CITRINE
INFORMATICS

EBook

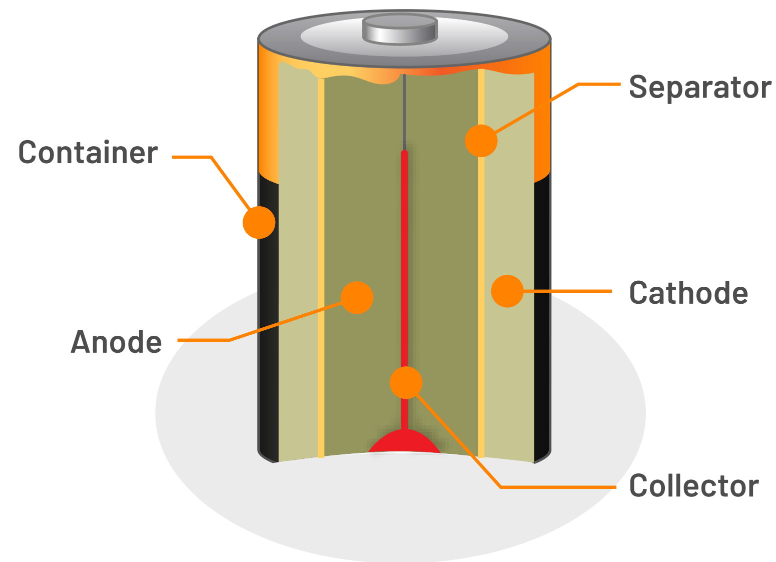
BETTER BATTERY DESIGN USING AI

Better Battery Design using AI

Introduction

Batteries with both high energy density (total electrical capacity) and high power density (ability to deliver electricity quickly) are critical for addressing climate change across future applications. As electricity production moves toward renewable energy sources, cheap, long-lasting energy storage methods are needed to decouple production and consumption. To move away from petrochemical-fuelled vehicles and enable fully electric transportation, smaller batteries with higher energy density and the ability to charge quickly are needed. There are complex challenges for each of these goals which span multiple scales from the molecular and chemical composition of the ceramics used in lithium-ion battery cathodes to the coatings on the cooling channels inside battery packs.

Modern lithium-ion batteries consist of several main components: an anode, a cathode, a separator & electrolyte, and current collectors, all held within a container. The materials used in each of these components can be optimized to improve the battery energy density, power density, and cost. However, their use cases and therefore requirements vary considerably. Optimization of each component spans several fields of research and must be considered in concert with the rest of the battery's constituent parts.



Battery Requirements

Whether the battery will be used in an electric vehicle or a pacemaker will determine the requirements for:

- Cost
- Safety
- Charge and discharge rate
- Voltage
- Specific energy
- Lifespan
- Size/Weight

Other factors are also important in battery design, including manufacturability, quality/variability of individual cell performances, and raw material considerations such as rare earth metal supply.

Additional considerations

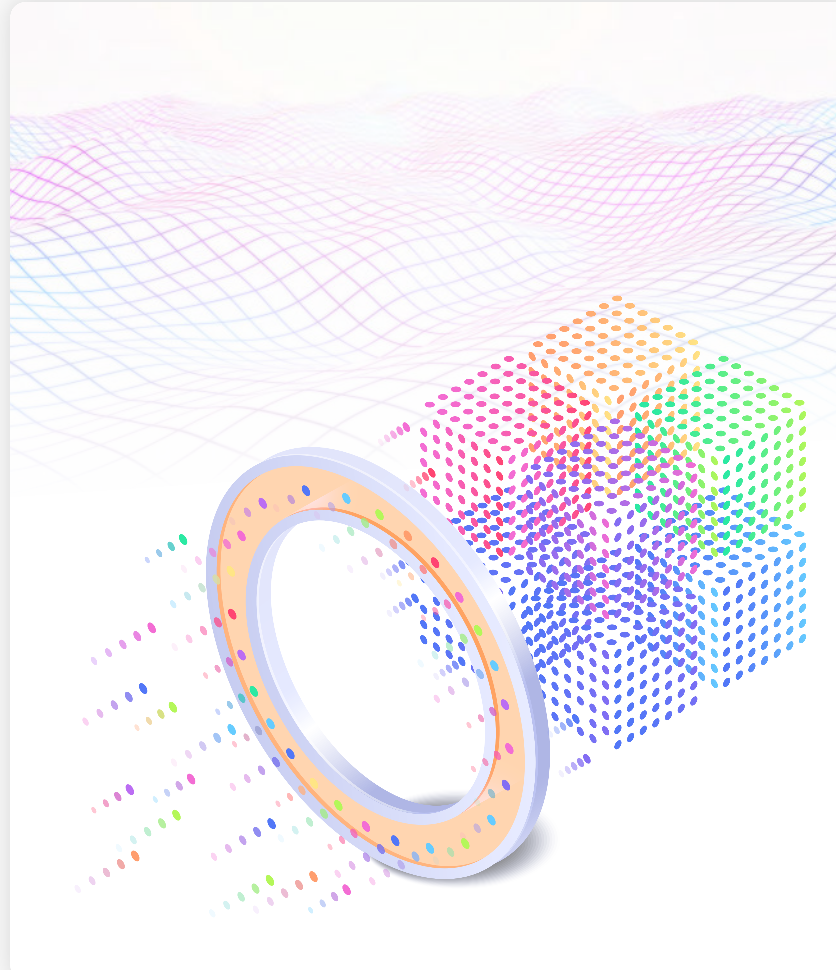
Long cycle-life is important for many applications, giving manufacturers who can produce and evidence such a battery an edge. Automotive OEM buyers require strong evidence of cycle life, such as >80% useful remaining capacity at 1,000 cycles. However, testing the performance of a battery over 1,000 cycles is very time-consuming and costly, especially considering that many emerging technologies (such as silicon anodes) introduce non-linear capacity fading mechanisms which may not be observable early in the battery's lifecycle. Additionally, as batteries are used in a wide variety of applications, testing often needs to be carried out under a variety of conditions such as extreme cold / heat, or demanding charge-discharge profiles, necessitating expensive test equipment. Validating predictive models of performance after 1,000 cycles without performing time-consuming tests is important and would greatly accelerate battery R&D.

AI loves high dimensional problems

From an experimentalist's point of view, these requirements, coupled with the wide variety of possible compositions for each of the battery components and long testing times, add up to a very complex, expensive, and time-consuming research project. Even with the best design-of-experiment methods, this is a lot of work.

This is exactly where materials informatics and AI-guided experimentation can accelerate battery R&D.

- AI-guided Sequential Learning is a way of efficiently exploring high-dimensional design spaces. It has been shown to reduce the number of experiments needed by 50–70%.
- AI can consider and track many more inputs than human intuition–led research and can therefore explore many more compositions and form-factors at the same time.
- Because more potential compositions can be considered, it is more likely that a novel, differentiated material will be discovered.
- AI can optimize multiple requirements at the same time (e.g., safety factors, battery performance and manufacturability).
- AI can identify ways of safely shortening long testing requirements.
- AI can identify properties that correlate to battery life for battery management purposes.



[1] https://link.springer.com/article/10.1007/s40192-017-0098-z

The last 5 years have seen multiple AI projects for accelerating battery research and battery testing both in universities and commercial companies.

CASE STUDY: CATHODE CONFIGURATION OPTIMIZATION

Being able to predict cycle life using only high-level cell information would reduce the need for time-consuming, expensive tests and be very valuable to battery producers. To demonstrate the general viability of AI for battery testing, Citrine used an open-source archive of battery cycling data (batteryarchive.org) to make cell cycle–life predictions. The goal was to predict discharge capacity remaining at 500 and 1,000 cycles, using only high-level cell information.

Input Data

Citrine's team acquired data from the Battery Archive which contains cycling data and cell configuration data, such as cathode/anode type, nominal cell capacity, and test cycling parameters (such as temperature, c-rate (charge current normalized to current required to charge the battery in 1 hour), etc). The cycling performance data contained voltage/time curves as well as raw discharge capacity per cycle. The discharge capacity was normalized to 100% and recorded at only cycles 1, 50, 100, 500, and 1,000 for this exercise. These simple inputs were used to train an AI model to predict the cell capacity (%) after 500 and 1,000 charge/discharge cycles. For additional information, Citrine's chemical formula featurizer produced 115 additional features which are descriptive of the cathode active material composition (for instance, LiFePO4, LiNiMnCoO2, LiNiCoAlO2, LiCoO2, and blends thereof).

An enumerated search space – a list of possible combinations of inputs – was used, which included 810 candidate configurations to obtain predictions from the AI model.

[2] Aykol, M., Herring, P. & Anapolsky, A. Machine learning for continuous innovation in battery technologies. *Nat Rev Mater* **5**, 725–727 (2020). https://doi.org/10.1038/s41578-020-0216-y

[3] https://batteryarchive.org

PREDICTOR

The AI model was trained to predict the normalized remaining discharge capacity after both 500 cycles and 1,000 cycles, using only chemical formula information and the testing parameters charge/discharge C-rate, min/max state-of-charge cut-off, nominal cell capacity, the cell form factor, temperature, and the canonical name of the cathode material (e.g., "NCA"). The results indicated that the model was not well-calibrated for predictions of cells with such a limited information input set.

To improve the model, the normalized remaining discharge capacity at cycle 1, 50, and 100 were used as latent variables for prediction of the capacity at 500 and 1,000 cycles. Citrine's approach of using latent variables allows for much cheaper-to-obtain information to be used as inputs when available, and predicted when unavailable, acting as a method of transfer learning from cheap to expensive output parameters. In this case, the normalized discharge capacity at 100 cycles was the most important feature for prediction of the capacity of the cell at 1,000 cycles, improving the prediction accuracy considerably. This raises the possibility of early stopping, saving time and freeing up valuable testing resources for new projects.

Predicting % discharge at 1000 cycles, using data from 100 cycles

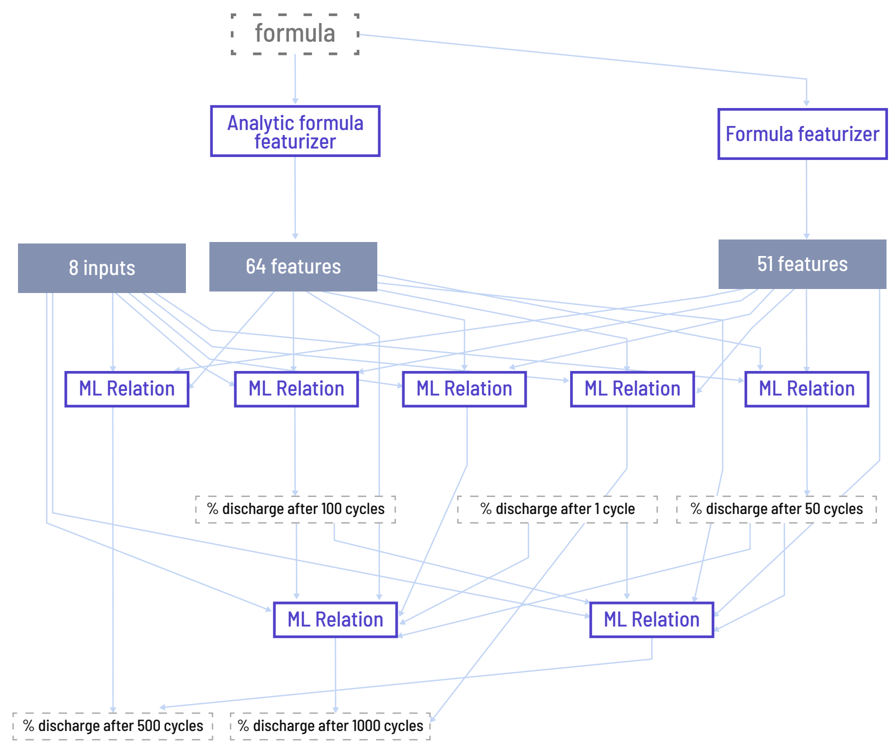


Figure 1: Citrine Graphical AI Model, showing automatic featurization of chemical formulas such as LiCoO2 in to 125 additional descriptors, and utilizing discharge capacity at cycles 1/10/50 as "latent variables" for discharge capacity at higher cycle numbers.

SELECTING CATHODE MATERIALS FOR LONG CYCLE LIFE

The Citrine Platform ranked battery and cycling configurations which satisfy cycle life constraints (>85% @ 1,000 cycles with a cycling discharge C-rate of 2) by their likelihood to achieve high performance properties both with respect to remaining cycle life at 1,000 cycles and discharge C-rate capability.

% discharge after 1000 cycles

* Note: This presents the results of combined models. Metrics use default cross validation settings.
* Note: Error bars represent 68% prediction intervals.

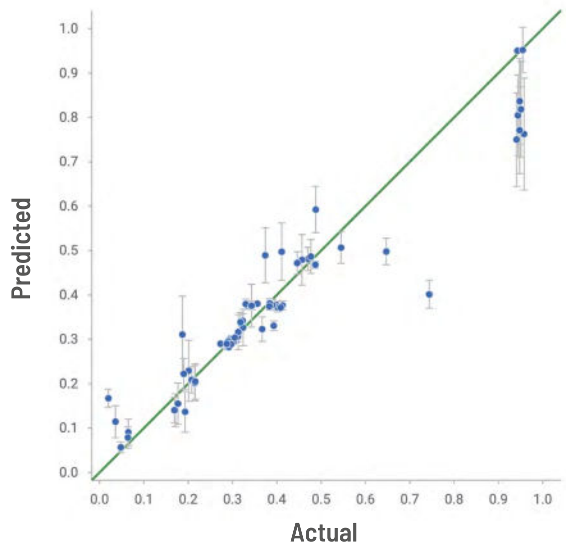


Figure 2: Cross-validation results showing the performance of the AI model shown in Figure 1 for normalized discharge capacity at 1,000 cycles. The predicted cell performance vs. actual cell performance for the training data are largely coincident, leading most points to lie on the line y=x, indicative of a predictive model.

Potential Performance

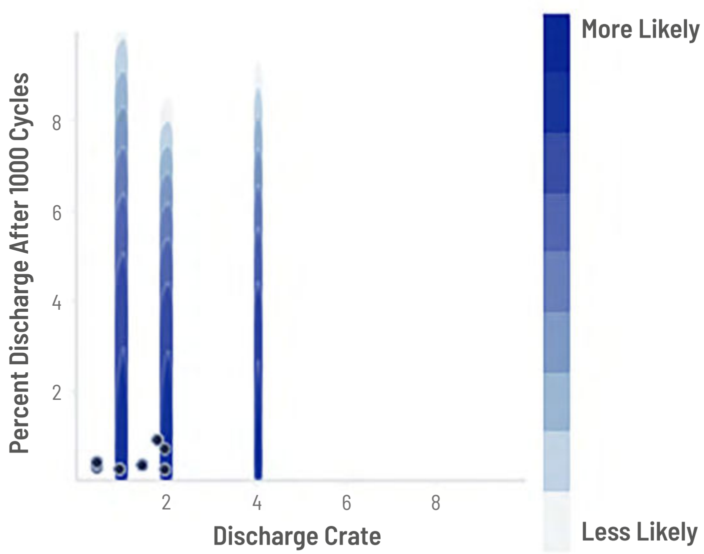
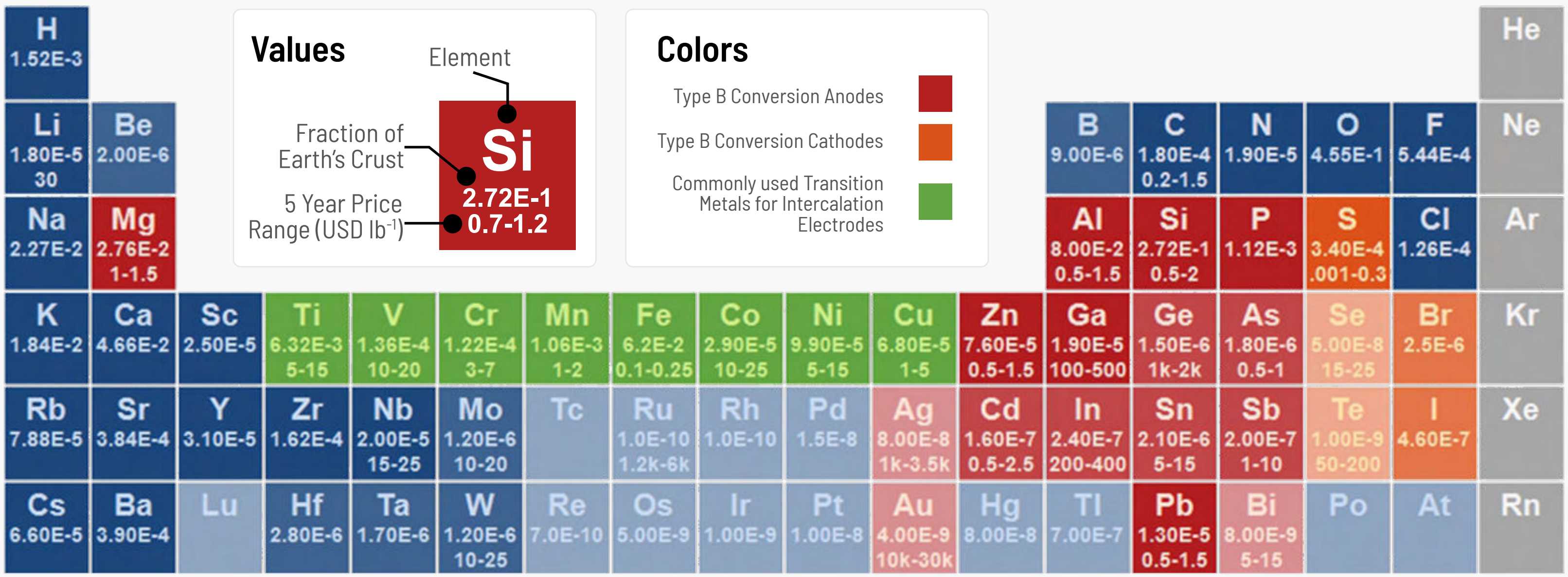


Figure 3: This capability map shows the likelihood of being able to hit target properties by one or more candidate battery configuration in the search space.

Many of the elements used in batteries, such as Lithium, are on the US and EU Critical Materials lists, meaning that there are threats to supply[4]. Lithium is highly reactive and light, which makes Li-ion batteries the go-to choice for high-end products needing rechargeable batteries. China currently dominates this market, because they have both easy access to Lithium and a large internal market. An estimated 80% of the world's Lithium raw material refining and 60% of Li-ion battery component manufacture happens in China, according the BNEF[5]. Large players like Tesla are squaring this circle by building manufacturing capacity in China, but others will be looking to optimize batteries without using critical materials.



This image from the paper Li-ion battery materials: present and future by **Naoki Nitta**[1,3] **Feixiang Wu**[1,2,3] **Jung Tae Lee**[1,3] and **Gleb Yushin**[1], nicely illustrates the abundance of elements and where they are used in batteries.

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https://doi.org/10.1016/j.mattod.2014.10.040

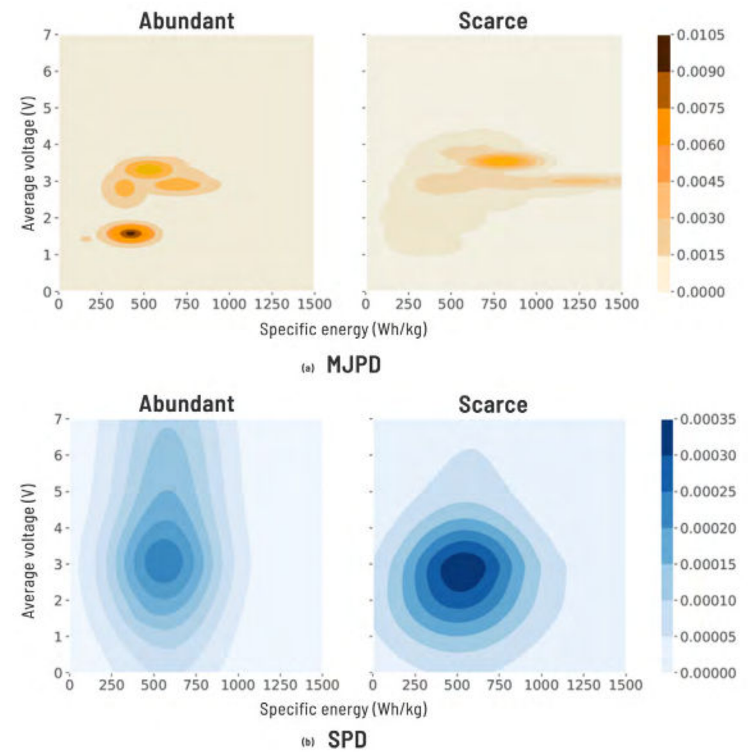
[4] H. Vikstr m, et al. Appl. Energy, 110 (2013), p.
[5] https://about.bnef.com/blog/china-dominates-the-lithium-ion-battery-supply-chain-but-europe-is-on-the-rise/

BATTERY PERFORMANCE OF ABUNDANT COMPOSITIONS

Citrine's patented technology enables companies to understand and compare the likelihood of achieving target material properties using different search spaces (the set of material candidates whose properties are predicted by an AI model). In this project, 3 existing databases of battery materials were combined and then sorted into two groups, scarce and abundant, depending on their composition and the availability of their elements in the earth's crust. An AI model was trained and used to predict the specific energy and voltage of all the materials. Uncertainty quantification was then used to visualize the likelihood of achieving target properties in the two design spaces. The visualizations show that a higher specific energy is more likely to be achievable with cathodes that use rare elements. Research leaders can now make data-driven business decisions about whether to invest in creating test samples and performing physical testing based on market size, application, research costs, and likelihood of success. This technology can be equally applied to other sustainable sourcing considerations such as how biodegradable ingredients affect materials properties.

Details of the project can be found here: James Peerless, Emre Sevgen, Stephen Edkins, Jason Koeller (Citrine Informatics) et al. "Design space visualization for guiding investments in biodegradable and sustainably sourced materials" MRS Comms (2020)

Battery materials



Higher specific energy is more likely in materials containing rare elements

SUMMARY

Battery design and performance testing is a high-dimensional challenge where multiple requirements need to be optimized simultaneously. Materials informatics is well suited to this challenge and Citrine has successfully worked on battery material and battery performance testing projects.

The Citrine Platform empowers materials scientists to leverage cutting-edge AI technology via a simple user interface. Citrine, founded in 2013, with 85+ employees across 3 continents and with the experience of 60+ customer engagements behind them, are the mature team that a global business needs to support them through this part of the digital transformation. Contact us to find out more.

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