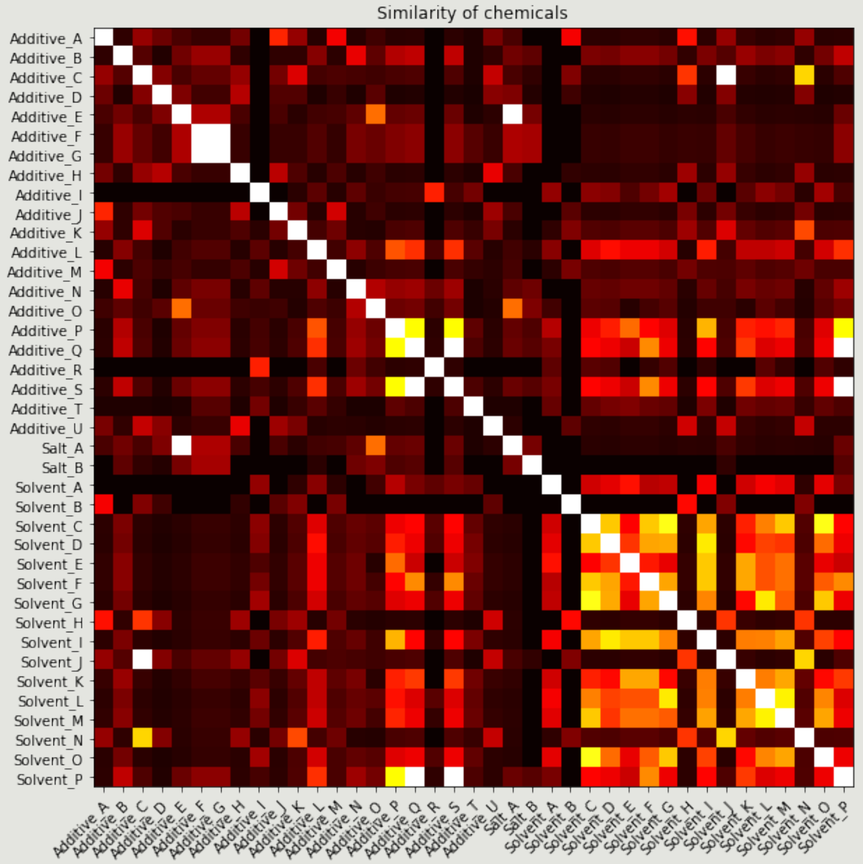
Case Study - Materials Search and Discovery

Battery Modeling and Design

- Key factors to improve in battery design include **energy density, power density, charging time, life, cost, and sustainability.**
  - Experiments to test battery performance give accurate results, but can be very expensive and time consuming.
  - Computer simulations can improve cost and speed. However, these require intricate multi-physics approach to achieve high accuracy: **thermal, chemical, electrical, and mechanical factors are all critical to battery performance.** Incorporating these factors in classical numerical simulations can still be very costly.
  - AI-accelerated physics-based modeling can give high accuracy at a fraction of the time and cost.
- In **Reactor**, we have developed AI models to predict **initial capacity** and **cycle life** for Li-Ion batteries based on their chemical composition of the anode, cathode, and electrolyte, and experimental conditions, such as temperature, trained on a dataset of ~1K battery experiments.

Advanced Chemical Featurization in Reactor

- We employ automated Deep Learning-based chemical featurization approaches using cutting edge AI methods adapted from natural language processing (NLP) to characterize chemical properties
- This allows us to find non-superficial similarities between different chemicals in the dataset, and leverage these to improve the model's predictive power
- Another benefit of featurization is that it allows the model to predict the performance of batteries involving **new chemicals** it has not seen before in training



Reactor AI models incorporate Chemistry, Chemistry+Experimental Conditions, and Experimental Certainty for Li-Ion Battery

- LiBatteryNet - AI model incorporating **experimental conditions and chemistry**
- LiChemistryNet - AI model incorporating **chemistry only**
- LiCertaintyNet - provides **certainty** scores, estimating the **standard deviation** for the provided conditions

These models can be used to efficiently search for highly performant battery designs

Reactor identified a potential ~50% improvement in cycle life in a sample battery design, while only sacrificing ~5% of initial capacity, by increasing the amount of a certain chemical additive by a specified percentage

Cycle Life increased 50% with minor reduction in Initial Capacity

Incorporating new chemicals

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- Result 1

A client provided us a list of chemical additives that they are interested in, but have not yet experimented with. Despite the absence of these chemicals from the training data, using chemical embeddings, we can predict the hypothetical performance of batteries with these chemicals. For one design, we find adding a certain Additive A with concentration 0.015 gives:

Capacity: 1.09 → 1.23 (+ 13 %), **Cycle life**: 601 → 593 (- 1 %)

- Result 2

In analyzing battery literature, we found a paper[1] claiming that **trivinylcyclotriboroxane (tVCBO)** can potentially enhance SEI stability for graphite anodes, increasing cycle life. Using chemical embeddings, we find adding this to a design with concentration 0.034 gives:

Capacity: 1.73 → 1.78 (+ 3 %), **Cycle life**: 541 → 716 (+ 32 %)

1 "**Evaluating electrolyte additives for lithium-ion cells: a new Figure of Merit Approach,"** Adam Tornheim, Cameron Peebles, James A. Gilbert, Ritu Sahore, Juan C. Garcia, Javier Bareño, Hakim Iddir, Chen Liao, Daniel P. Abraham