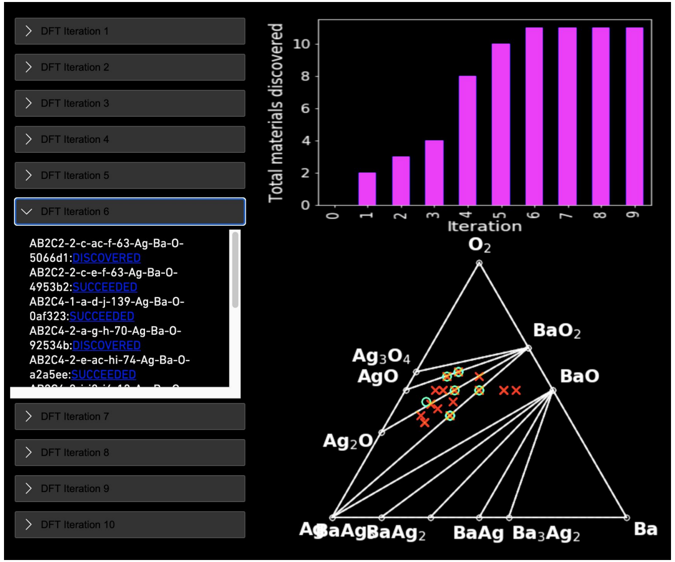


CAMD: Computational Autonomy for Materials Discovery

User **chooses chemical system**, e.g. Ag-Ba-O



CAMD **displays real-time results on frontend**



CAMD **stores structures and data**

https://github.com/TRI-AMDD/CAMD

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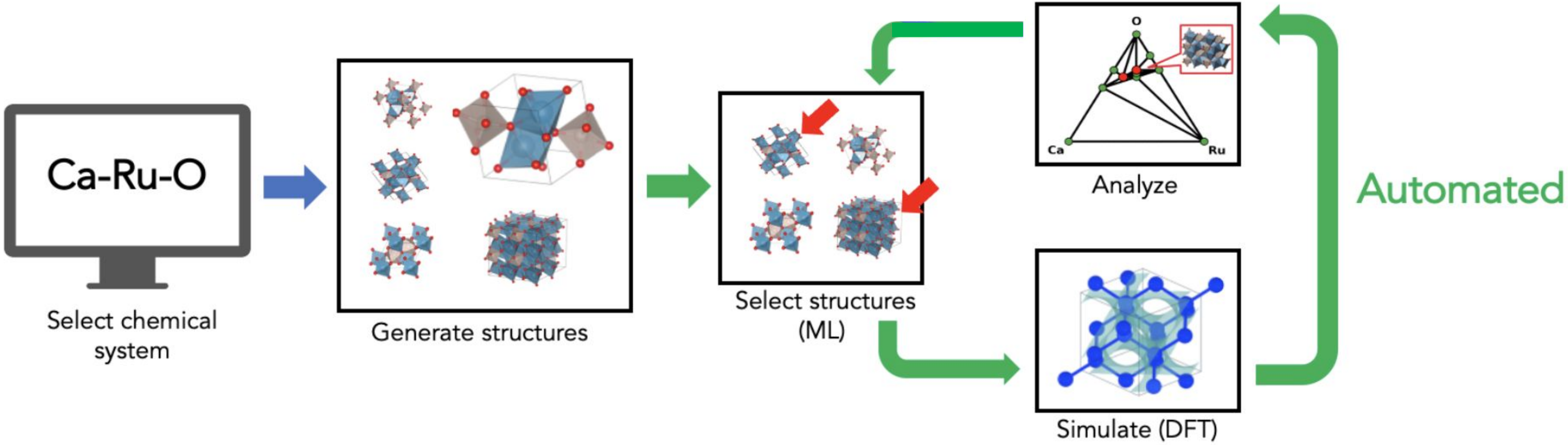
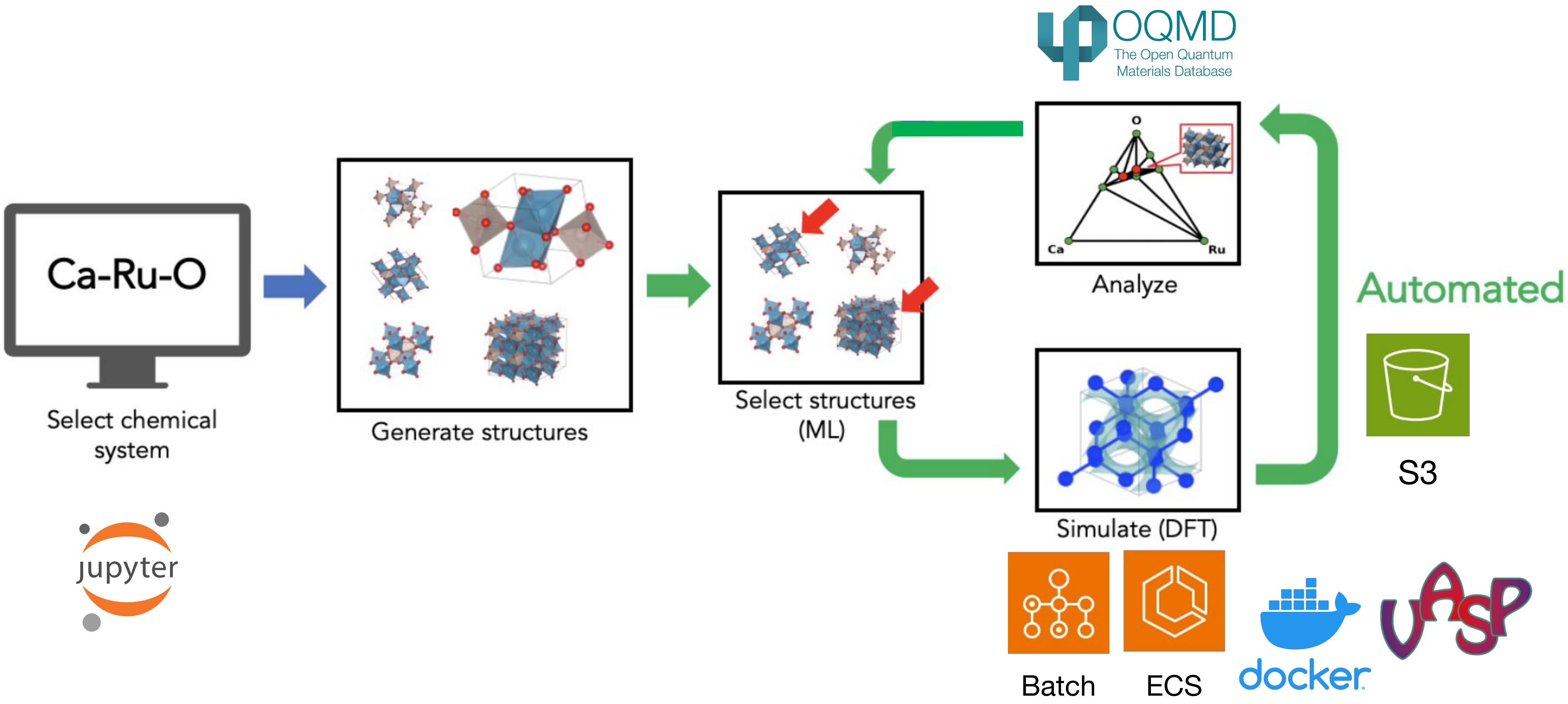
Active learning to discover materials



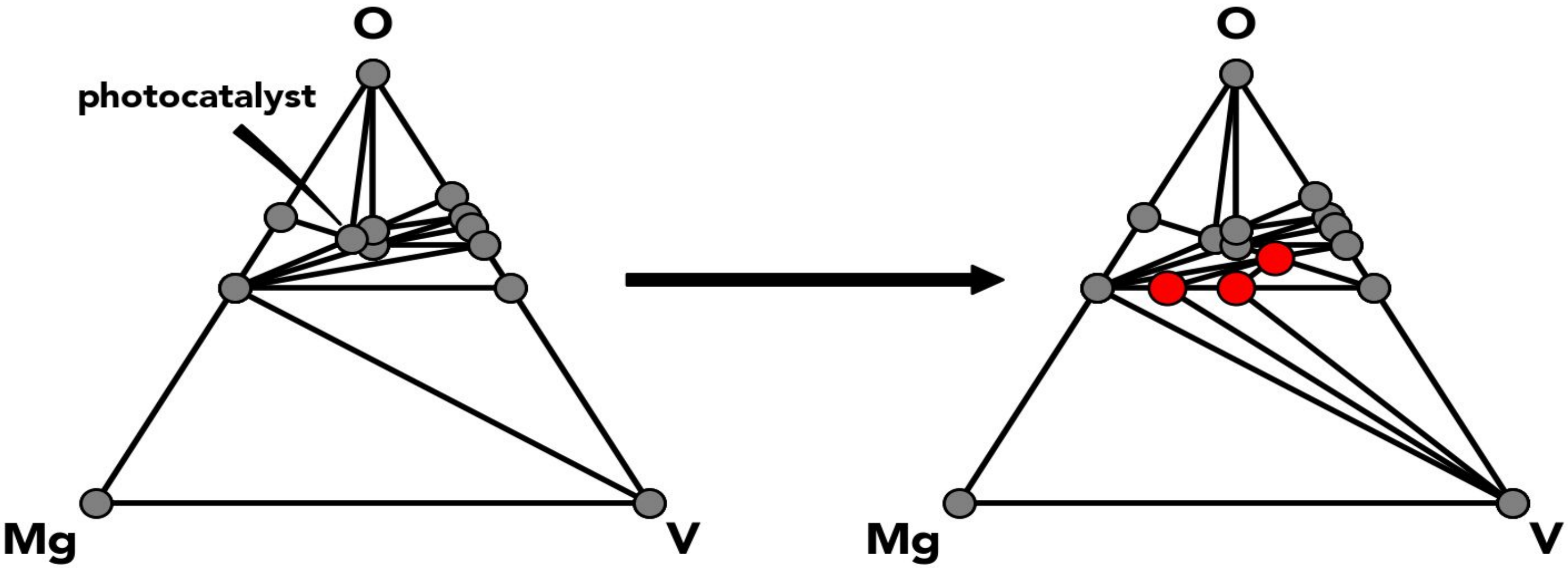
"Autonomous Intelligent Agents for Accelerated Materials Discovery" J.H. Montoya *et al.*, *Chem Sci* **11**, 8517-8532 (2020).

Active learning to discover materials



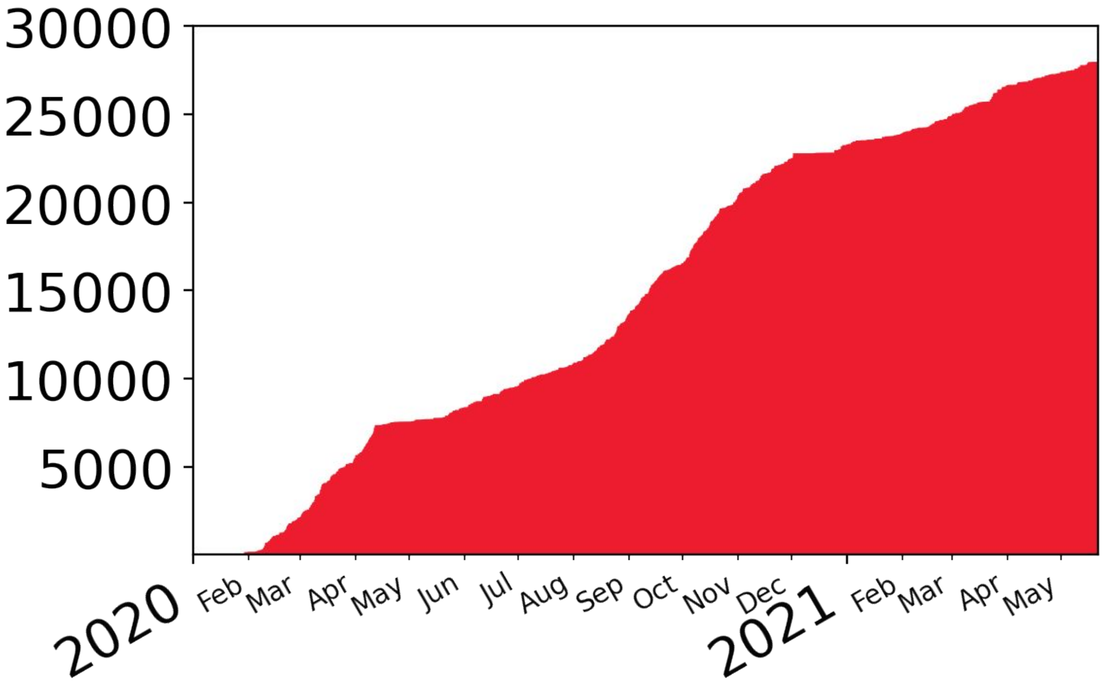
"Autonomous Intelligent Agents for Accelerated Materials Discovery" J.H. Montoya *et al.*, *Chem Sci* **11**, 8517-8532 (2020).

CAMD finds new (meta)stable structures



“Novel inorganic crystal structures predicted using autonomous simulation agents”, W. Ye, X. Lei, *et al.*, *Sci Data* **9**, 302 (2022).

CAMD finds a lot of metastable structures



https://data.matr.io/7/

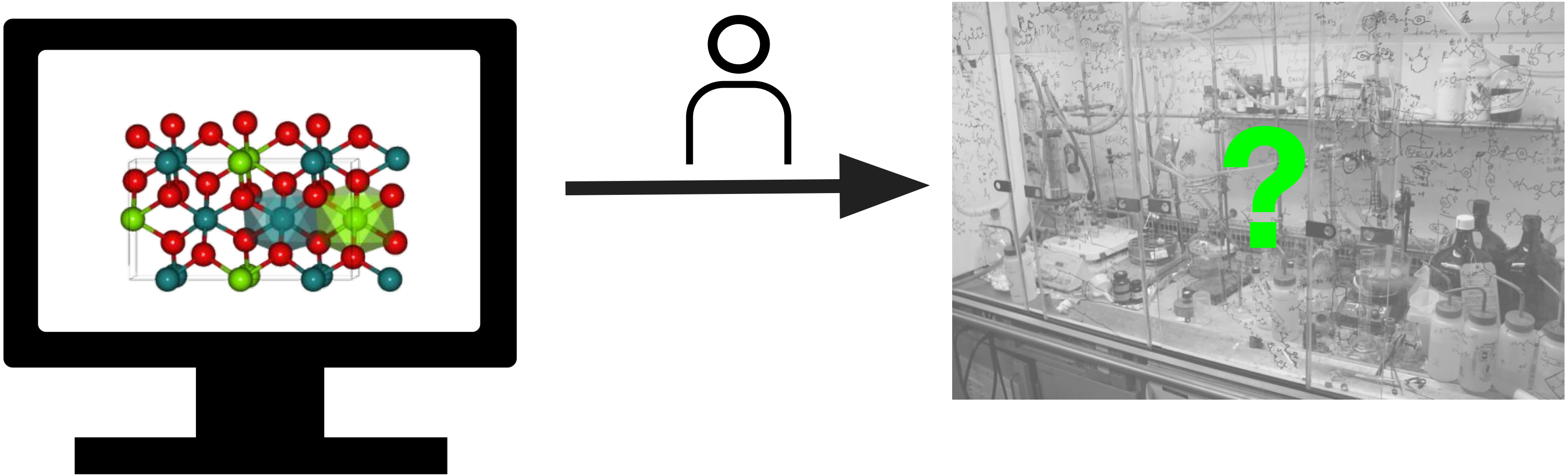
CAMD discovers 2-3 new structures within 200 meV of the convex hull per hour

CAMD spends $3.00 per metastable structure

CAMD's infrastructure is scalable

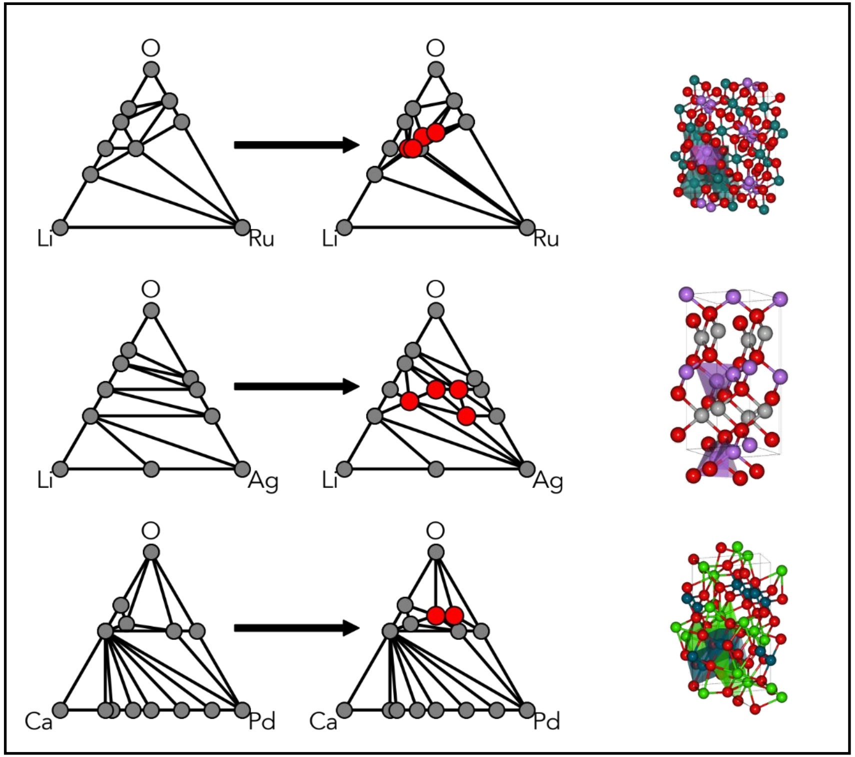
"Novel inorganic crystal structures predicted using autonomous simulation agents", W. Ye, X. Lei, *et al.*, *Sci Data* **9**, 302 (2022).

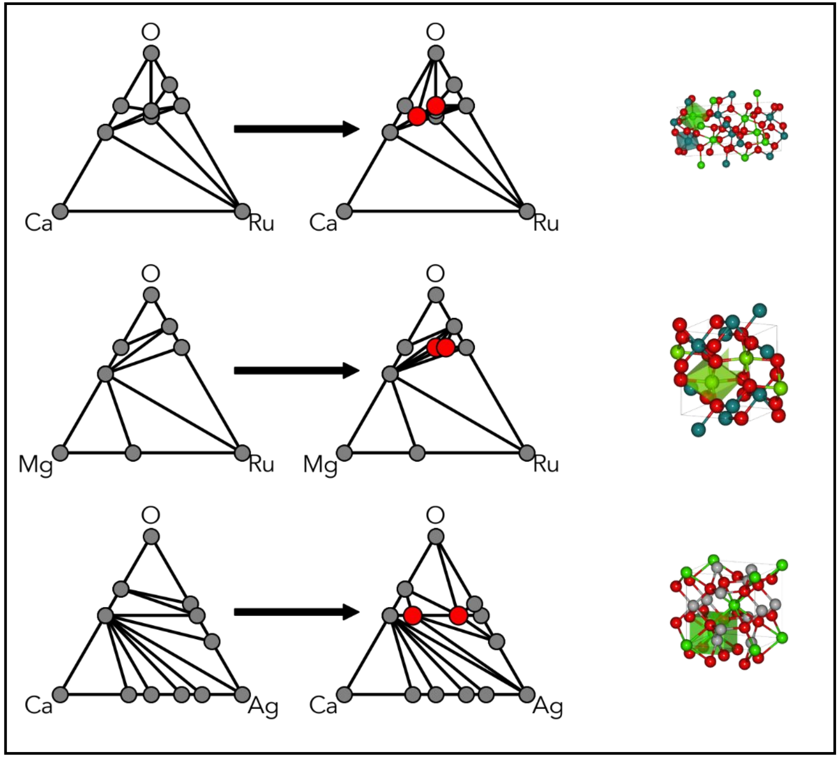
We tried to make CAMD materials



“Computer-assisted discovery and rational synthesis of ternary oxides”, J.H. Montoya *et al.*, DOI: [10.26434/chemrxiv-2023-n4pz9](https://doi.org/10.26434/chemrxiv-2023-n4pz9) (2023).

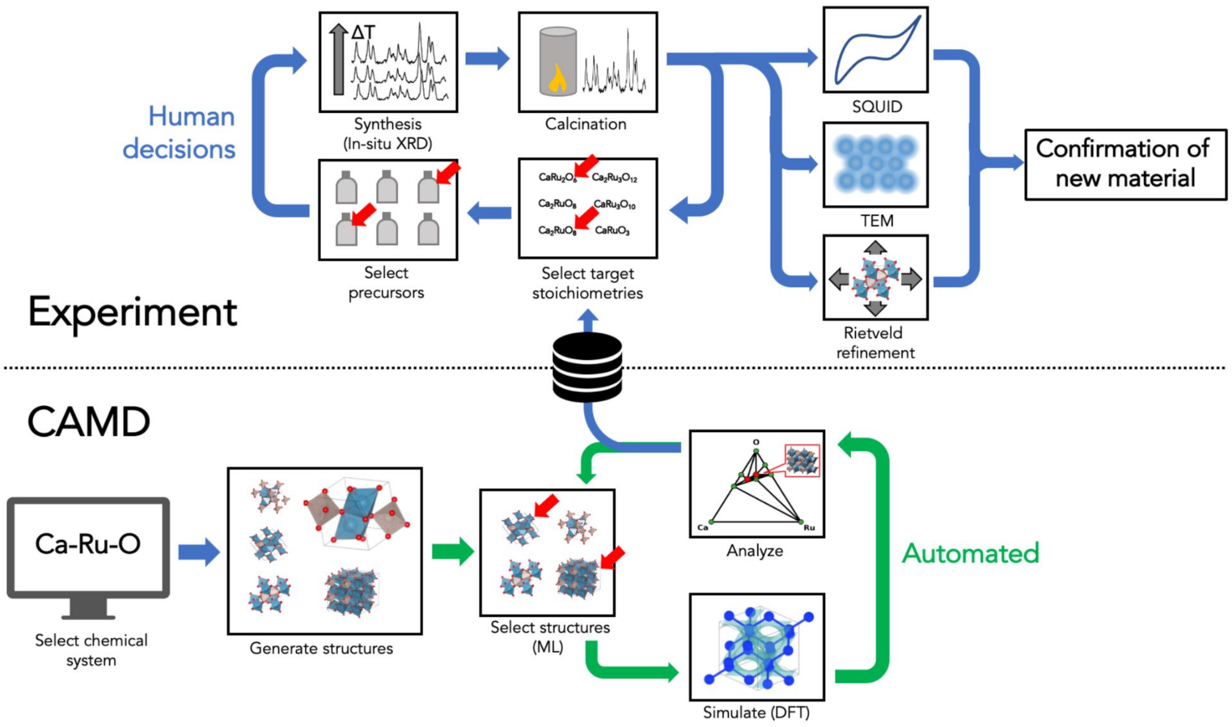
Six CAMD inspired systems were selected





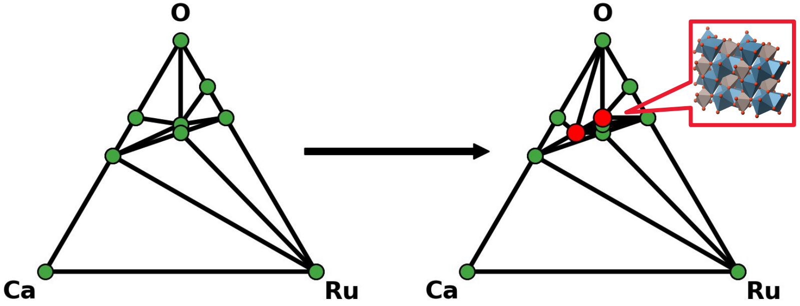
“Computer-assisted discovery and rational synthesis of ternary oxides”, J.H. Montoya *et al.*, DOI: 10.26434/chemrxiv-2023-n4pz9 (2023).

Materials discovery workflow



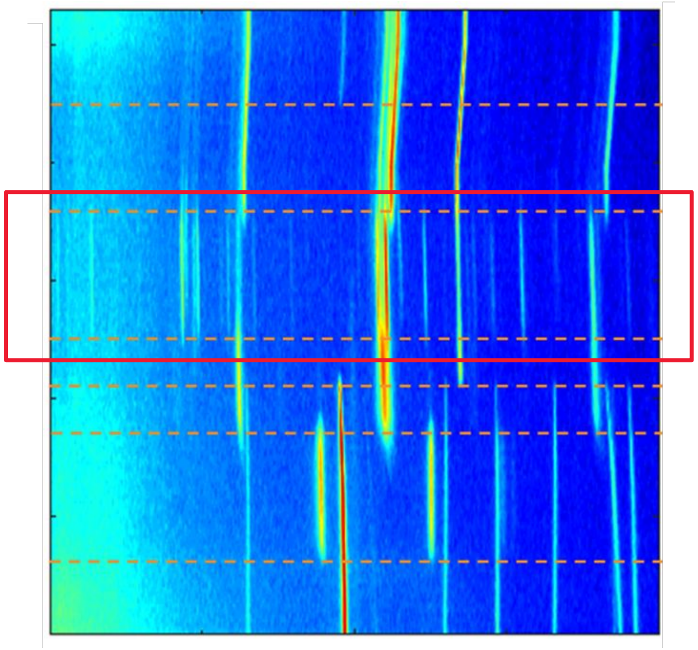
"Computer-assisted discovery and rational synthesis of ternary oxides", J.H. Montoya *et al.*, DOI: 10.26434/chemrxiv-2023-n4pz9 (2023).

A new material predicted by CAMD was synthesized



CAMD predicted a novel material containing Ru, a common element in catalyst materials.

In-situ, variable temp XRD experiments confirm a new phase exists, appears 700-1100°C



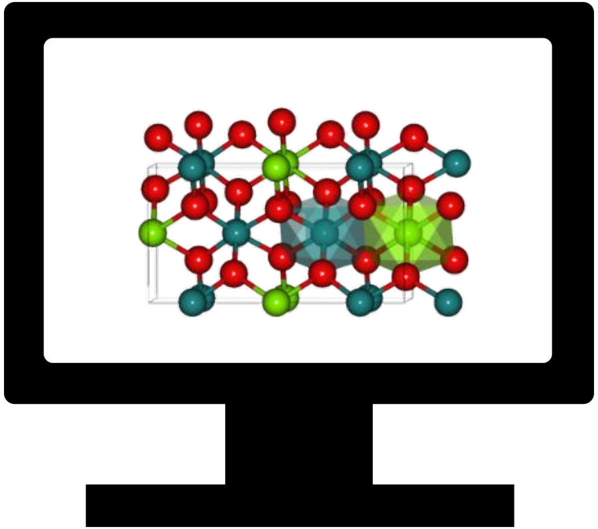
in-situ XRD

“Computer-assisted discovery and rational synthesis of ternary oxides”, J.H. Montoya *et al.*, DOI: 10.26434/chemrxiv-2023-n4pz9 (2023).

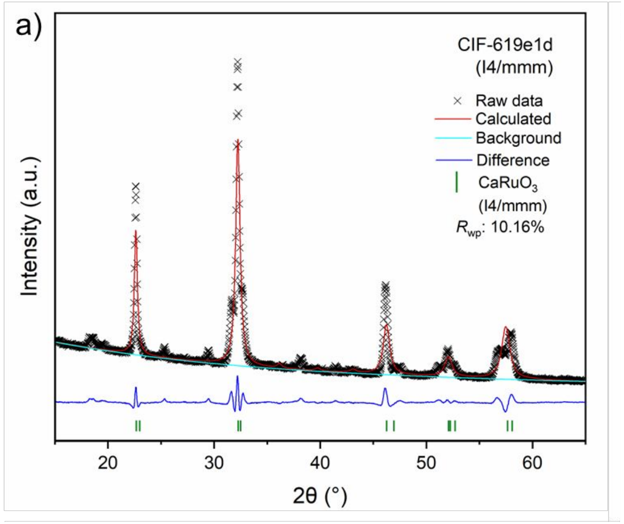
Other examples start to sound the same

10^4 designed on the computer

10^0 confirmed in the lab



~2 years pass



Computation-mediated discovery - challenges

Efficiency is too low

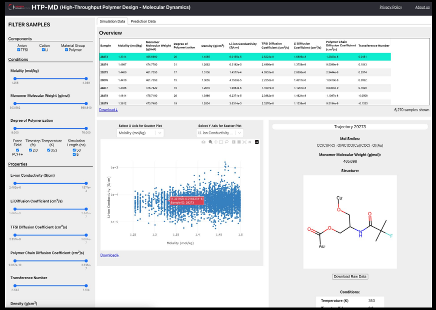
- Automating expt and expt analyses

Experimental feedback is very difficult

- Datasets: dark data
- Data-driven analyses

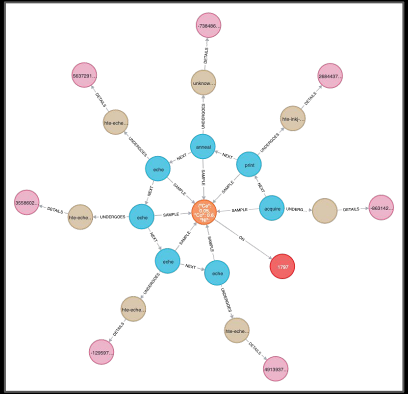
Lack of theory to enable design

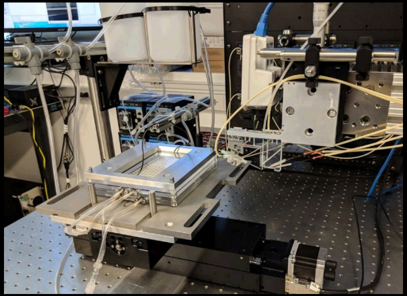
- Datasets: defect structures
- Datasets: kinetic properties
- Integrate data-theory
- Multiscale models



...and more research

Polymers, catalysts, ML





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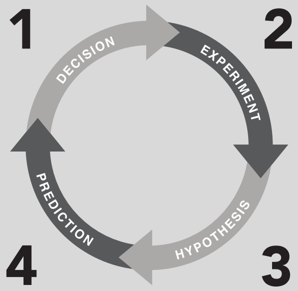
Outlook

Bridging the gap between experiment & simulation

Challenges with accelerating materials discovery

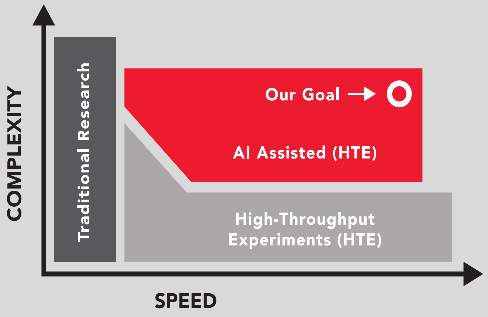
Efficiency is too low

Our approach
Automation & closed loop discovery.



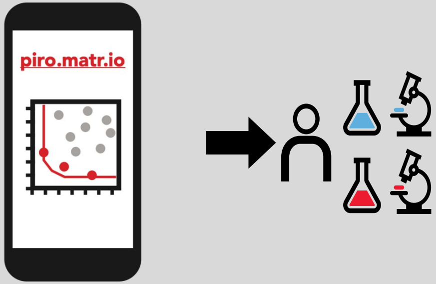
Experimental feedback is very difficult

Our approach
AI powered data analysis.



Lack of theory to enable design

Our approach
Actionable input to experiments



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Outlook

- Highlights
  - Battery lifetime
  - Novel materials
- Workflow software allows better integration of compute and experiment
- Industry research uses minimal or mid-scale compute -- but also will benefit from exascale compute to address fundamental questions

Thank You