intellegens

# Machine learning for battery discovery

Gareth Conduit

# Alchemite™ for materials design

Train from sparse datasets with technology from University of Cambridge

Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

# Nickel-Cobalt-Manganese (NCM) battery materials

# Properties of interest

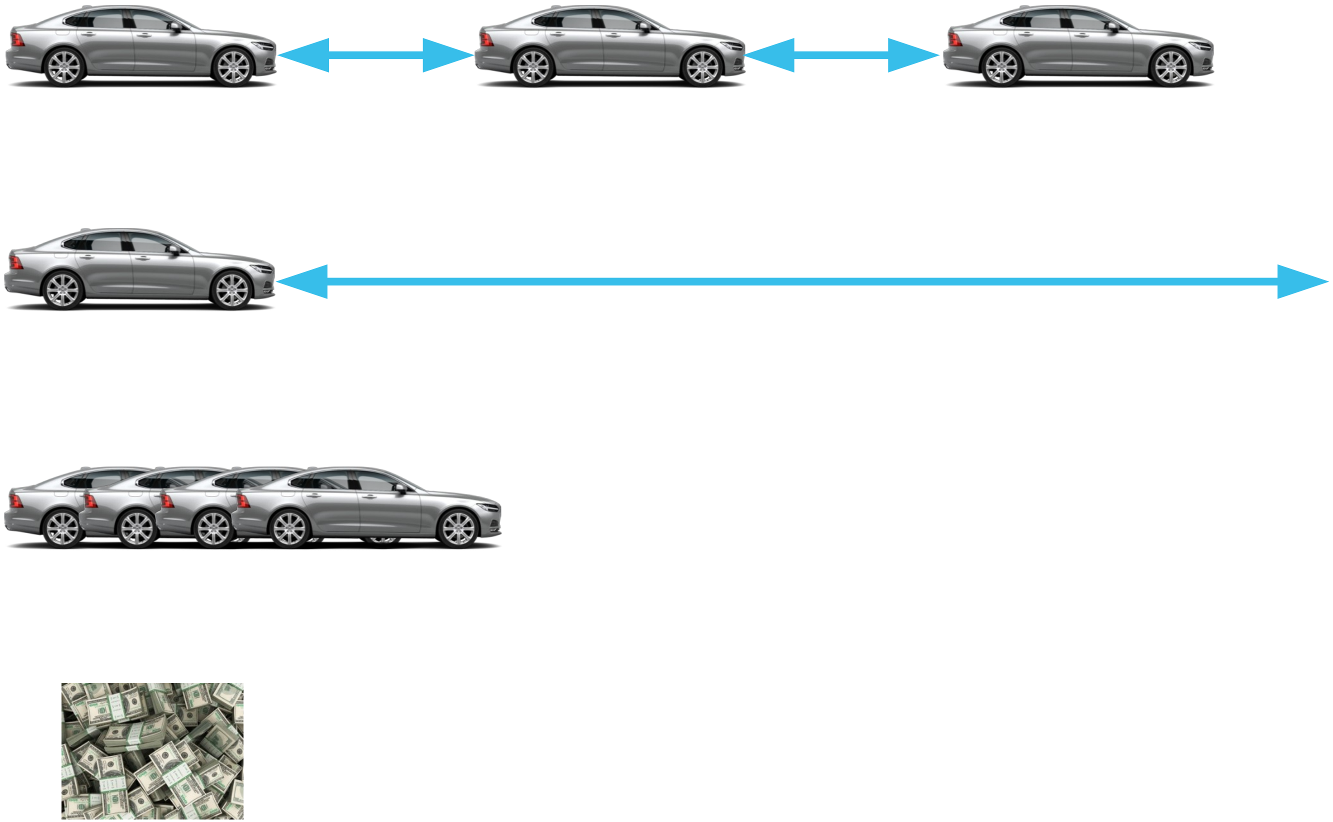
Number of uses

Range

Speed

Cost

# Battery properties of interest



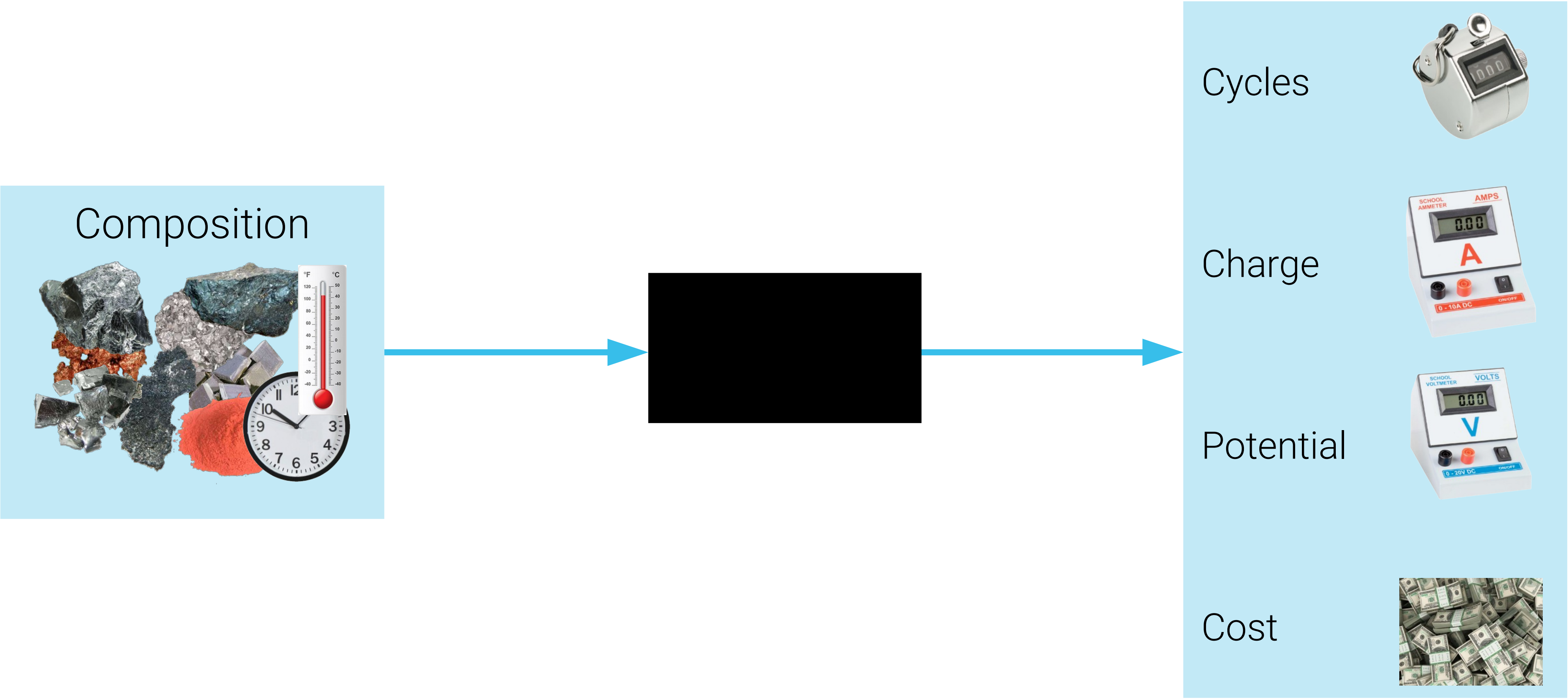
Cycles

Charge


Potential

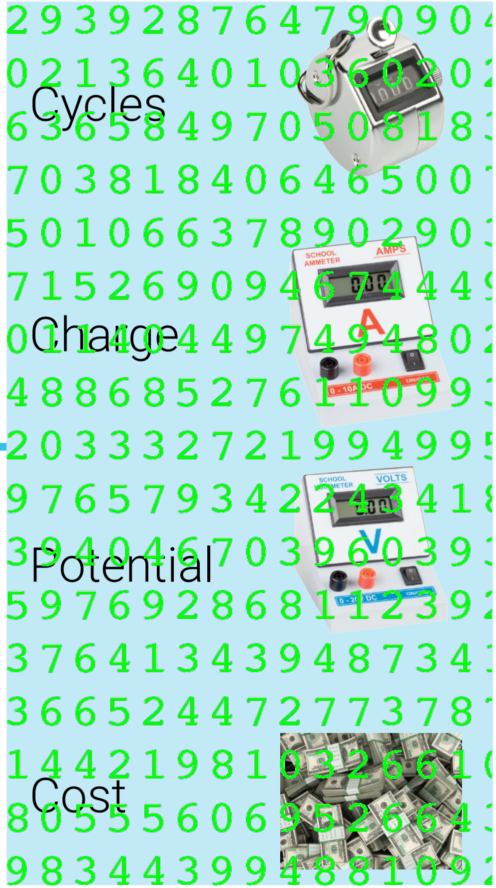

Cost

# Black box machine learning for materials design



# Training machine learning

Composition



# Machine learning for materials design

Composition

Cycles

Charge

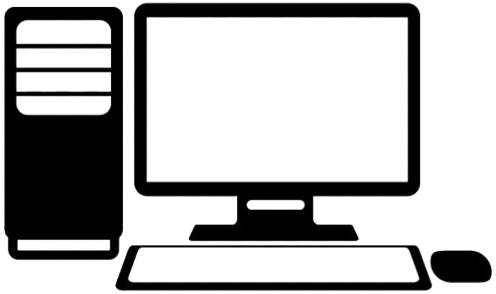

Potential


Cost

# Two sources of information

## Experiment

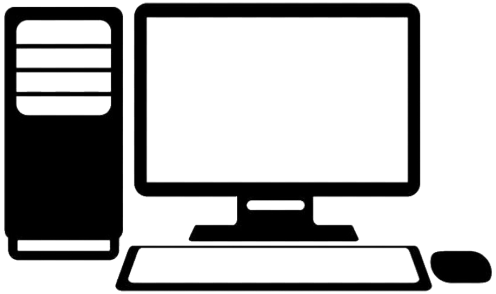
Accurate
Quantities of interest
Lack of data
Expensive



## Computational

Less accurate
Atom level insights
Perform on demand
Cheap to perform

# Merge information with machine learning



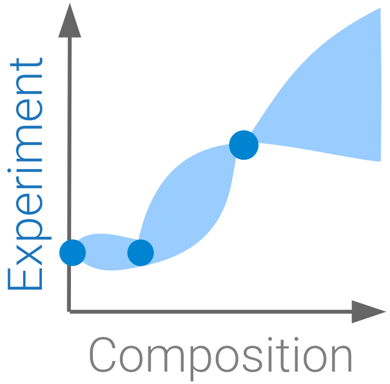
## Experiment

Accurate
Quantities of interest
Lack of data
Expensive

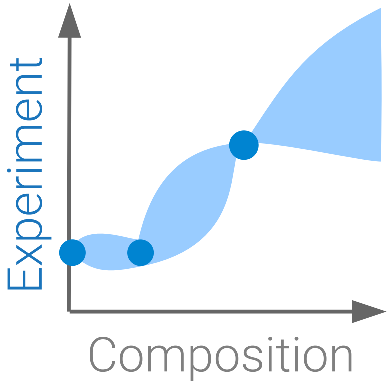
## Computational

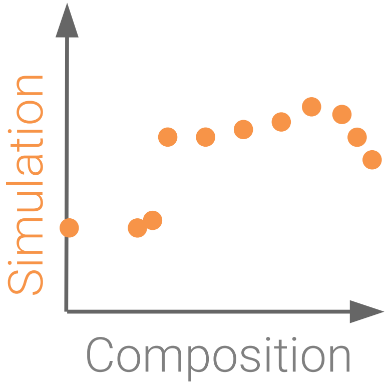
Less accurate
Atom level insights
Perform on demand
Cheap to perform

# Little data to train machine learning model

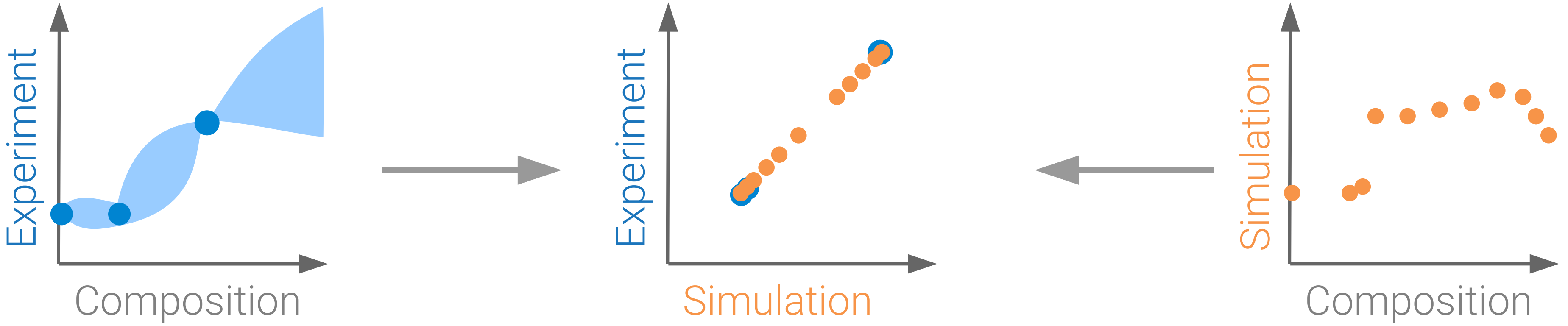


# Complementary computer simulations

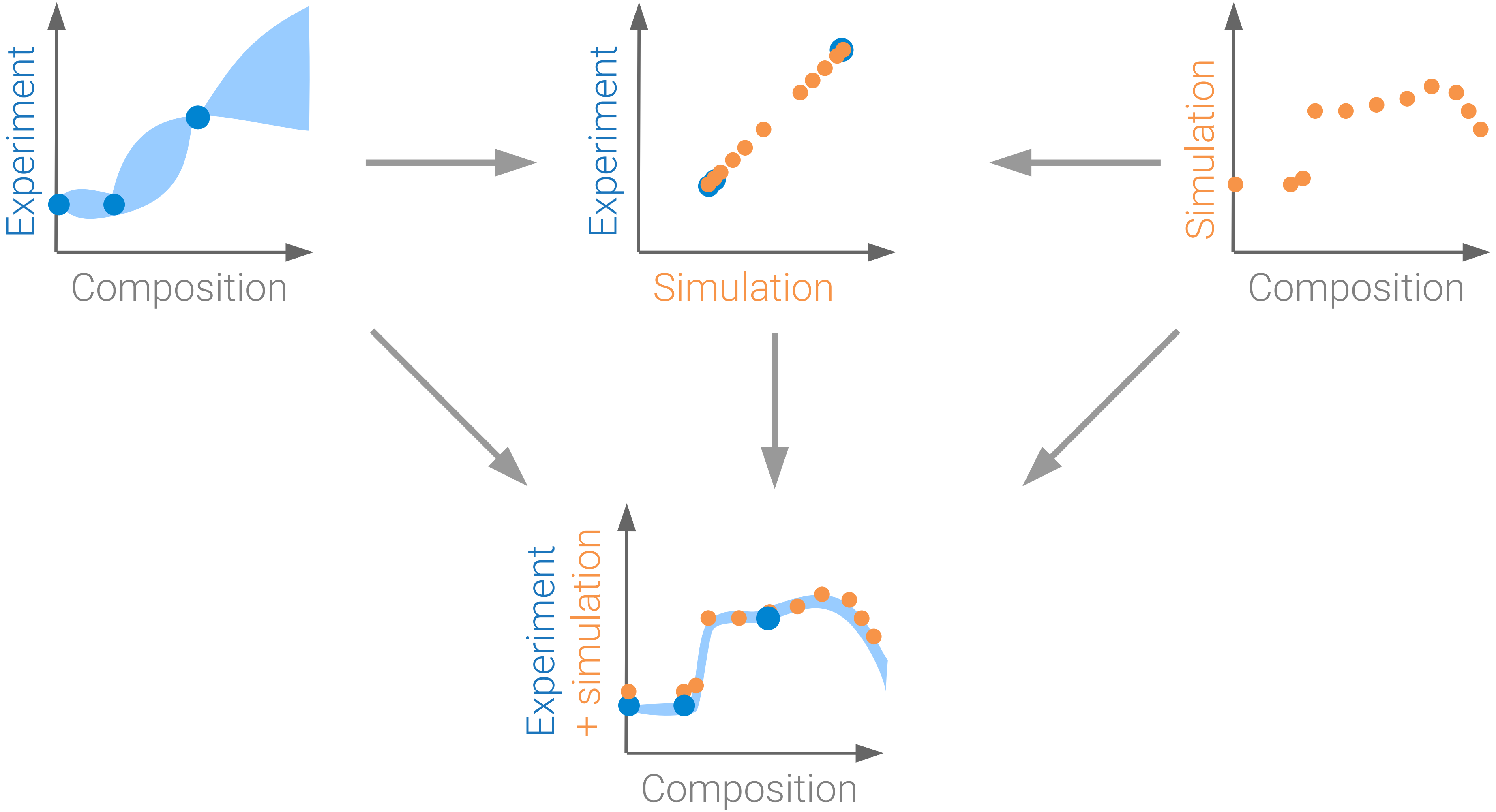


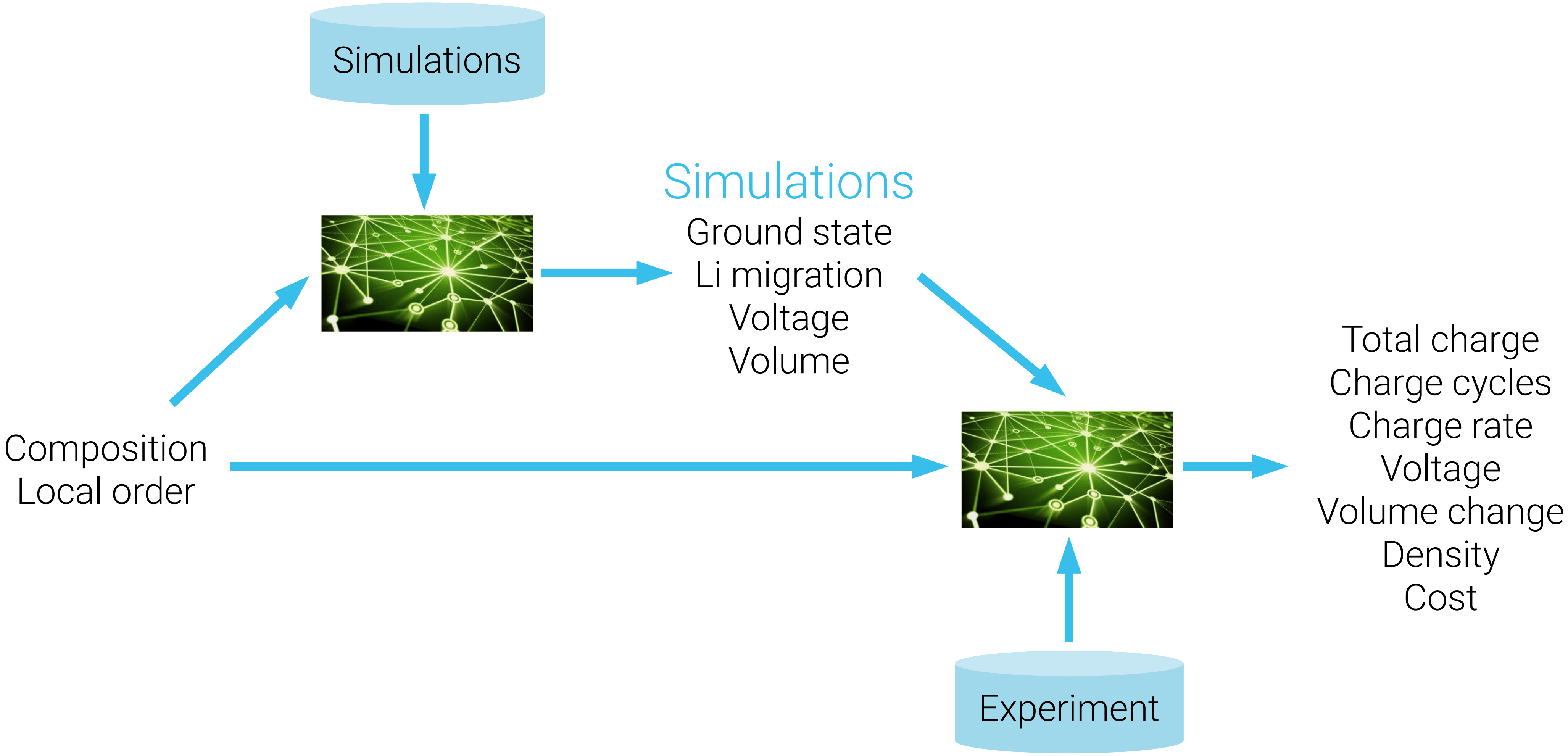
# Simulations make accurate but not perfect predictions



# Simulations guide extrapolation of experimental data



# Merge computational and experimental data



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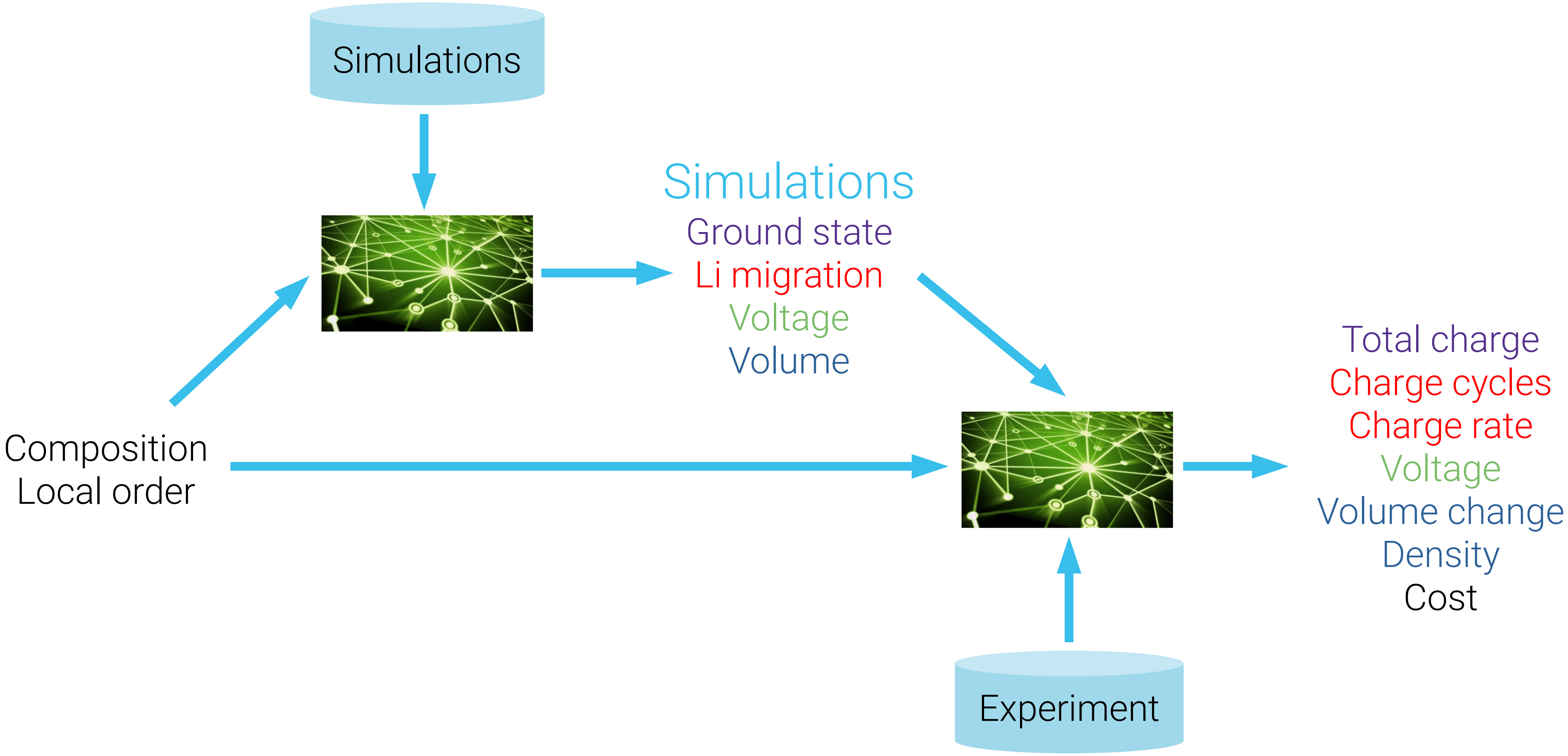
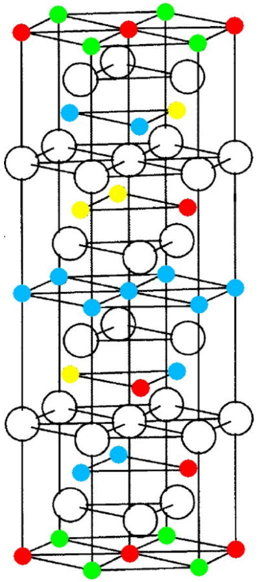


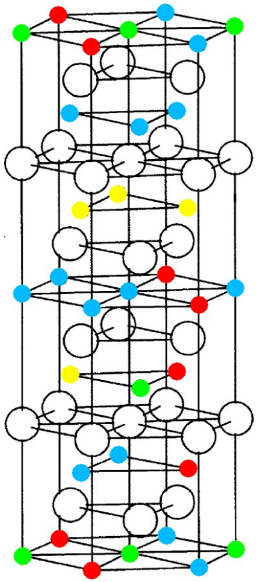
# Battery cathode design

Reduce Li migration so improve battery life



Original

82% robust



Proposed

100% robust

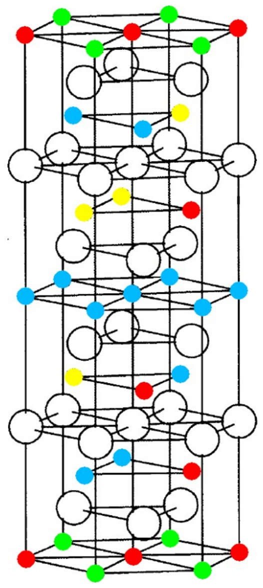
# Battery cathode design

Reduce Li migration so improve battery life

Maintain voltage, charge stored, density, and cost

Empowers specification of the optimal components

Bespoke battery design for each customer



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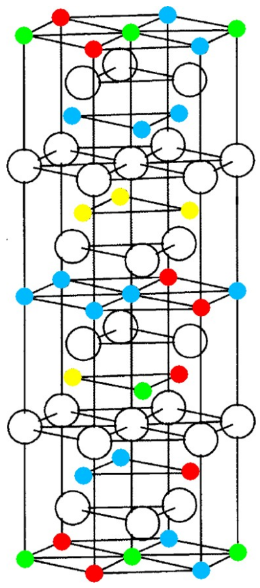

Proposed

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# Battery management system

In-service data from a particular battery and others deployed to make bespoke predictions of remaining useful life

nature machine intelligence

REVIEW ARTICLE
https://doi.org/10.1038/s42256-020-0156-7

Check for updates

## Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2]✉, Gareth J. Conduit[3]✉ and Zhi Wei Seh[4]✉

**Machine learning is a specific application of artificial intelligence that allows computers to learn and improve from data and experience via sets of algorithms, without the need for reprogramming. In the field of energy storage, machine learning has recently emerged as a promising modelling approach to determine the state of charge, state of health and remaining useful life of batteries. First, we review the two most studied types of battery models in the literature for battery state prediction: the equivalent circuit and physics-based models. Based on the current limitations of these models, we showcase the promise of various machine learning techniques for fast and accurate battery state prediction. Finally, we highlight the major challenges involved, especially in accurate modelling over length and time, performing in situ calculations and high-throughput data generation. Overall, this work provides insights into real-time, explainable machine learning for battery production, management and optimization in the future.**

With rising concerns about global warming, electrification of transport has recently emerged as an important vision in many countries. The successful development of electric vehicles (EVs) depends highly on the cycling performance, cost and safety of the batteries. Rechargeable lithium-ion (Li-ion) batteries are currently the best choice for EVs due to their reasonable

where $C_{curr}$ is the capacity of the battery in its current state, $C_{full}$ is the capacity of the battery in its fully charged state, $C_{nom}$ is the nominal capacity of the brand-new battery[2].

In essence, SOC denotes the capacity of the battery in its current state compared to the capacity in its fully charged state (equivalent of a fuel gauge), while SOH describes the capacity of the battery

Predicting the State of Charge and Health of Batteries using Data-Driven Machine Learning
Nature Machine Intelligence 2, 161 (2020)

# Battery management system

In-service data from a particular battery and others deployed to make bespoke predictions of remaining useful life

Model that spans time-scales to permit simultaneous state-of-health and state-of-charge predictions

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# Battery management system

In-service data from a particular battery and others deployed to make bespoke predictions of remaining useful life

Model that spans time-scales to permit simultaneous state-of-health and state-of-charge predictions

Data from testing in first few cycles with in-house long-term testing to predict long-term battery performance

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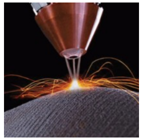
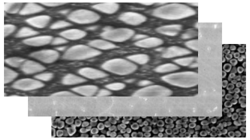
# Other materials designed

Titanium additive manufacturing



High temperature alloys



Lubricants

Pharmaceuticals

Journal of Chemical Physics 153, 014102 (2020)
Fluid Phase Equilibria 501, 112259 (2019)
Materials & Design 168, 107644 (2019)
Computational Materials Science 147, 176 (2018)

Physical Review Applied 12, 034024 (2019)
Matter 1, 219 (2019)
Scripta Materialia 146, 82 (2018)
Materials & Design 131, 358 (2017)

# Prospects for the future

Alchemite™, a full stack machine learning solution to merge sparse data, including computational simulations and experimental data

Design battery cathode materials with longer life

Embedded battery management software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Website https://intellegens.ai
Demo https://app.intellegens.ai/steel_optimise
Papers https://www.intellegens.ai/paper.html