UNIVERSITY OF CAMBRIDGE

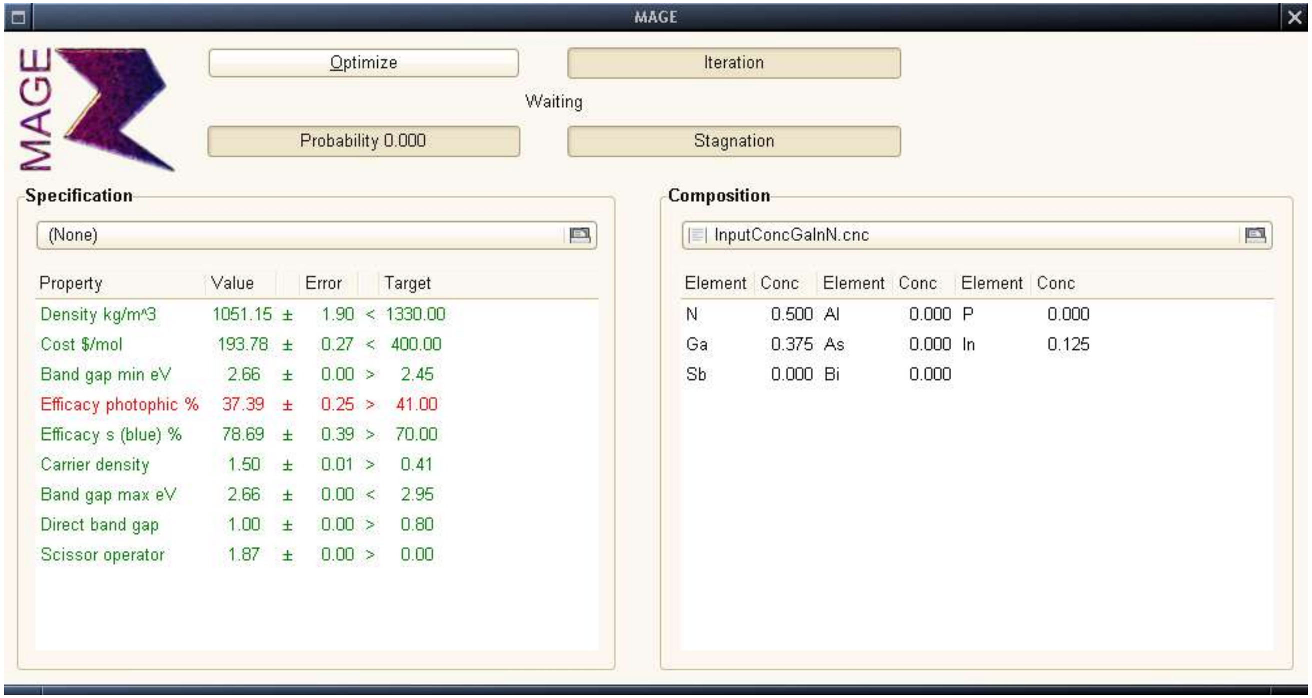
Breakthroughs in data driven materials design

EP14153898.3; US 2014/177578; GB1302743.8
EP14161255.6; US 2014/223465; GB1307533.8
EP14161529.4; US 2014/224885; GB1307535.3
EP14157622.3; amendment to US 2013/0052077 A1; GB1408536.9
Acta Materialia **61**, 3378 (2013)
Intermetallics **48**, 62 (2014)
Phys. Rev. B **90**, 184302 (2014)

Samsung GRO 2013
Theory of Condensed Matter Group, Department of Physics

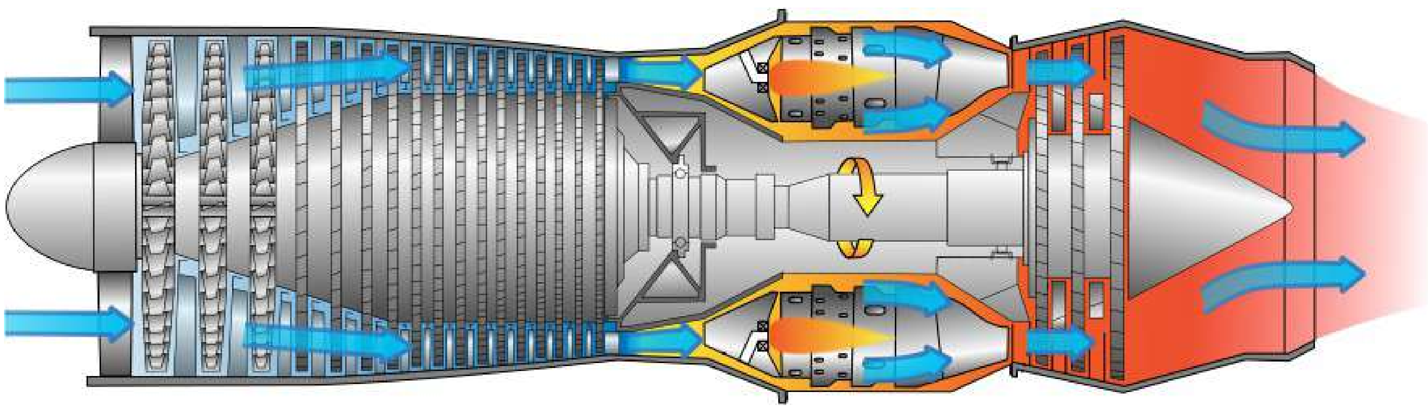
Materials design using machine learning

Experimental data | First principles calc | Physical models



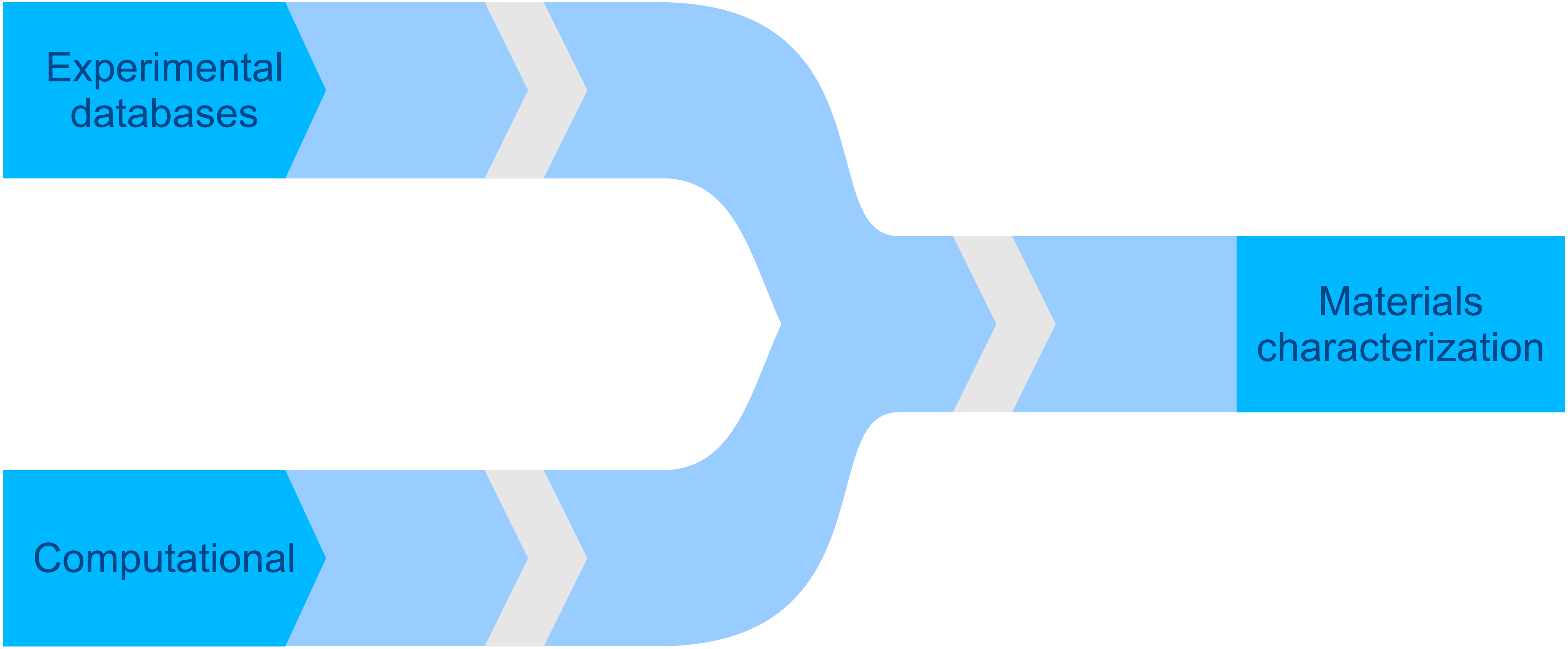
Alloys | Semiconductors | NCM battery | Oil discovery

Schematic of a jet engine

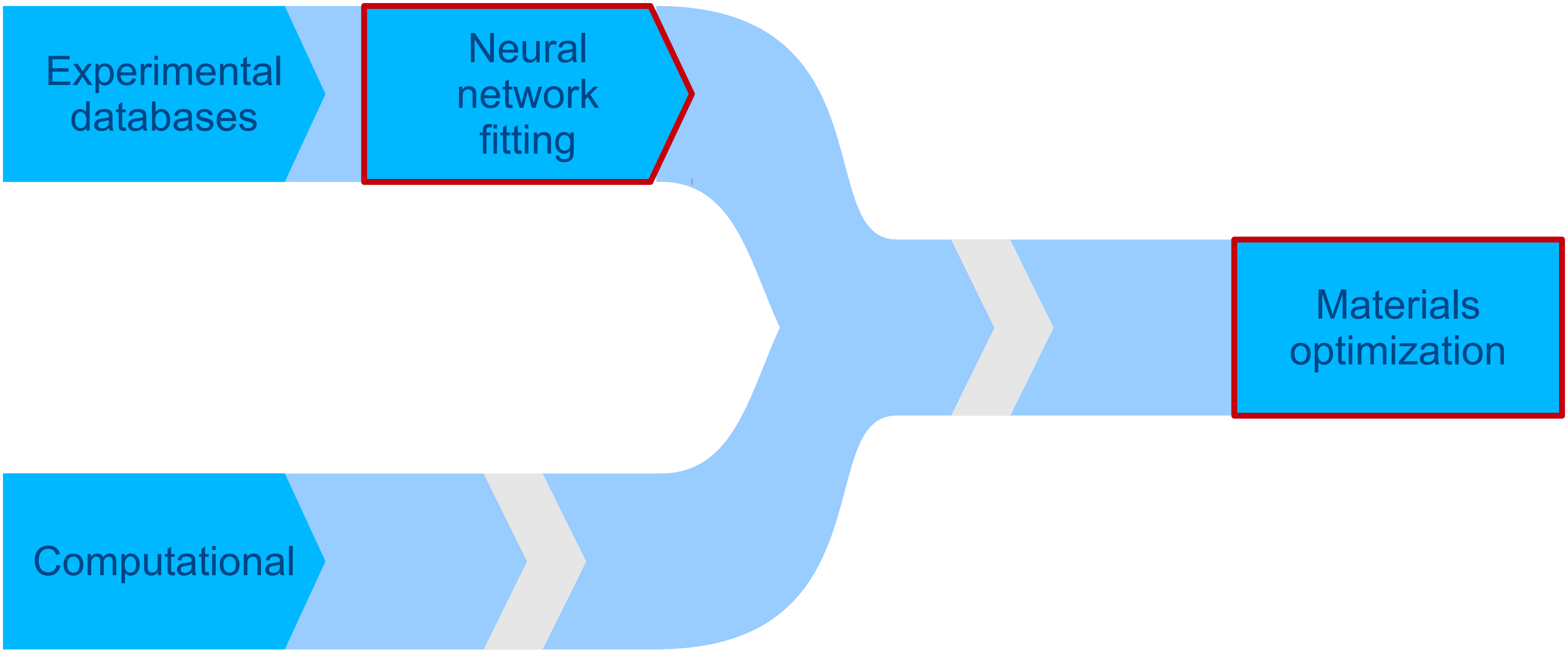


Designing a new alloy – what is required?

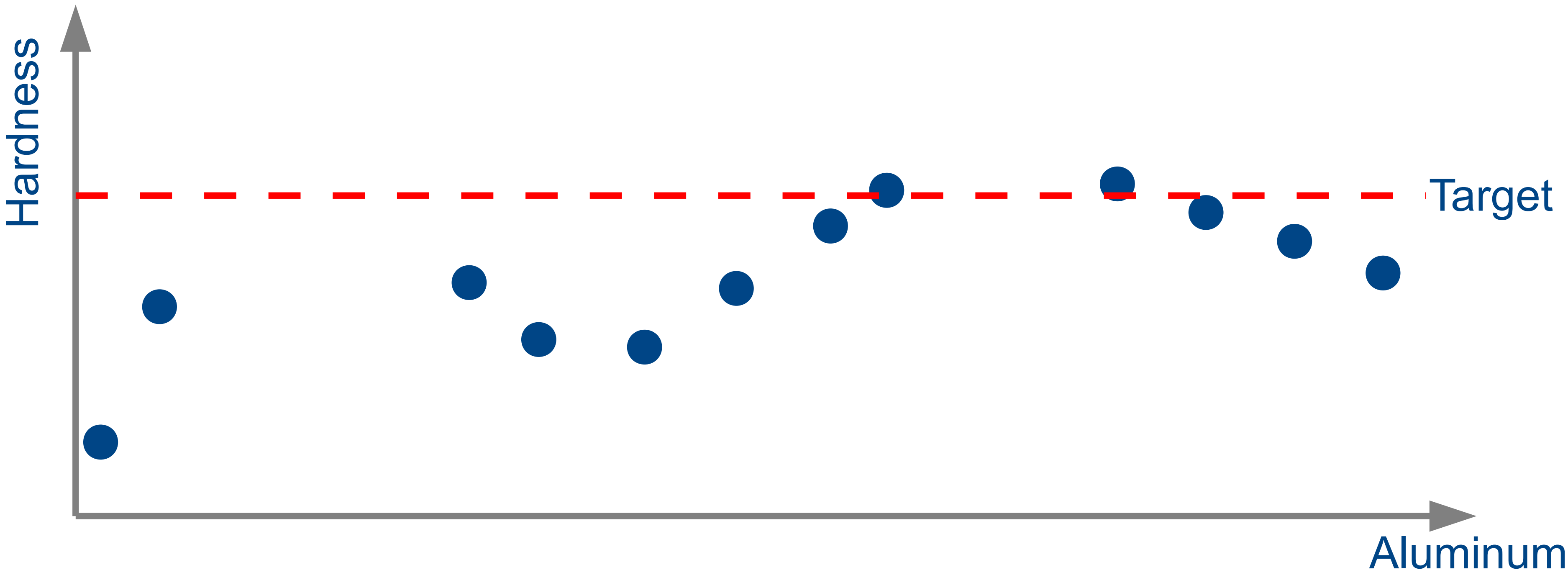
Materials design pipeline



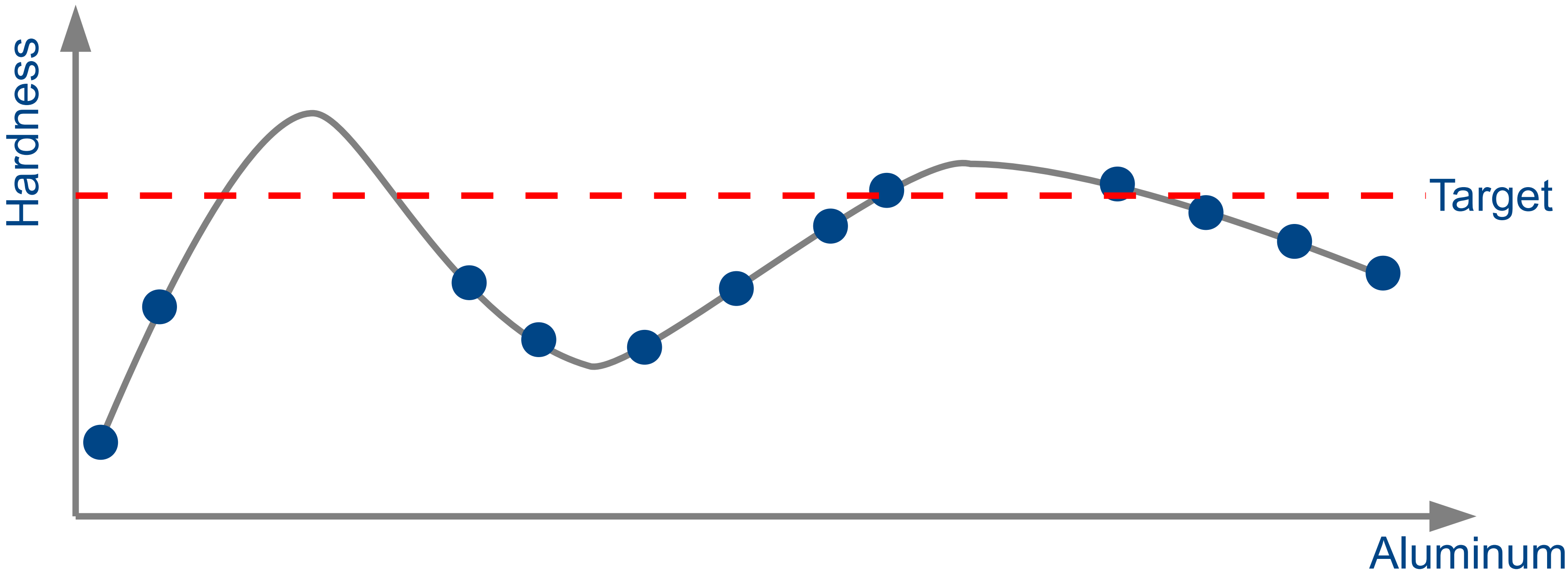
Two new tools in the materials design pipeline



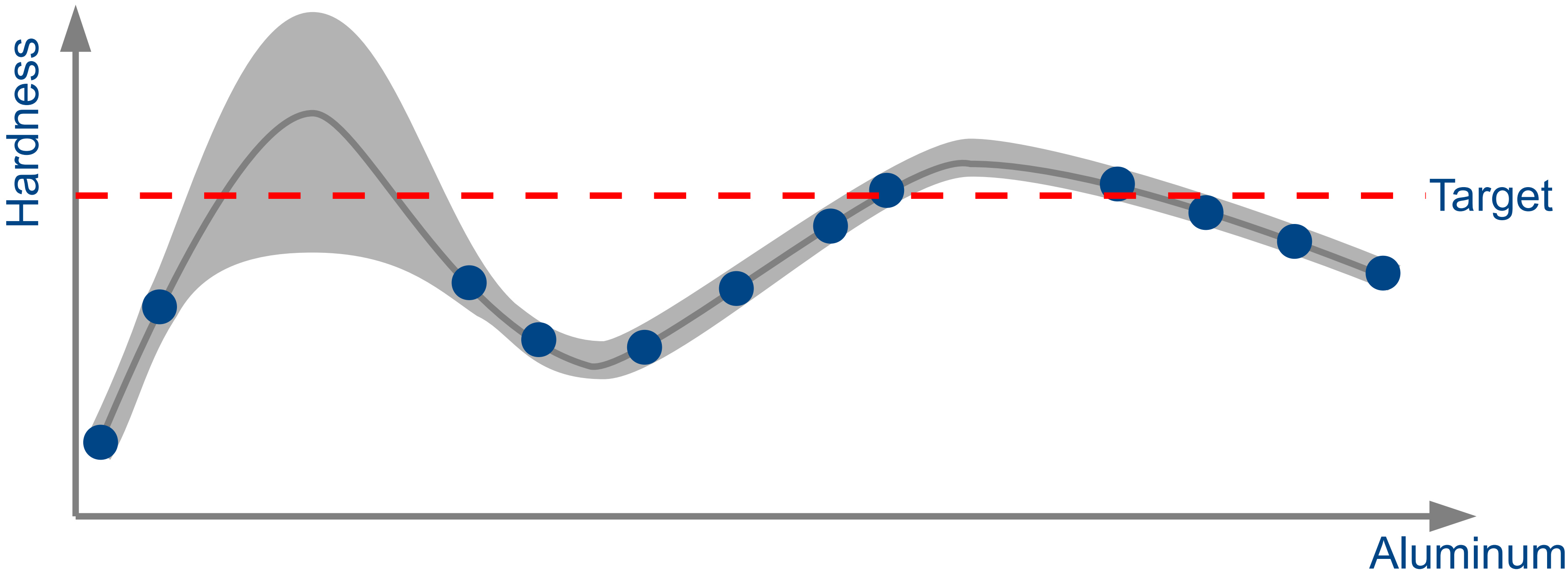
Neural network fitting & optimization



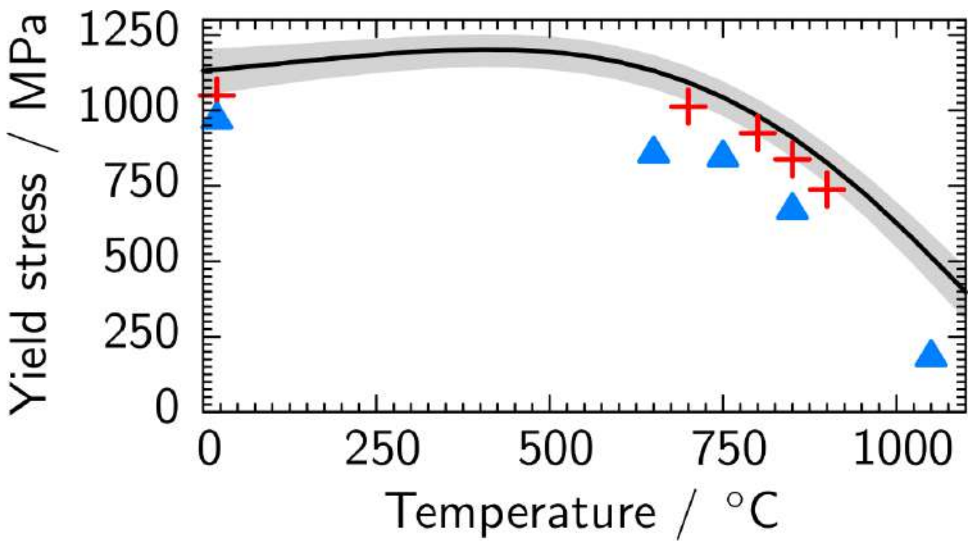
Neural network fitting & optimization



Neural network fitting & optimization

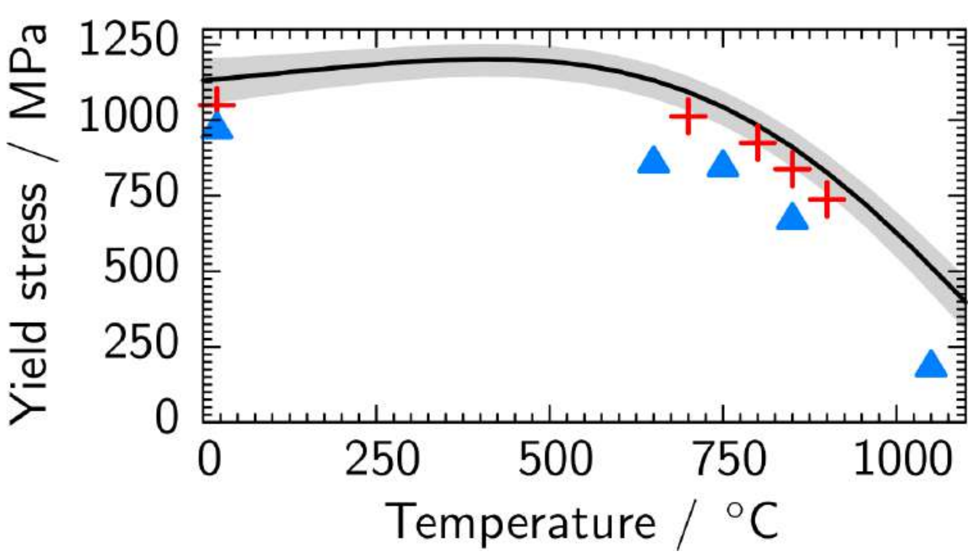


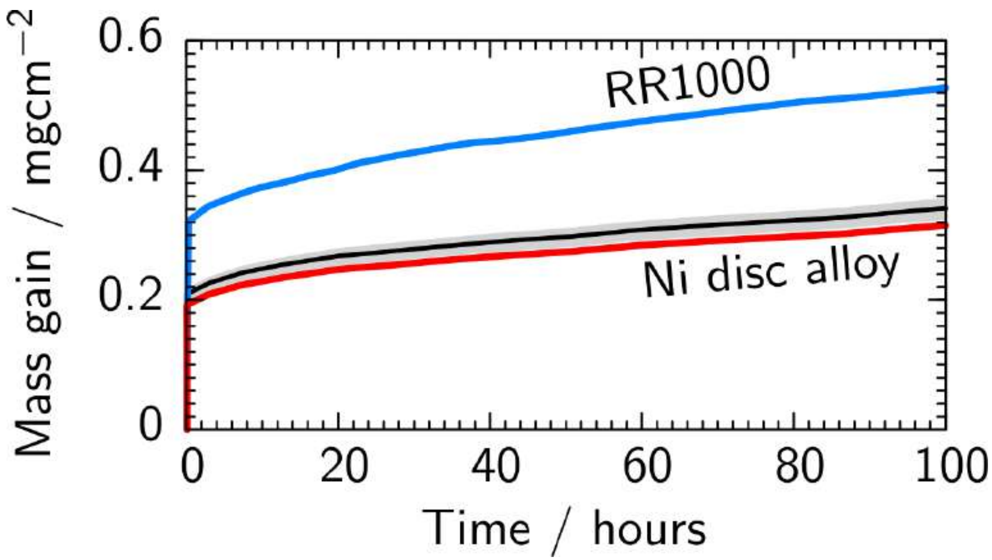
Experimental verification of a Ni-base superalloy



Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

Experimental verification of a Ni-base superalloy

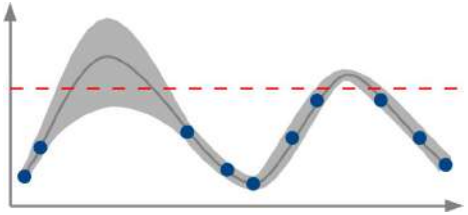




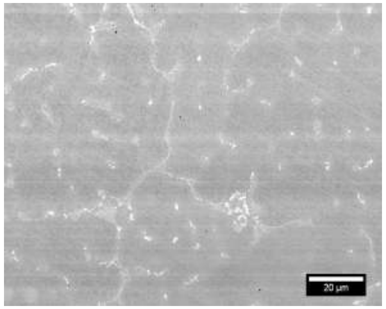
Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

Alloys discovered

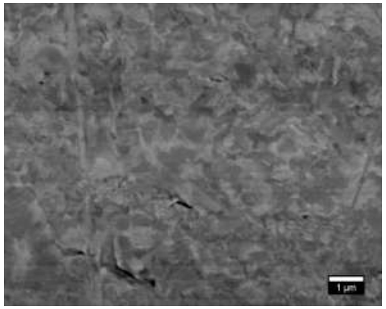
Discovery algorithm
EP14153898.3
US 2014/177578
GB1302743.8



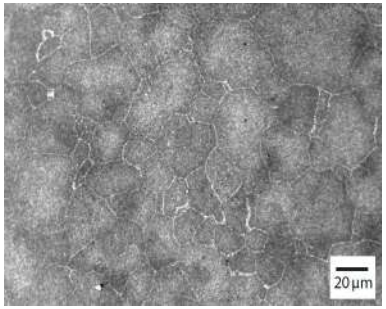
Mo-Hf forging alloy
EP14161255.6
US 2014/223465
GB1307533.8



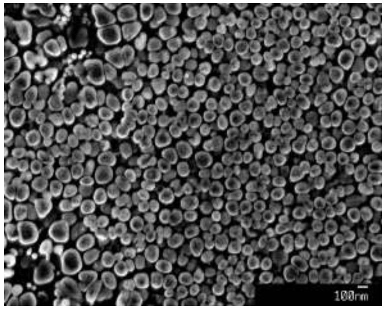
Mo-Nb forging alloy
EP14161529.4
US 2014/224885
GB1307535.3



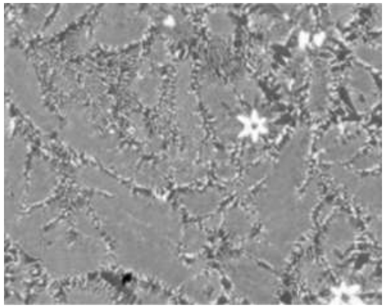
RR1000 grain growth
Acta Materialia, 61, 3378



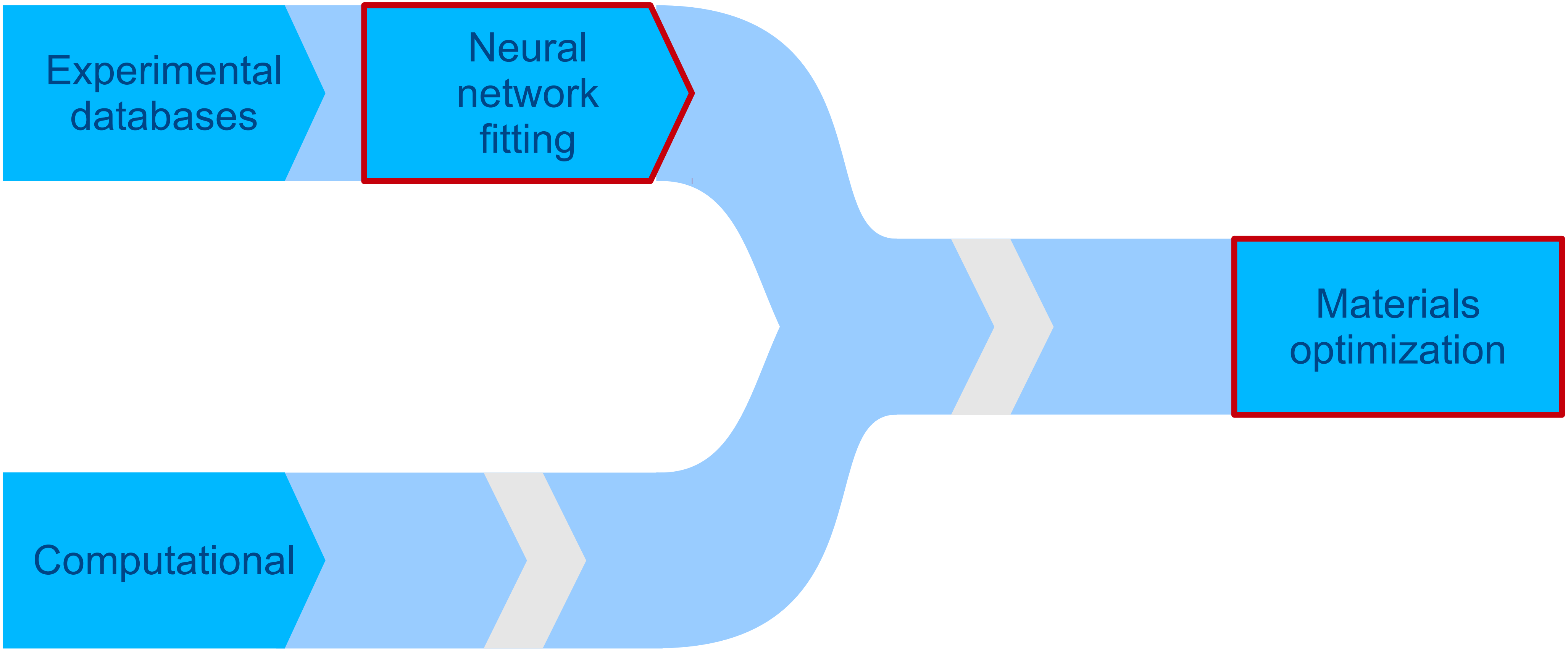
Ni disc alloy
EP14157622.3
US 2013/0052077 A2
GB1408536.9



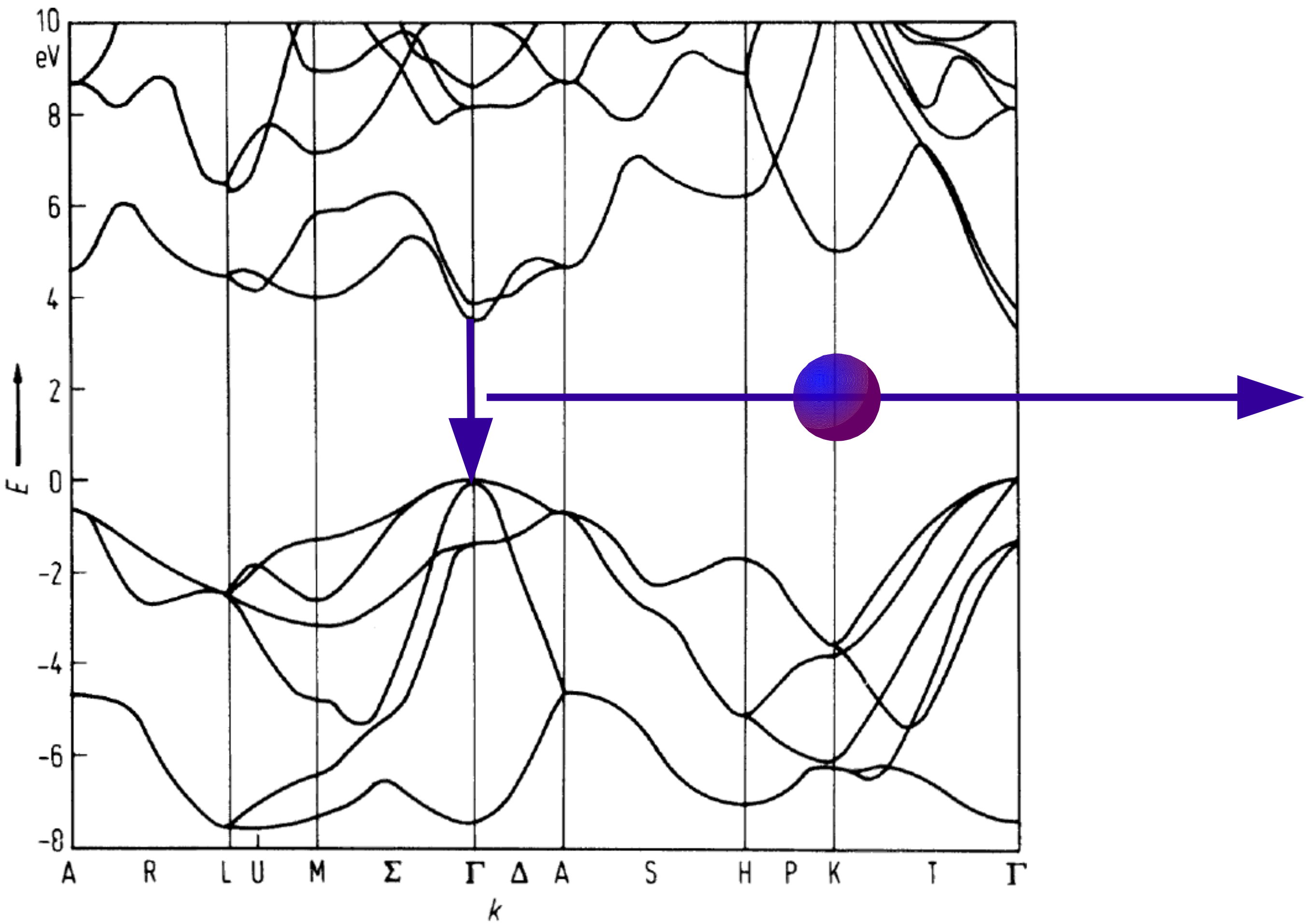
Cr-Cr2Ta alloys
Intermetallics 48, 62



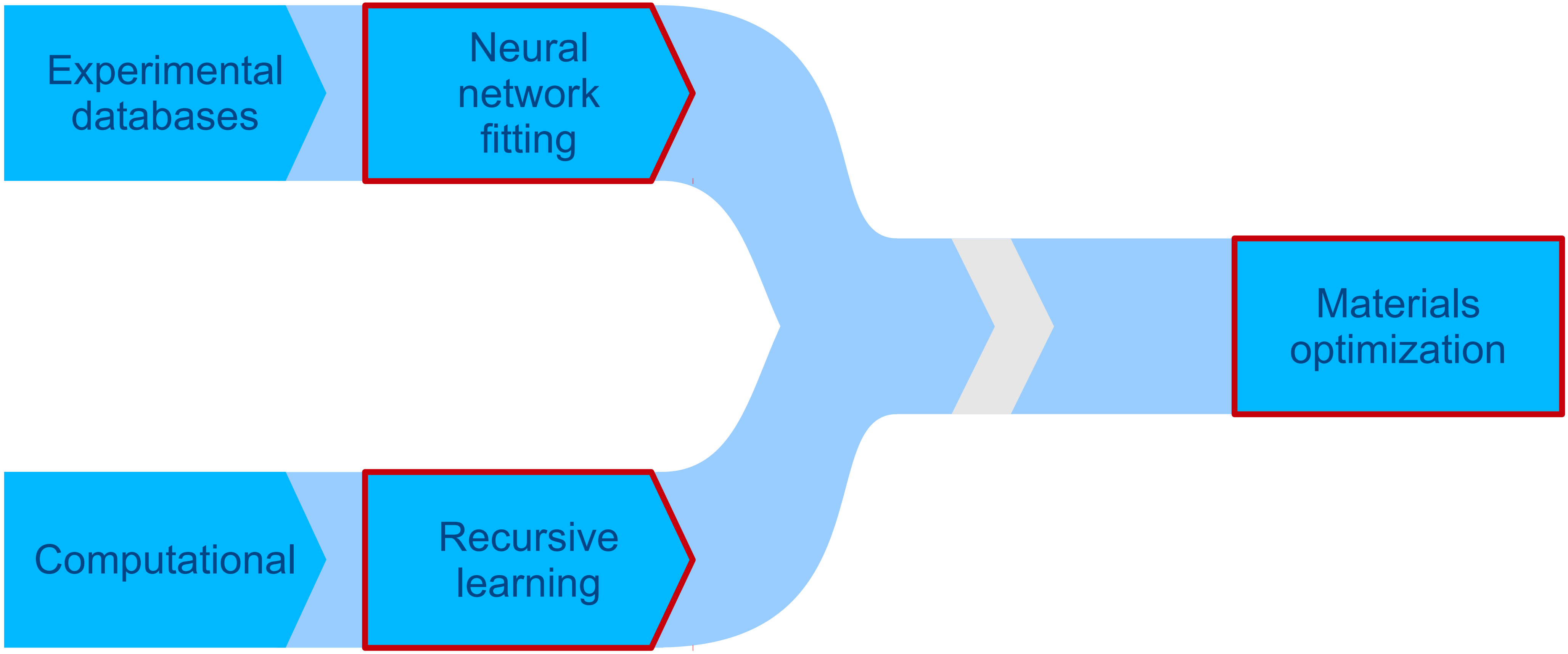
Two new tools in the materials design pipeline



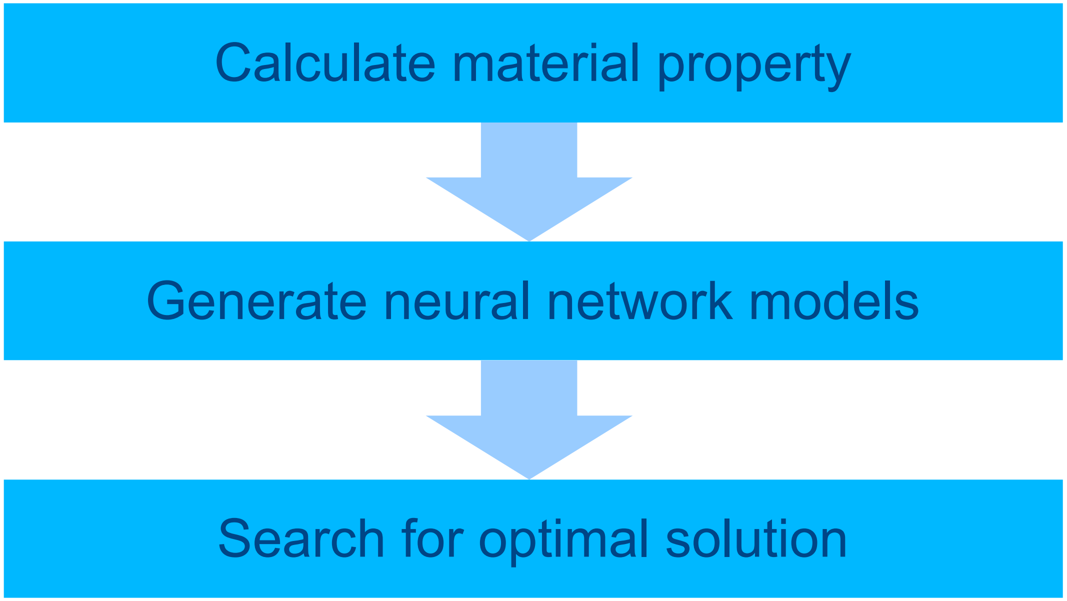
InGaN-base semiconductors for blue LEDs

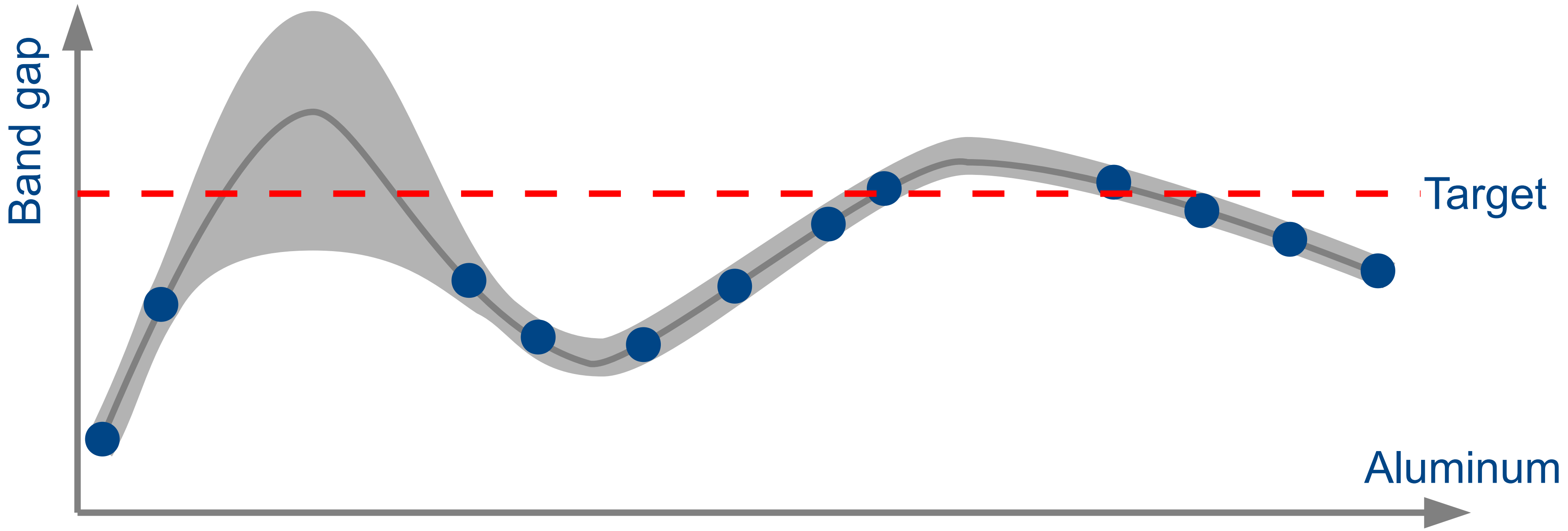


Three new tools in the materials design pipeline

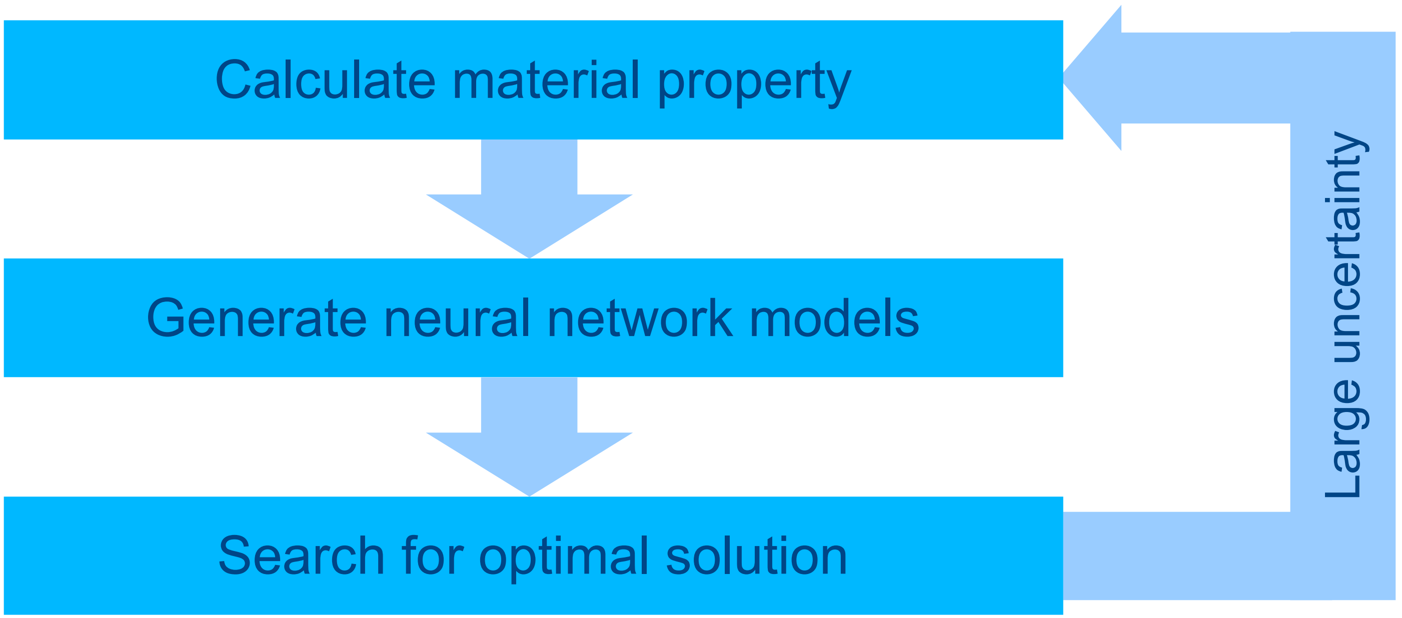


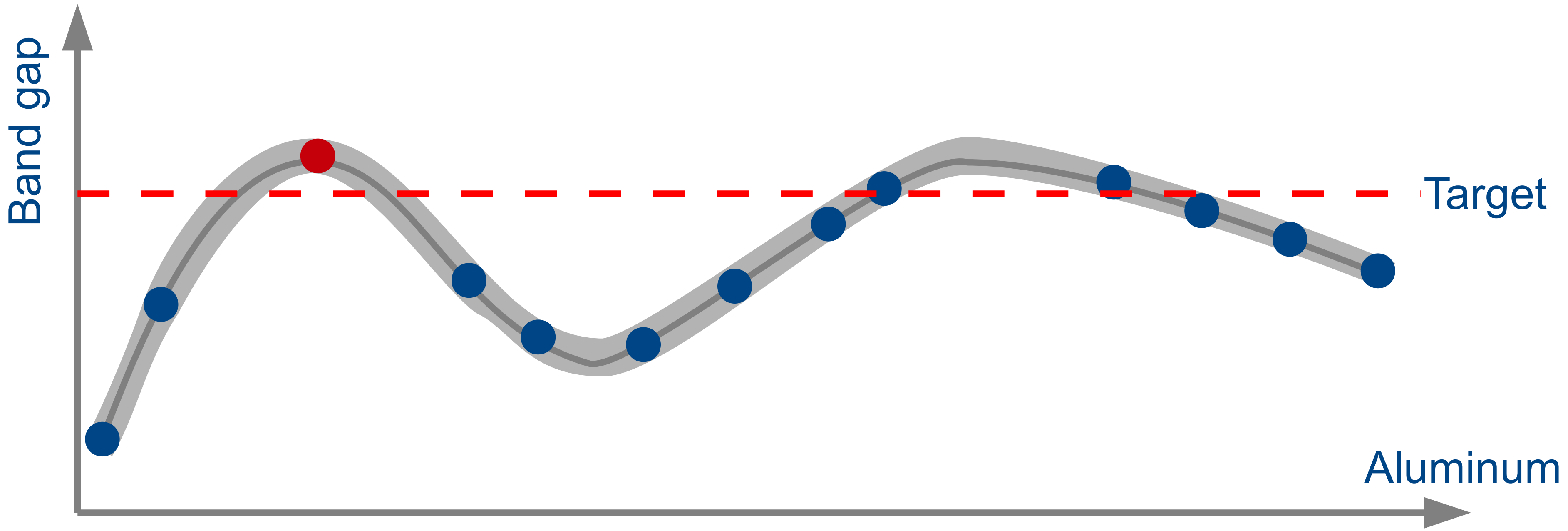
Recursive learning in neural networks



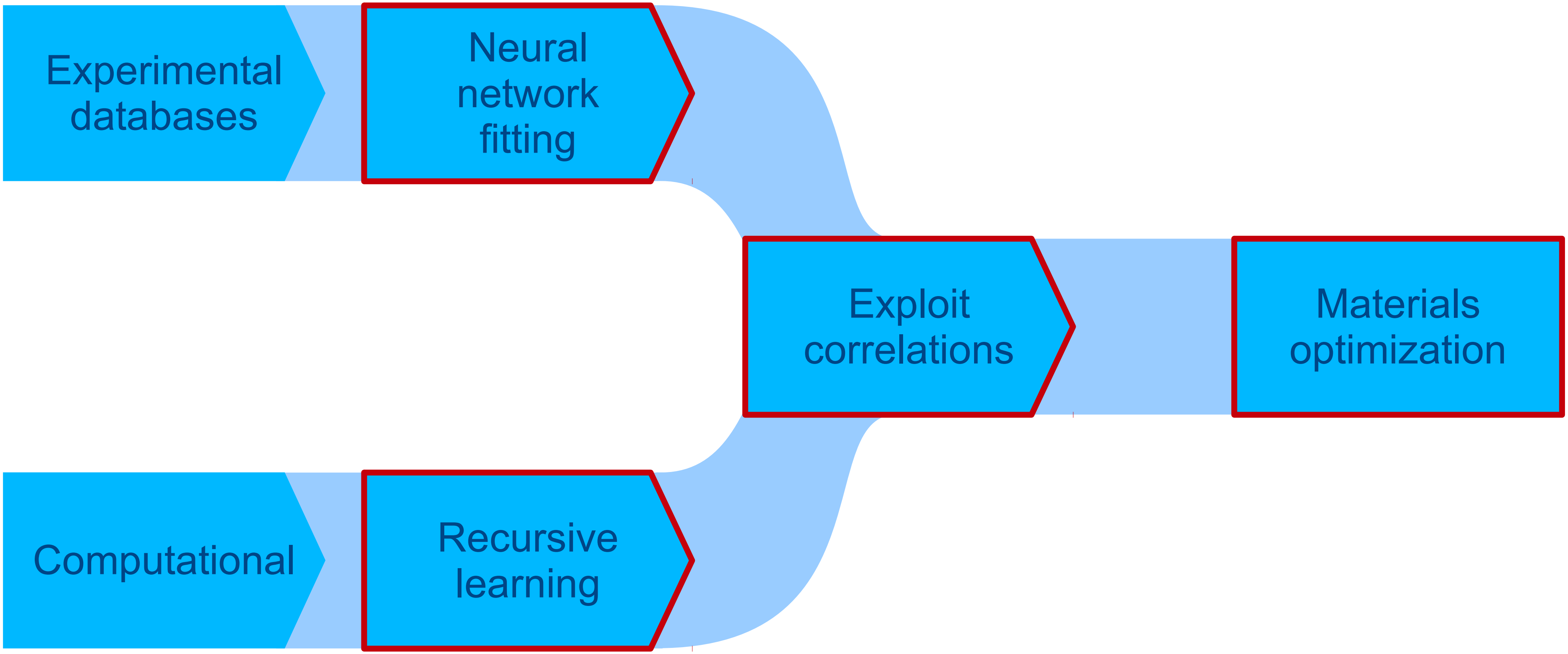


Recursive learning in neural networks

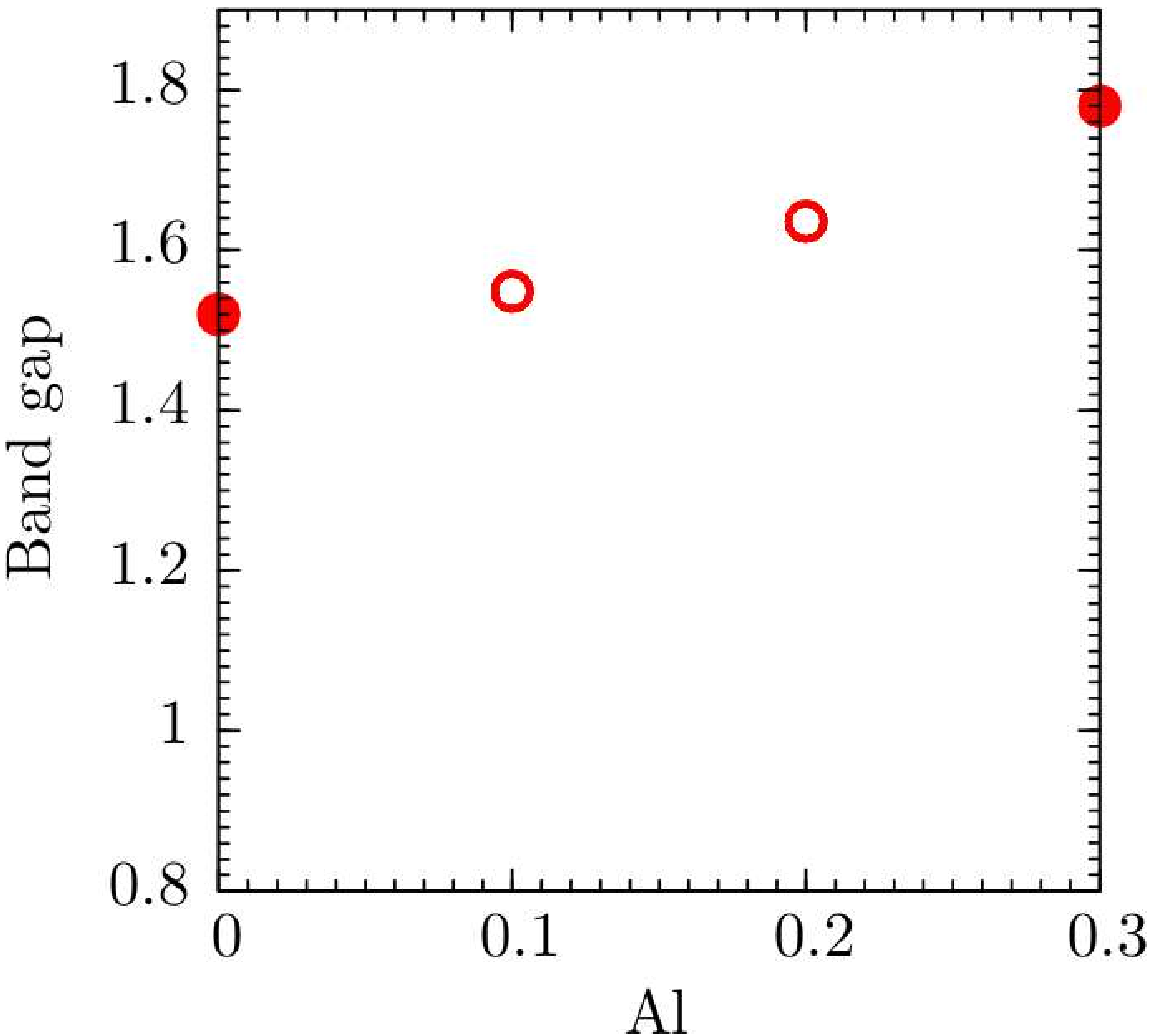




Four new tools in the materials design pipeline

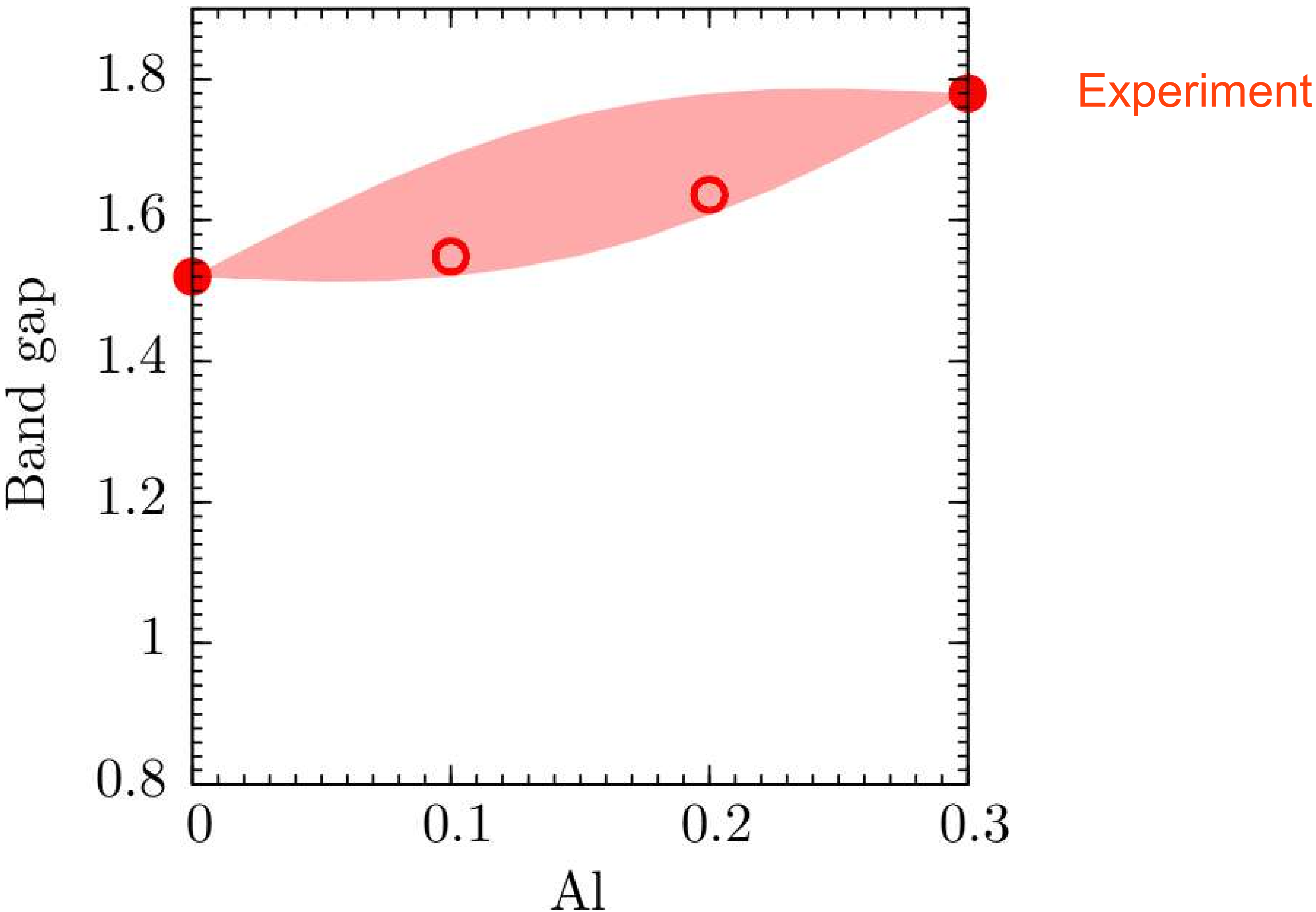


InGaN-base semiconductors: exploiting correlations

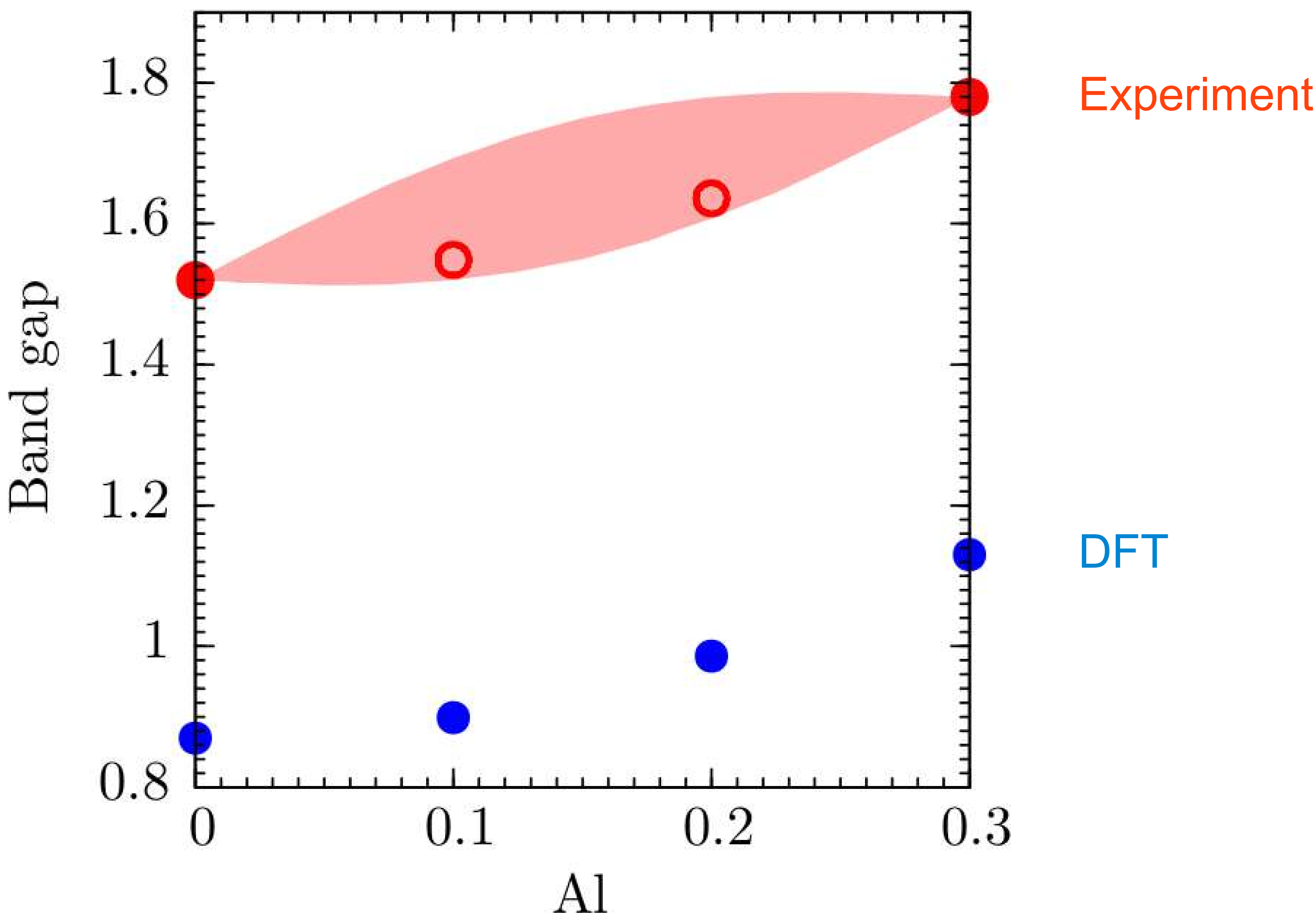


Experiment

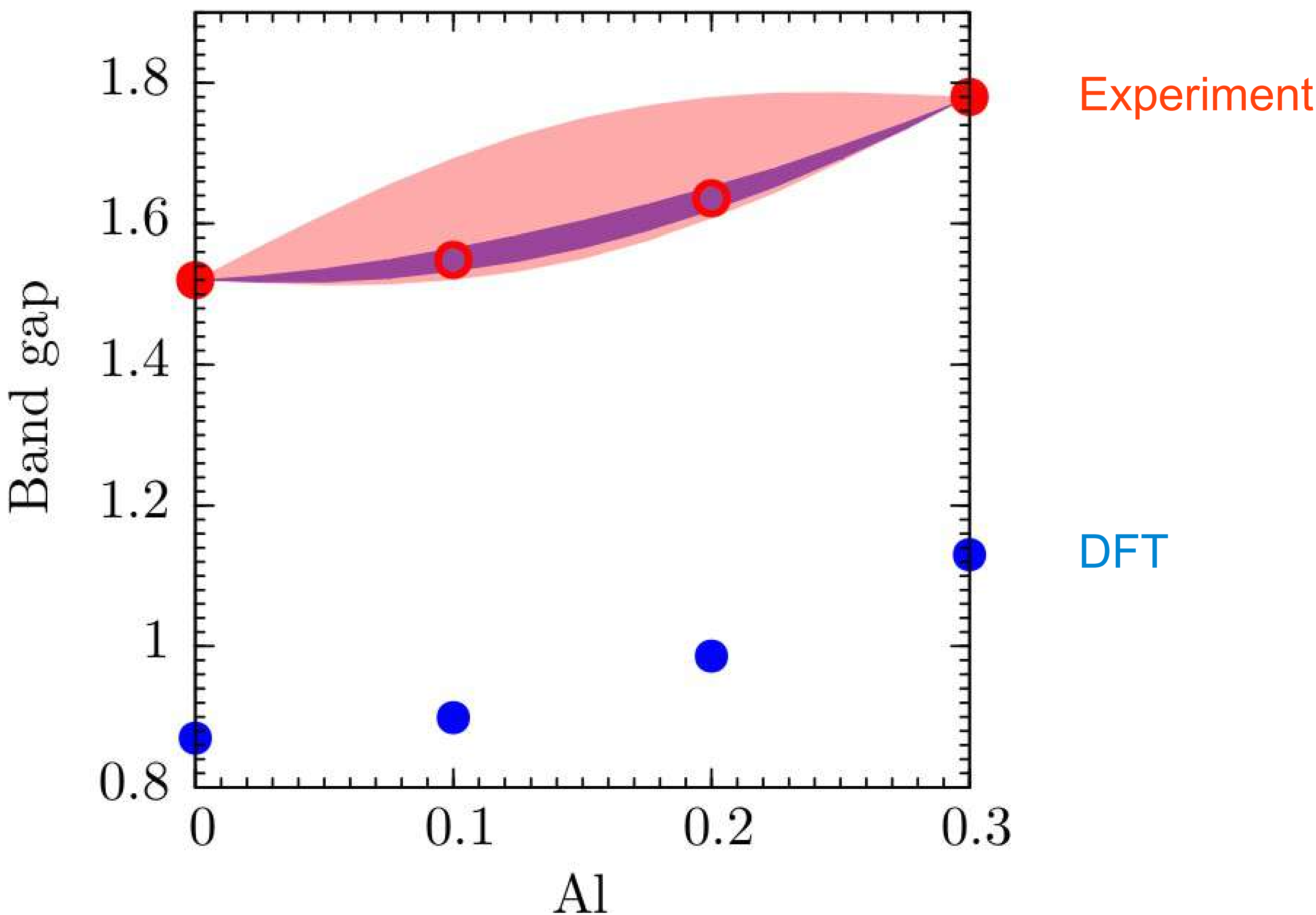
InGaN-base semiconductors: exploiting correlations



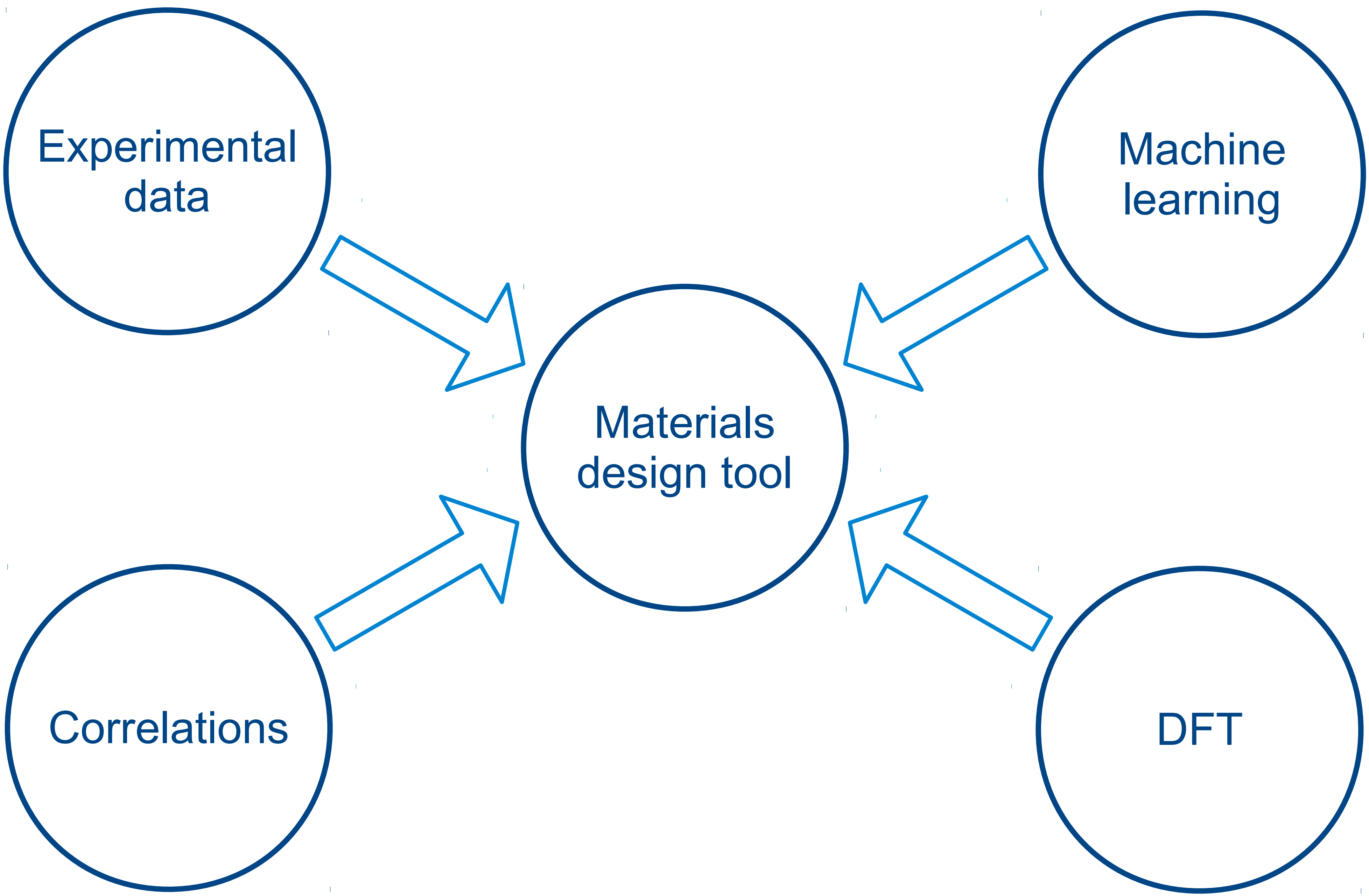
InGaN-base semiconductors: exploiting correlations



InGaN-base semiconductors: exploiting correlations

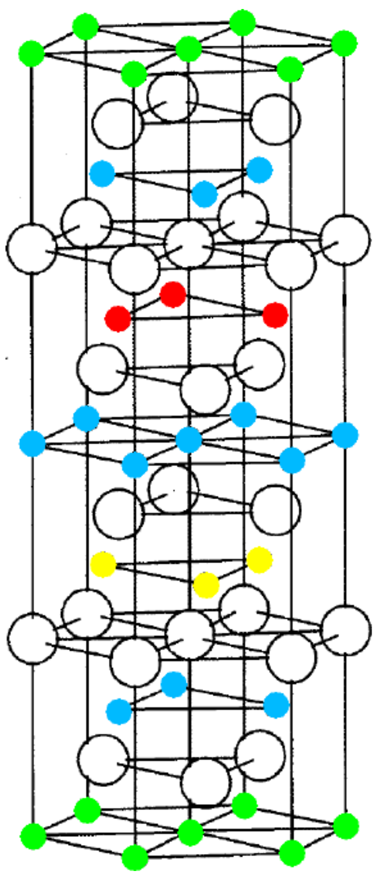


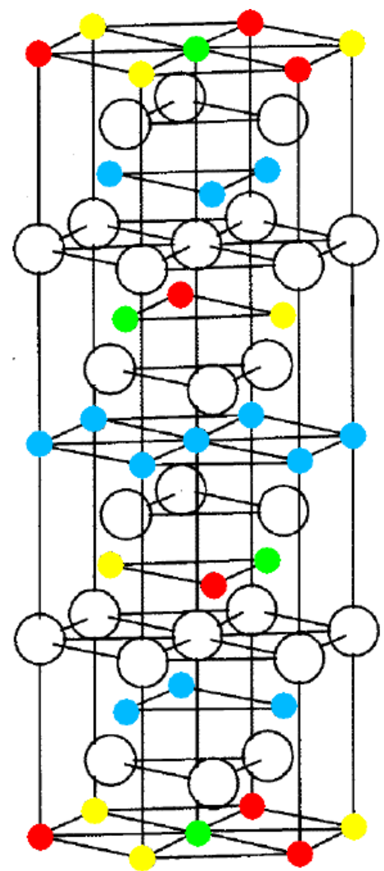
Unification of approaches



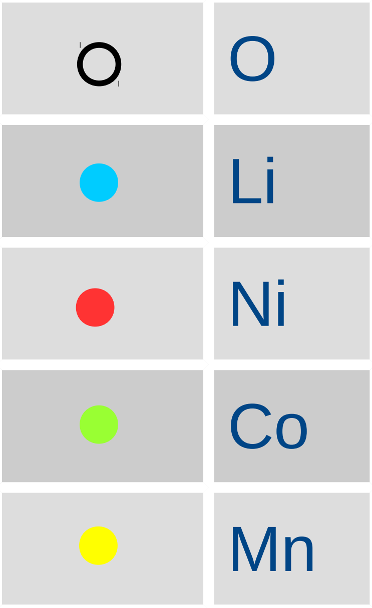
Nickel-Cobalt-Manganese (NCM) battery materials

Nickel-Cobalt-Manganese (NCM-424) battery materials

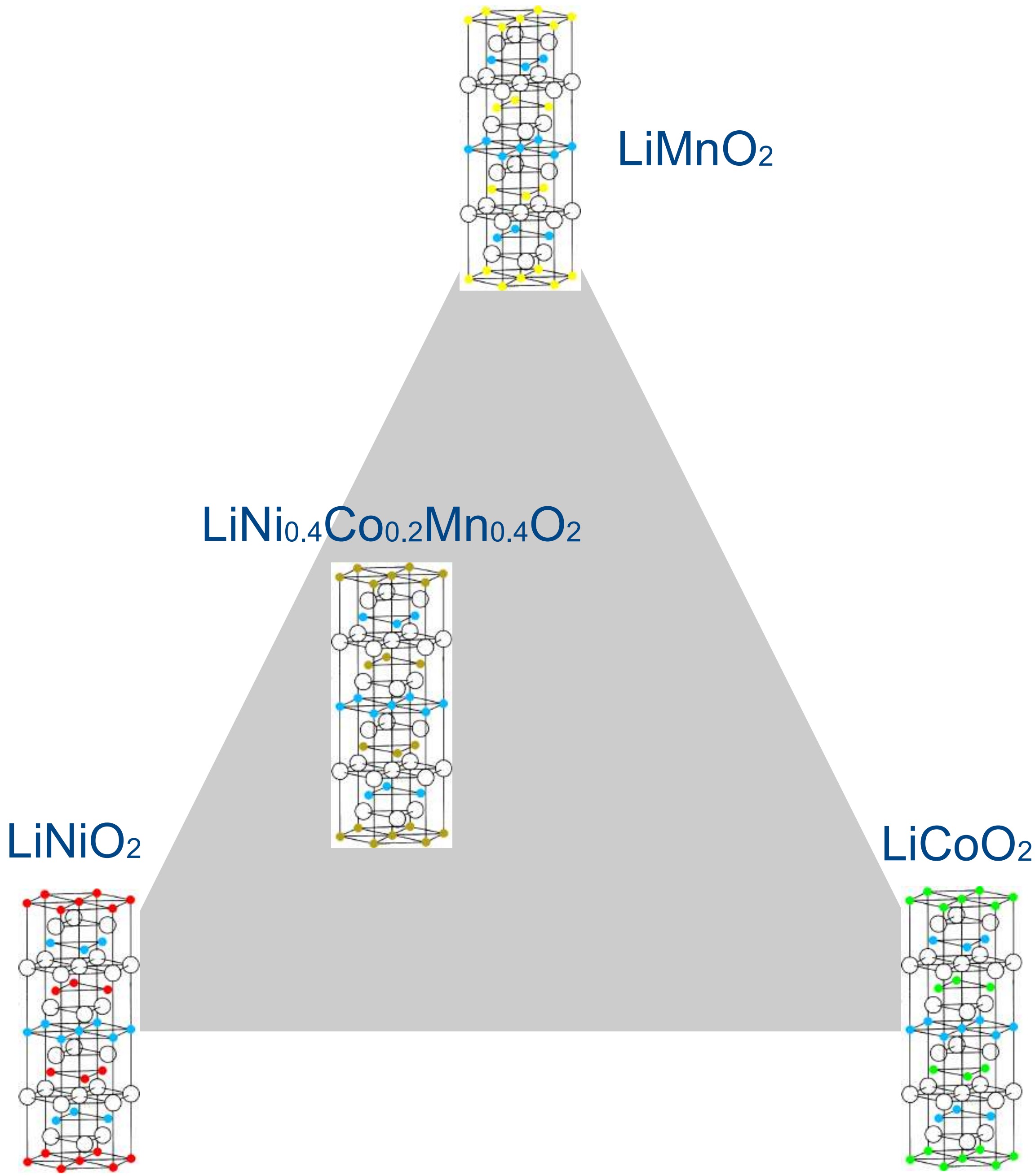




$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$



Approach: Lego: previous approach

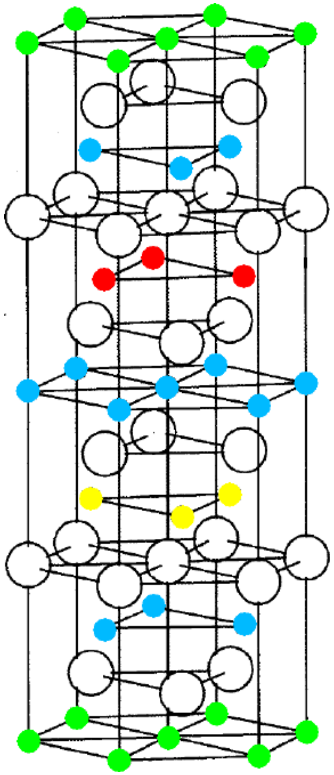


Access any composition

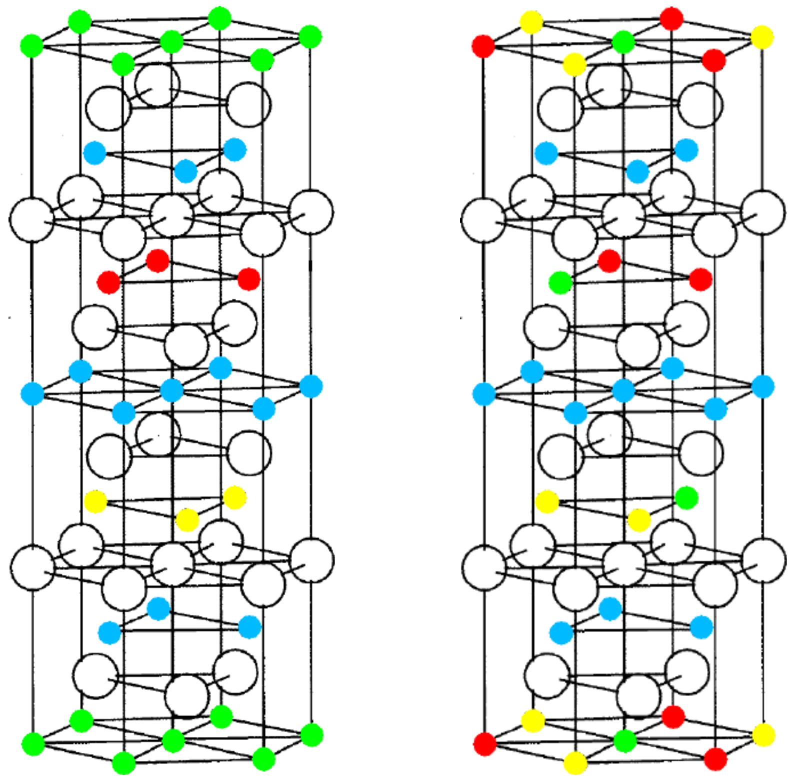
No information on order

No Li migration

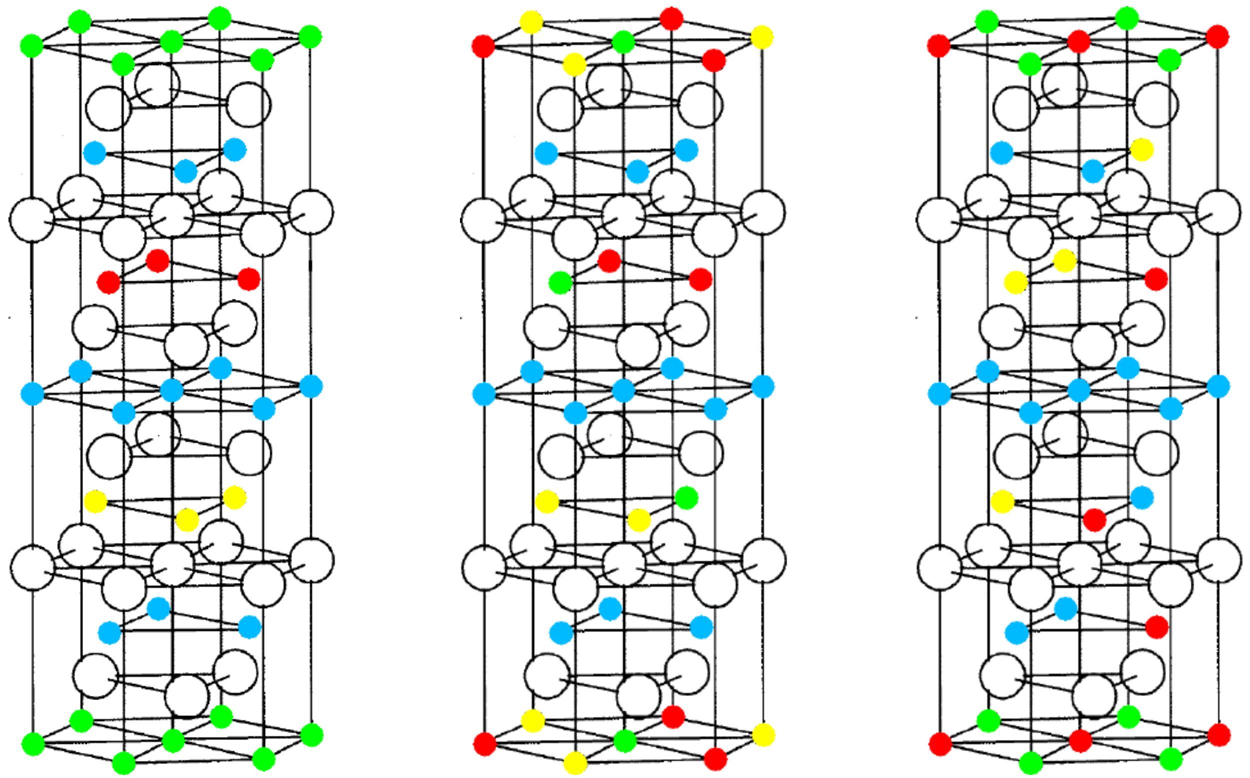
Approach: exhaustive exploration of unit cells



Approach: exhaustive exploration of unit cells



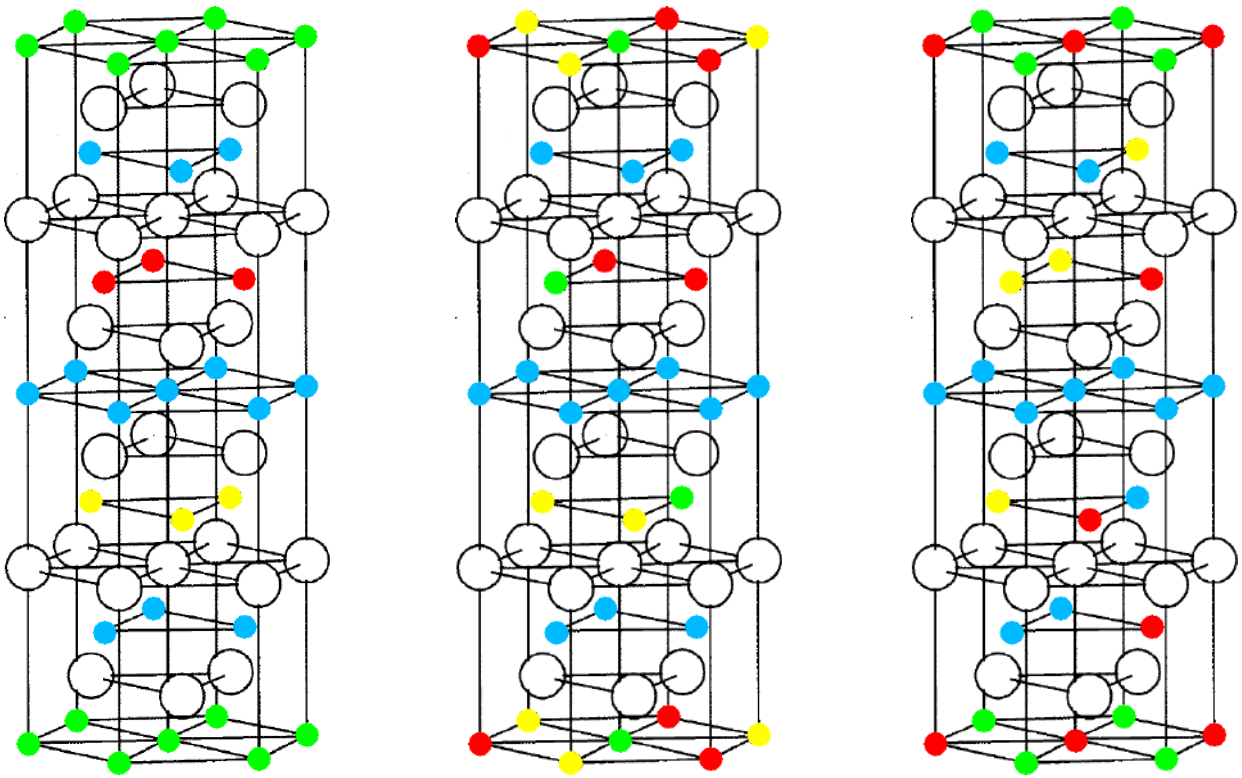
Approach: exhaustive exploration of unit cells



Approach: exhaustive exploration of unit cells

153153000
possible
permutations
=42000 years

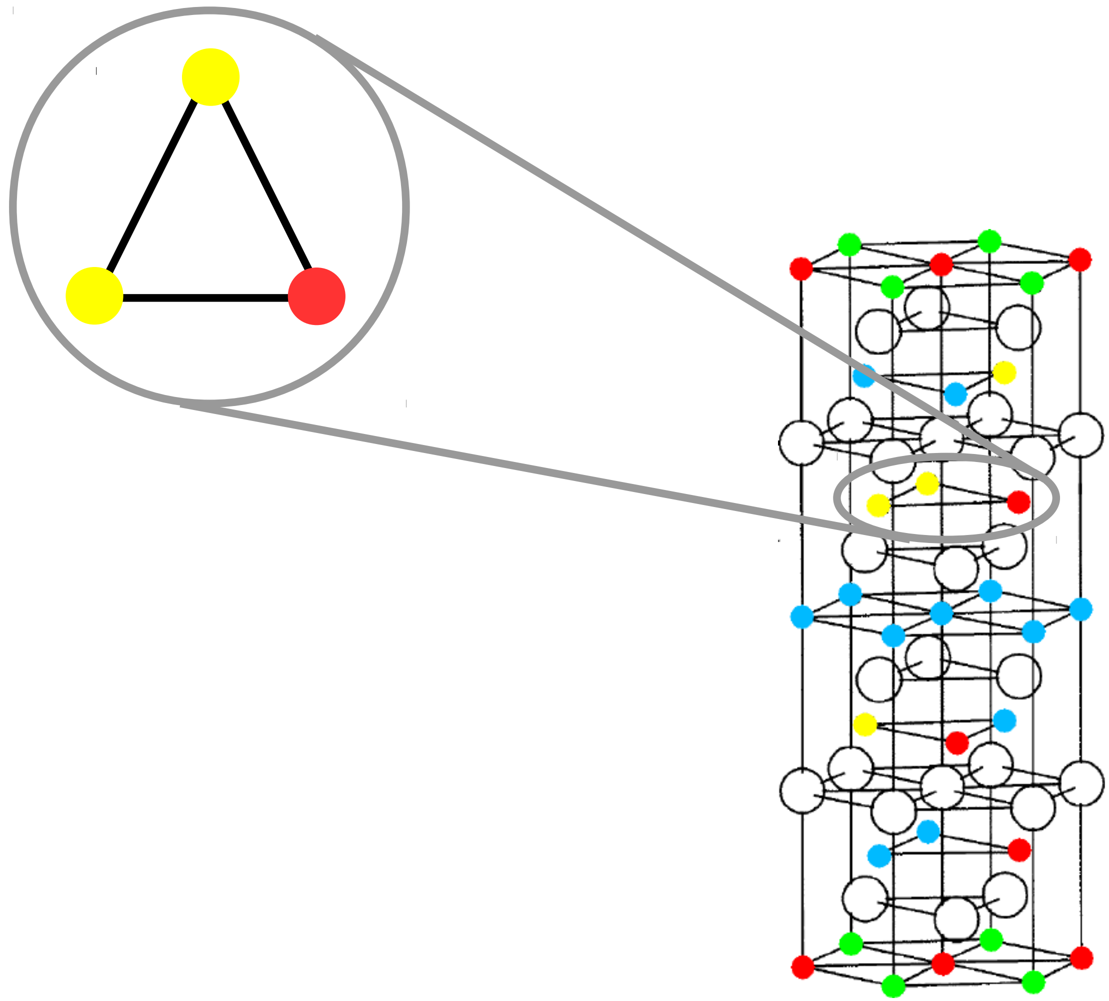
Only examine
order that fits
into the unit cell



Approach: characterize with a local order matrix

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

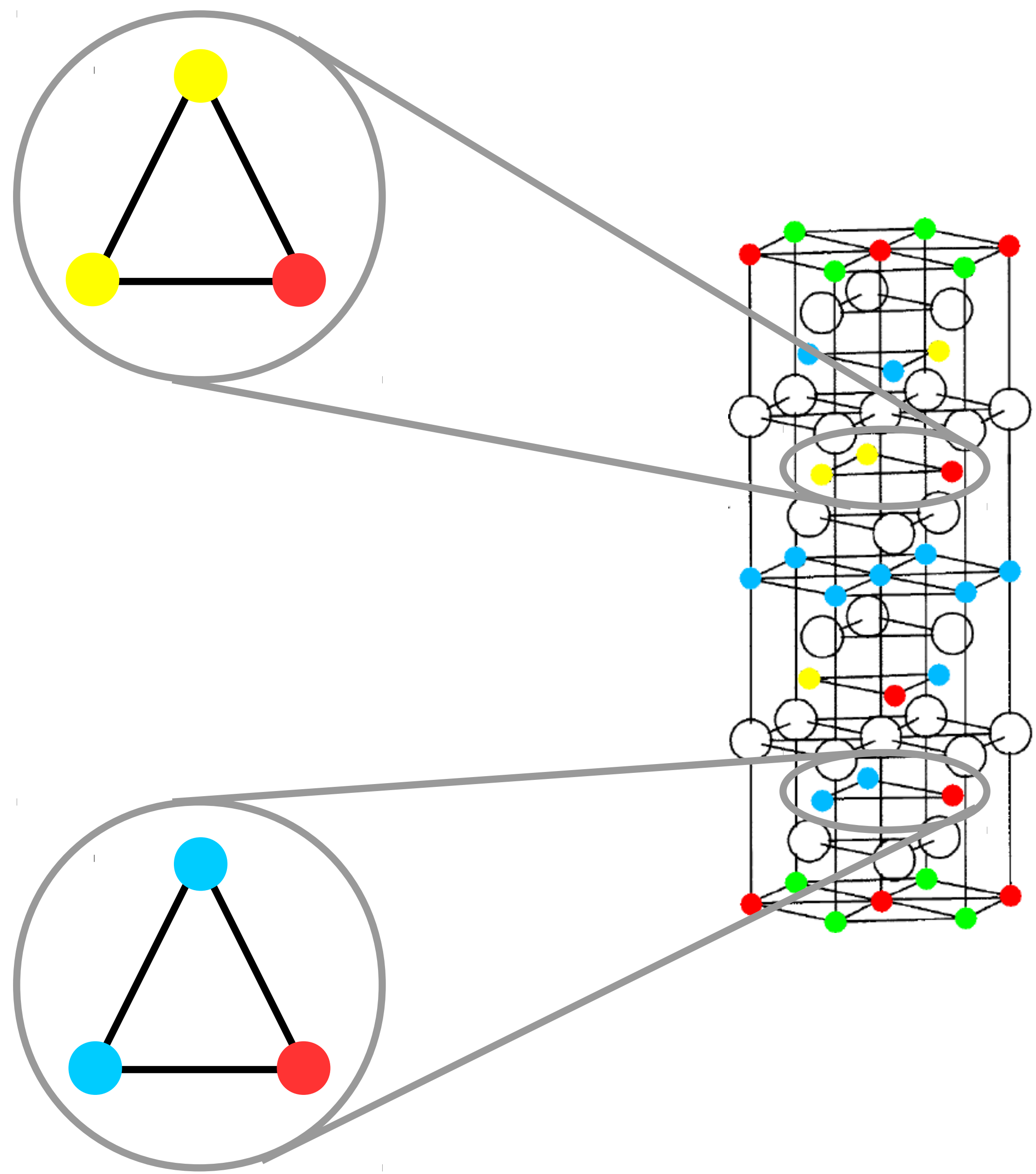
$N_{\text{yellow-red}}=2$



Approach: characterize with a local order matrix

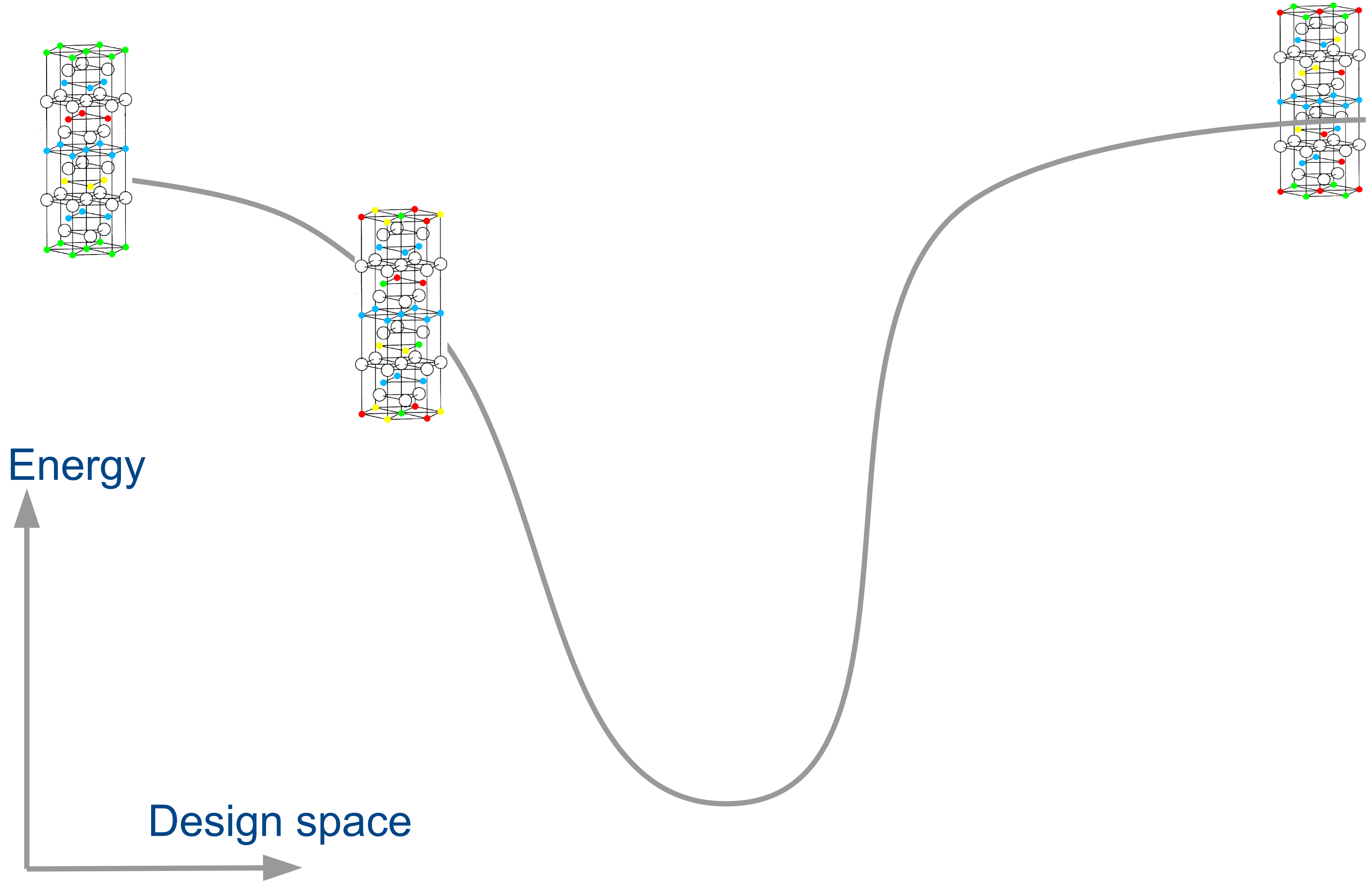
$N_{\text{yellow-yellow}}$=1

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

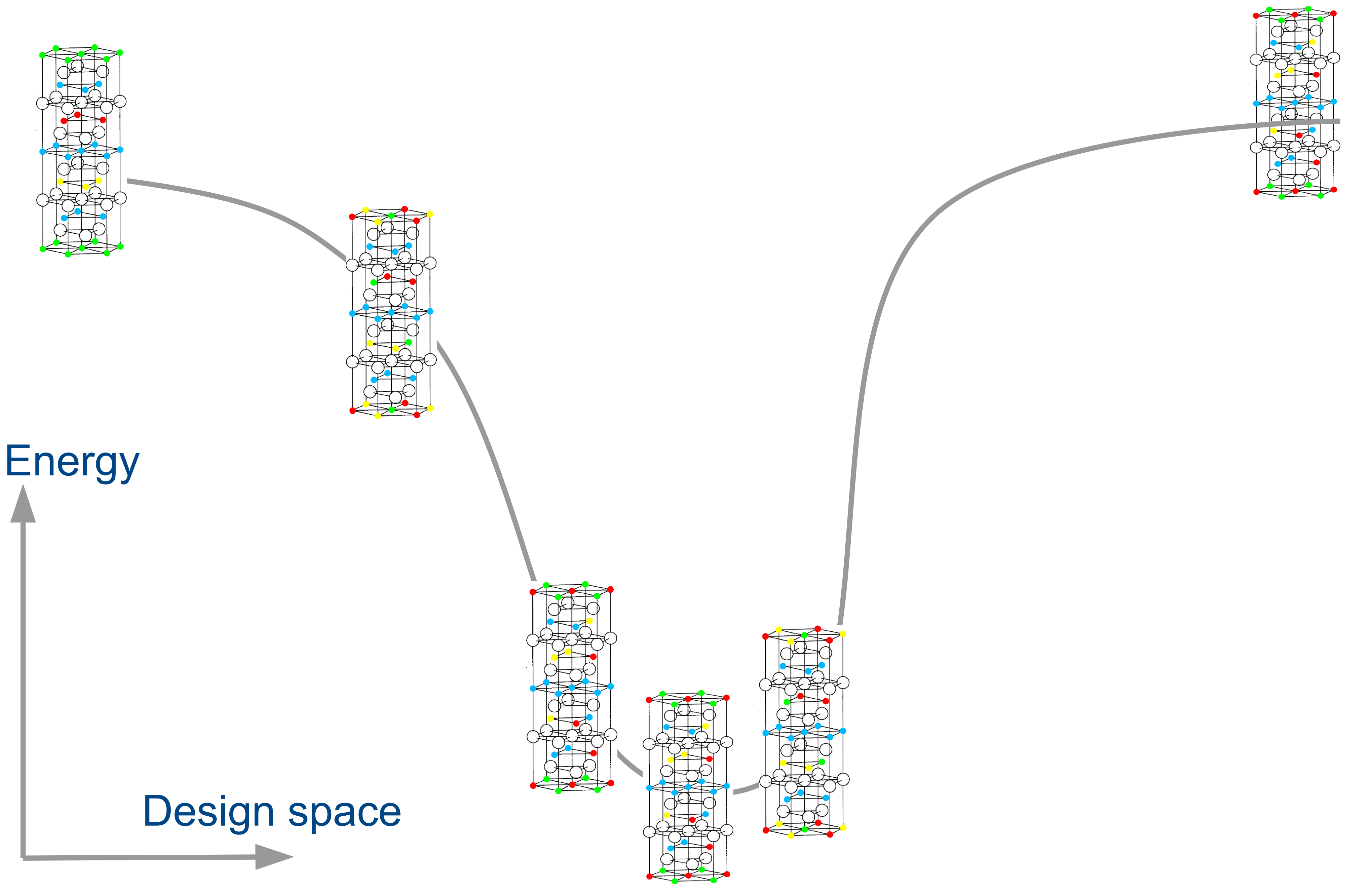


$N_{\text{red migrate}}$=1

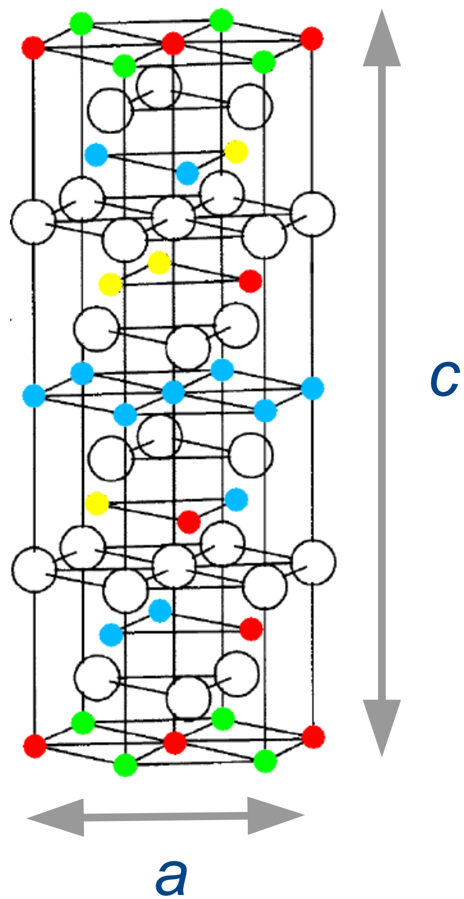
Recursive learning



Recursive learning



Lattice constants



Predictions from the neural network

Structure	a (Å)	c (Å)
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ neural net	2.851	14.269
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ experiment	2.866	14.254

Structure	a (Å)	c (Å)
$LiNiO_2$	2.9108	14.1099
$LiCoO_2$	2.8473	13.9214
$LiMnO_2$	2.7614	14.7740
$LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ layered	2.8827	14.1067

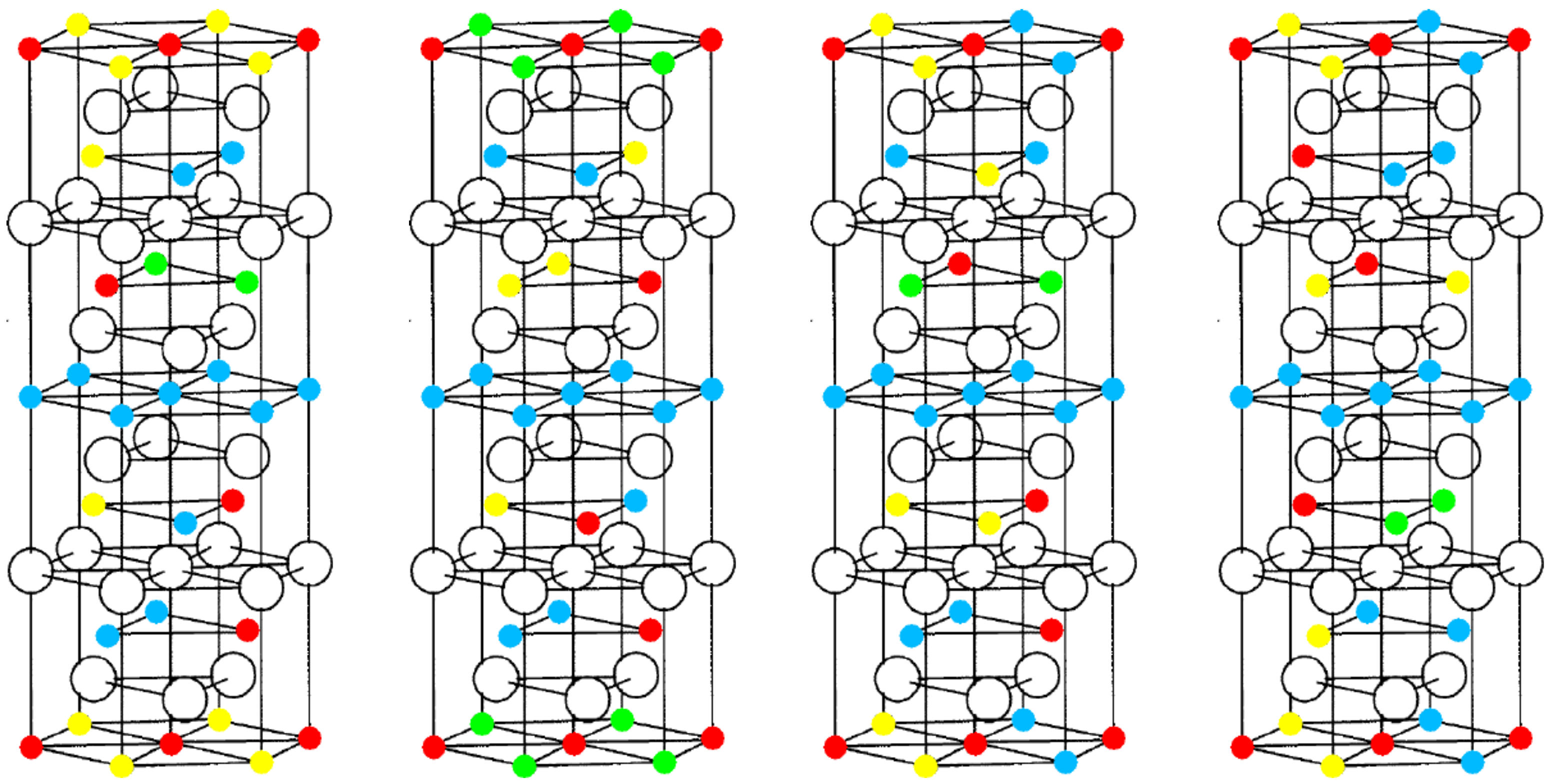
Local order matrix

Matrix element	Optimal	Expected if random
$N_{Co\text{-}Co}$	0.34	0.75
$N_{Ni\text{-}Ni}$	0.16	0.75
$N_{Mn\text{-}Mn}$	0.09	0.75
$N_{Li\text{-}Li}$	0.08	0.75
$N_{Co\text{-}Ni}$	2.5	2.25
$N_{Co\text{-}Mn}$	0.2	2.25
$N_{Ni\text{-}Mn}$	3.4	2.25
$N_{Ni\text{-}Li}$	0.32	2.25
$N_{Co\text{-}Li}$	0.21	2.25
$N_{Mn\text{-}Li}$	1.37	2.25
N_{Ni}	1.82	0
N_{Co}	0.02	0
N_{Mn}	0.01	0

Local order matrix within a single unit cell

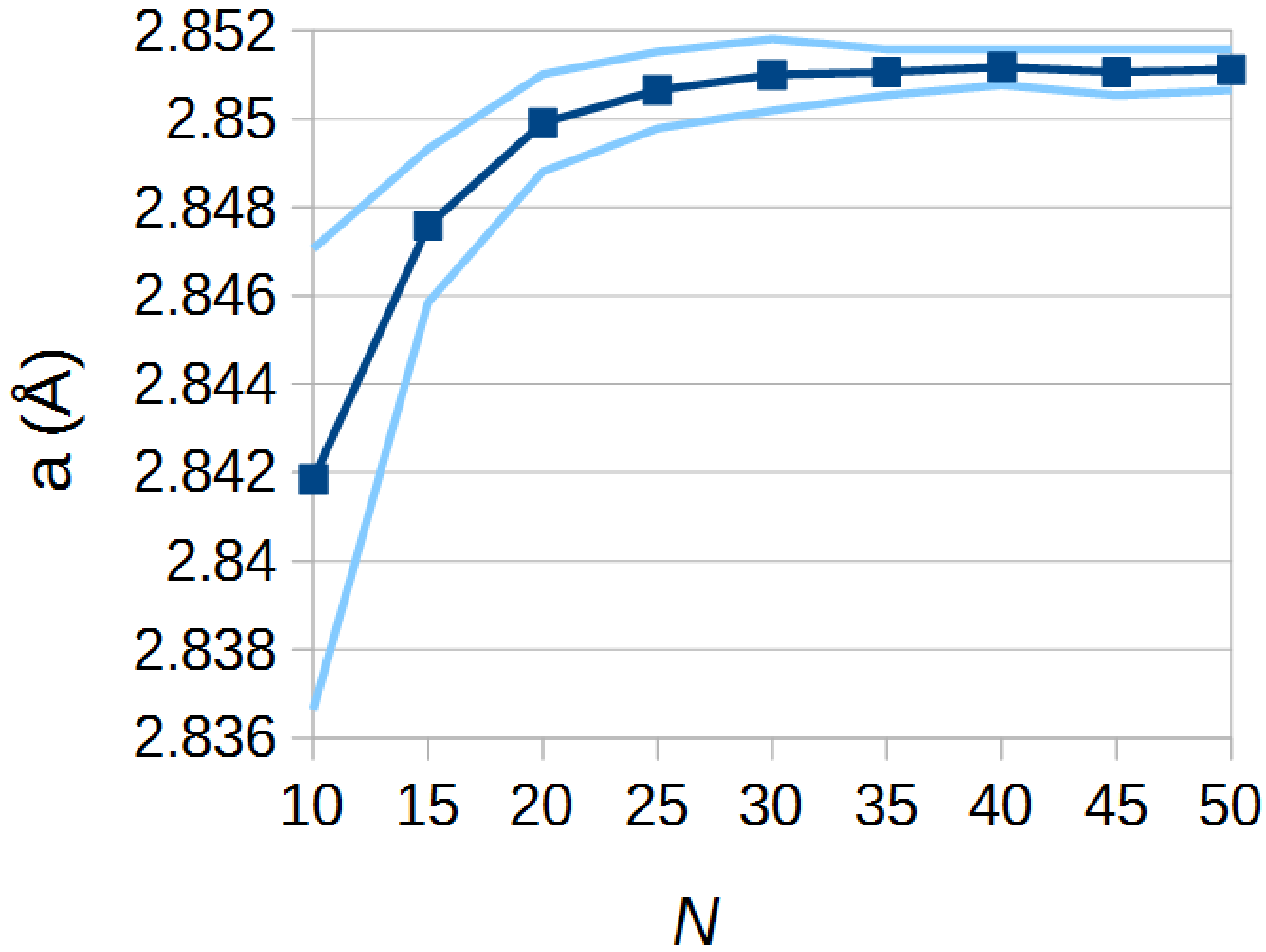
Matrix element	Optimal	Achievable in single unit cell
$N_{Co\text{-}Co}$	0.34	1
$N_{Ni\text{-}Ni}$	0.16	0
$N_{Mn\text{-}Mn}$	0.09	1
$N_{Li\text{-}Li}$	0.08	0
$N_{Co\text{-}Ni}$	2.5	2
$N_{Co\text{-}Mn}$	0.2	0
$N_{Ni\text{-}Mn}$	3.4	3
$N_{Ni\text{-}Li}$	0.32	1
$N_{Co\text{-}Li}$	0.21	0
$N_{Mn\text{-}Li}$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

Four representative unit cells



E=-18430.0eV	*E*=-18428.2eV	*E*=-18428.1eV	*E*=-18429.0eV	Experiment
a=2.863Å	*a*=2.852Å	*a*=2.857Å	*a*=2.860Å	*a*=2.866Å
c=14.212Å	*c*=14.274Å	*c*=14.254Å	*c*=14.221Å	*a*=14.254Å

How many calculations are required



Prospects for the future

Test four new tools uniquely unified within a materials design tool to maximize learning from data

Build on these platforms to respond to future GRO and Samsung collaboration needs

Continue high-level interaction with SAIT Europe and SAIT HQ teams to work on most relevant needs and outcomes