intellegens

Machine learning for battery discovery

Gareth Conduit

Alchemite™ for materials design

Train from sparse datasets

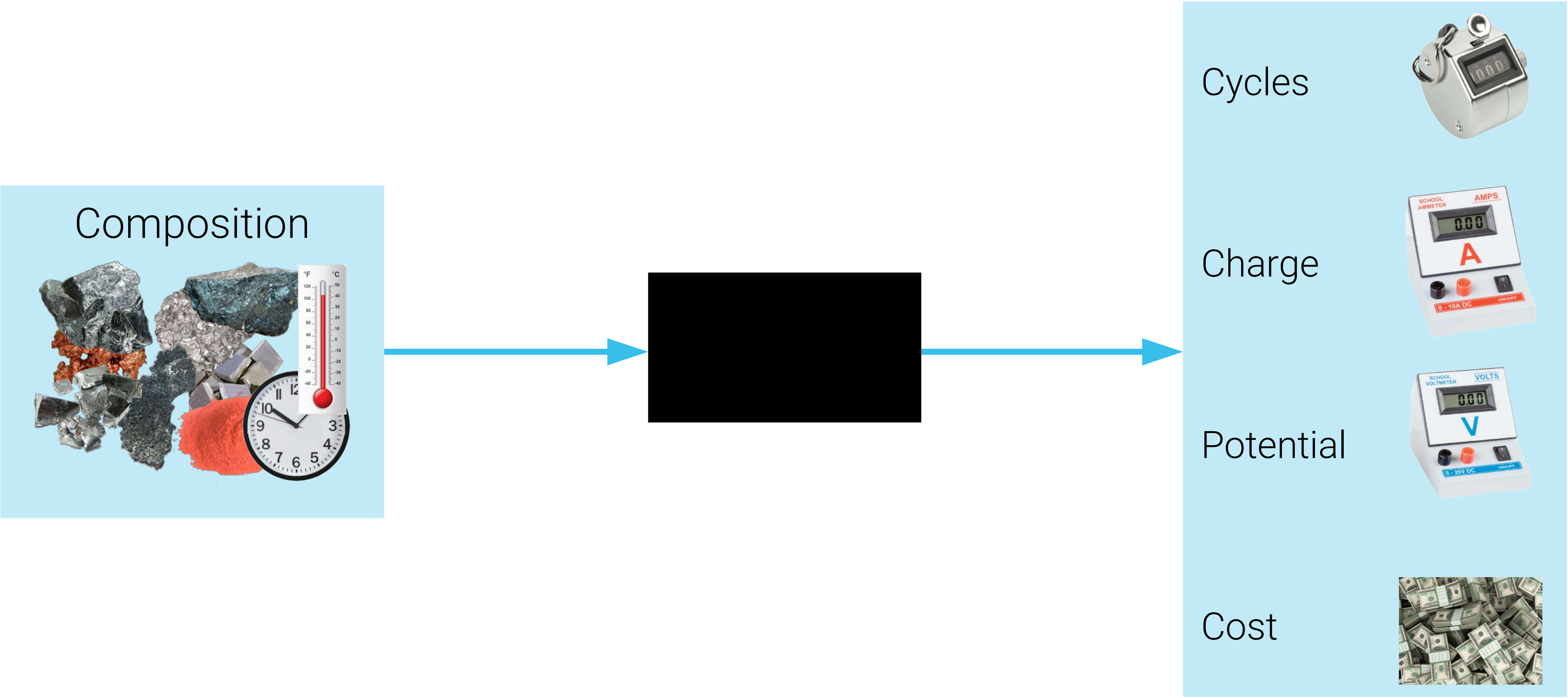
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

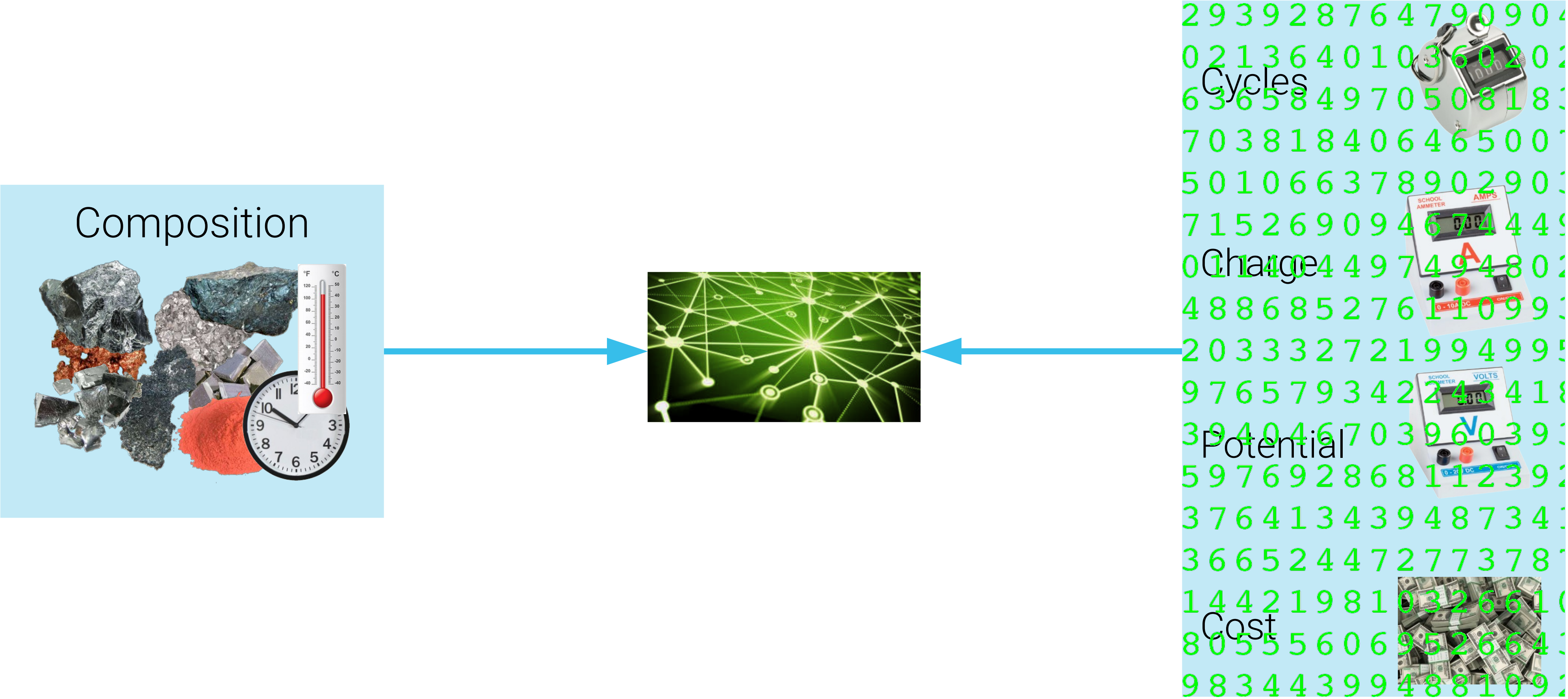
Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

Black box machine learning for materials design



Training machine learning



Machine learning for materials design

Composition

Cycles

Charge

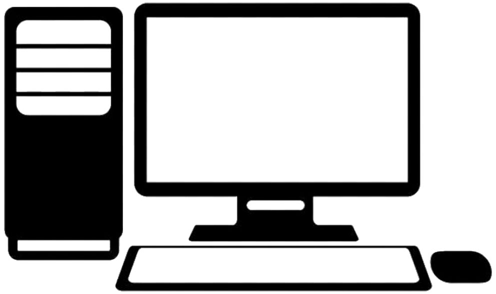
Potential

Cost

Two sources of information

Experiment

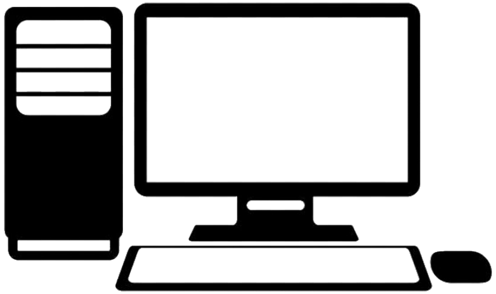
Accurate
Quantities of interest
Lack of data
Expensive



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

Nickel-Cobalt-Manganese (NCM) battery materials

Design variables and target properties

Concentration of Ni, Mn, Co

Location of atoms

Charge cycles

Voltage

Total charge

Volume change

Li migration

Ground state

Charge rate

Design variables and target properties with DFT

Concentration of Ni, Mn, Co

Location of atoms

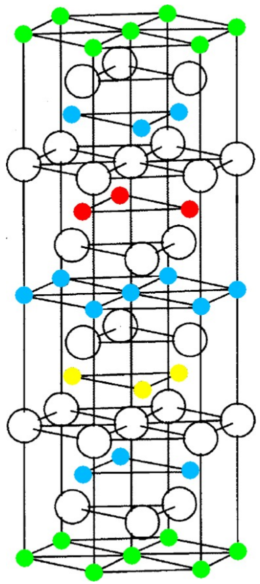
Volume change

Li migration

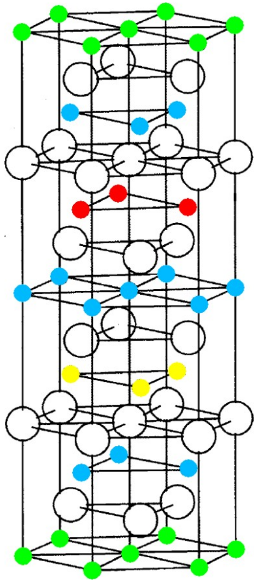
Voltage

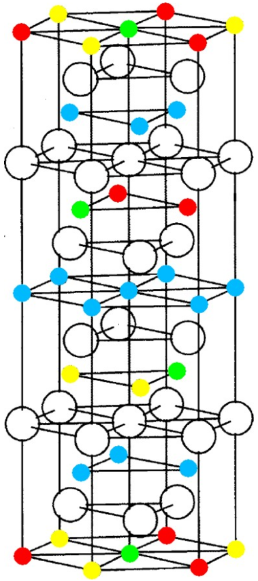
Ground state

Approach: exhaustive exploration of unit cells

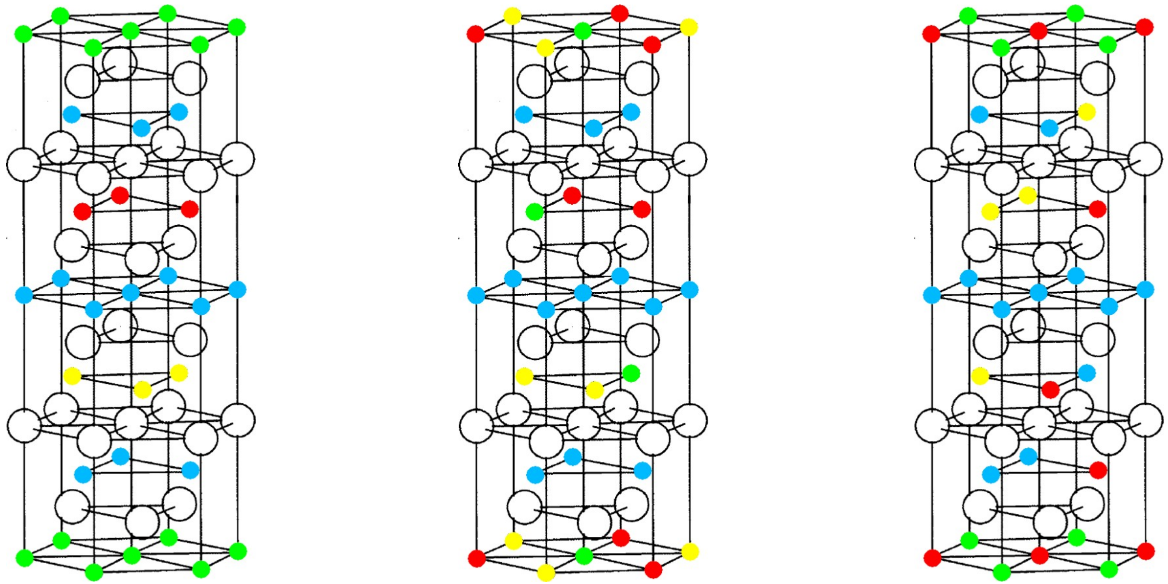


Approach: exhaustive exploration of unit cells





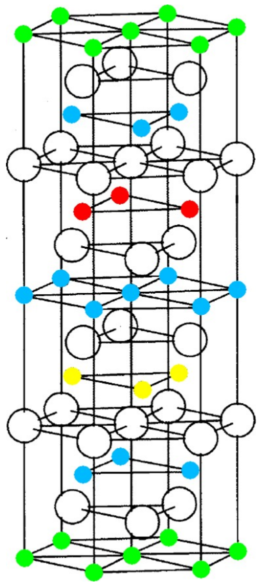
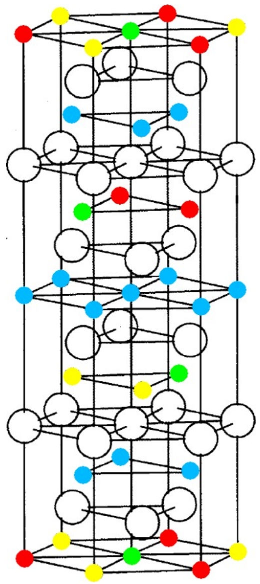
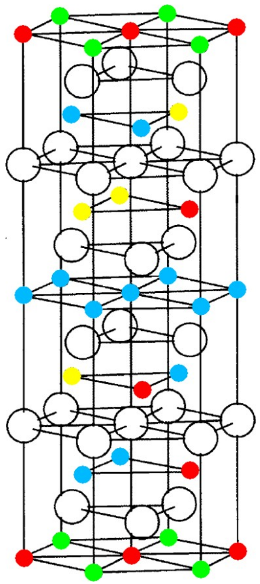
Approach: exhaustive exploration of unit cells



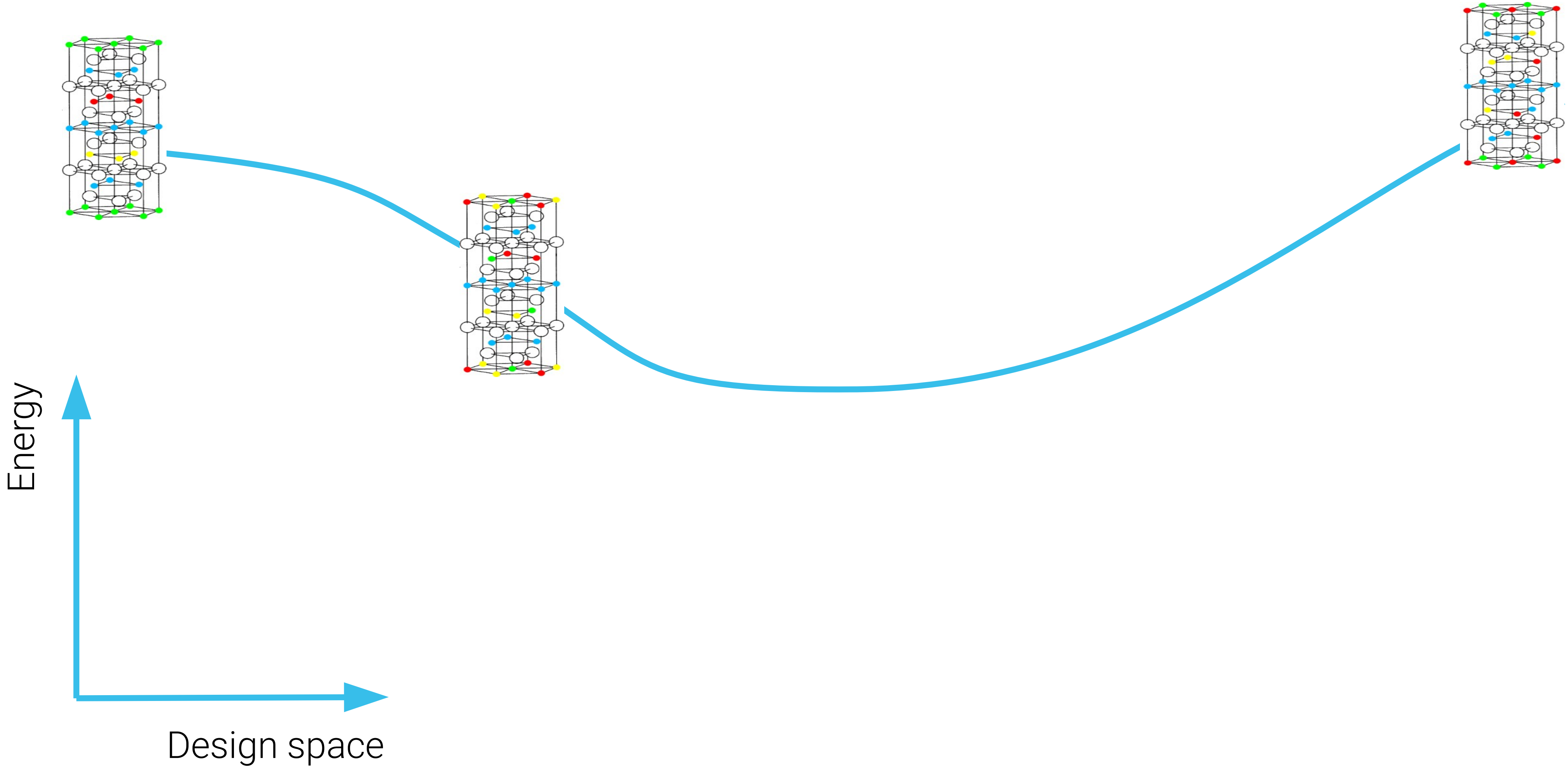
Approach: exhaustive exploration of unit cells

153153000 permutations =42000 years

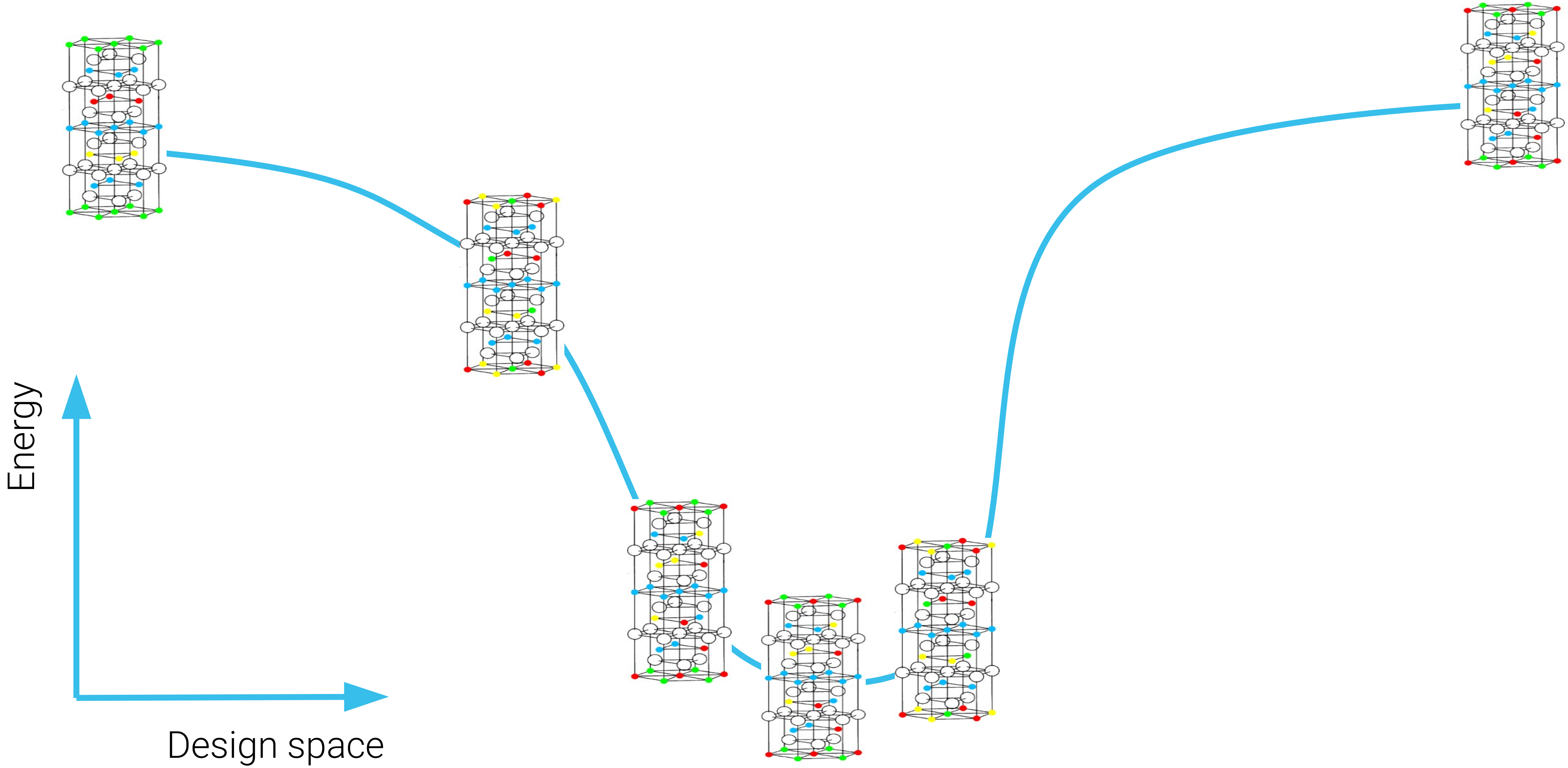
Only examine order that fits into the unit cell

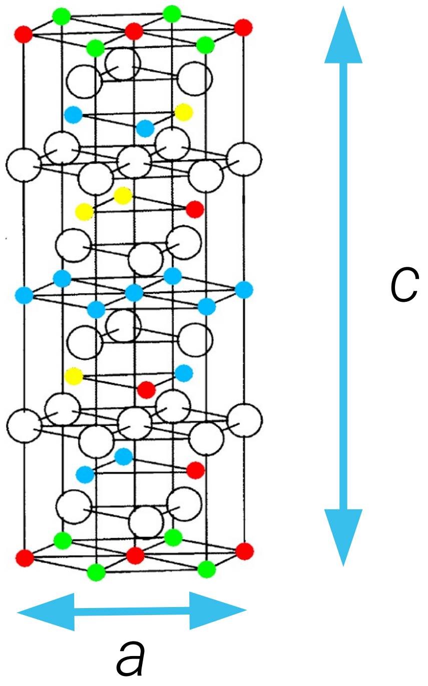
Train on initial results



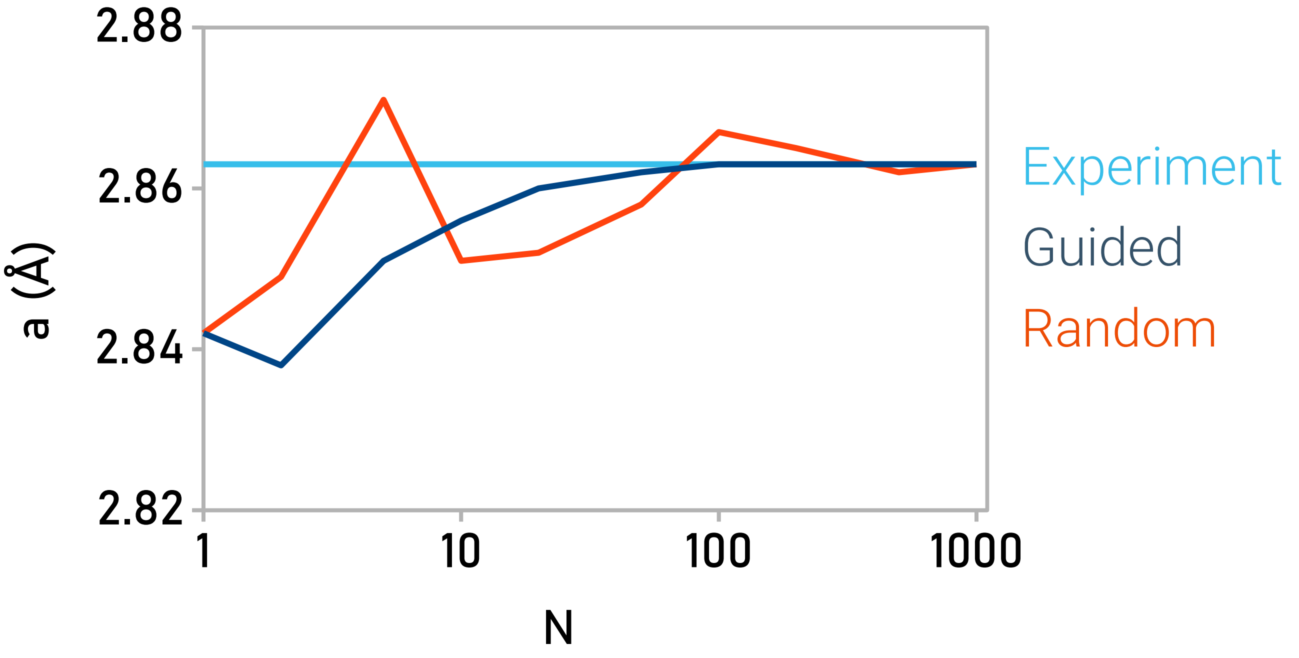
Guided calculation for recursive learning



Lattice constants

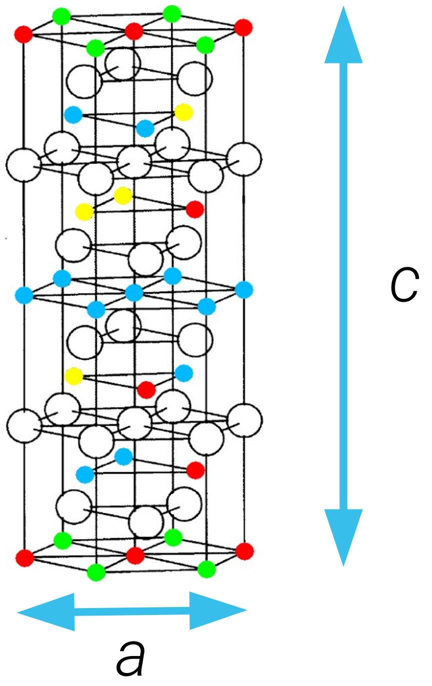


How many calculations are required



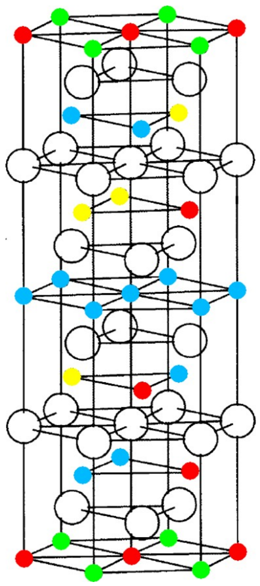
Machine learning guidance requires 5-times fewer calculations

Predicting the lattice constant from DFT

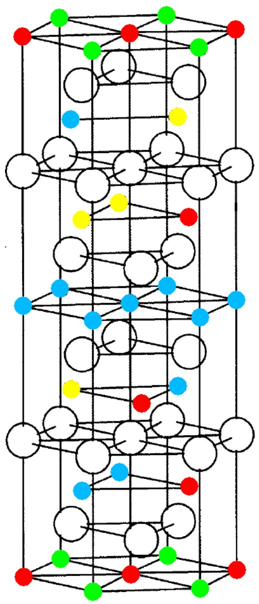


Structure	a (Å)	c (Å)
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ prediction	2.863	14.257
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ experiment	2.866	14.254

Tracking Li migration

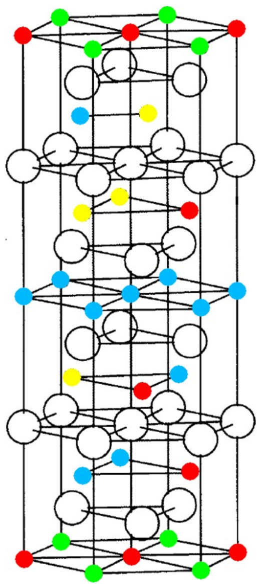


Original structure



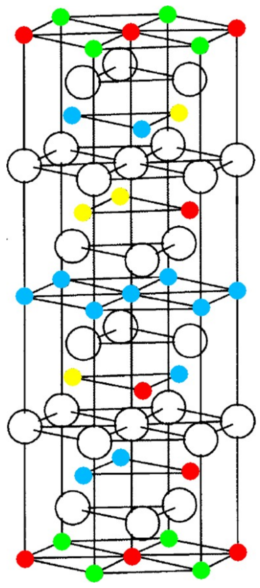
Remove Li

+ Li



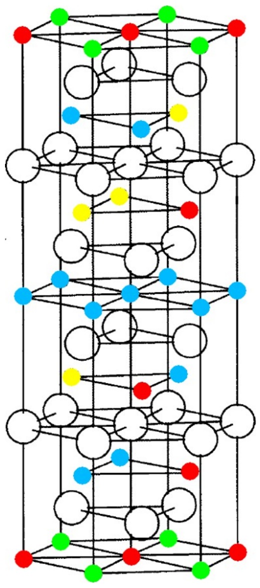
Relax atoms

+ Li



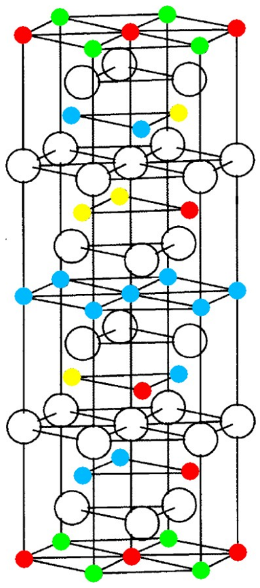
Reinsert Li

+ Li



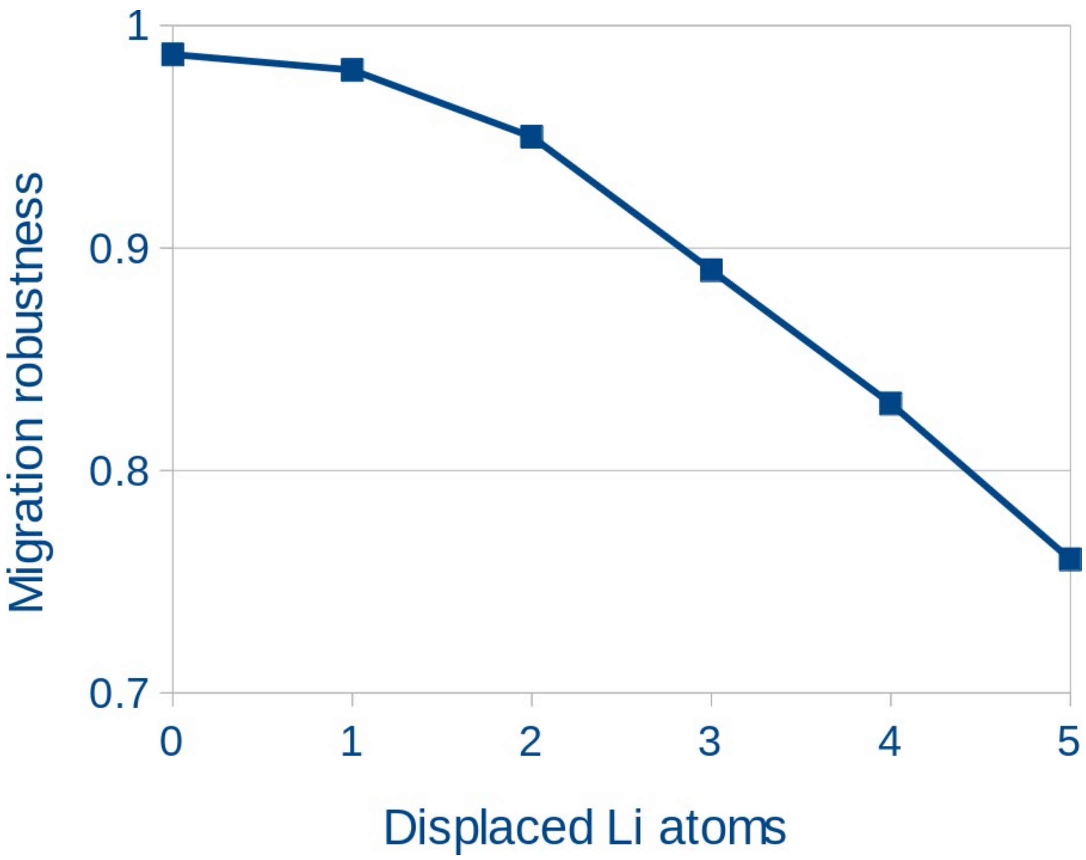
Relax atoms

Li migration optimal structures

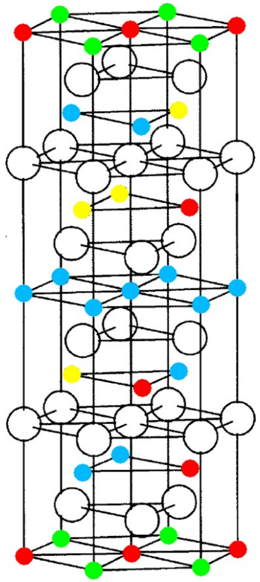


Ground state

82% robust

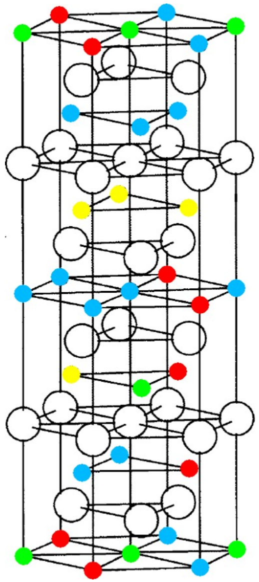


Li migration optimal structures displacing 4xLi



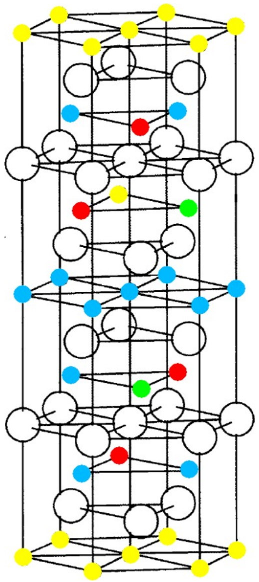
Ground state

82% robust



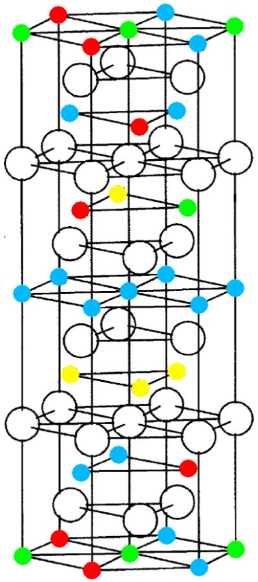
Configuration 1

100% robust



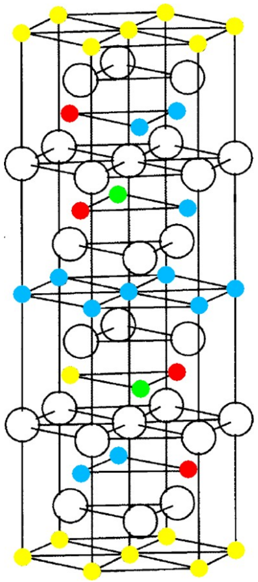
Configuration 2

100% robust



Configuration 3

100% robust



Configuration 4

100% robust

Merge computational and experimental data

DFT

DFT

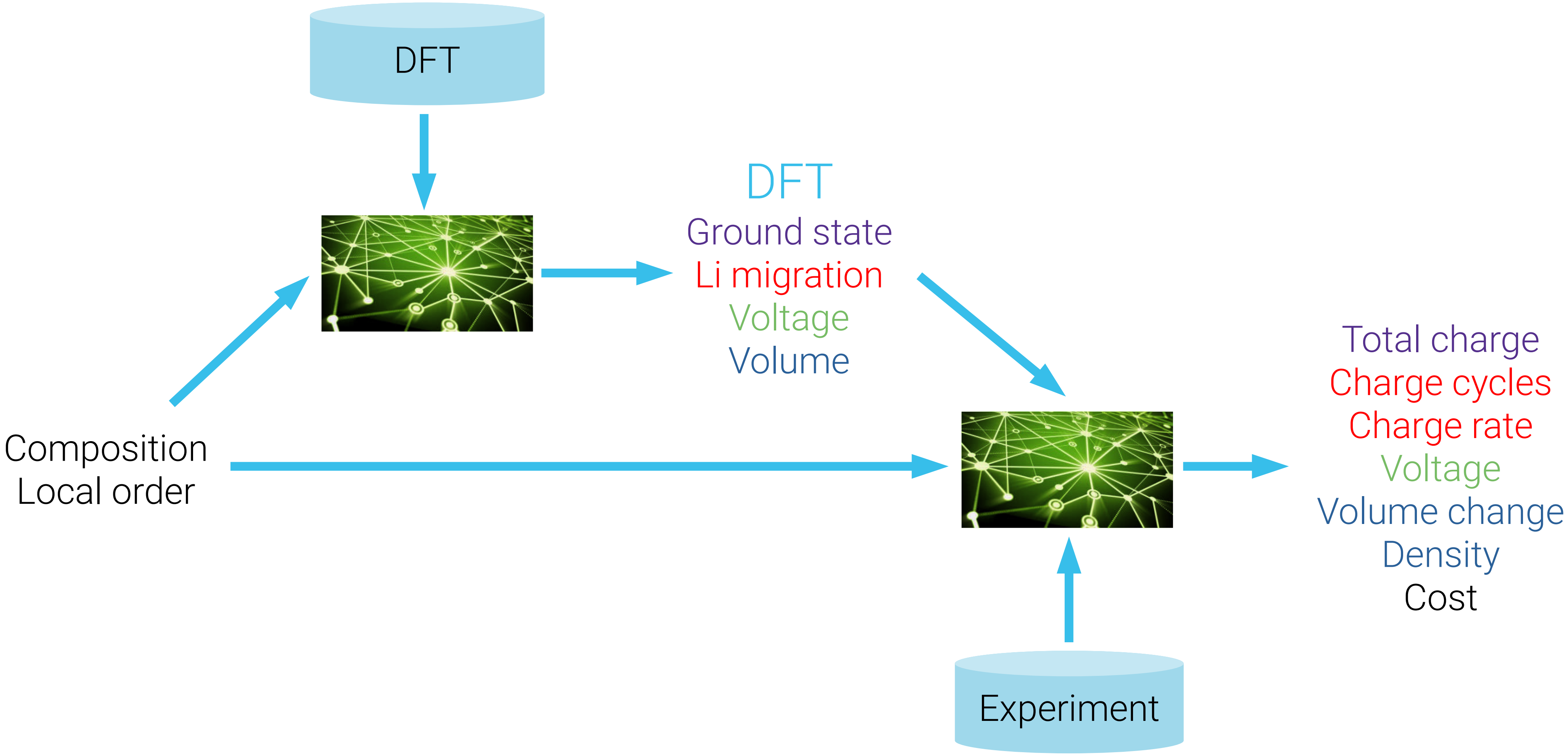
Ground state
Li migration
Voltage
Volume

Composition
Local order

Experiment

Total charge
Charge cycles
Charge rate
Voltage
Volume change
Density
Cost

Merge computational and experimental data



Battery management system

Juxtapose physics-based modeling with machine learning

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 to predict long-term battery performance

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 component specification

Improved understanding of battery properties

Empowers specification of the optimal components

Bespoke battery design for each customer

nature machine intelligence

REVIEW ARTICLE

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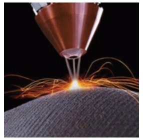
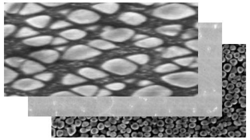
Other materials designed

Steel welding consumables

Titanium additive manufacturing



High temperature alloys

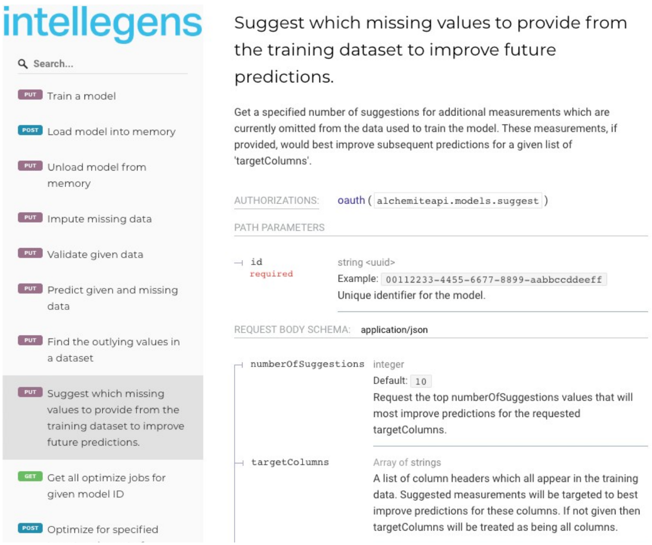


Lubricants

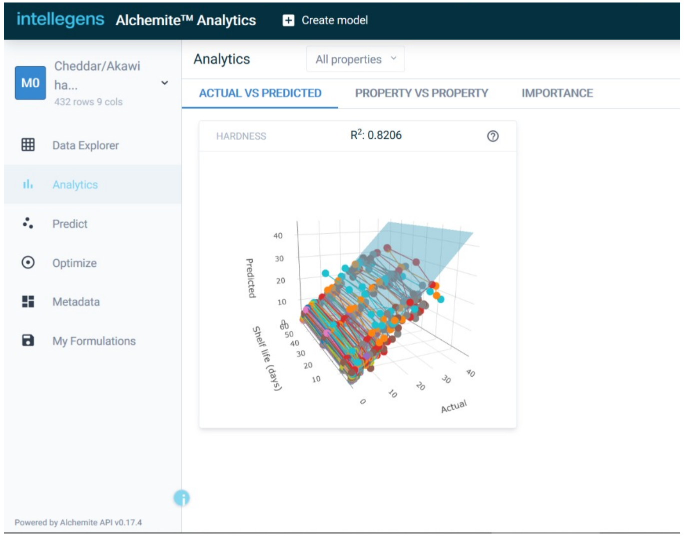
Journal of Chemical Physics 153, 014102 (2020)
Fluid Phase Equilibria 501, 112259 (2019)
Materials & Design 168, 107644 (2019)
Computational Materials Science 147, 176 (2018)
Physical Review Applied 12, 034024 (2019)
Matter 1, 219 (2019)
Scripta Materialia 146, 82 (2018)
Materials & Design 131, 358 (2017)

Delivery

API for integration



Within the browser



Prospects for the future

Merge computational simulations and experimental data

Design battery materials

Guided simulations and experiments leads to 5x speedup

Embedded battery management software