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

Composition

Cycles

Charge

Potential

Cost

Training machine learning

Composition

Cycles

Charge

Potential

Cost

Machine learning for materials design

Composition

Cycles

Charge

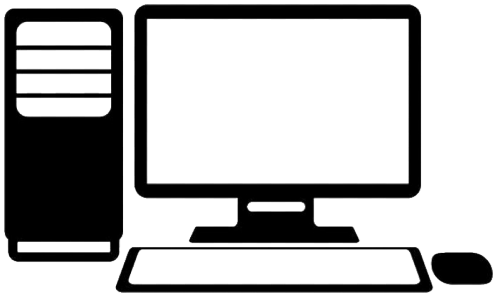
Potential

Cost

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

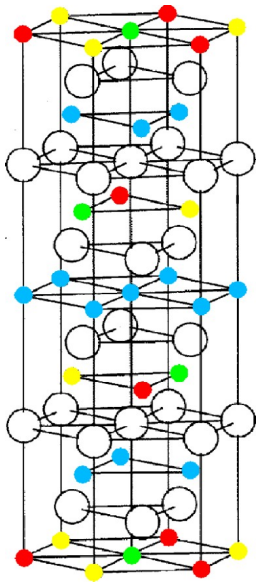
Volume change

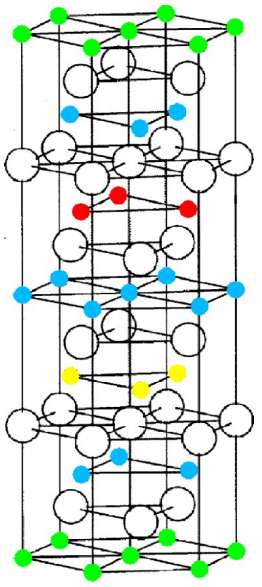
Li migration

Ground state

Charge rate

Nickel-Cobalt-Manganese NCM-424 material

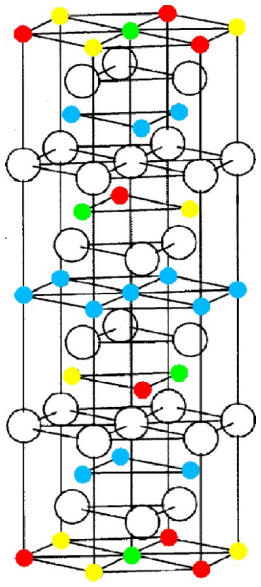


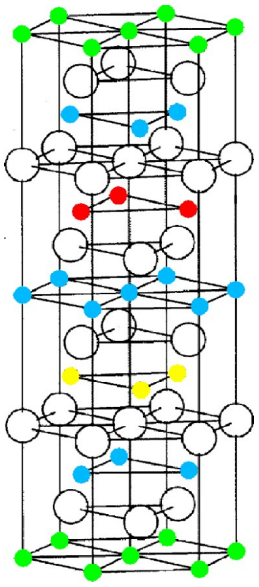


$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$

- O
- Li
- Ni
- Co
- Mn

Nickel-Cobalt-Manganese NCM-424 material



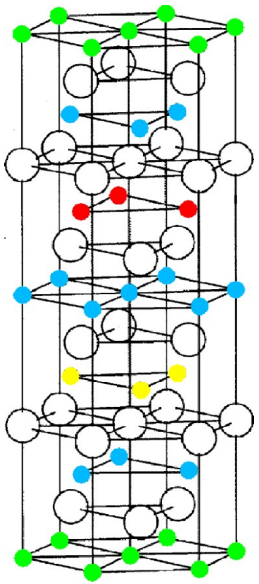


$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$

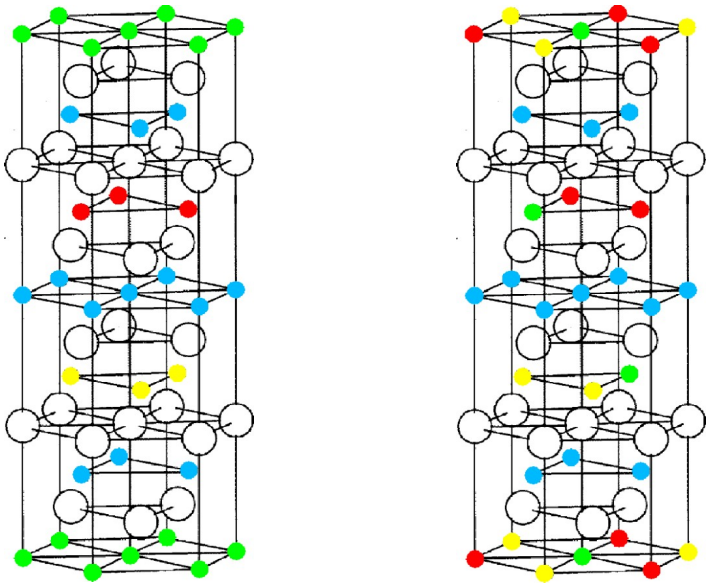
- O
- Li
- Ni
- Co
- Mn

Calculate properties with DFT simulations

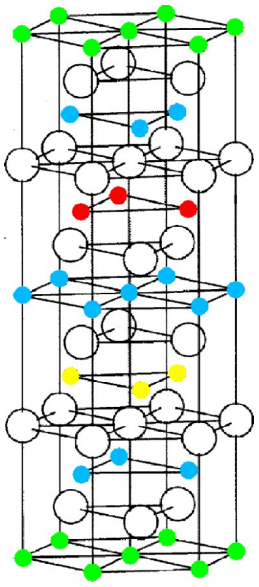
Approach: exhaustive exploration of unit cells

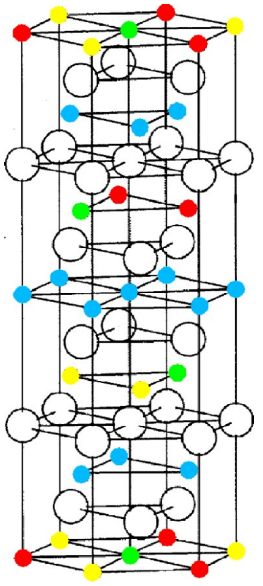


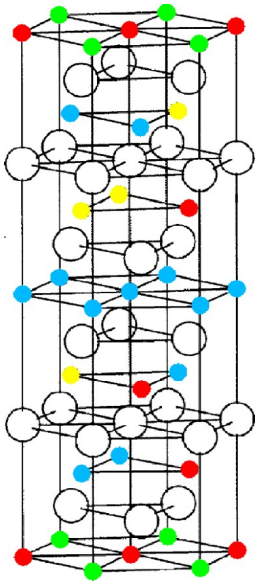
Approach: exhaustive exploration of unit cells



Approach: exhaustive exploration of unit cells



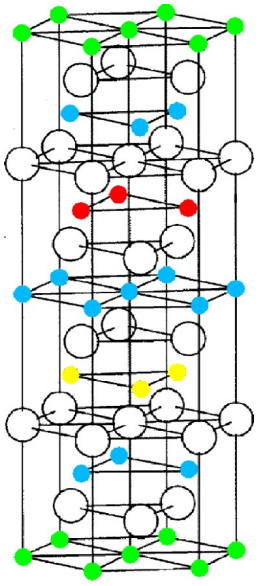


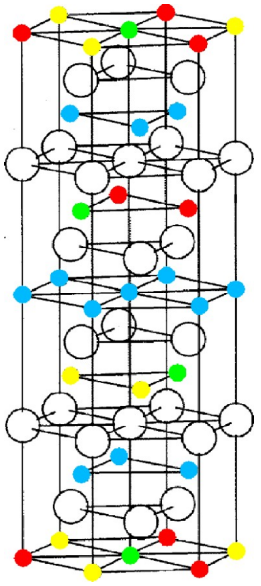


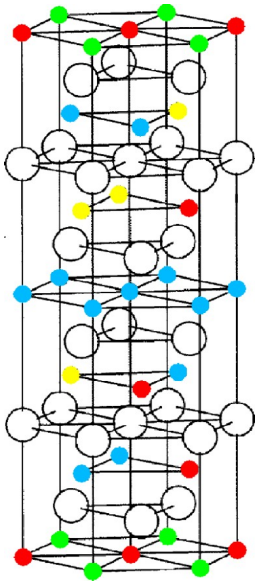
Approach: exhaustive exploration of unit cells

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

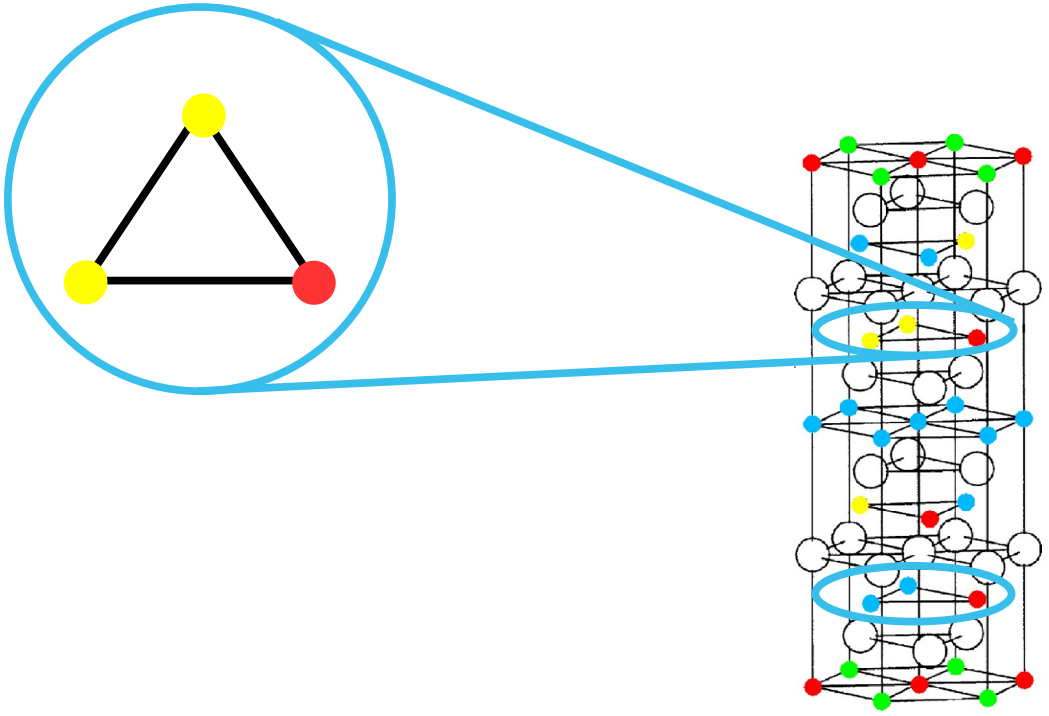
Voltage

Ground state

Approach: characterize with a local order matrix

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

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

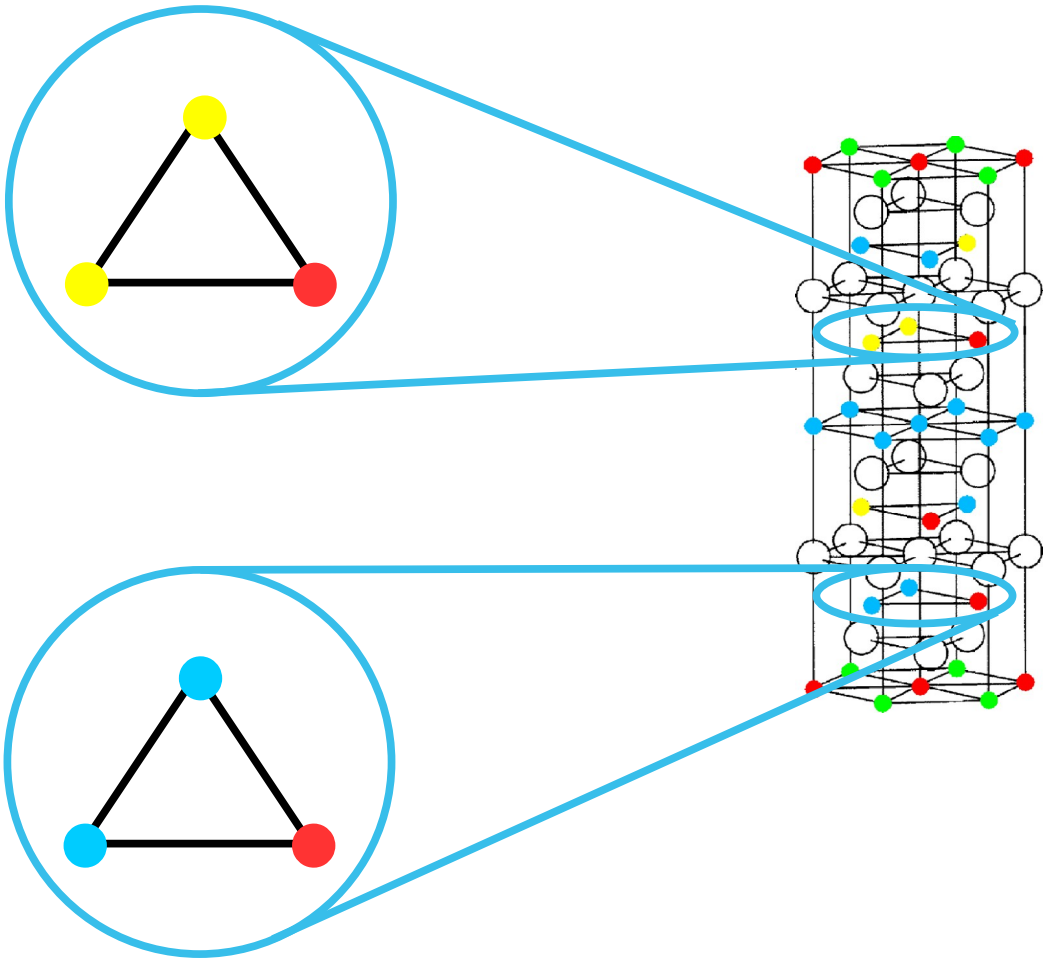


Approach: characterize with a local order matrix

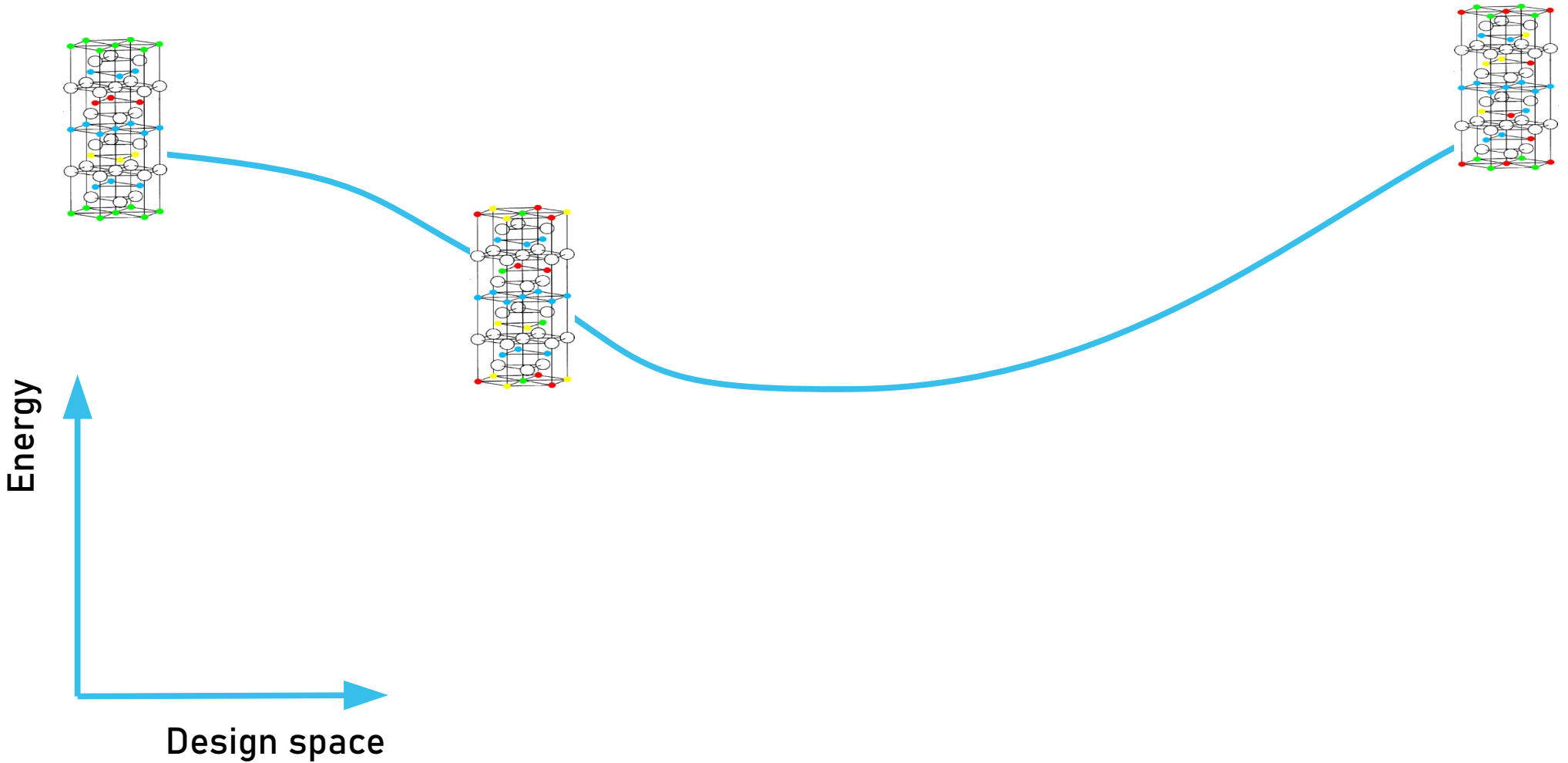
$N_{\text{yellow-yellow}}=1$

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

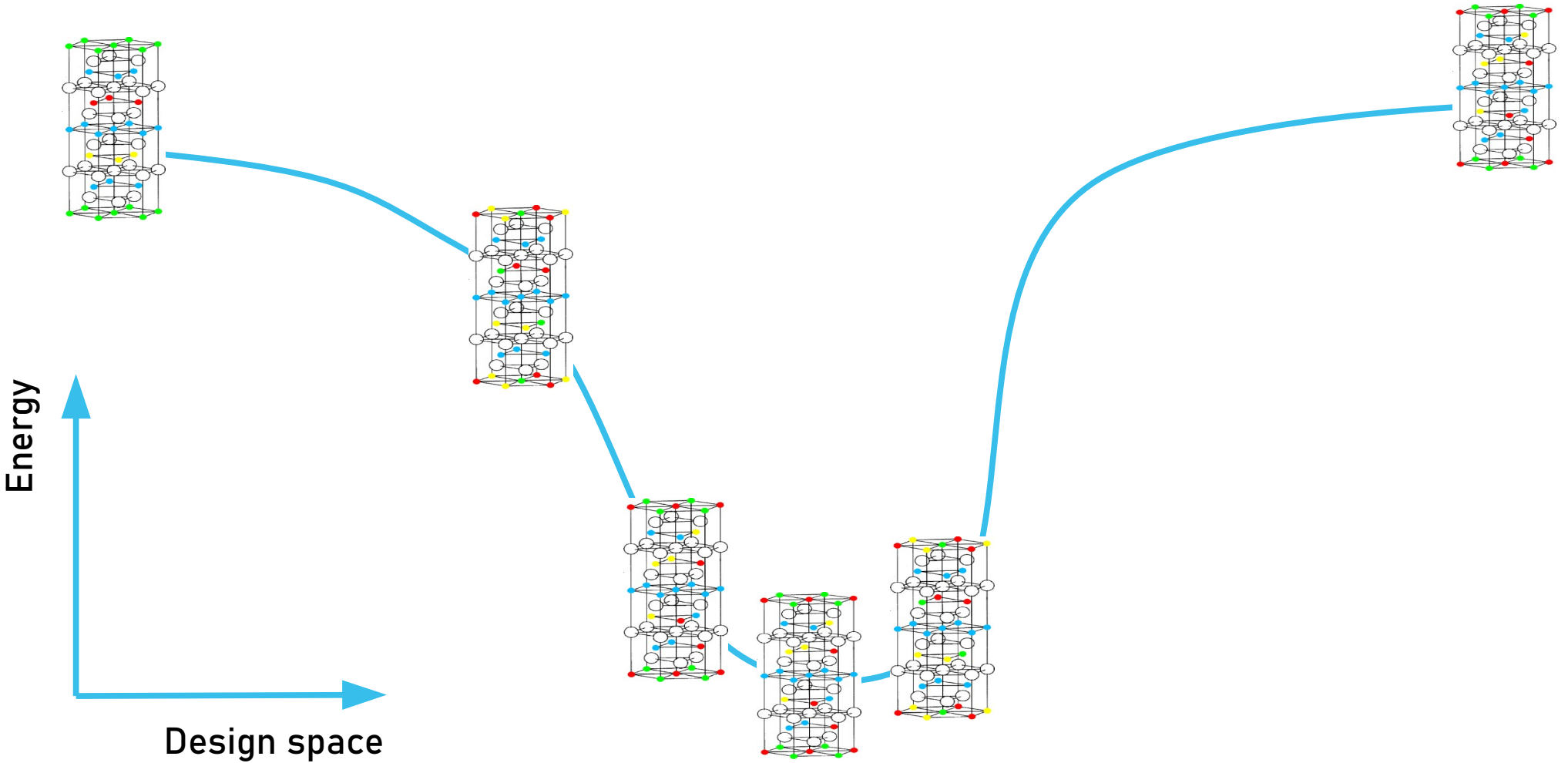
$N_{\text{red-blue}}=1$



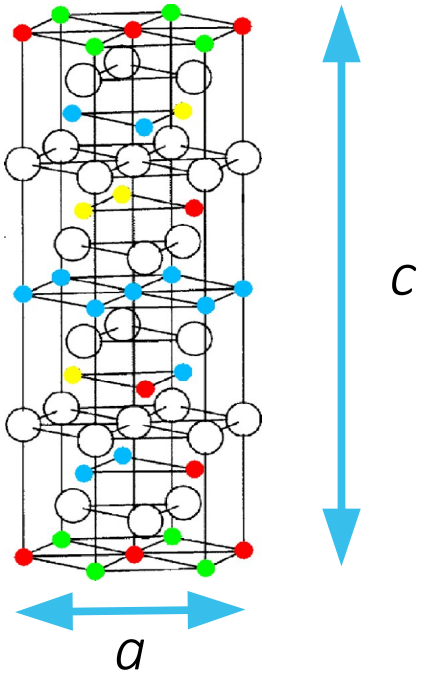
Train on initial results



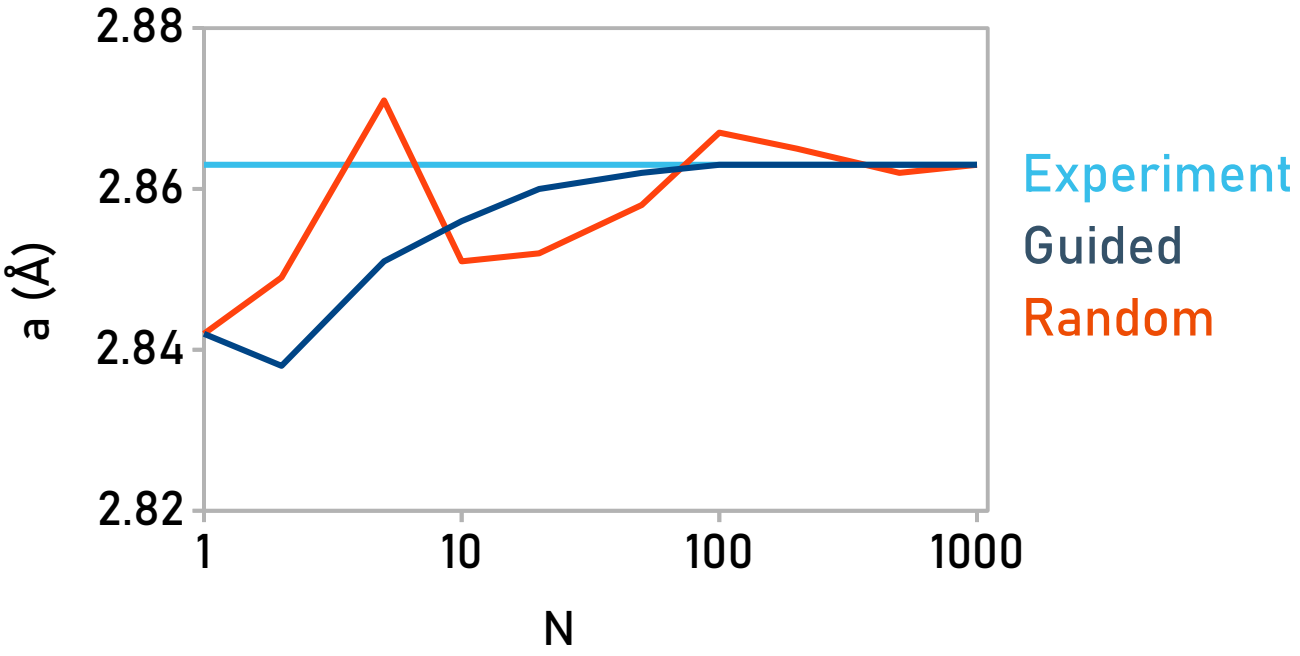
Guided calculation for recursive learning



Lattice constants

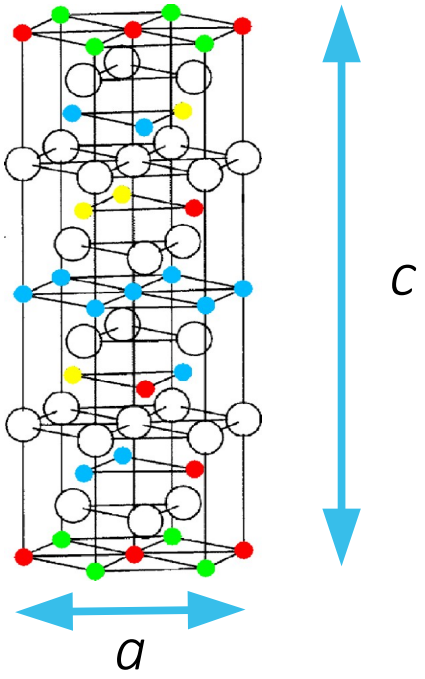


How many calculations are required



Machine learning guidance requires 5-times fewer calculations

Predicting the lattice constant from DFT



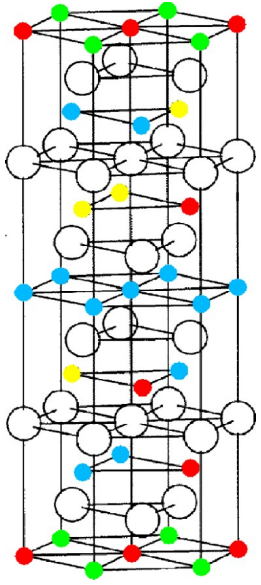
Structure	a (Å)	c (Å)
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ prediction	2.863	14.257
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ experiment	2.866	14.254

Local order matrix within a single unit cell

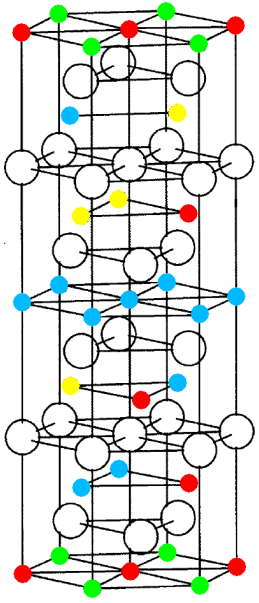
Matrix element	Optimal	Achievable in cell
$N_{Co\text{-}Co}$	0.34	1
$N_{Ni\text{-}Ni}$	0.16	0
$N_{Mn\text{-}Mn}$	0.09	1
$N_{Li\text{-}Li}$	0.08	0
$N_{Co\text{-}Ni}$	2.5	2
$N_{Co\text{-}Mn}$	0.2	0
$N_{Ni\text{-}Mn}$	3.4	3
$N_{Ni\text{-}Li}$	0.32	1
$N_{Co\text{-}Li}$	0.21	0
$N_{Mn\text{-}Li}$	1.37	1
N_{Ni}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

Machine learning can predict cells inaccessible to DFT

Tracking Li migration

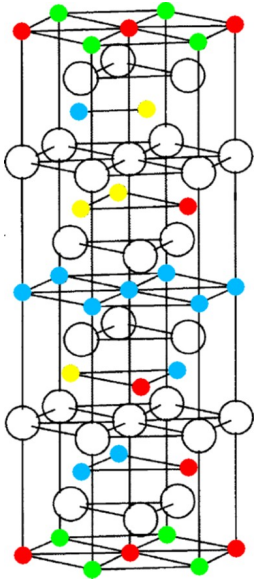


Original structure



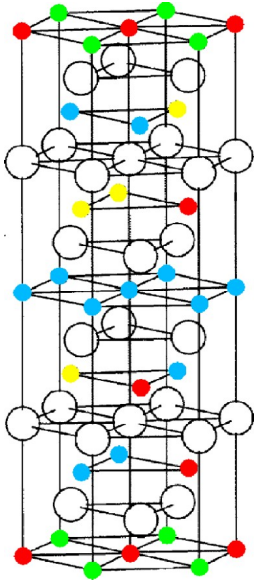
Remove Li

+ Li



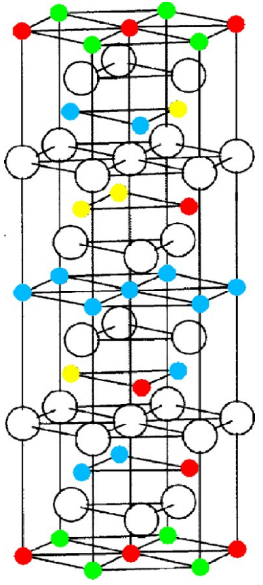
Relax atoms

+ Li



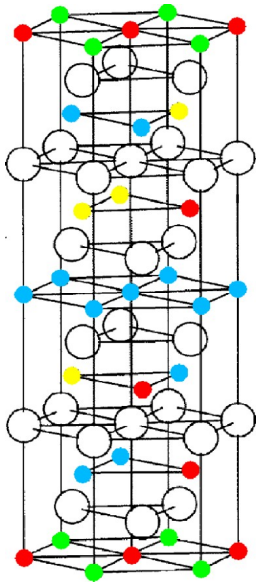
Reinsert Li

+ Li



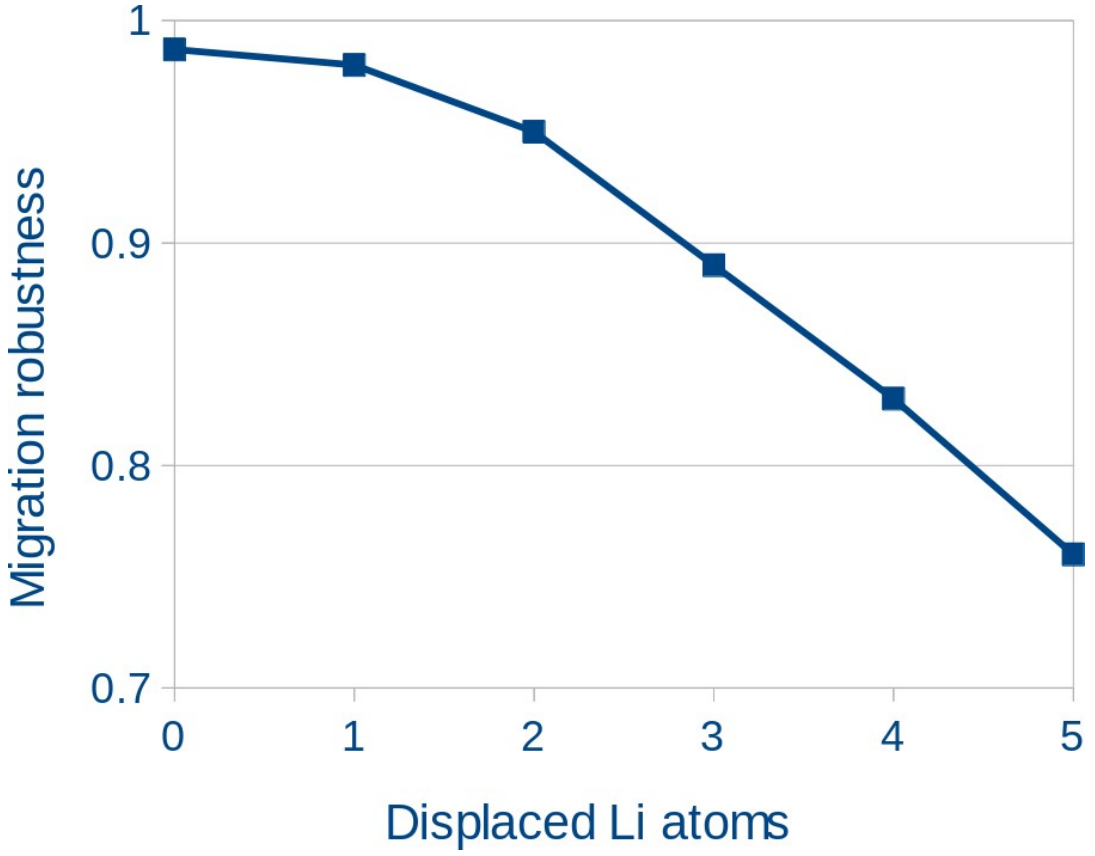
Relax atoms

Li migration optimal structures

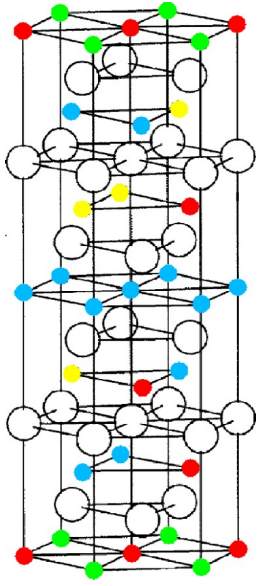


Ground state

82% robust

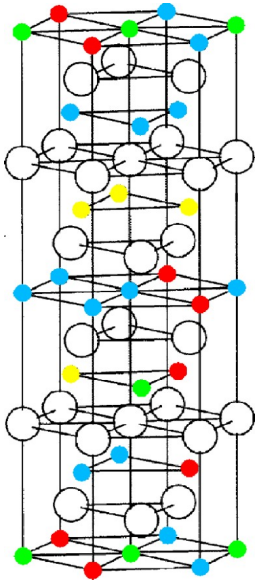


Li migration optimal structures displacing 4xLi



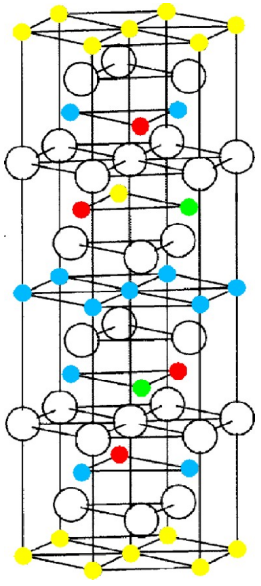
Ground state

82% robust



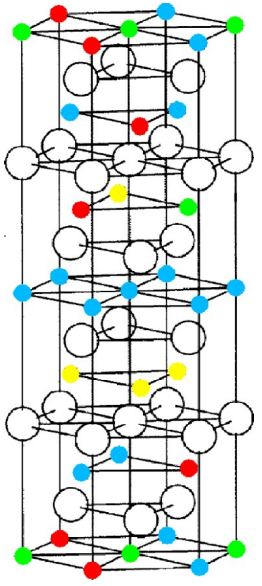
Configuration 1

100% robust



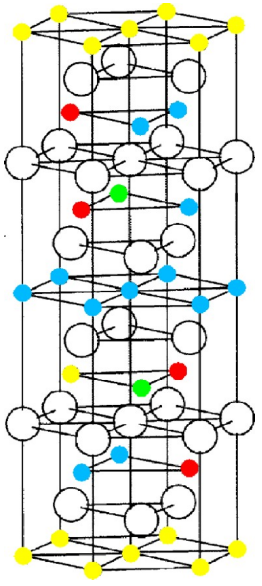
Configuration 2

100% robust



Configuration 3

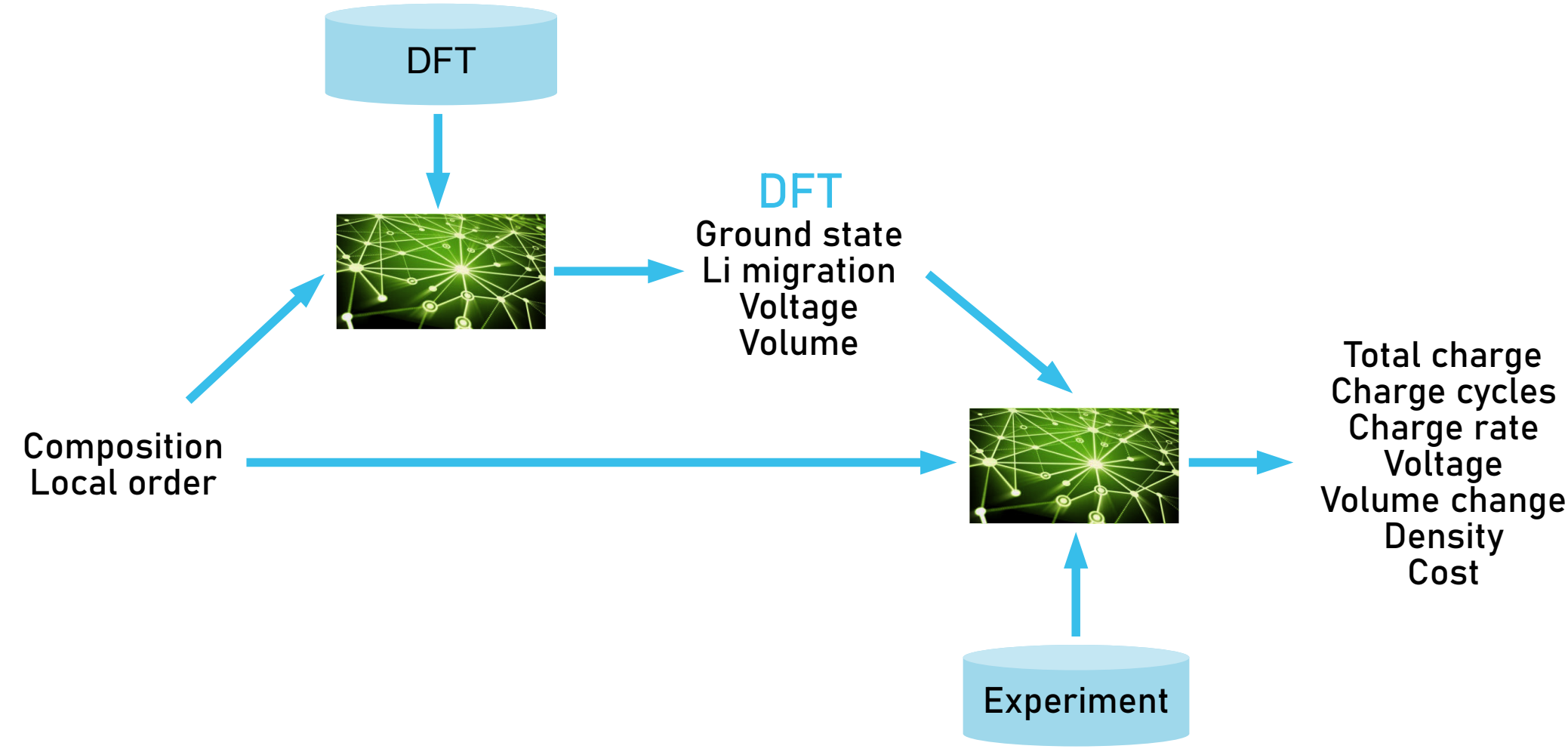
100% robust



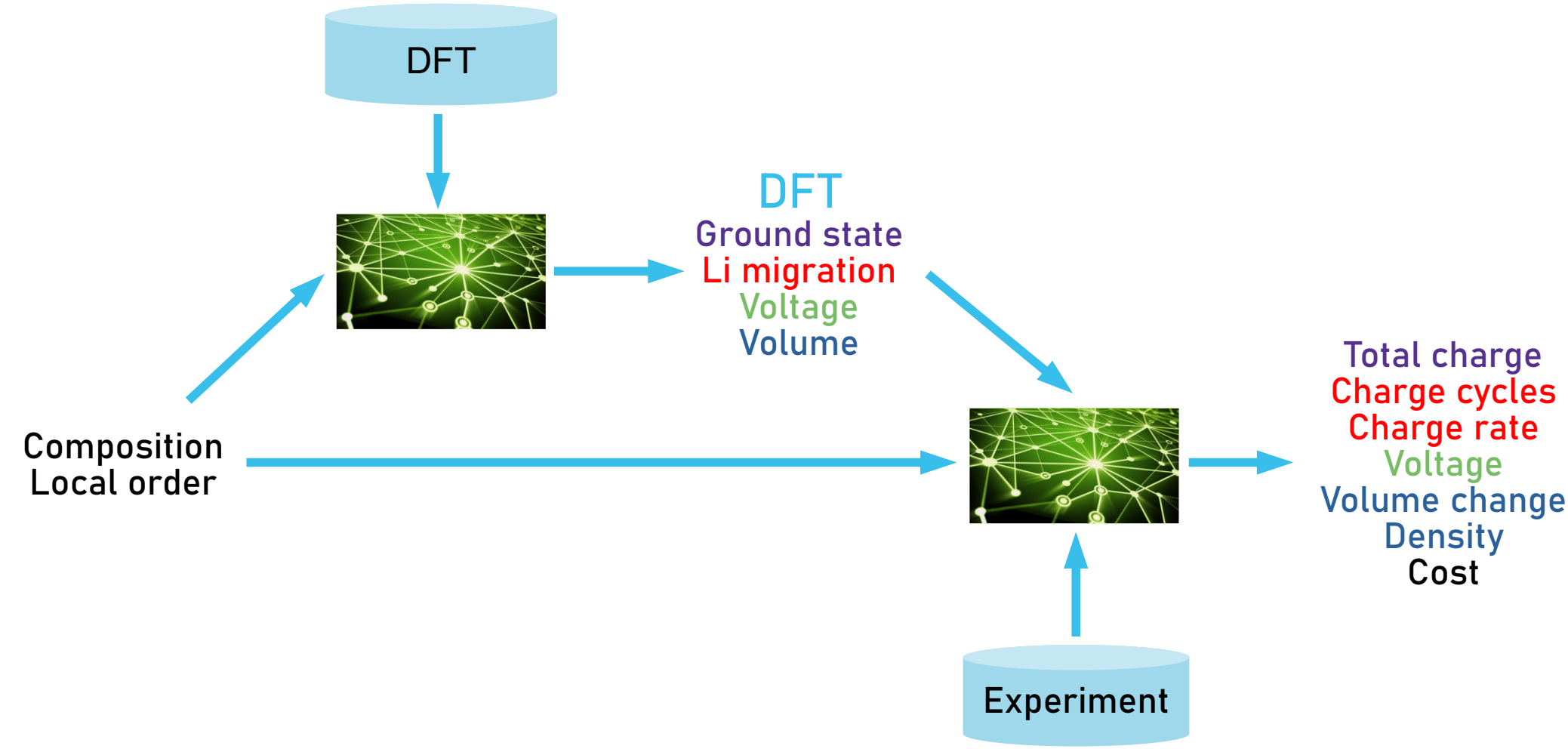
Configuration 4

100% robust

Merge computational and experimental data



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