



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

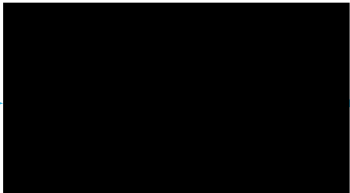
Accelerate materials and drugs discovery

Generic with **proven** applications in materials discovery and drug design

Black box machine learning for materials design



Composition

A collection of icons representing material composition, including various types of rocks and minerals, a pile of red powder, a thermometer with both Fahrenheit and Celsius scales, and a circular clock face.

Cycles

A silver digital counter with a small LCD screen showing '000' and a push button.

Charge

A white digital ammeter with a red LCD screen showing '0.00', labeled 'SCHOOL AMPMETER' and 'A', with a range of '0-10A DC'.

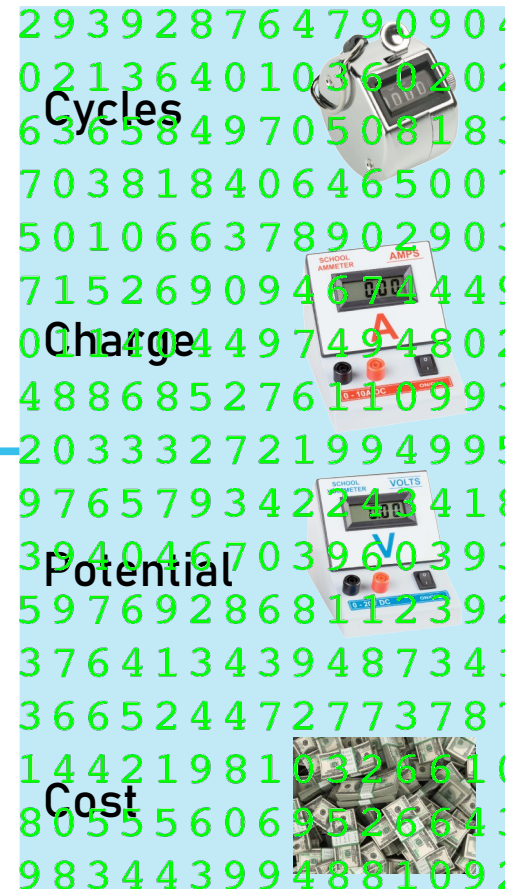
Potential

A white digital voltmeter with a blue LCD screen showing '0.00', labeled 'SCHOOL VOLTMETER' and 'VOLTS', with a range of '0-20V DC'.

Cost

A pile of US dollar bills, representing the cost of the materials or the process.

Training machine learning



Machine learning for materials design



Cycles A silver digital counter with a display showing '000'.

Charge A white school ammeter with a digital display showing '0.00' and a red 'A' symbol. It is labeled 'SCHOOL AMPMETER' and '0-10A DC'.

Potential A white school voltmeter with a digital display showing '0.00' and a blue 'V' symbol. It is labeled 'SCHOOL VOLTMETER' and '0-20V DC'.

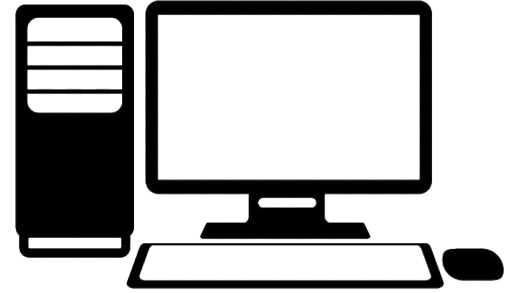
Cost A pile of US dollar bills.

Two sources of information in the design pipeline



Experiment

Accurate
Quantities of interest
Lack of data
Expensive



Computational

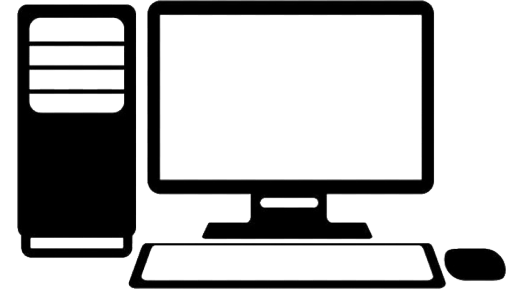
Less accurate
Atom level insights
Perform on demand
Cheap to perform

Merge the 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

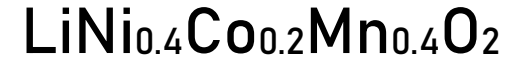
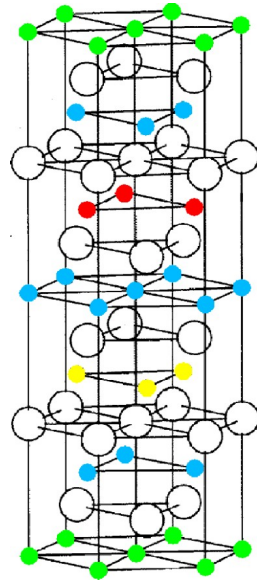
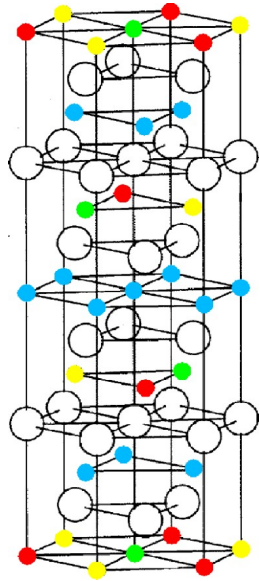
Volume change

Li migration

Ground state

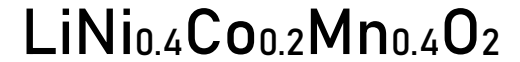
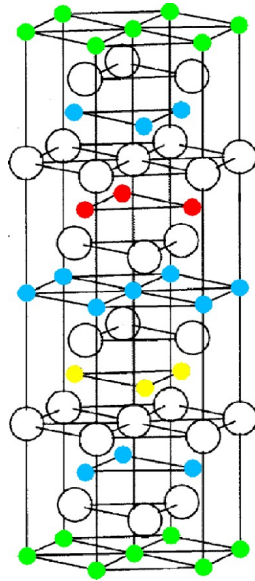
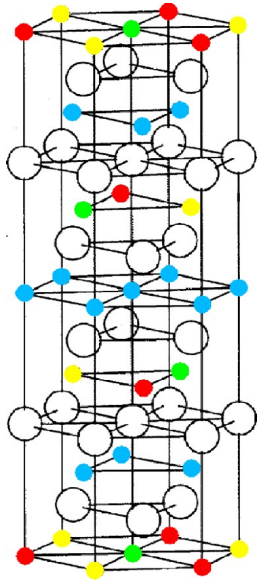
Charge rate

Nickel-Cobalt-Manganese NCM-424 material



- O
- Li
- Ni
- Co
- Mn

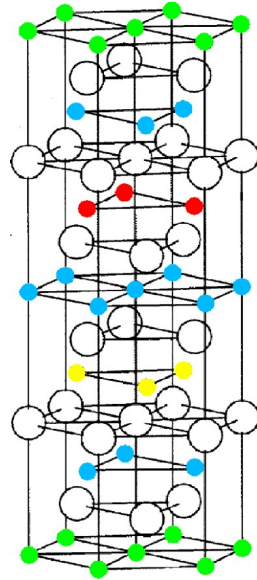
Nickel-Cobalt-Manganese NCM-424 material



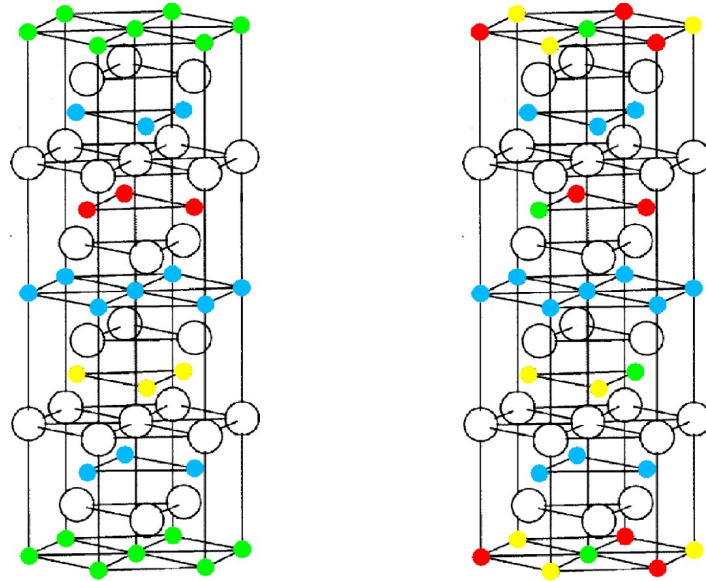
○	O
●	Li
●	Ni
●	Co
●	Mn

Calculate properties with **DFT** simulations

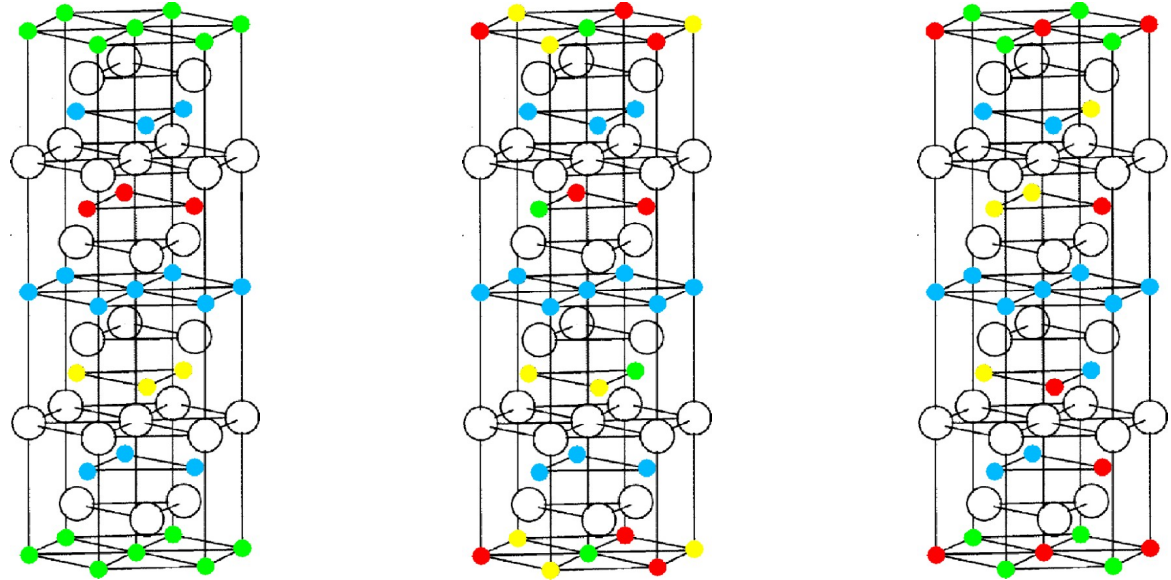
Approach: exhaustive exploration of unit cells



Approach: exhaustive exploration of unit cells



Approach: exhaustive exploration of unit cells

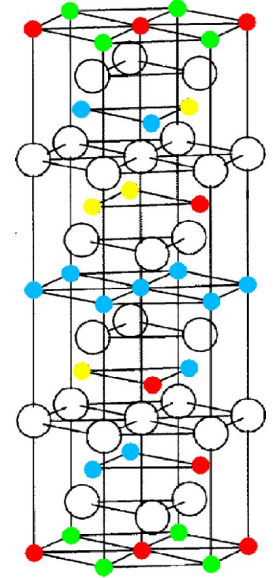
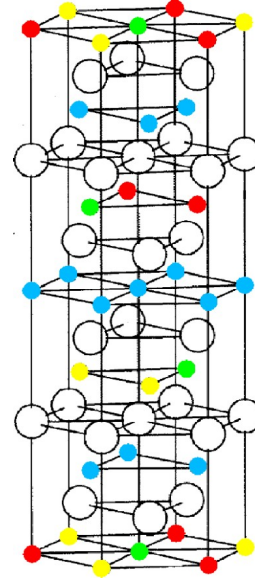
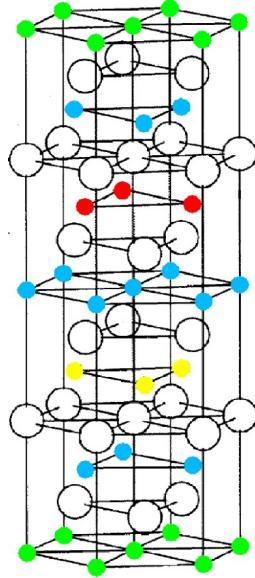


Approach: exhaustive exploration of unit cells



153153000
permutations
=42000 years

Only examine
order that fits
into the unit cell



Design variables and target properties with DFT



Concentration
of Ni, Mn, Co

Location of
atoms



Volume change

Li migration

Voltage

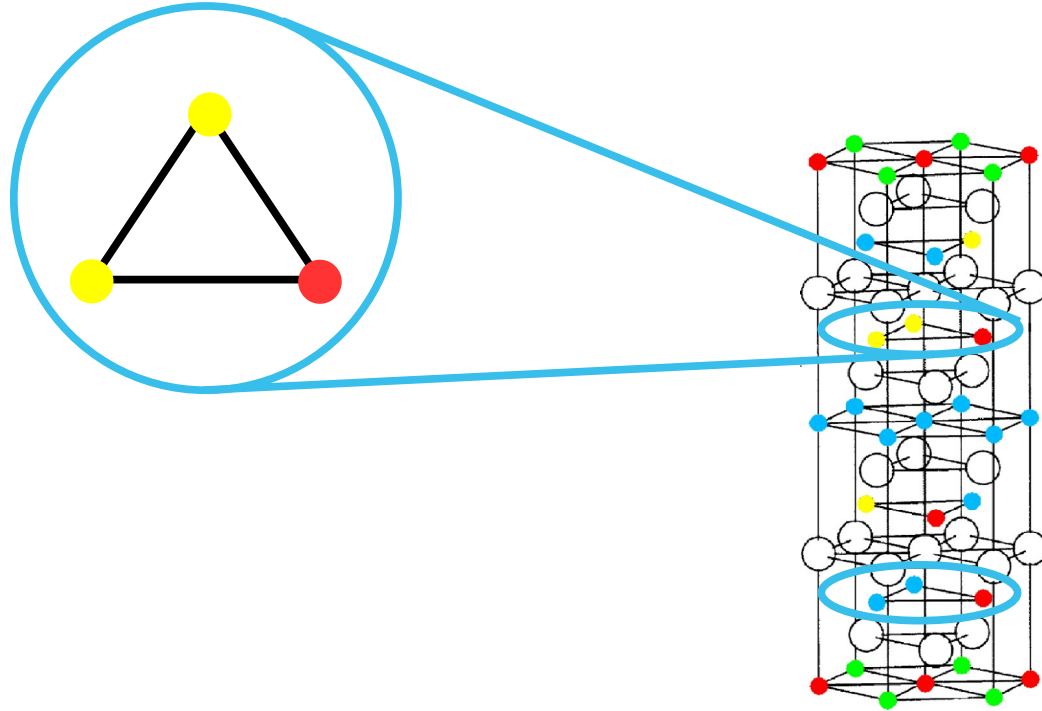
Ground state

Approach: characterize with a local order matrix



$$N_{\text{yellow-yellow}}=1$$

$$N_{\text{yellow-red}}=2$$

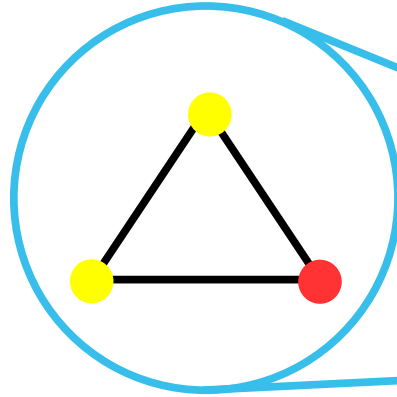


Approach: characterize with a local order matrix

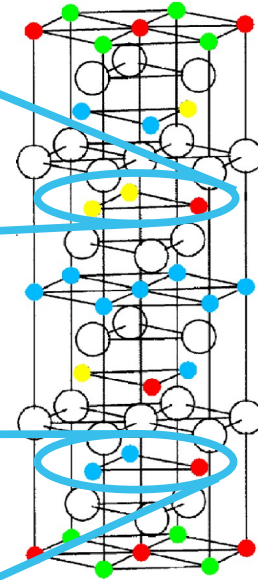
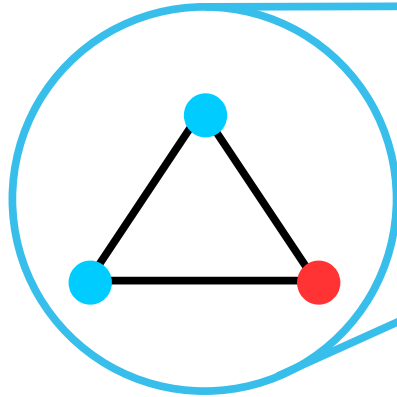


$$N_{\text{yellow-yellow}}=1$$

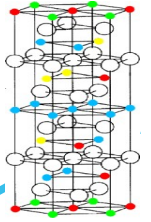
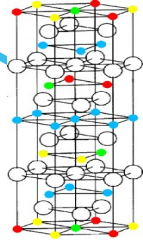
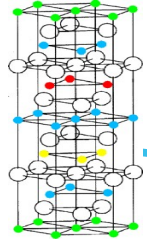
$$N_{\text{yellow-red}}=2$$



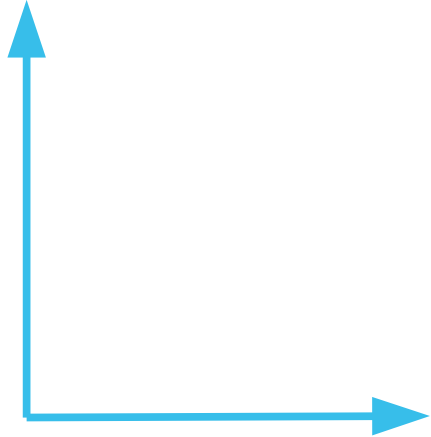
$$N_{\text{red-blue}}=1$$



Train on initial results

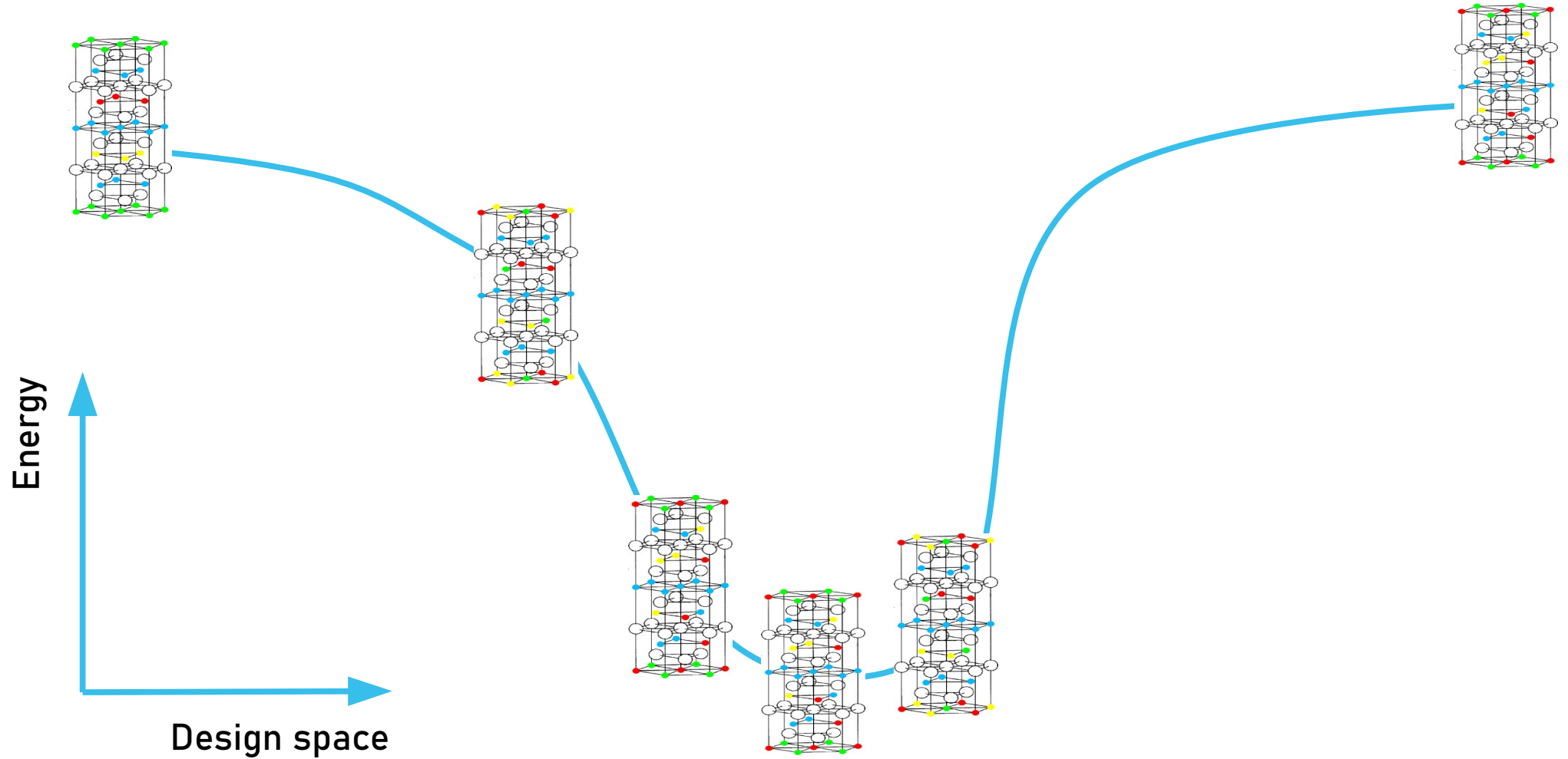


Energy

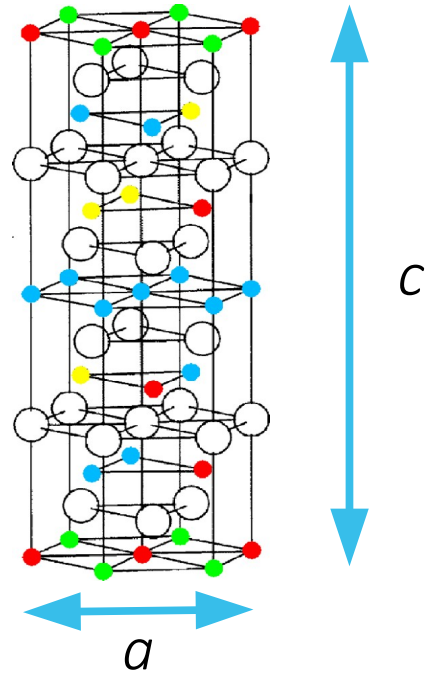


Design space

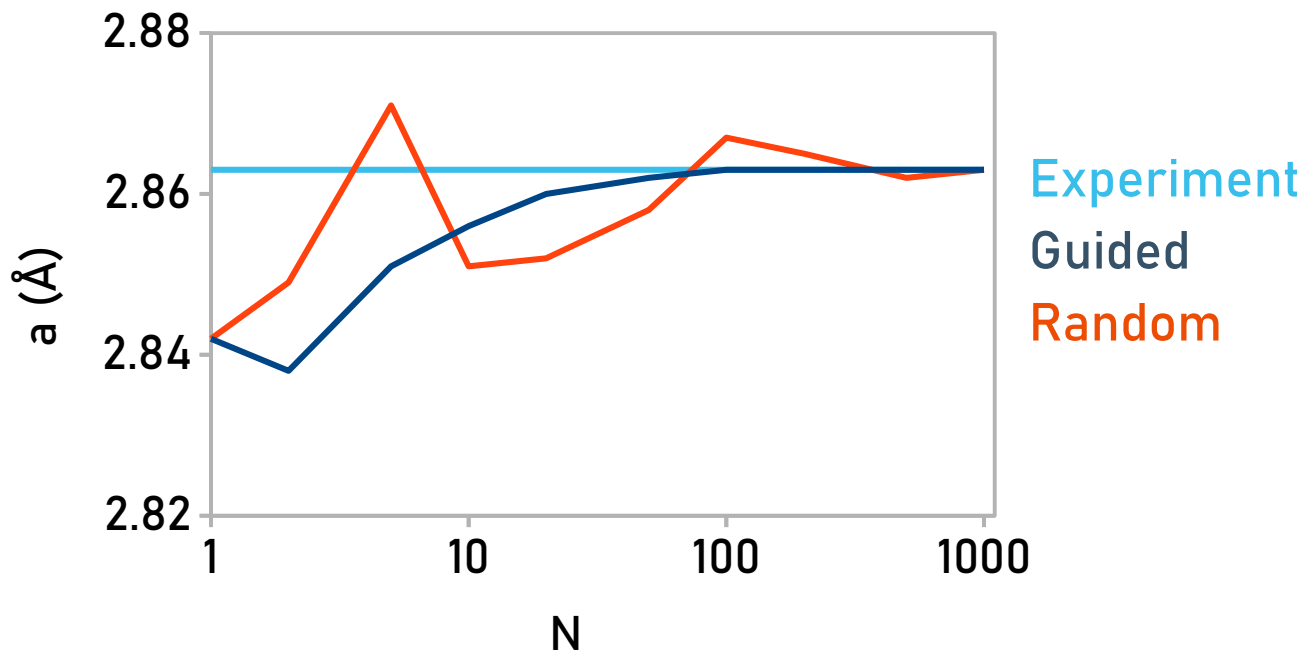
Guided calculation for recursive learning



Lattice constants

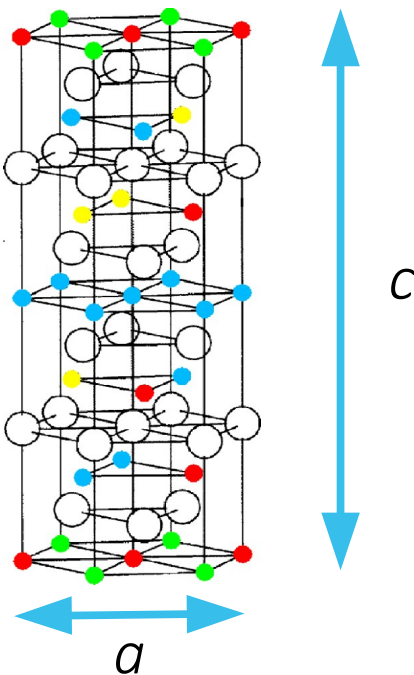


How many calculations are required



Machine learning guidance requires **5-times fewer** calculations

Predicting the lattice constant from DFT



Structure

$\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$ prediction

$\text{LiNi}_{0.4}\text{Co}_{0.2}\text{Mn}_{0.4}\text{O}_2$ experiment

a (Å)

2.863

2.866

c (Å)

14.257

14.254

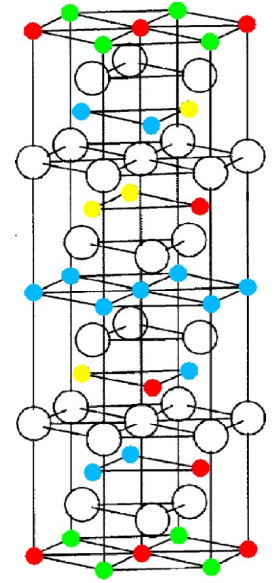
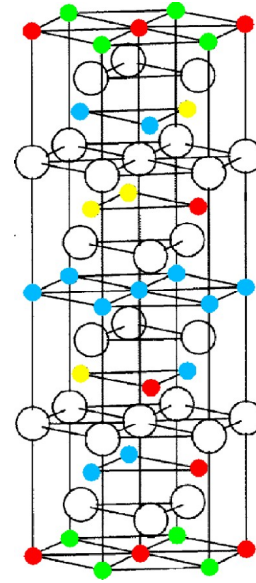
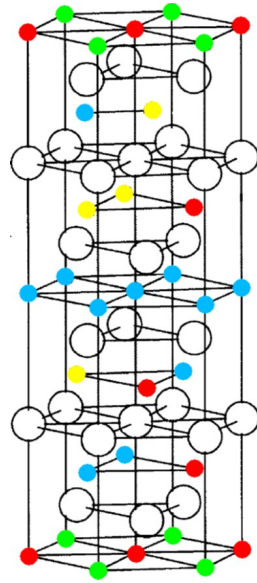
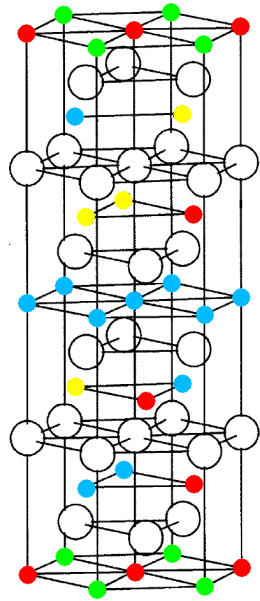
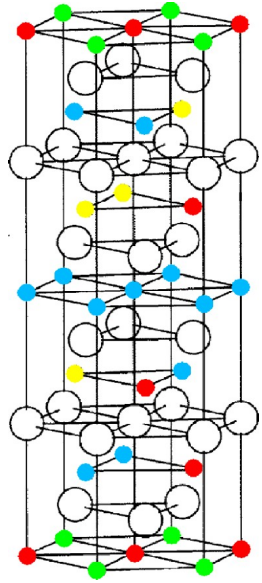
Local order matrix within a single unit cell



Matrix element	Optimal	Achievable in cell
$N_{\text{Co-Co}}$	0.34	1
$N_{\text{Ni-Ni}}$	0.16	0
$N_{\text{Mn-Mn}}$	0.09	1
$N_{\text{Li-Li}}$	0.08	0
$N_{\text{Co-Ni}}$	2.5	2
$N_{\text{Co-Mn}}$	0.2	0
$N_{\text{Ni-Mn}}$	3.4	3
$N_{\text{Ni-Li}}$	0.32	1
$N_{\text{Co-Li}}$	0.21	0
$N_{\text{Mn-Li}}$	1.37	1
N_{Ni}	1.82	1
N_{Co}	0.02	0
N_{Mn}	0.01	1

Machine learning can predict cells **inaccessible** to DFT

Tracking Li migration



Original structure

Remove Li

Relax atoms

Reinsert Li

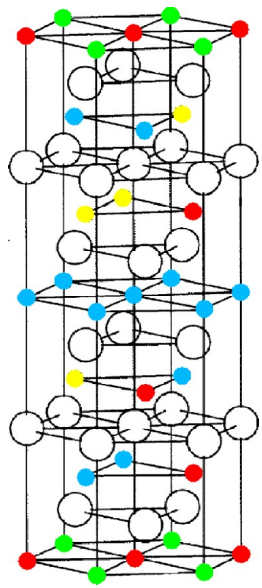
Relax atoms

+ Li 

+ Li 

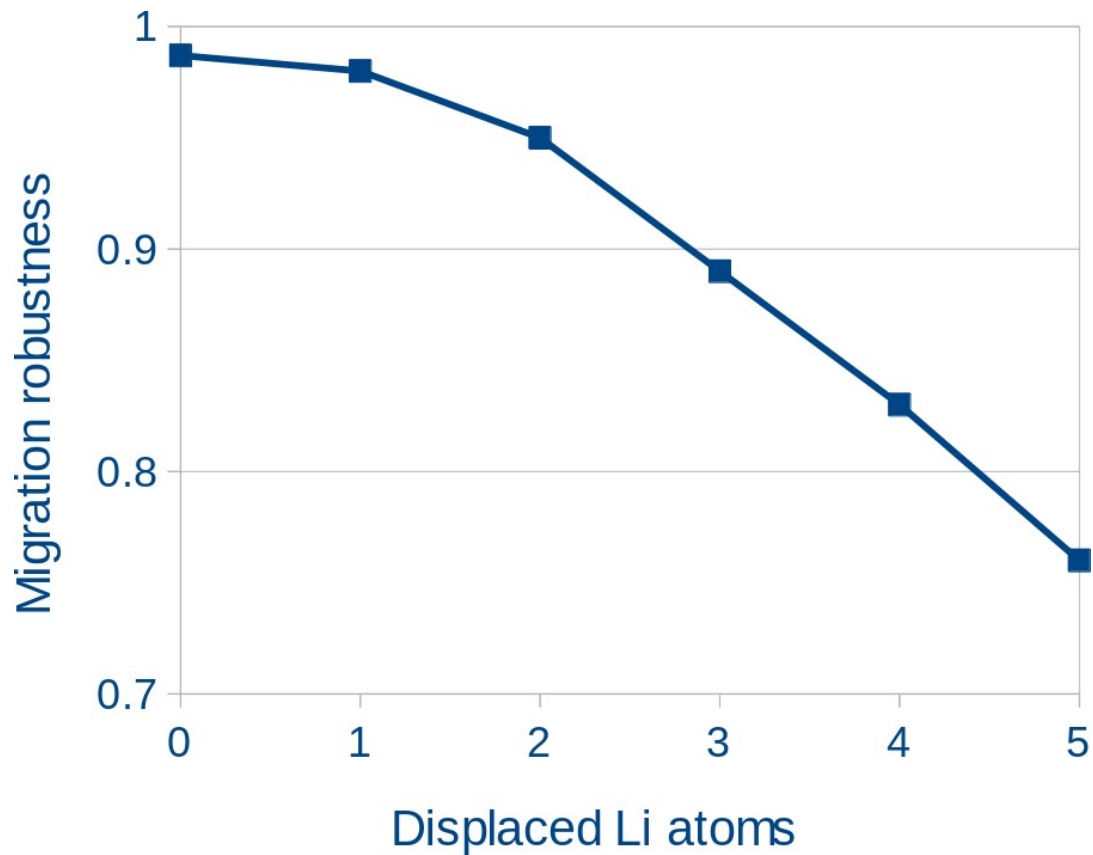
+ Li 

Li migration optimal structures

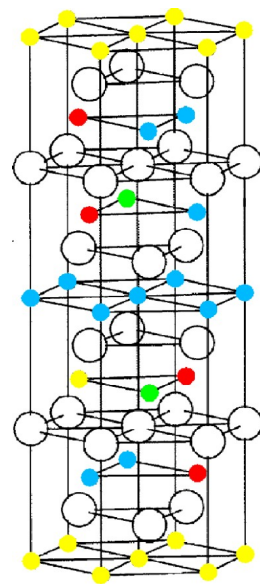
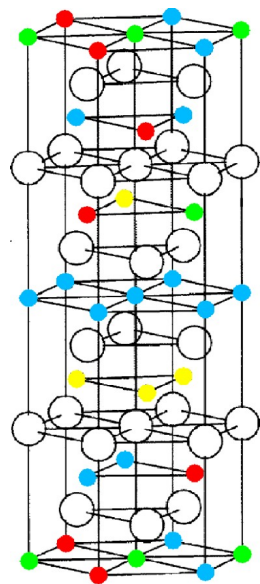
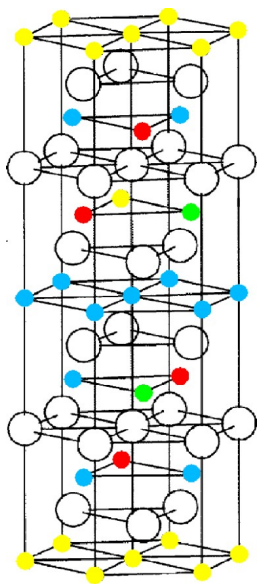
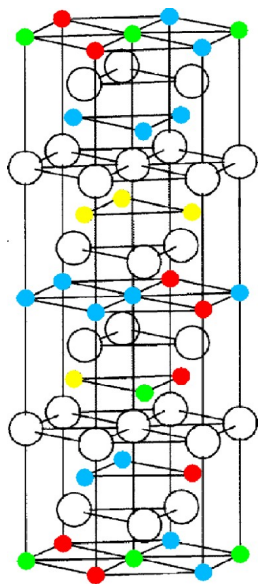
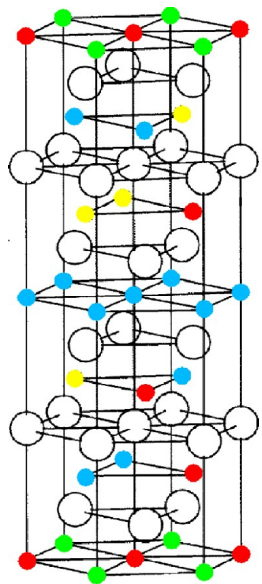


Ground state

82% robust



Li migration optimal structures displacing 4xLi



Ground state

Configuration 1

Configuration 2

Configuration 3

Configuration 4

82% robust

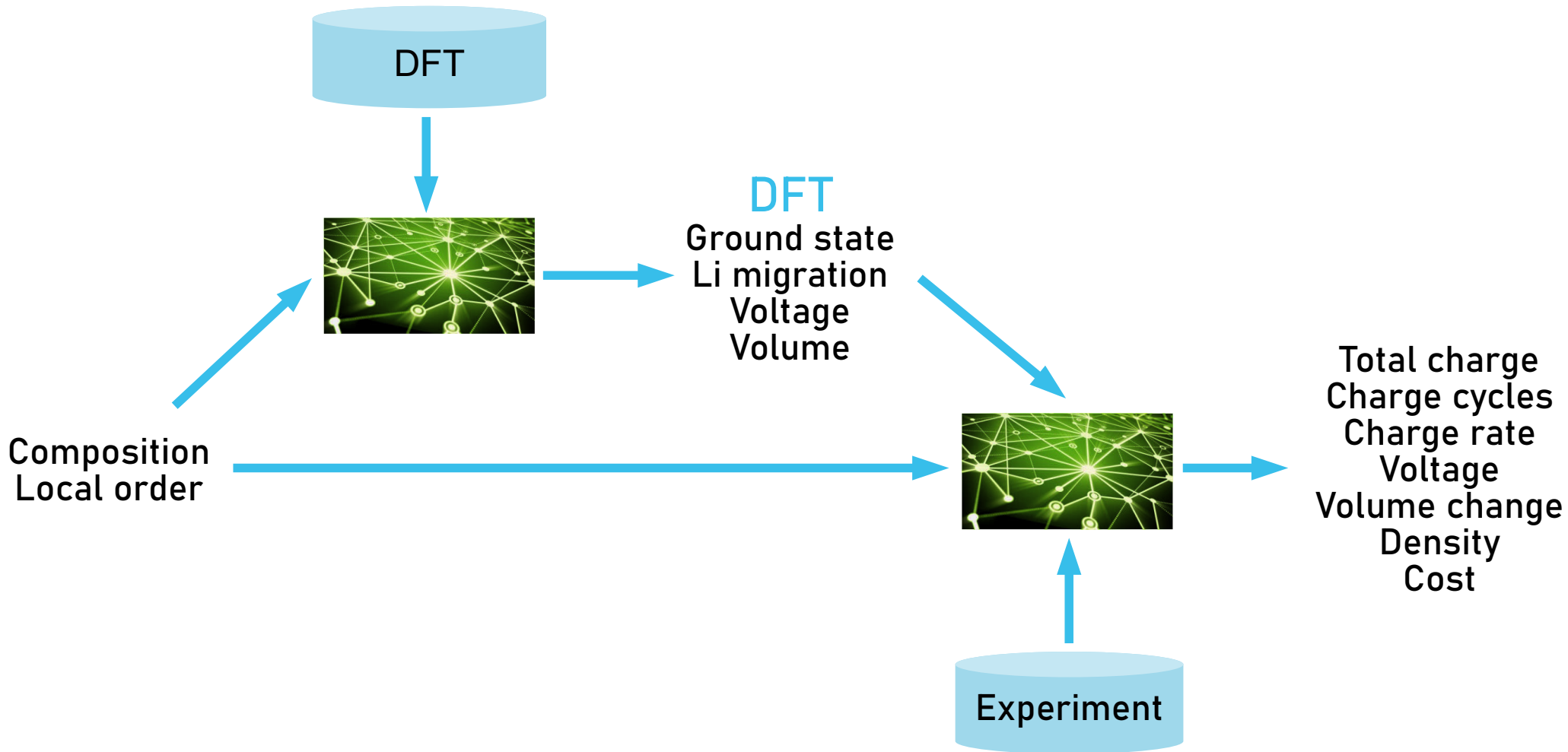
100% robust

100% robust

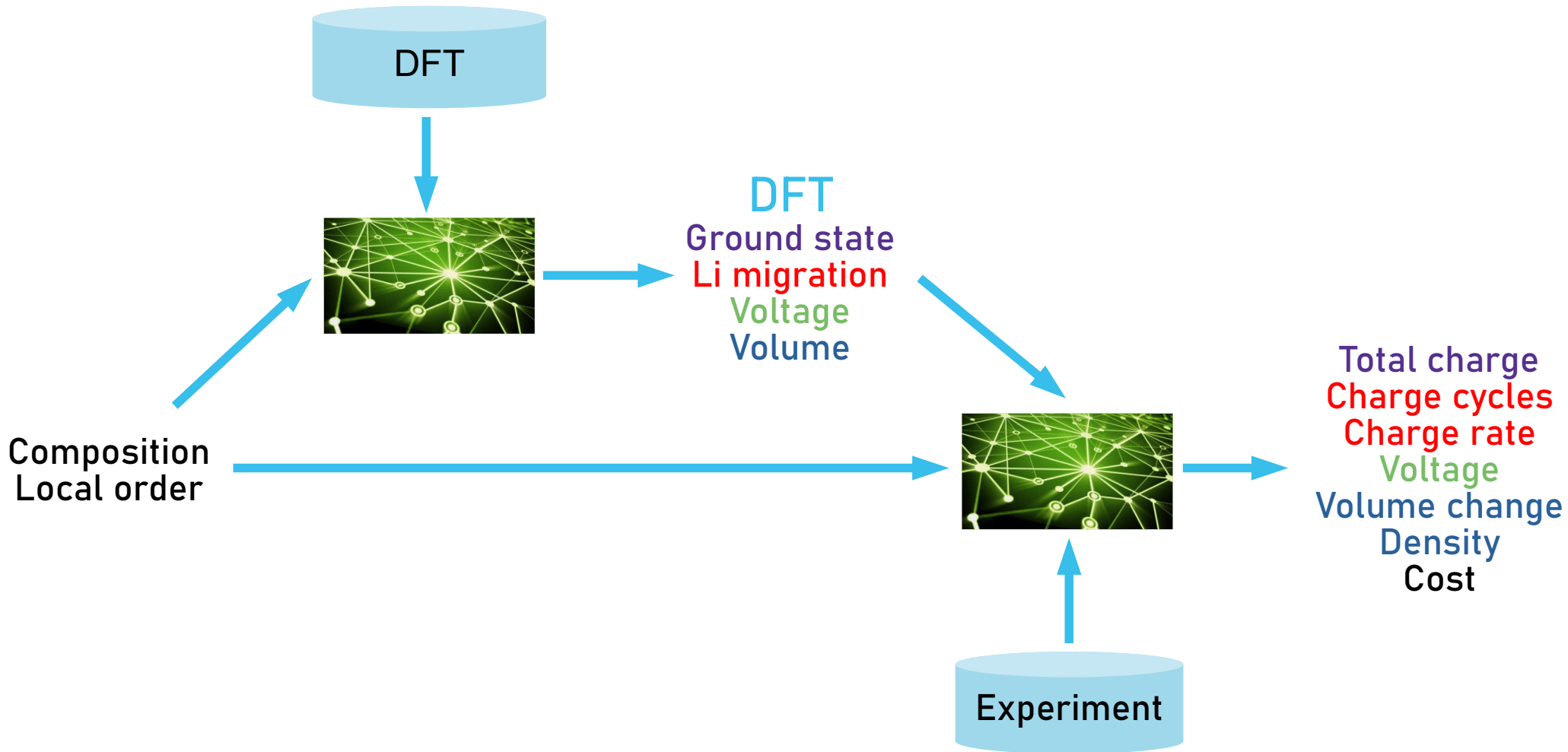
100% robust

100% robust

Merge computational and experimental data



Merge computational and experimental data



Prospects for the future



Merge computational simulations and experimental data

Design battery materials

Guided simulations and experiments leads to 5x speedup

Predict **complex** cells inaccessible to DFT