UNIVERSITY OF CAMBRIDGE

Machine learning in materials design, oil exploration, and beyond

Gareth Conduit & Bartomeu Monserrat

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)

Theory of Condensed Matter Group, Department of Physics

Stone age: 3.4 million BC – 2000 BC

1.9 million BC
Stone age

Bronze age: 2000 BC – 1000 BC

1.9 million BC
Stone age

1200 BC
Bronze age

Iron age: 1000 BC – 1850 AD

1.9 million BC
Stone age

1200 BC
Bronze age

300 BC
Iron age

Steel age: 1850 AD – 1930 AD

1.9 million BC
Stone age

1200 BC
Bronze age

300 BC
Iron age

1906
Steel age

Scientific age

1930s
Plastics

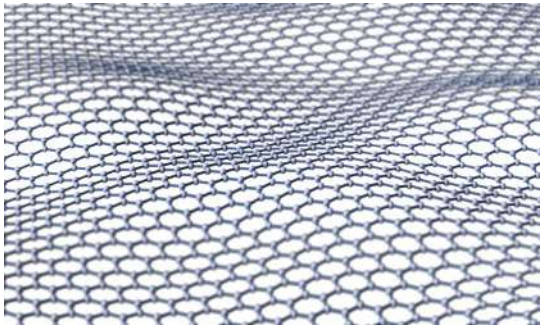
1940s
Semiconductors

Scientific age

1930s
Plastics

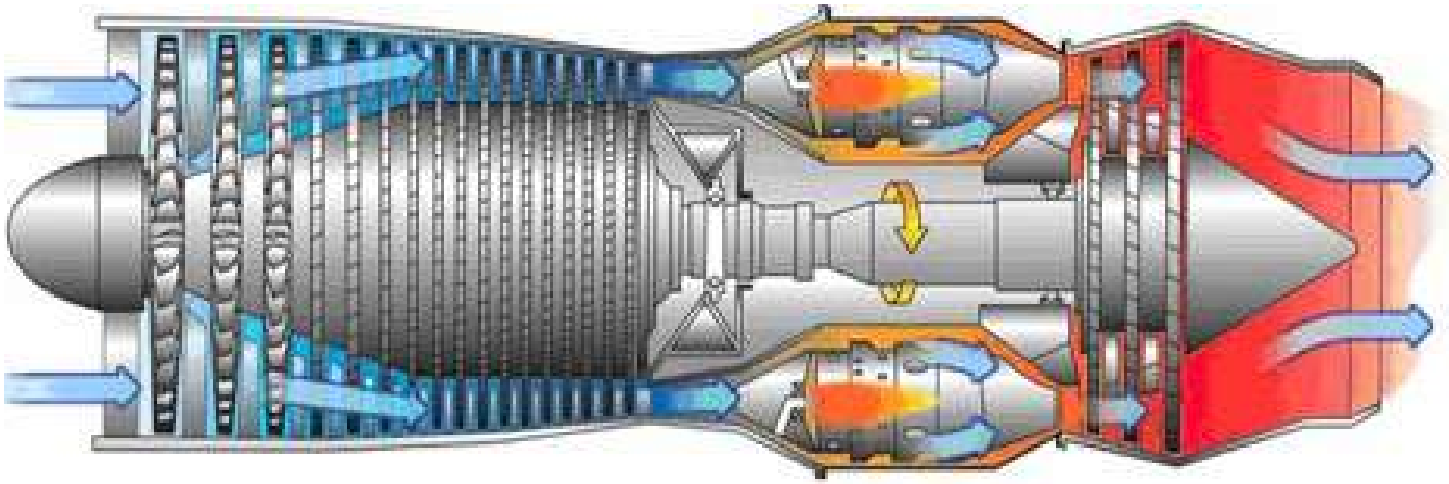
1940s
Semiconductors

1990s
High temperature superconductors

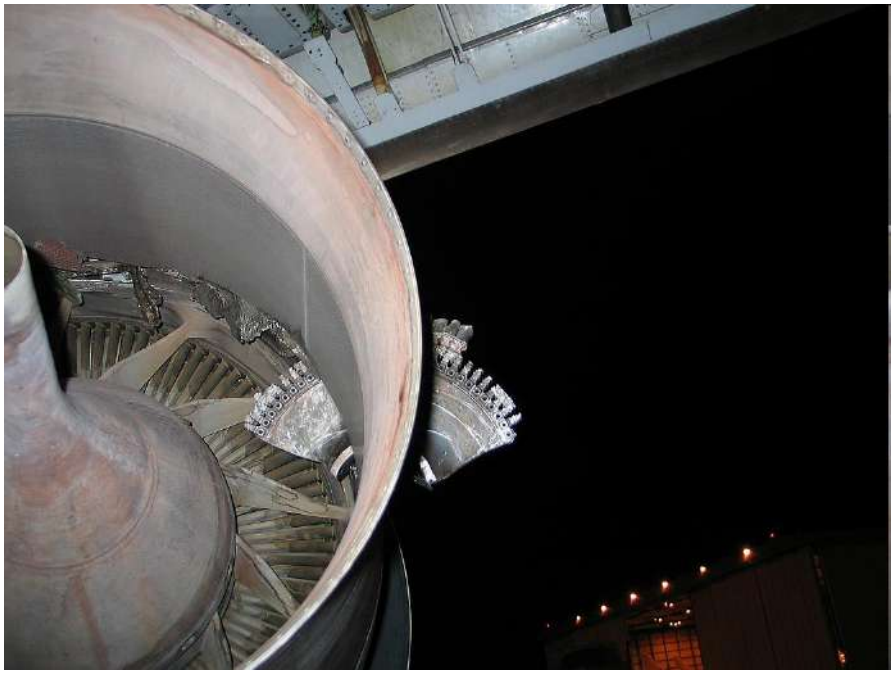


2000s
Graphene

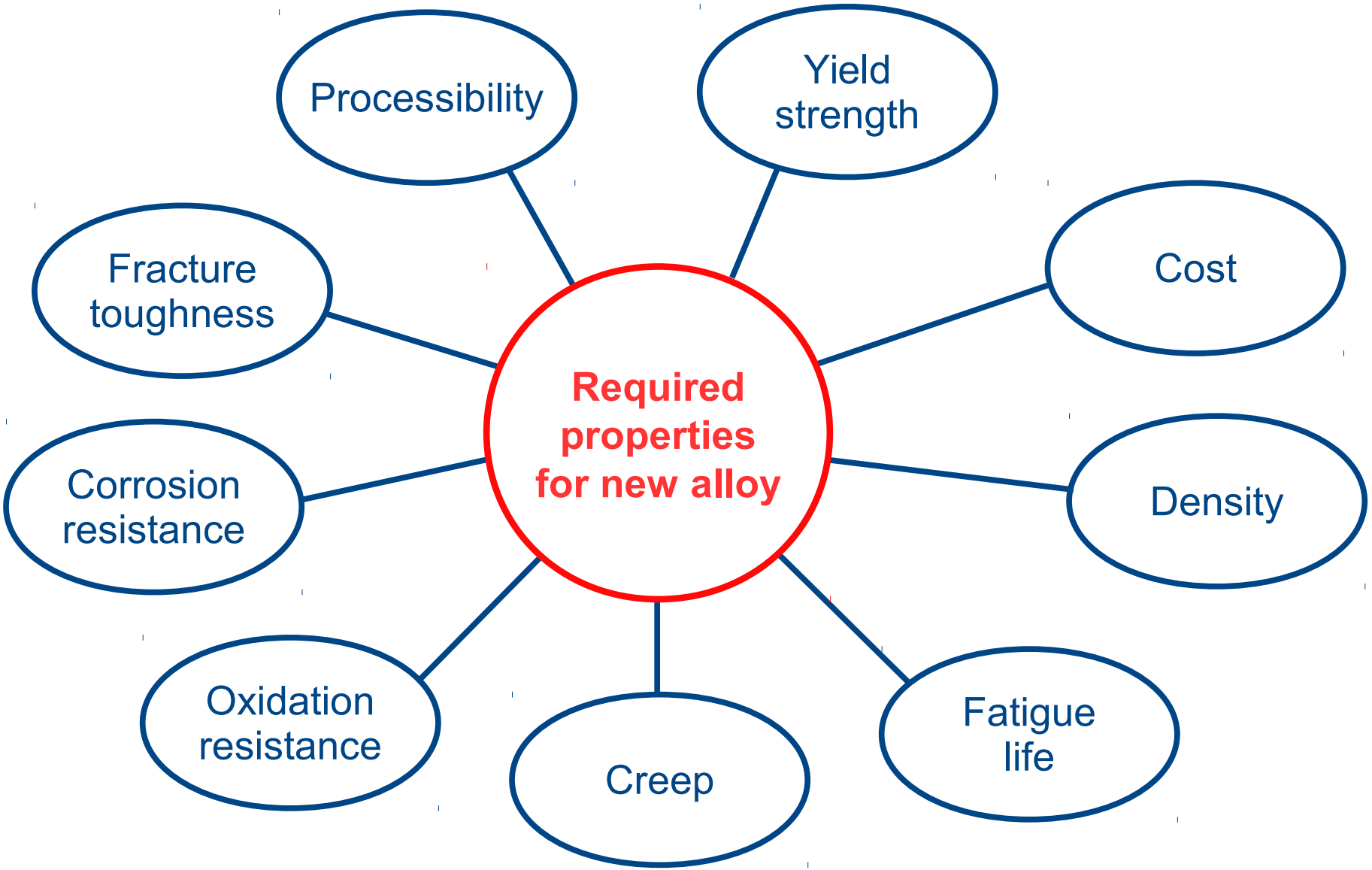
Jet engine



Jet engine



Designing a new alloy – what is required?



Materials pipeline

Cr 

Co 

Mo 

W 

Ta 

Nb 

Al 

Ti 

Fe 

Mn 

Si 

C 

B 

Zr 

Cu 

N 

P 

V 

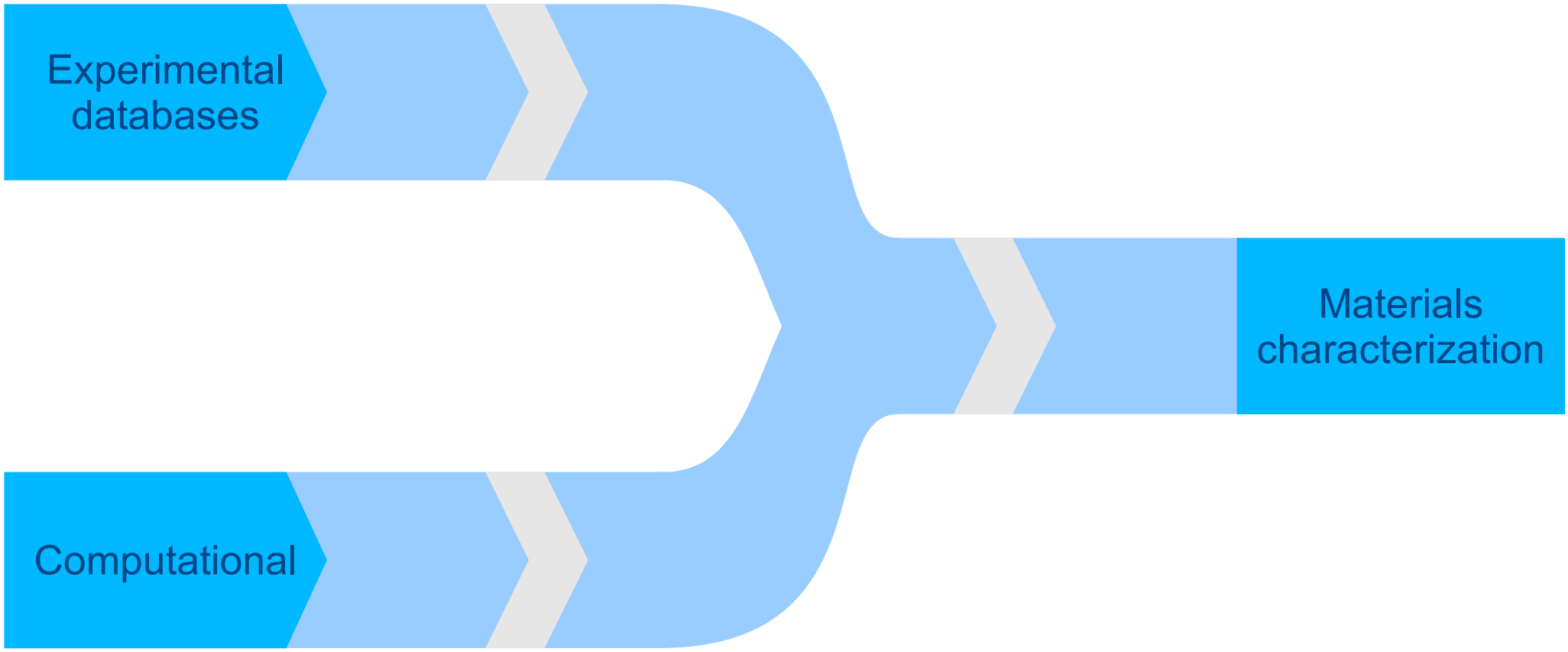
Hf 

Mg 

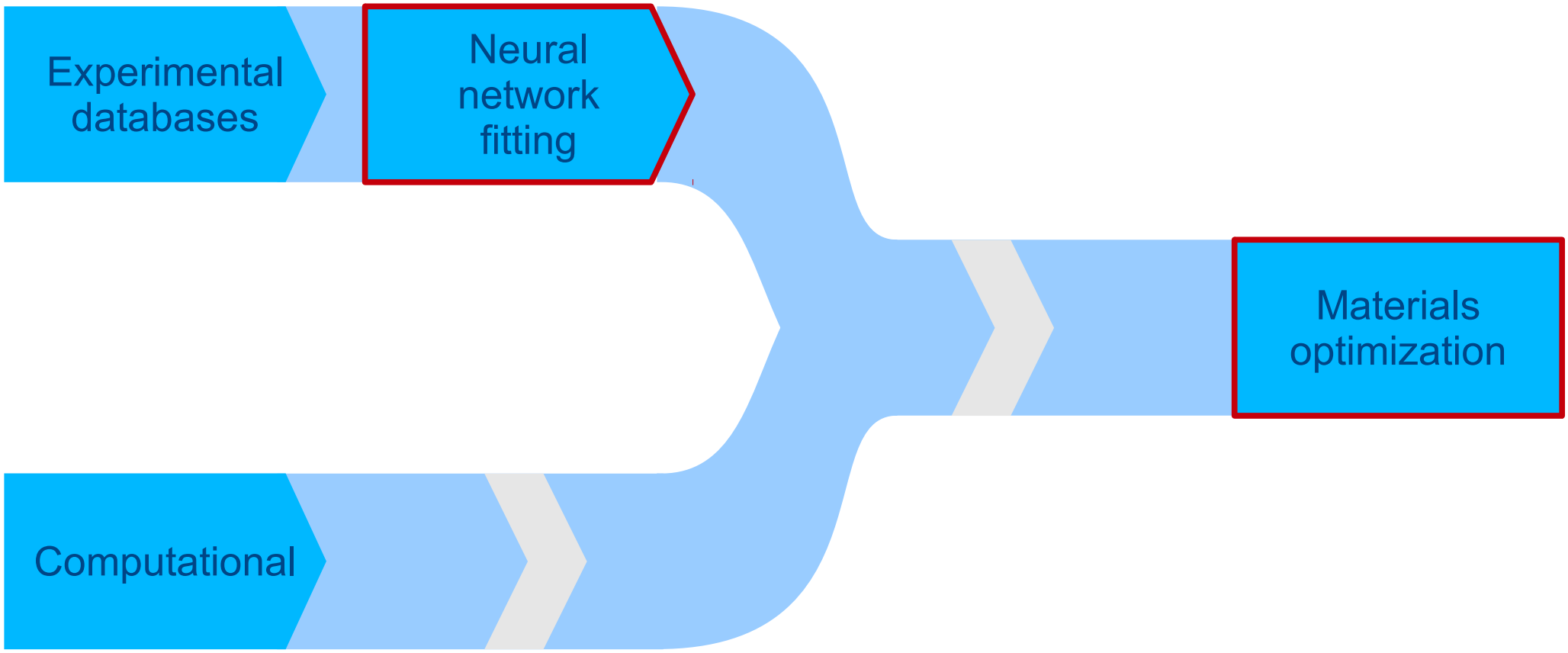
Ni 

and 4 different manufacturing processes

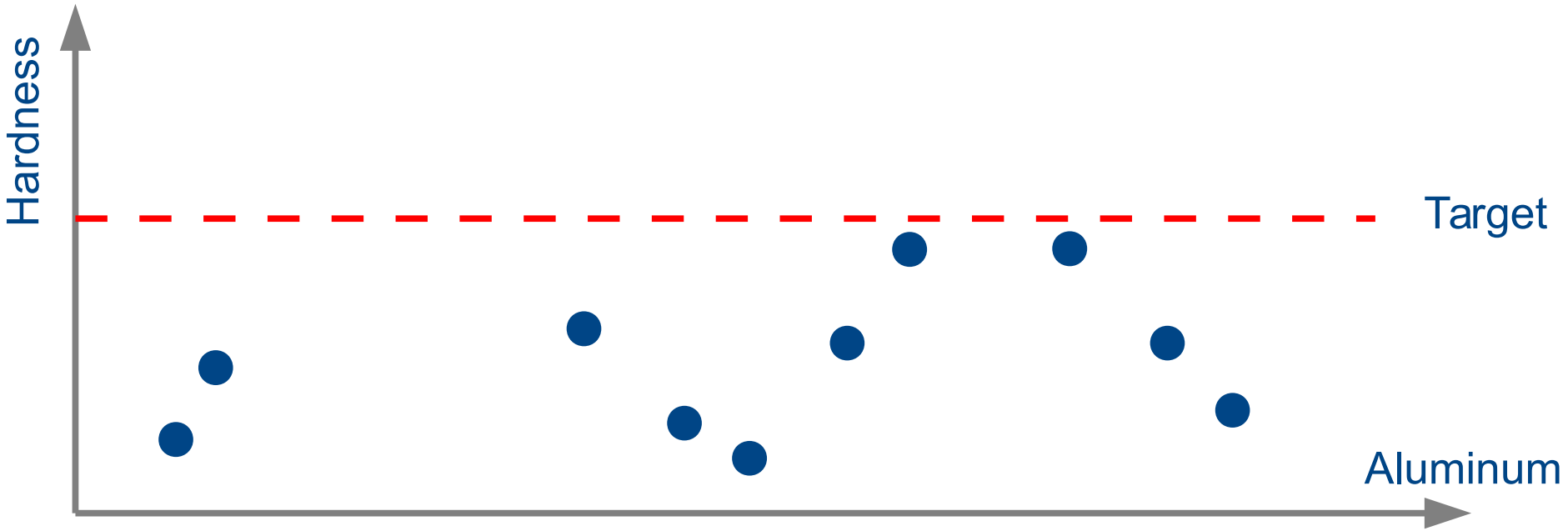
Materials pipeline



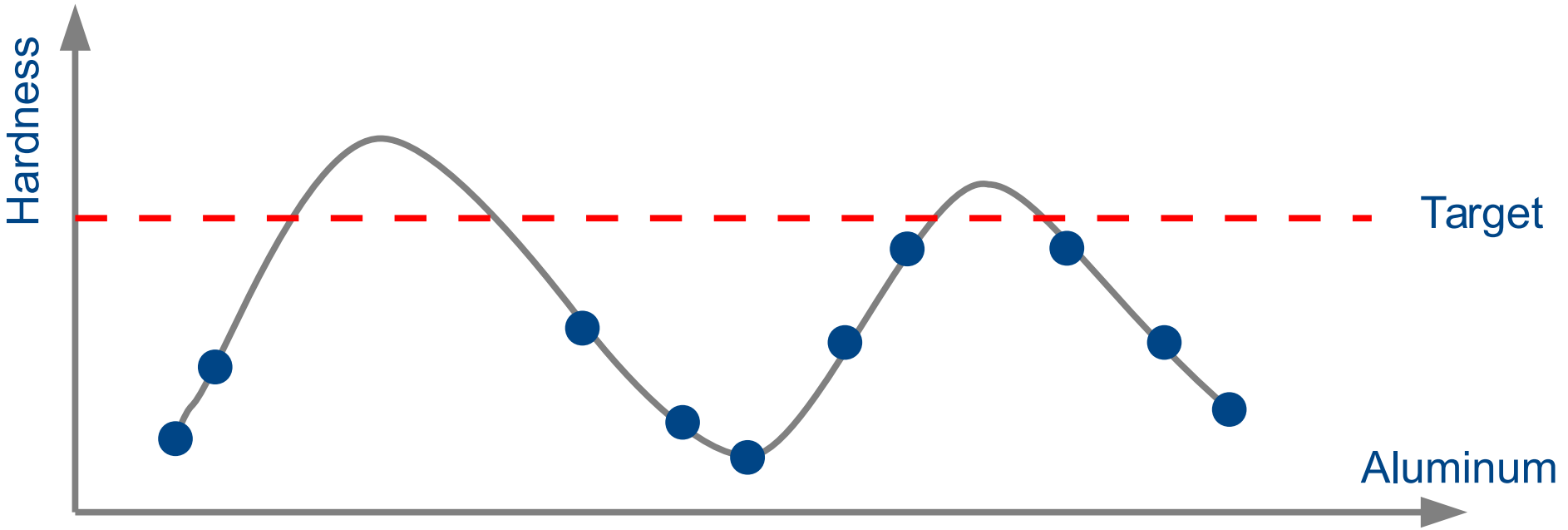
Two new tools



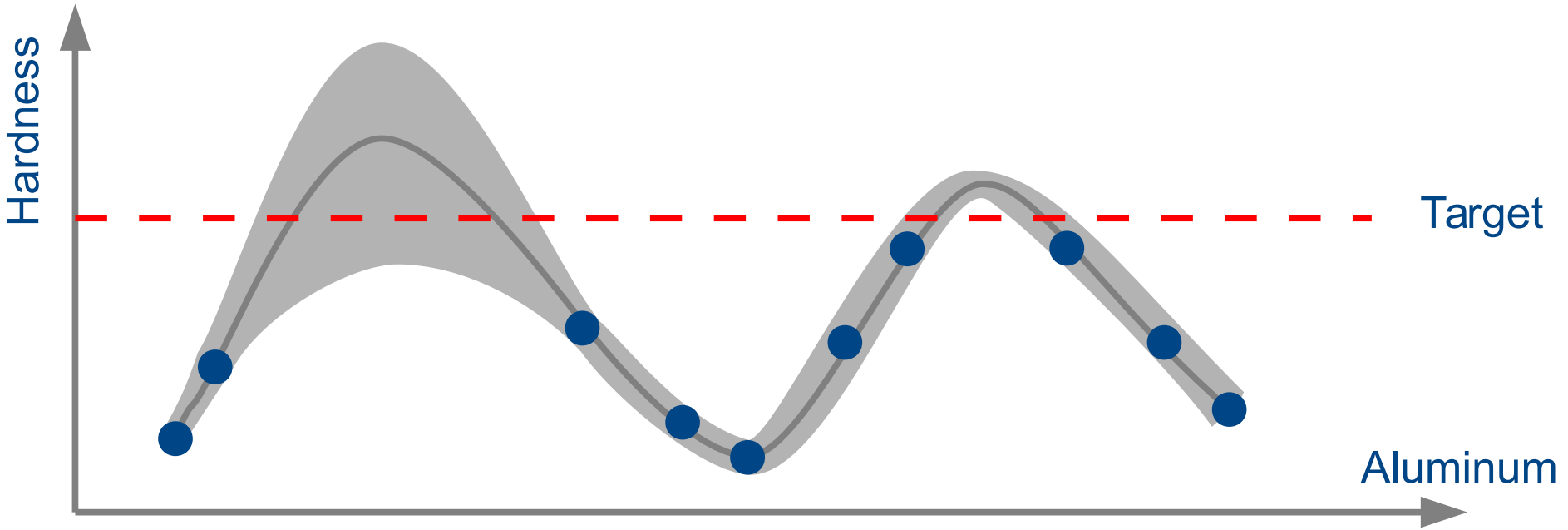
Neural network fitting & optimization



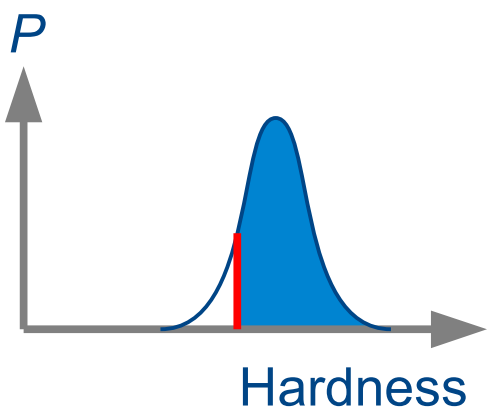
Neural network fitting & optimization

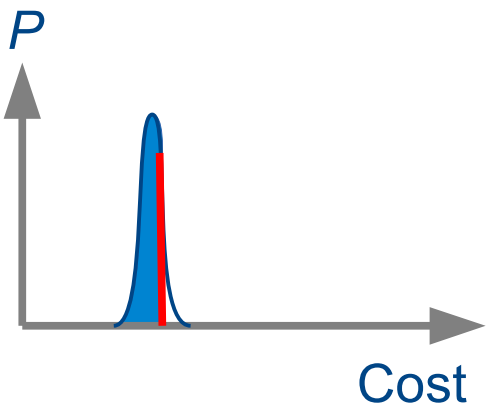


Neural network fitting & optimization

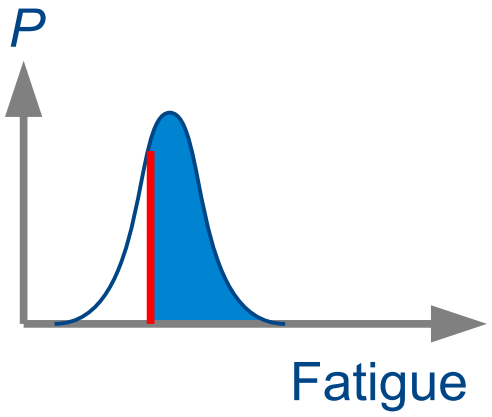


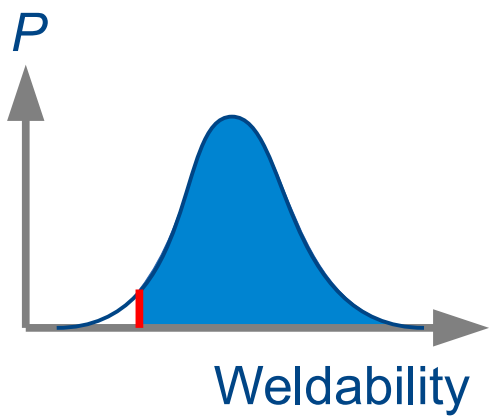
Optimizing the likelihood





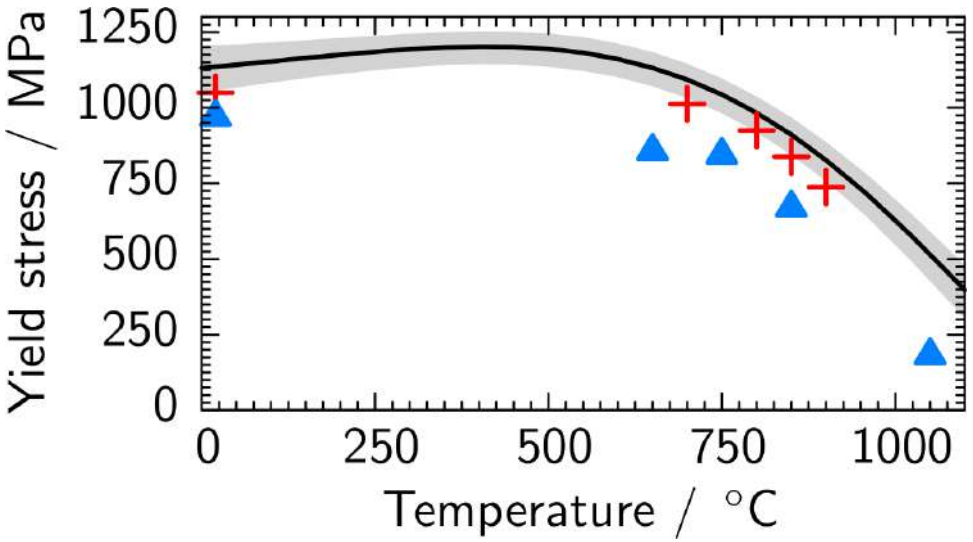
Likelihood of alloy satisfying all targets





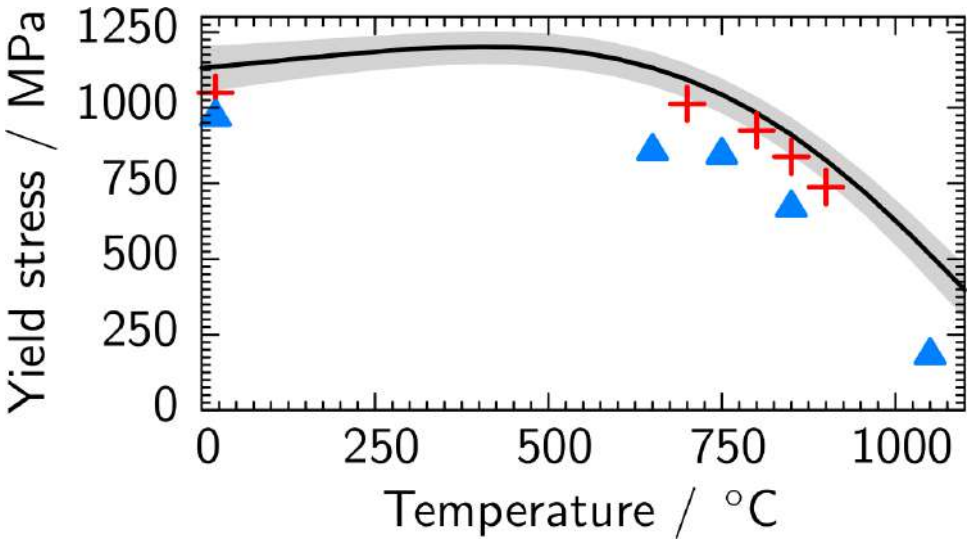
EP14153898.3; US 2014/177578; GB1302743.8

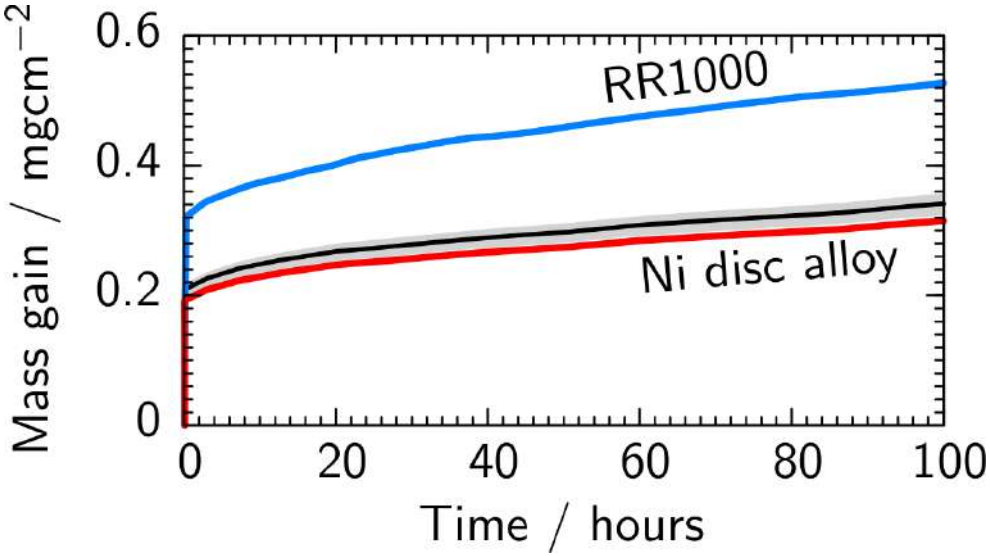
Ni-base superalloy



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

Ni-base superalloy

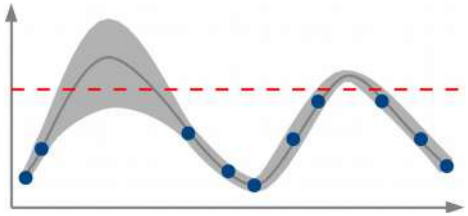




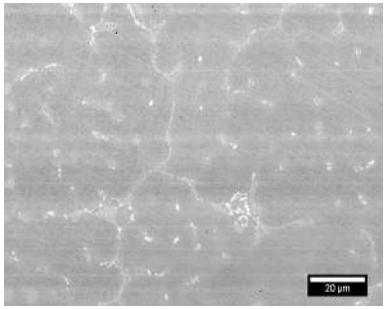
Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

Alloys discovered

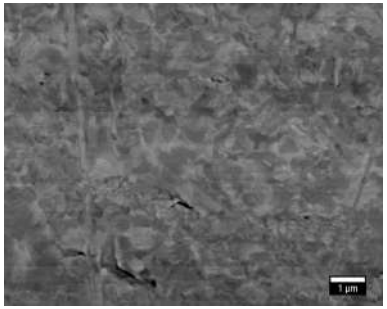
Discovery algorithm
EP14153898.3
US 2014/177578
GB1302743.8



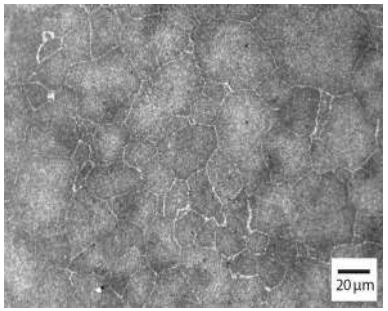
Mo-Hf forging alloy
EP14161255.6
US 2014/223465
GB1307533.8



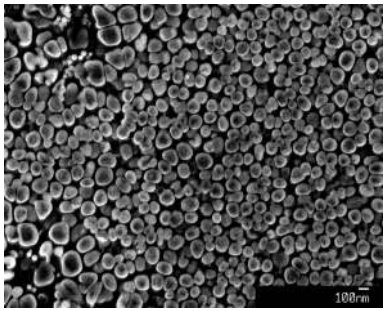
Mo-Nb forging alloy
EP14161529.4
US 2014/224885
GB1307535.3



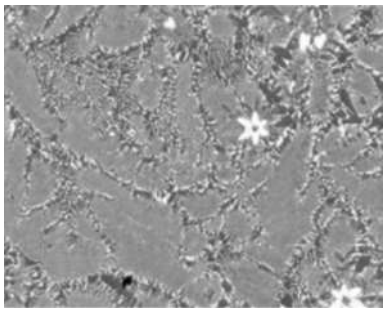
RR1000 grain growth
Acta Materialia, 61, 3378



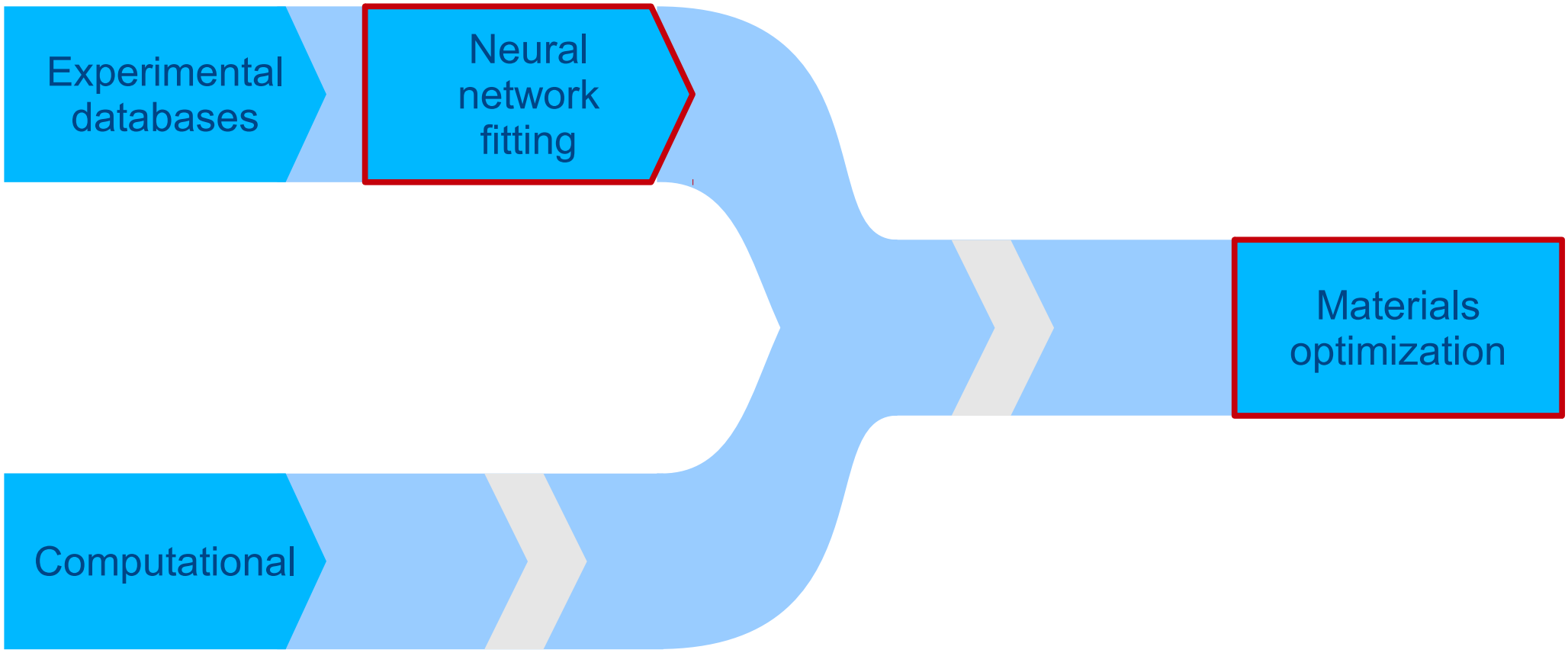
Ni disc alloy
EP14157622.3
US 2013/0052077 A2
GB1408536.9



Cr-Cr2Ta alloys
Intermetallics 48, 62



Two new tools



Light emitting diodes

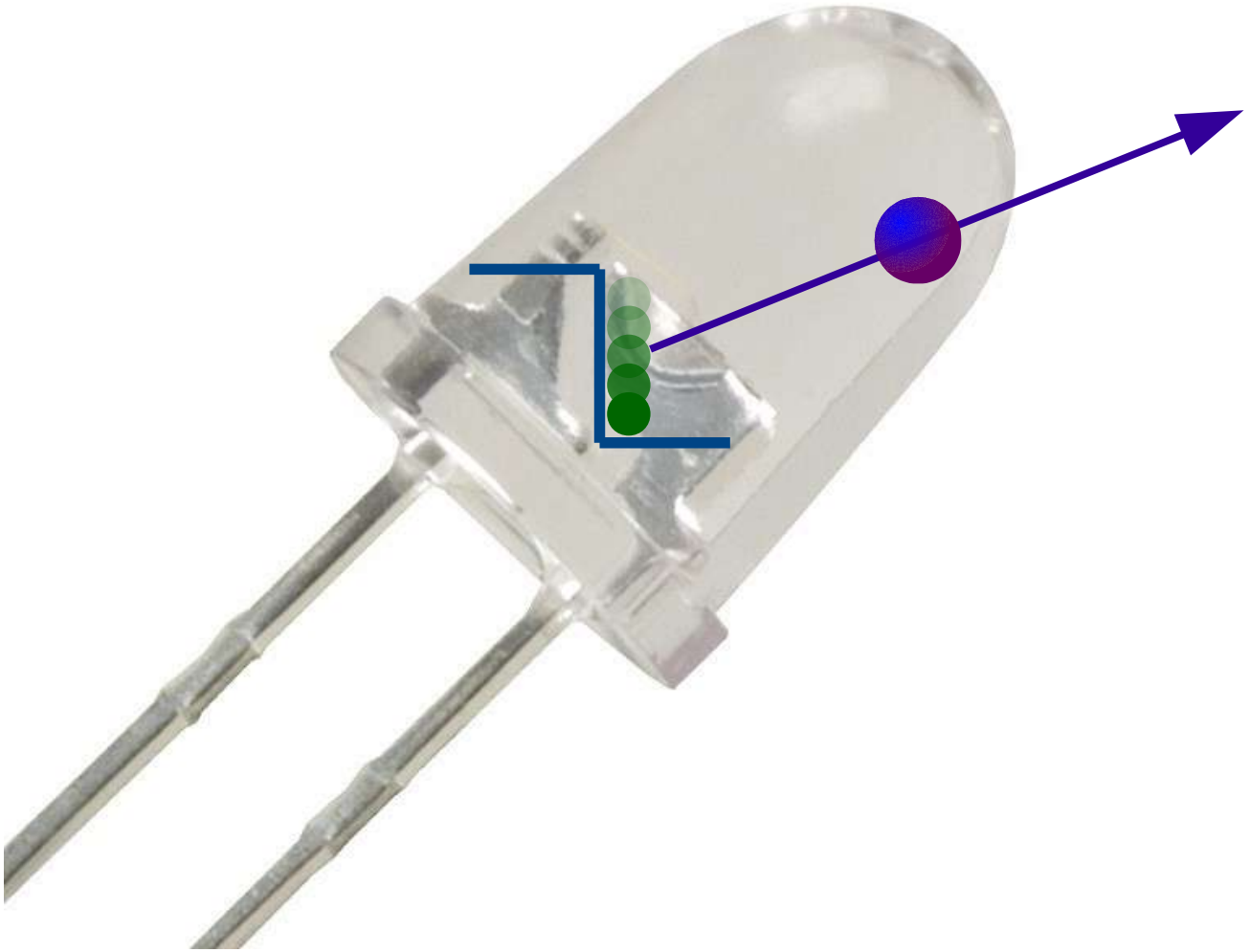
Cost

Efficiency

Color

Band gap

Light emitting diodes



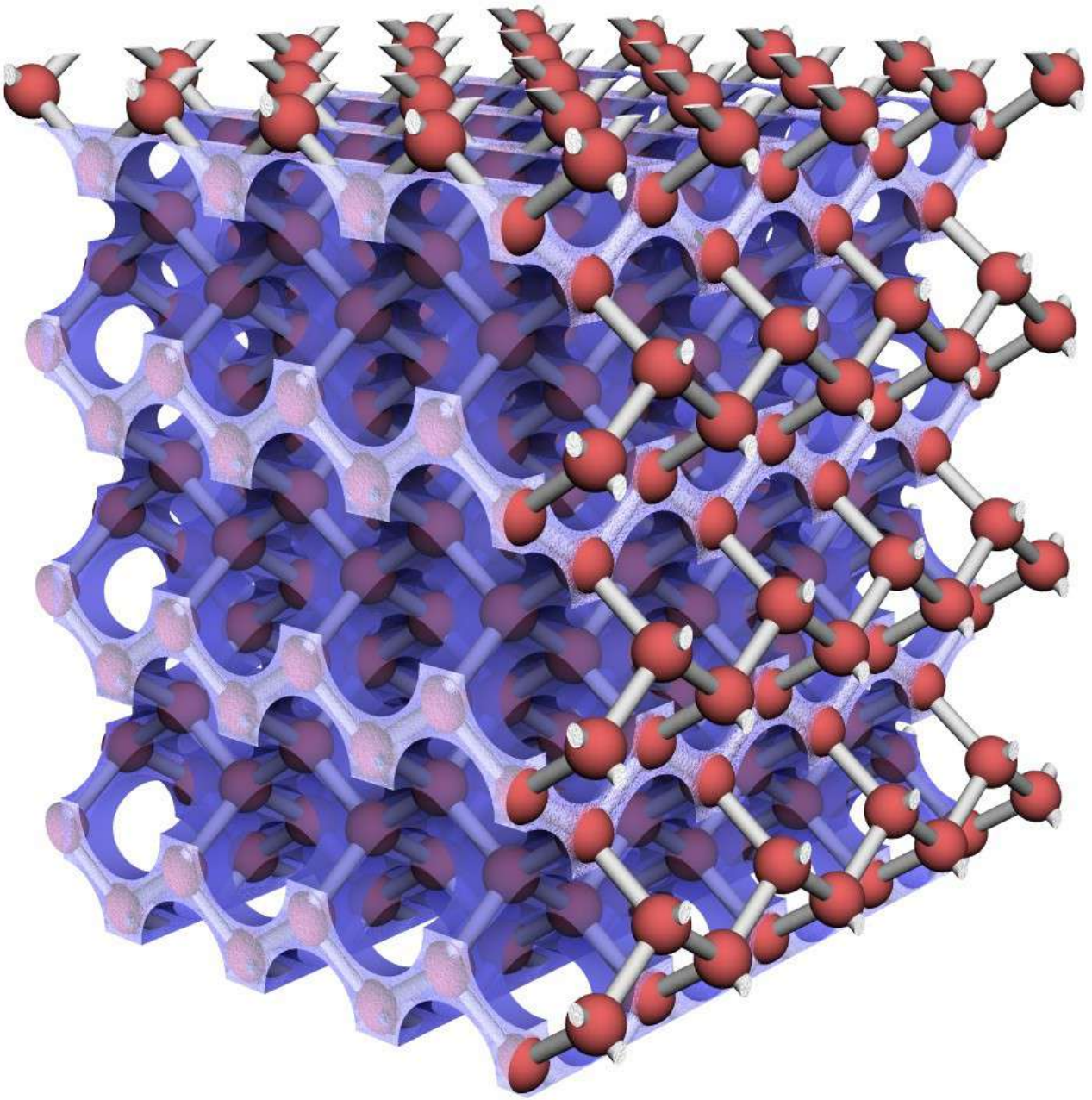
Cost

Efficiency

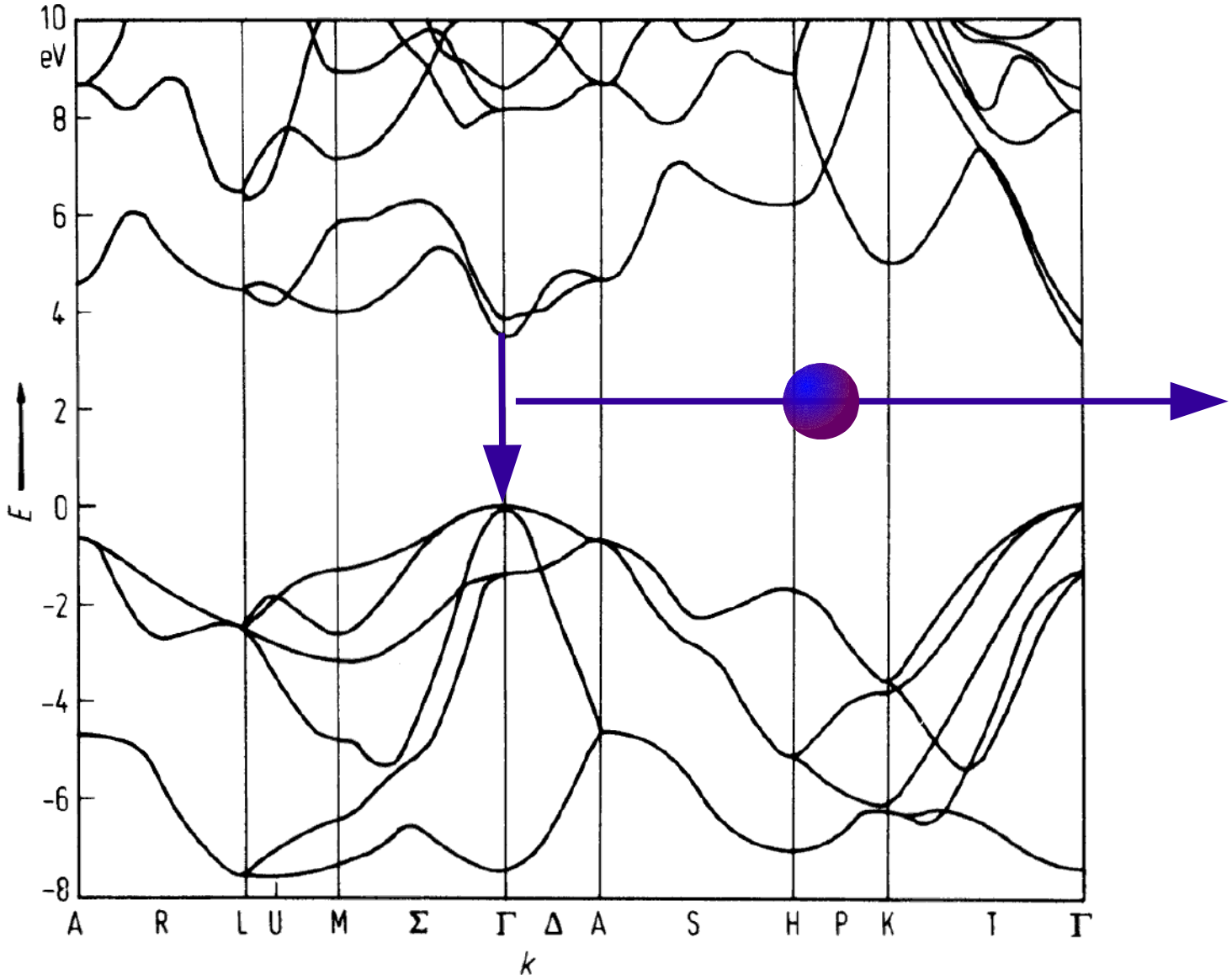
Color

Band gap

Computer simulations



Band gap

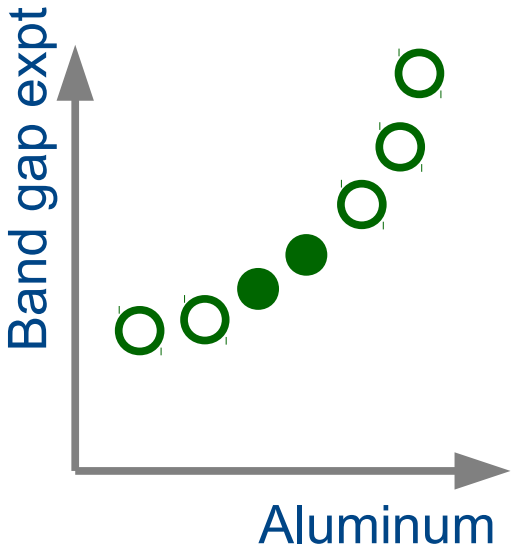


Computational challenges

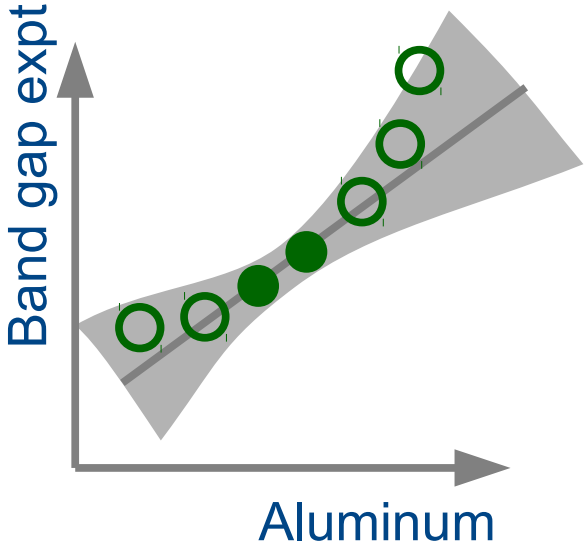
Inevitable approximations behind first principles simulations

Reducing number of simulations performed

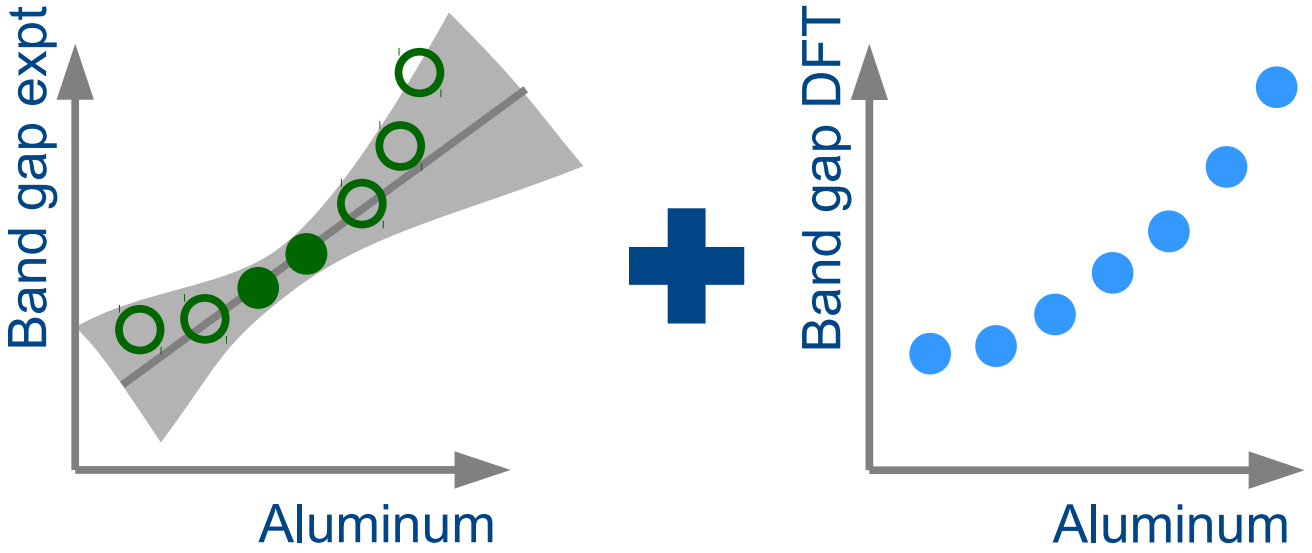
Correlations between properties



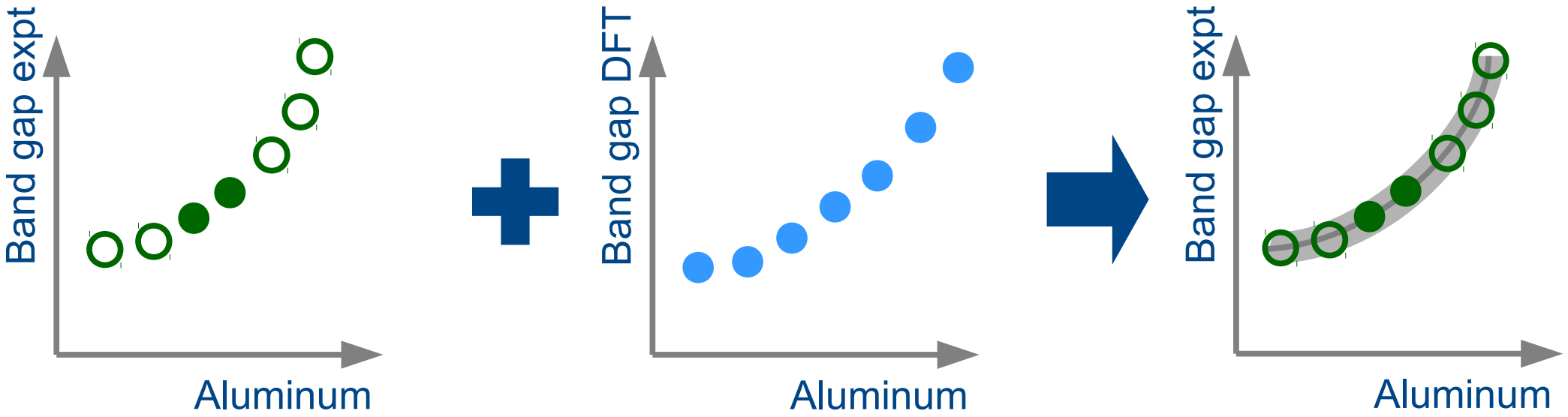
Correlations between properties



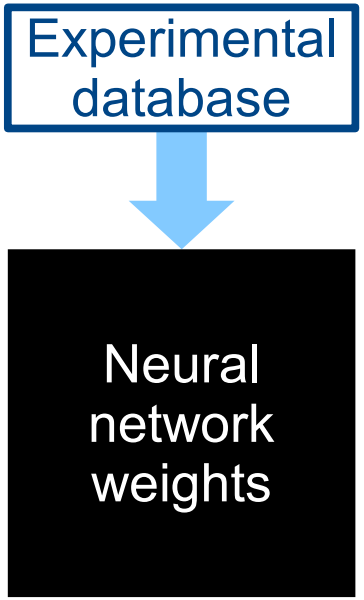
Correlations between properties



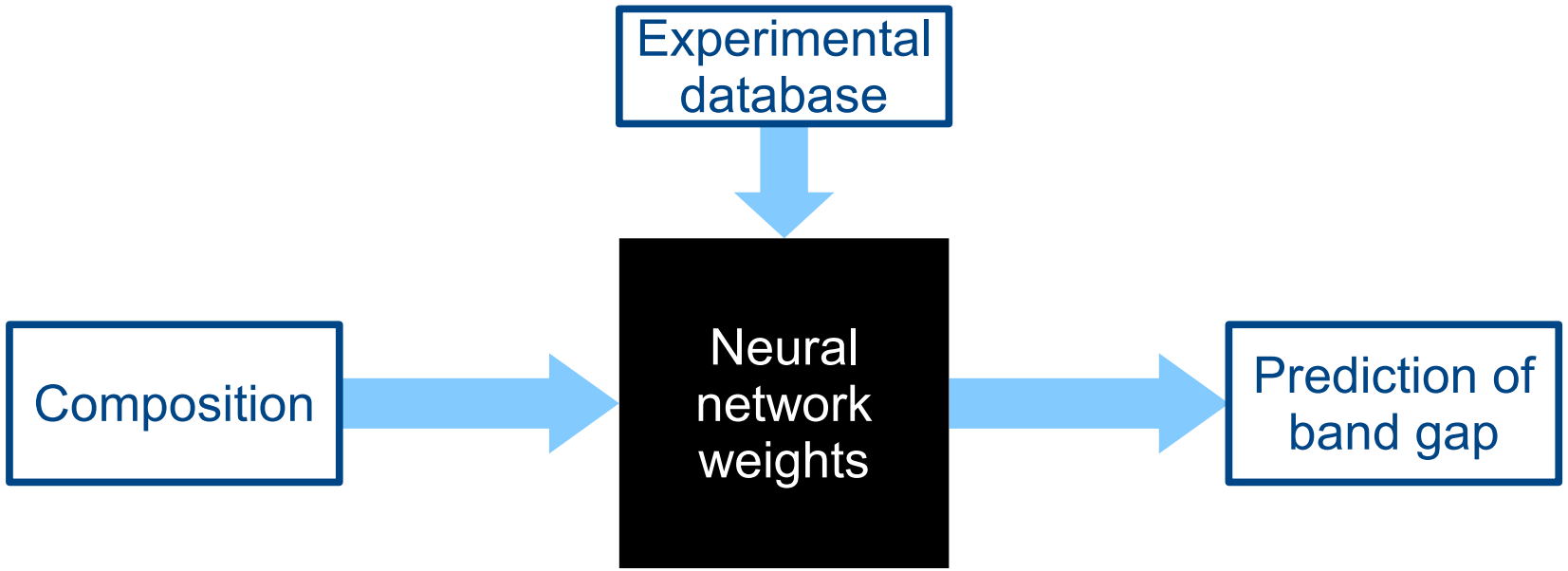
Correlations between properties



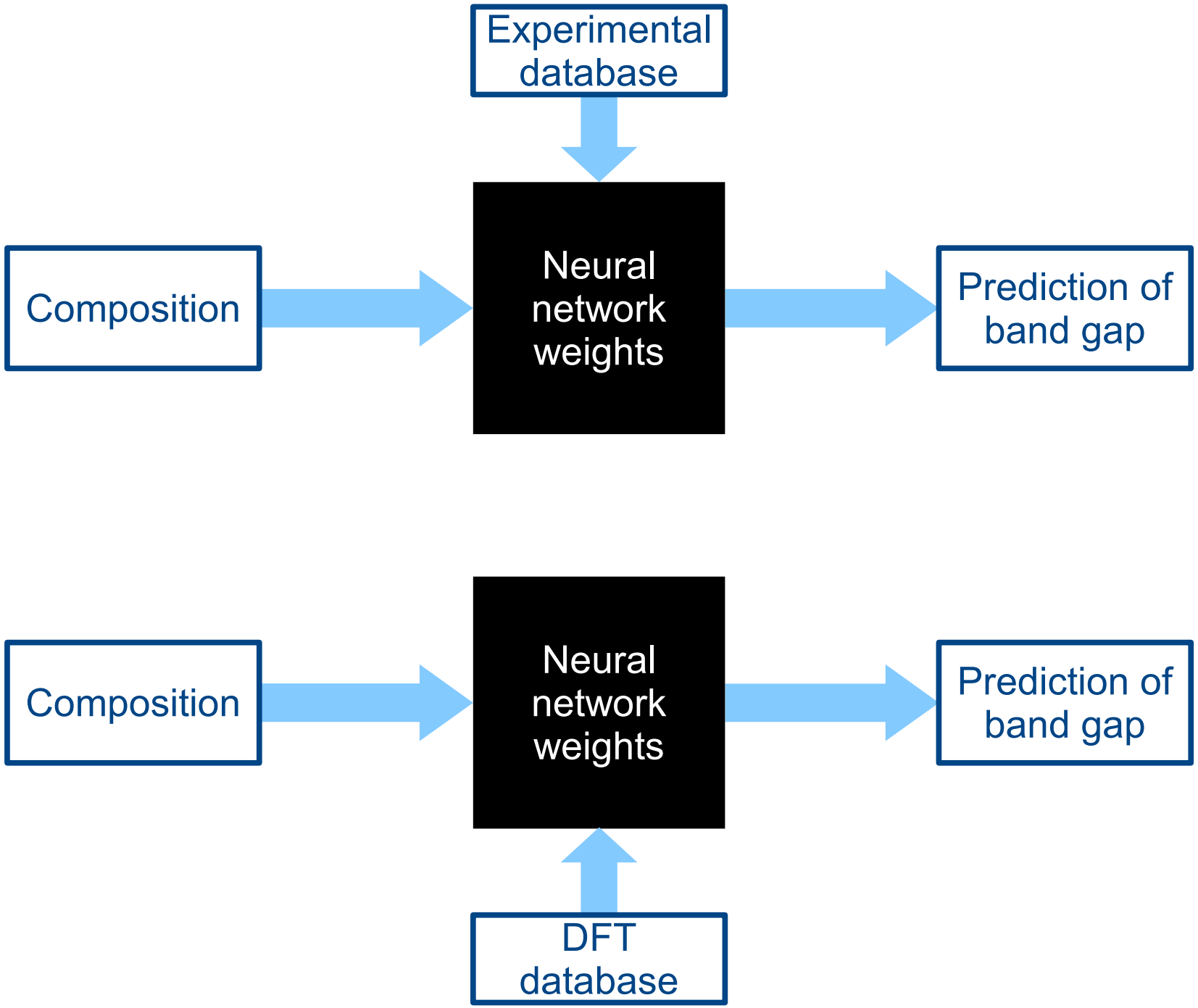
Correlations between properties



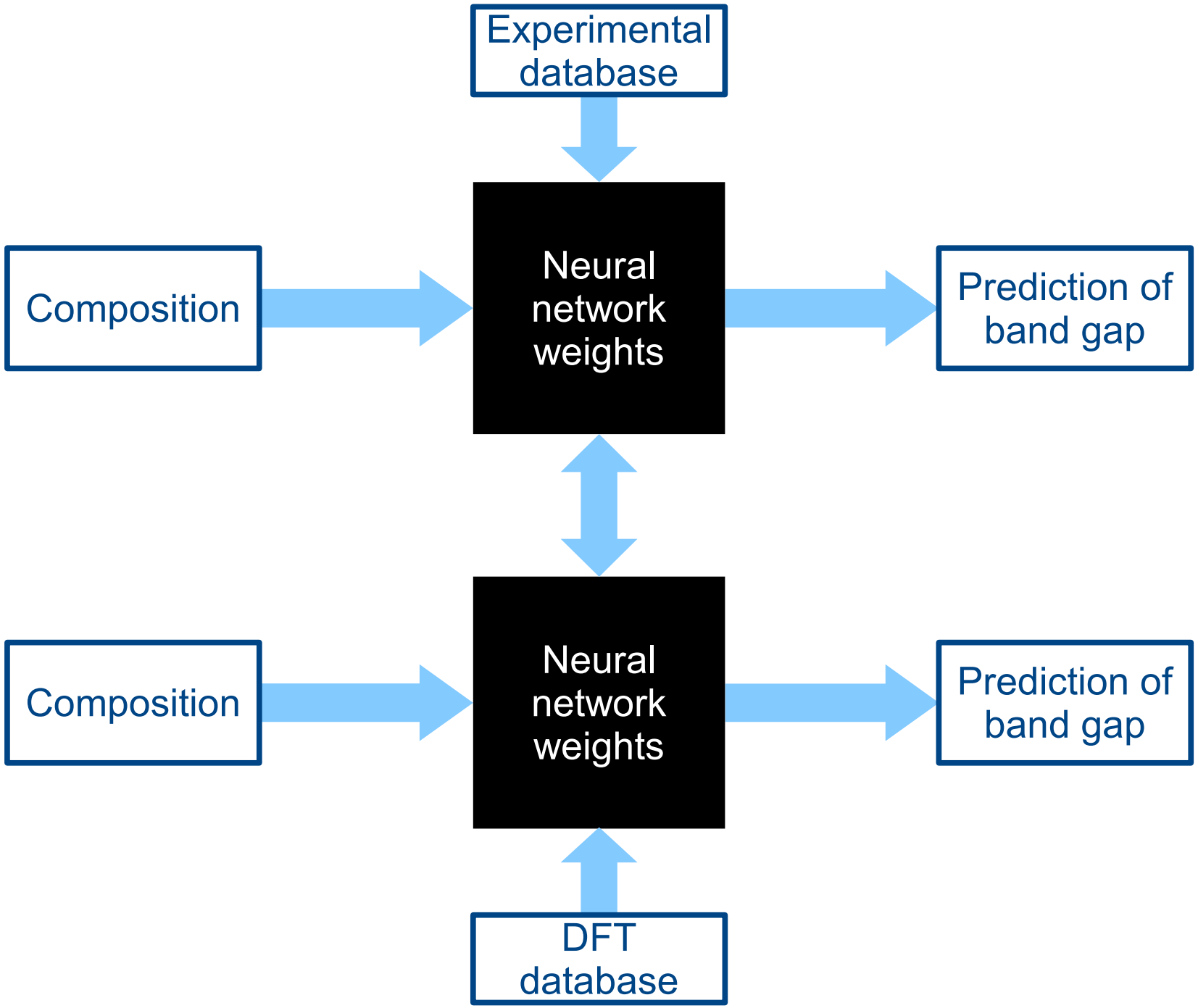
Correlations between properties



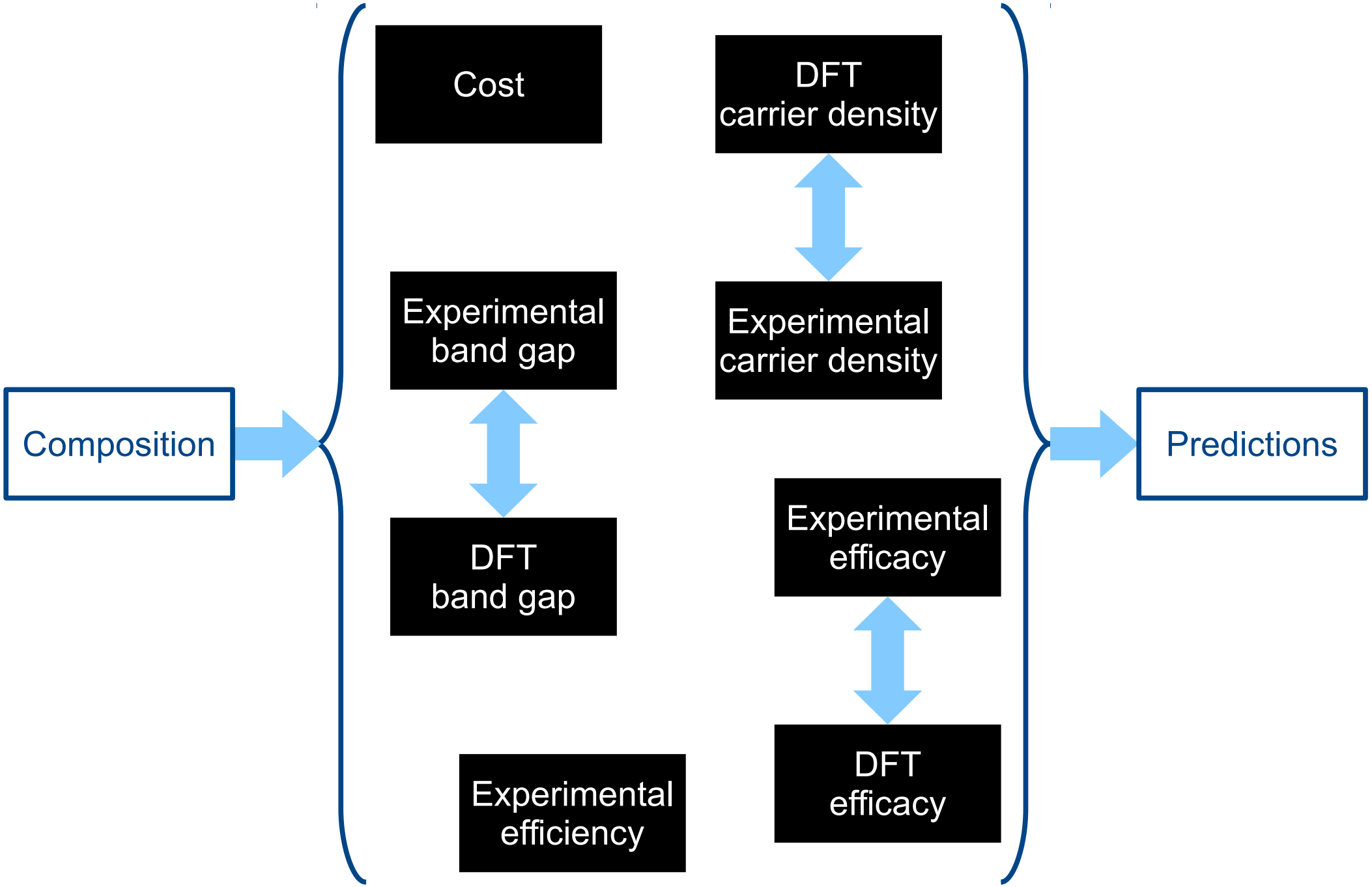
Correlations between properties



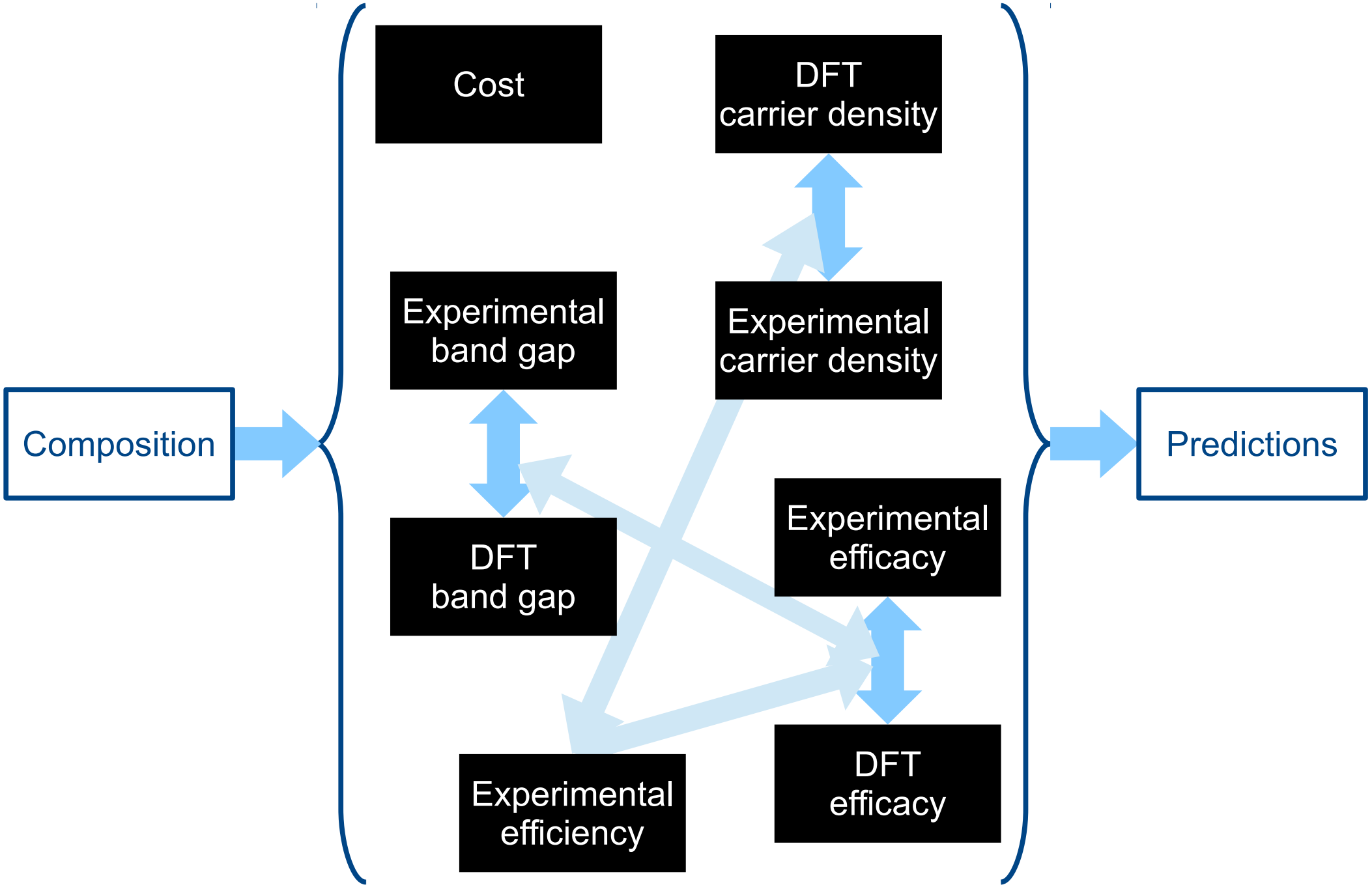
Correlations between properties



Correlations between properties



Correlations between properties

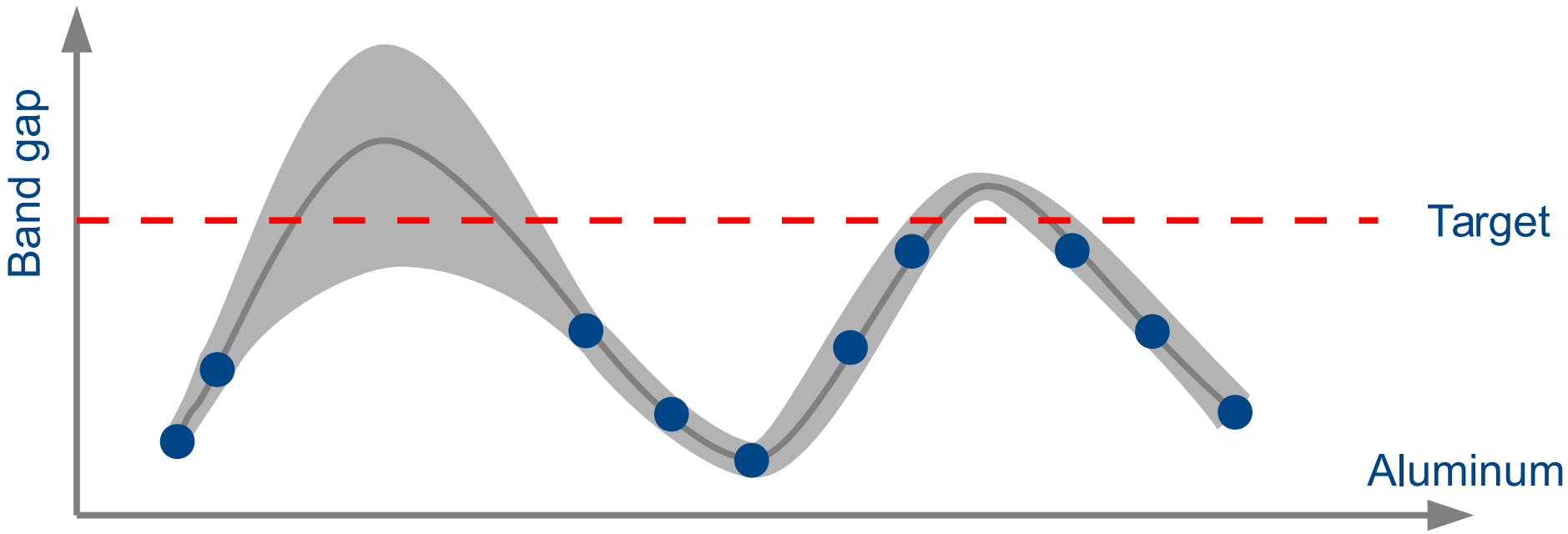


Recursive learning

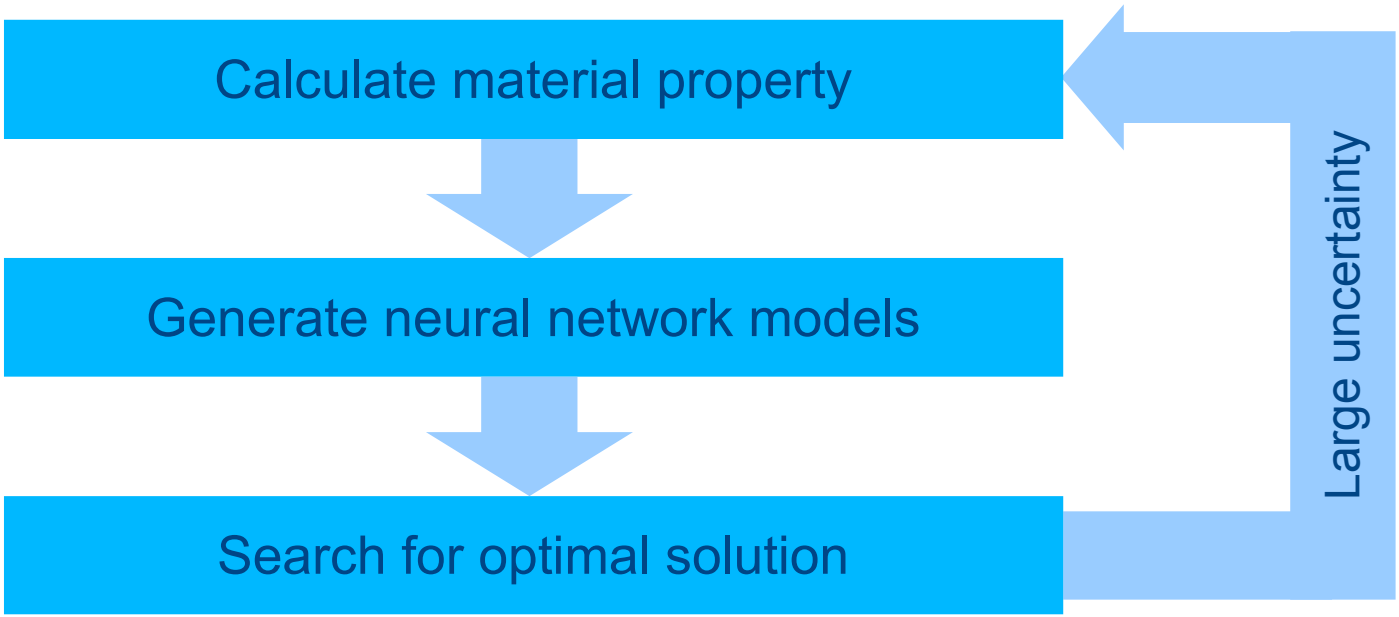
Calculate material property

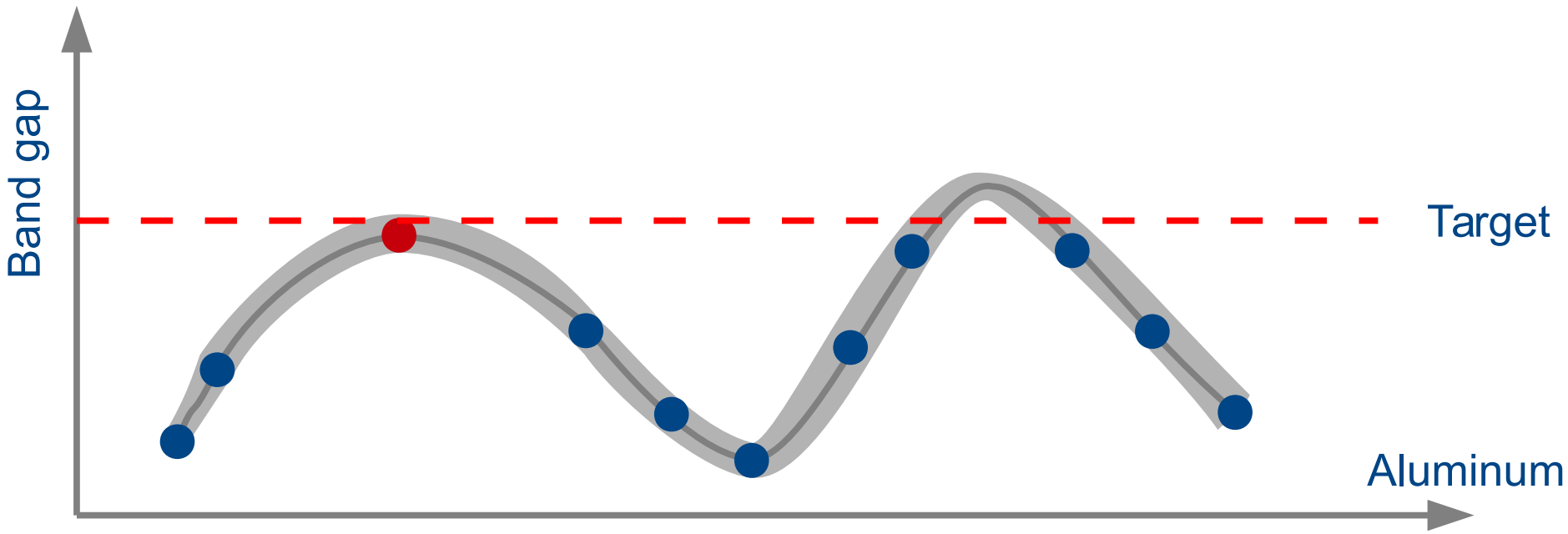
Generate neural network models

Search for optimal solution

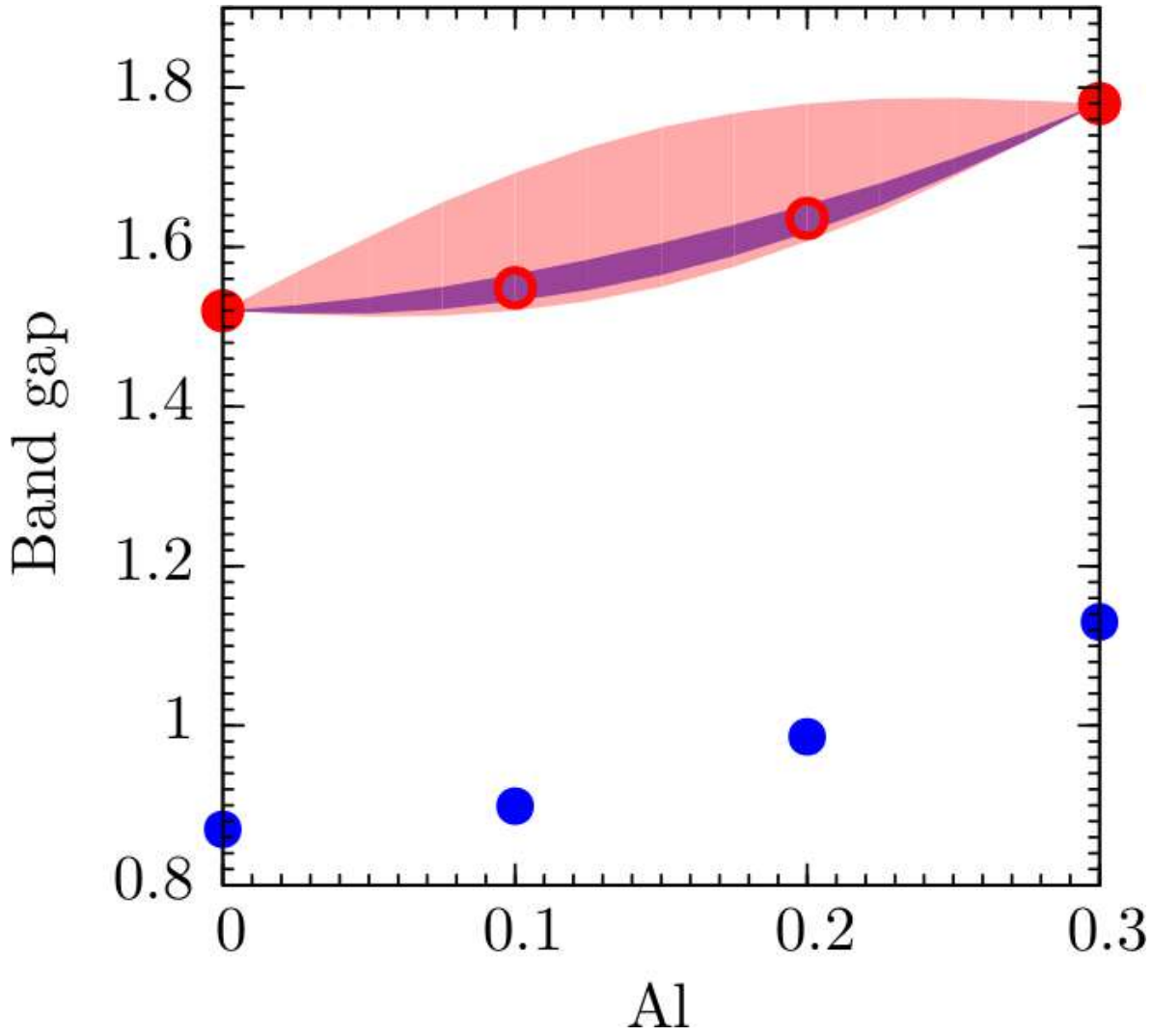


Recursive learning

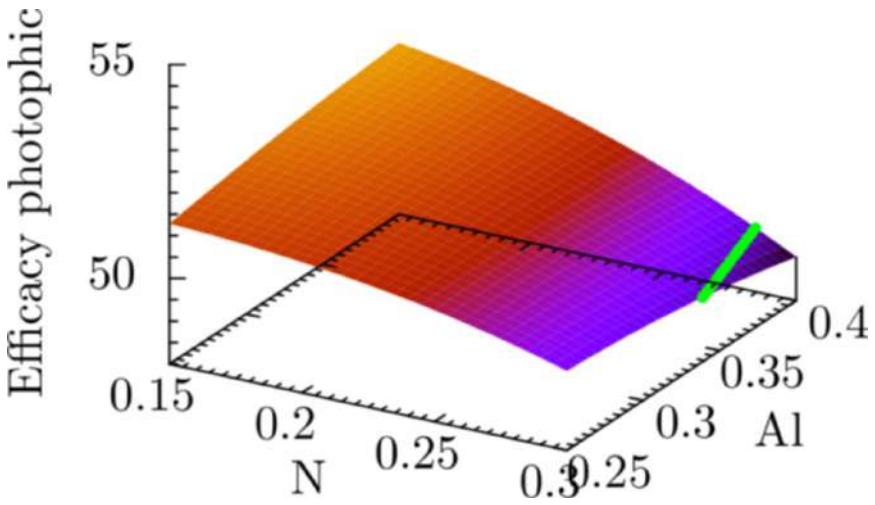




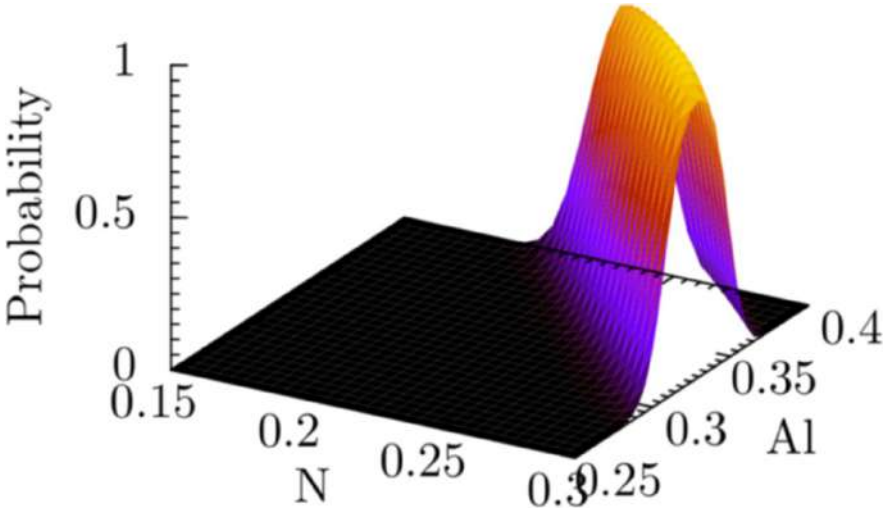
Case study: III-V InGaN-base semiconductors

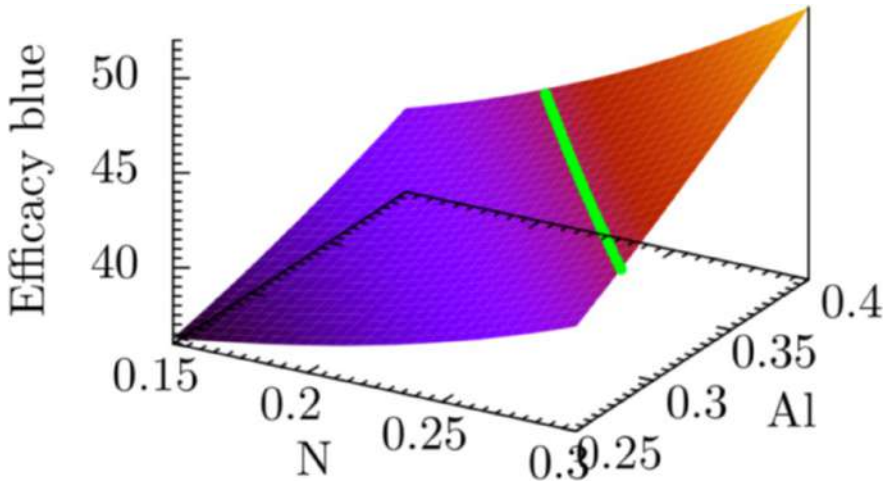


Case study: III-V InGaN-base semiconductors

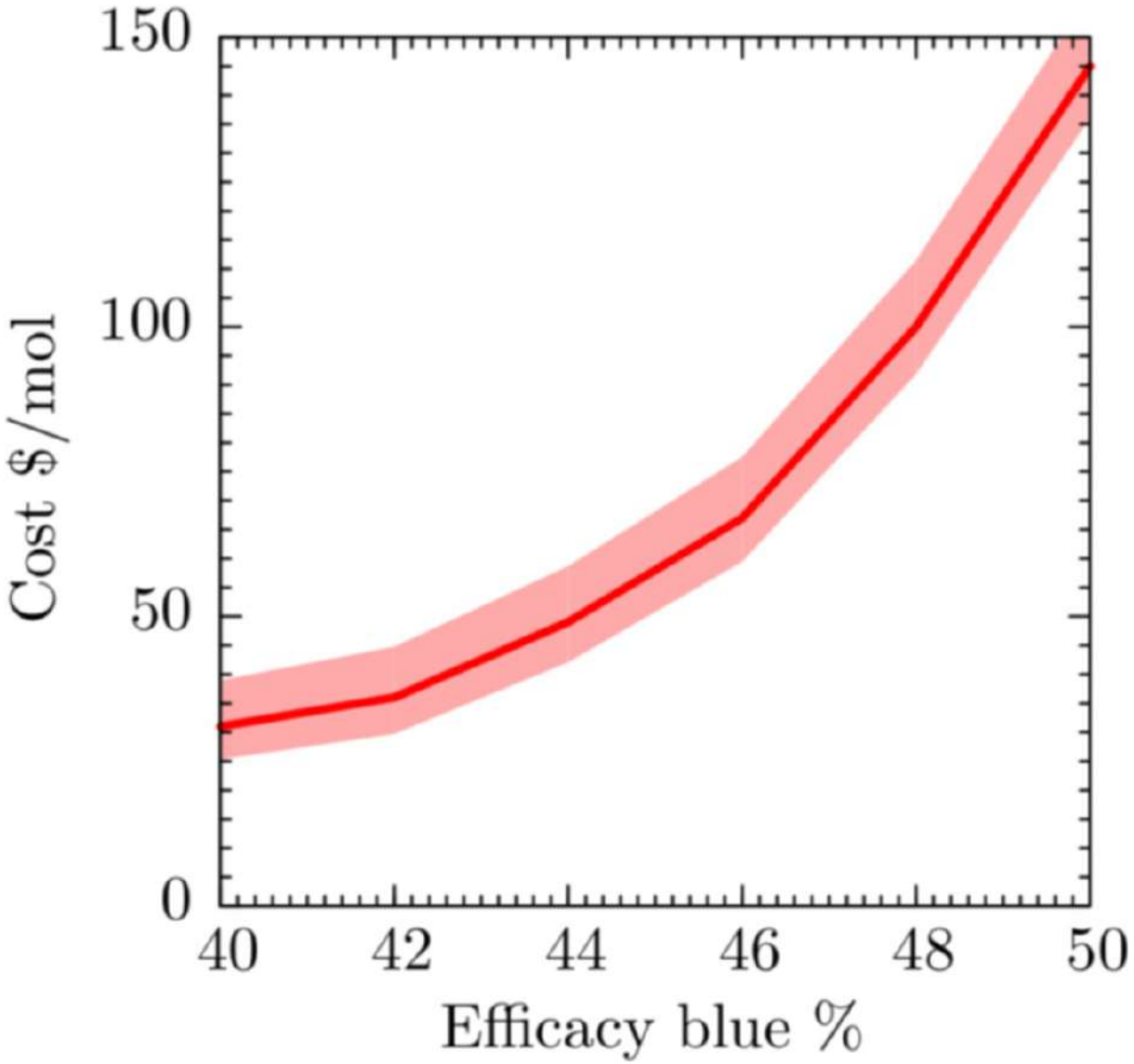


Combine

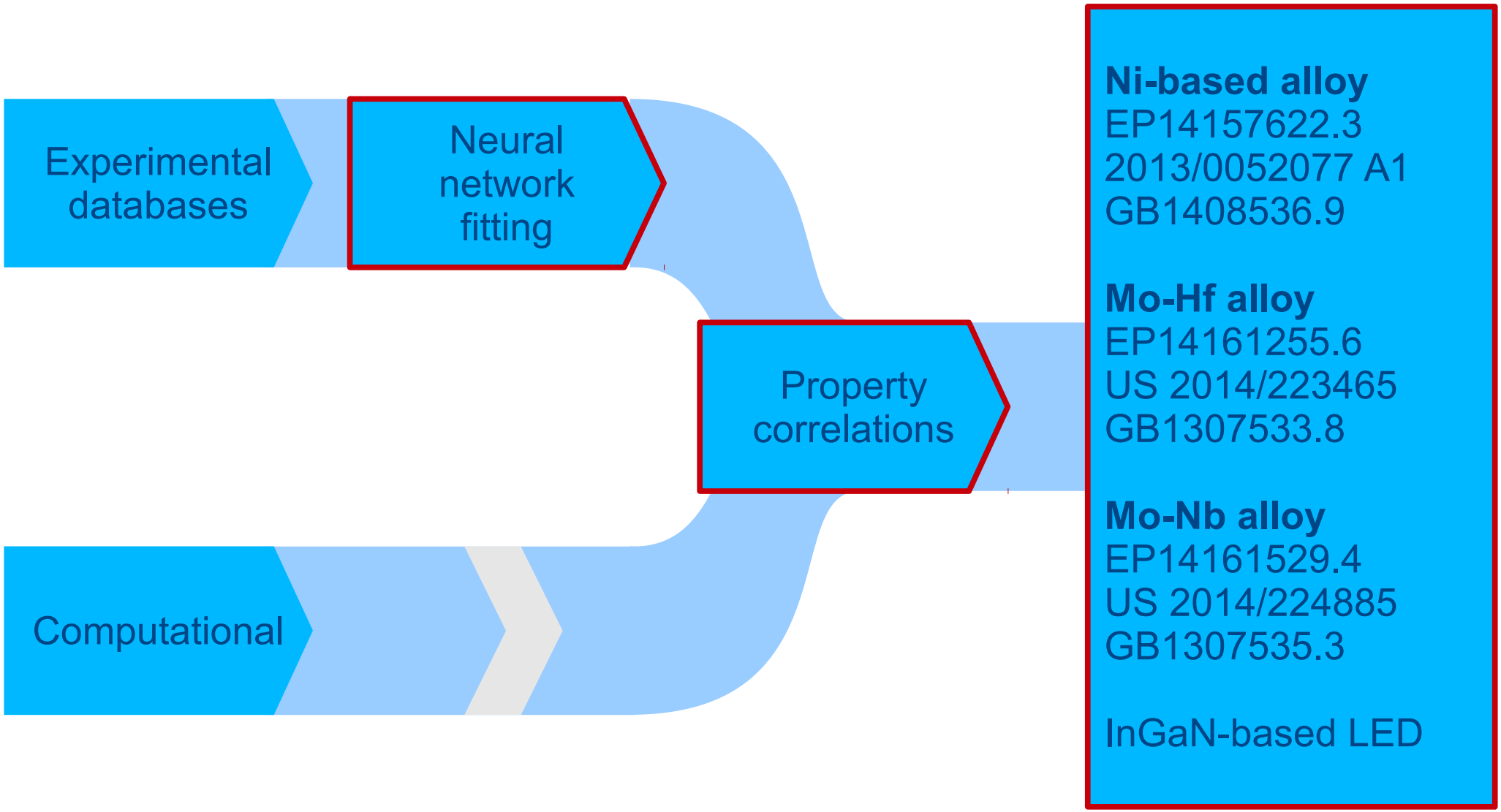




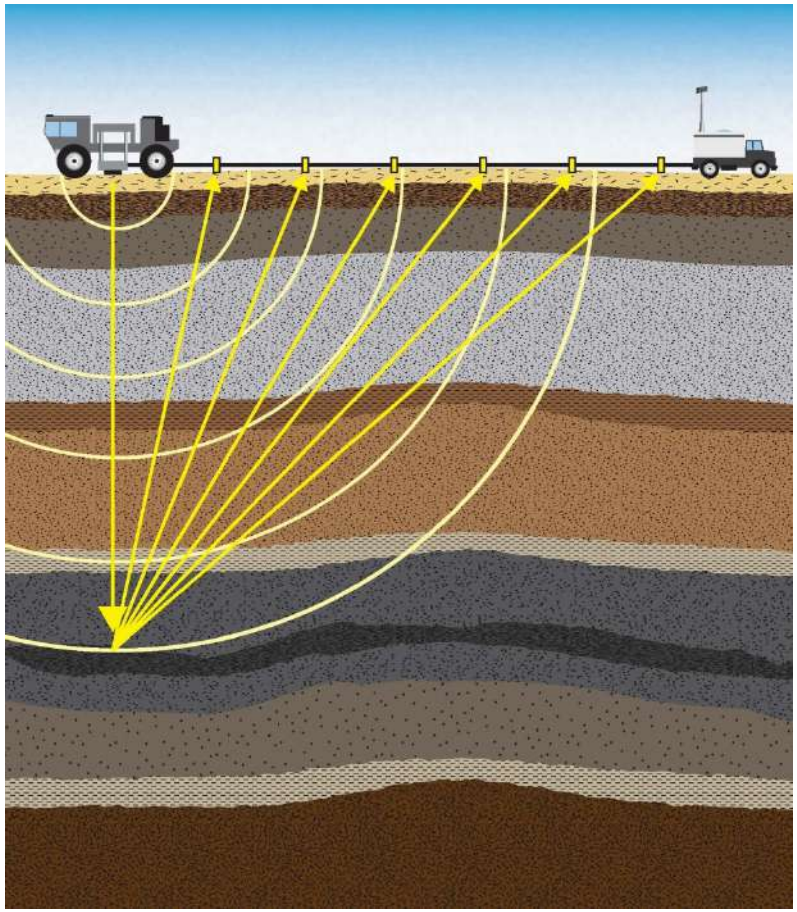
Case study: III-V InGaN-base semiconductors



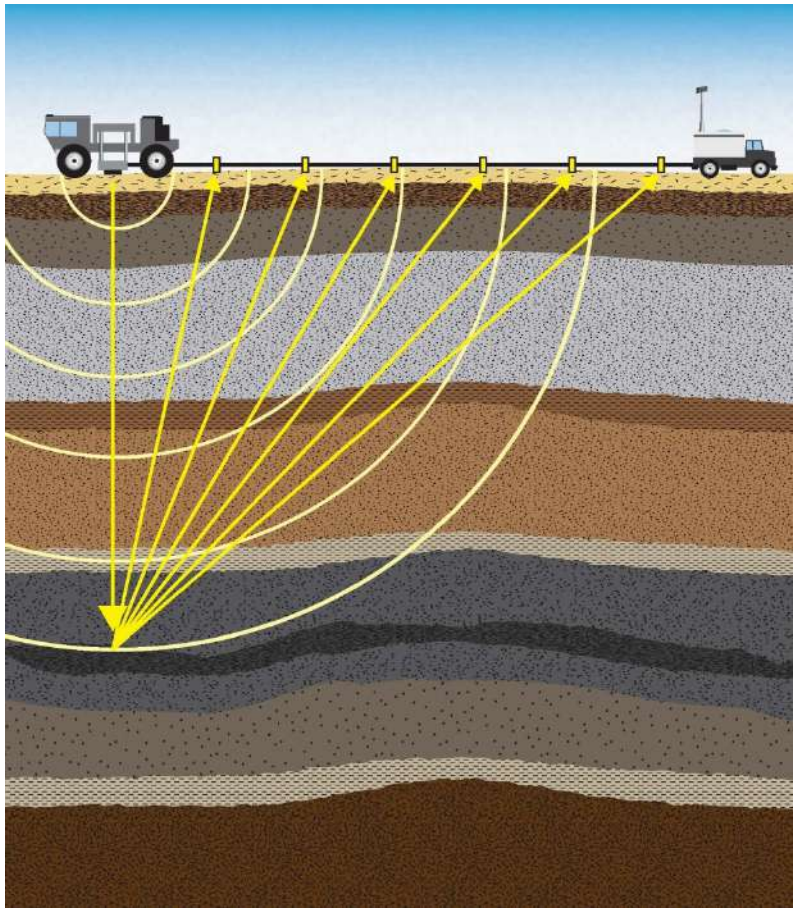
Three new tools

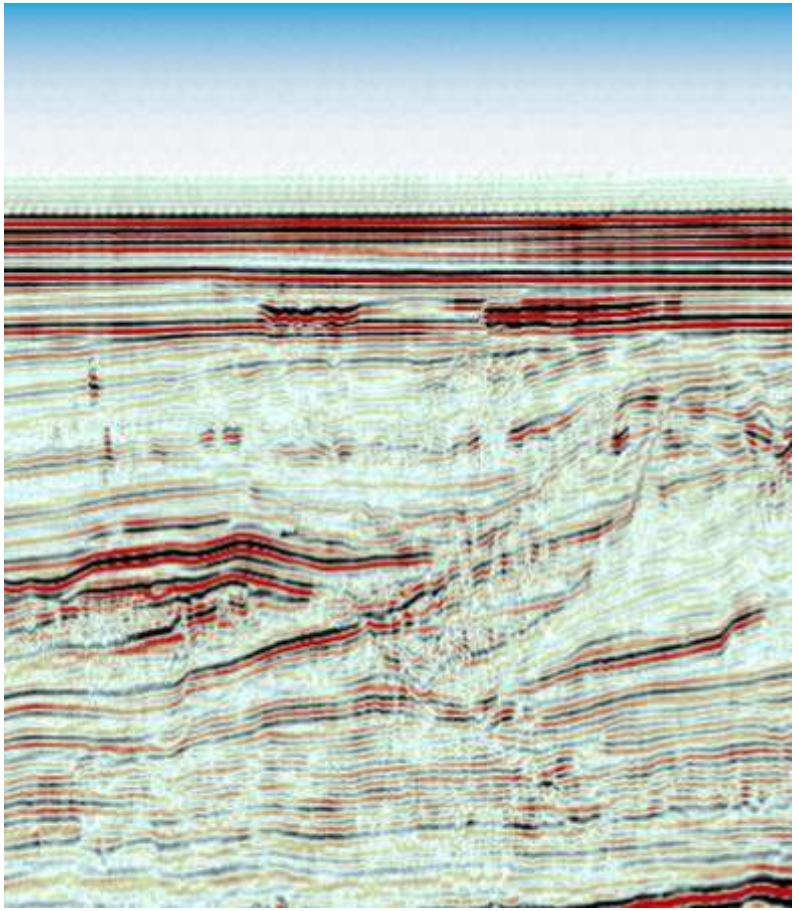


Search for oil

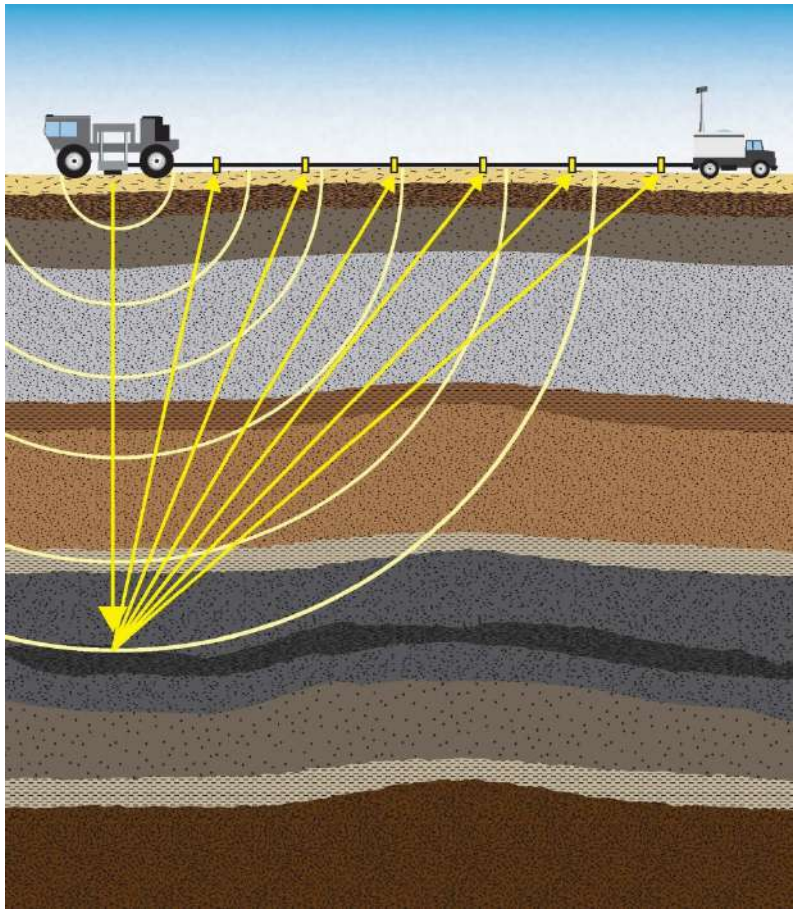


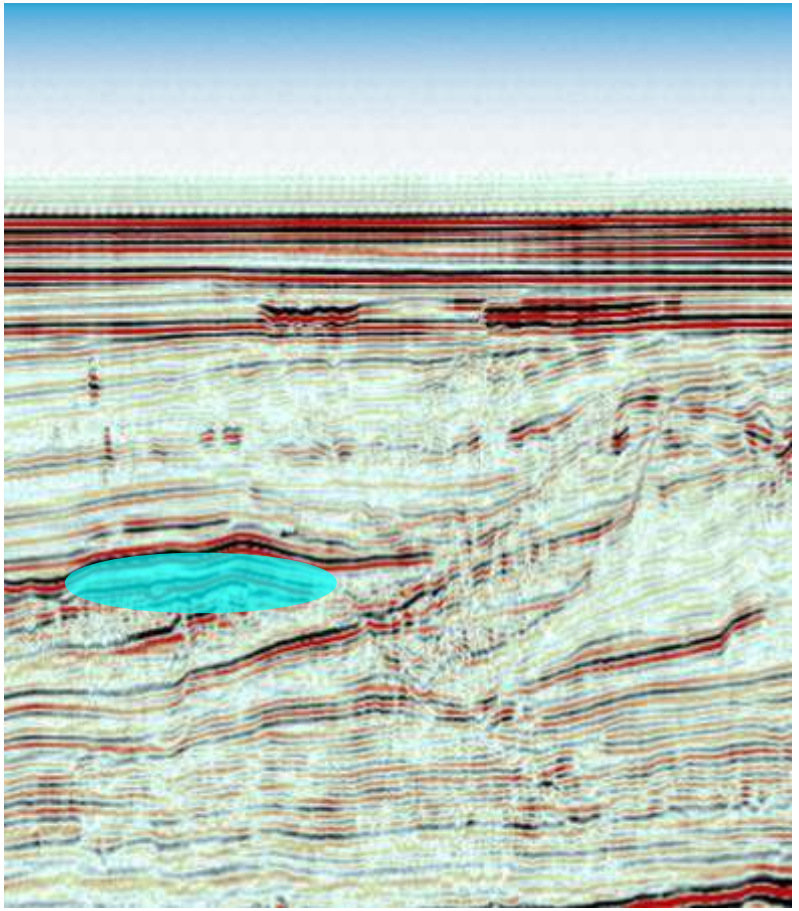
Search for oil



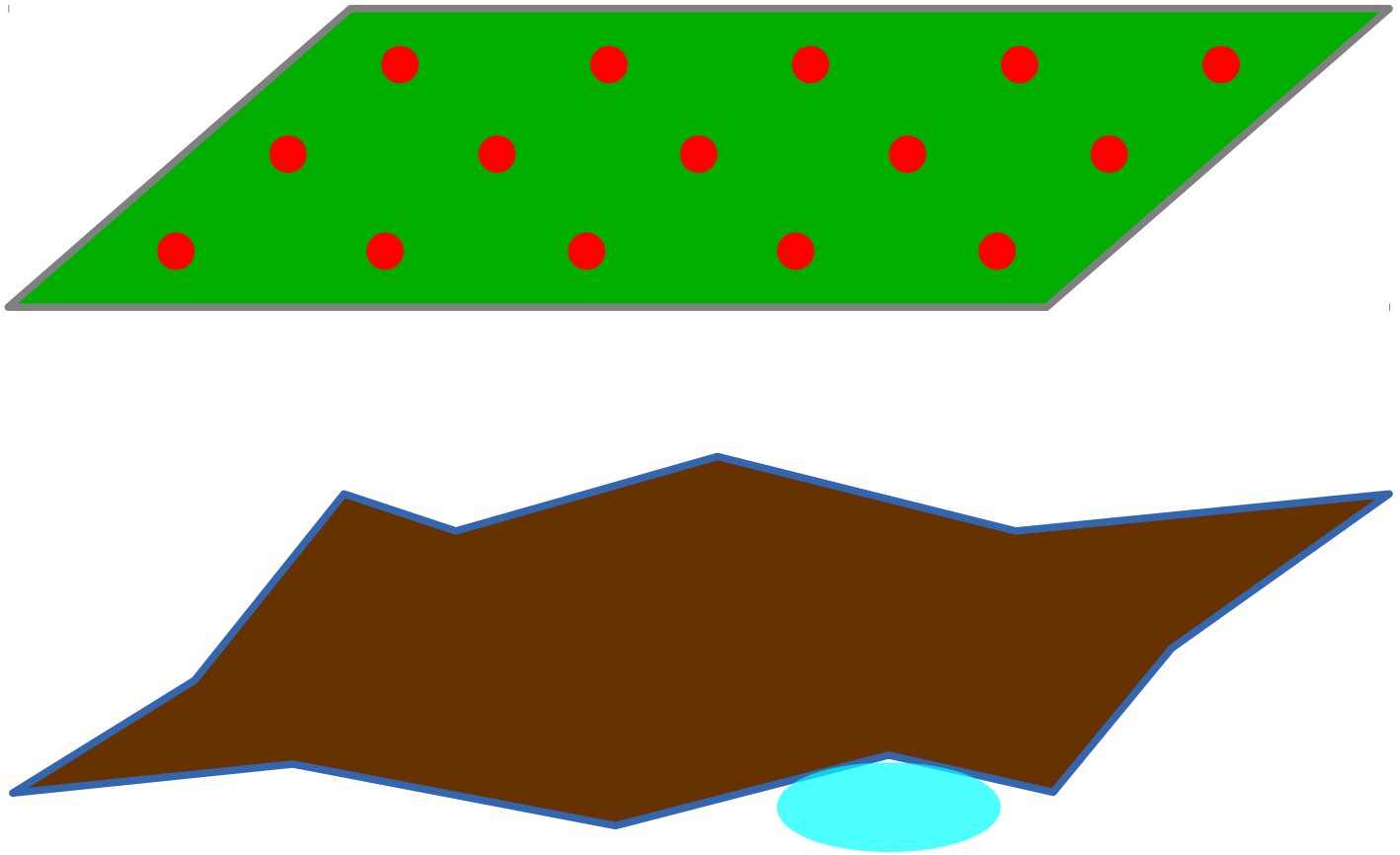


Search for oil

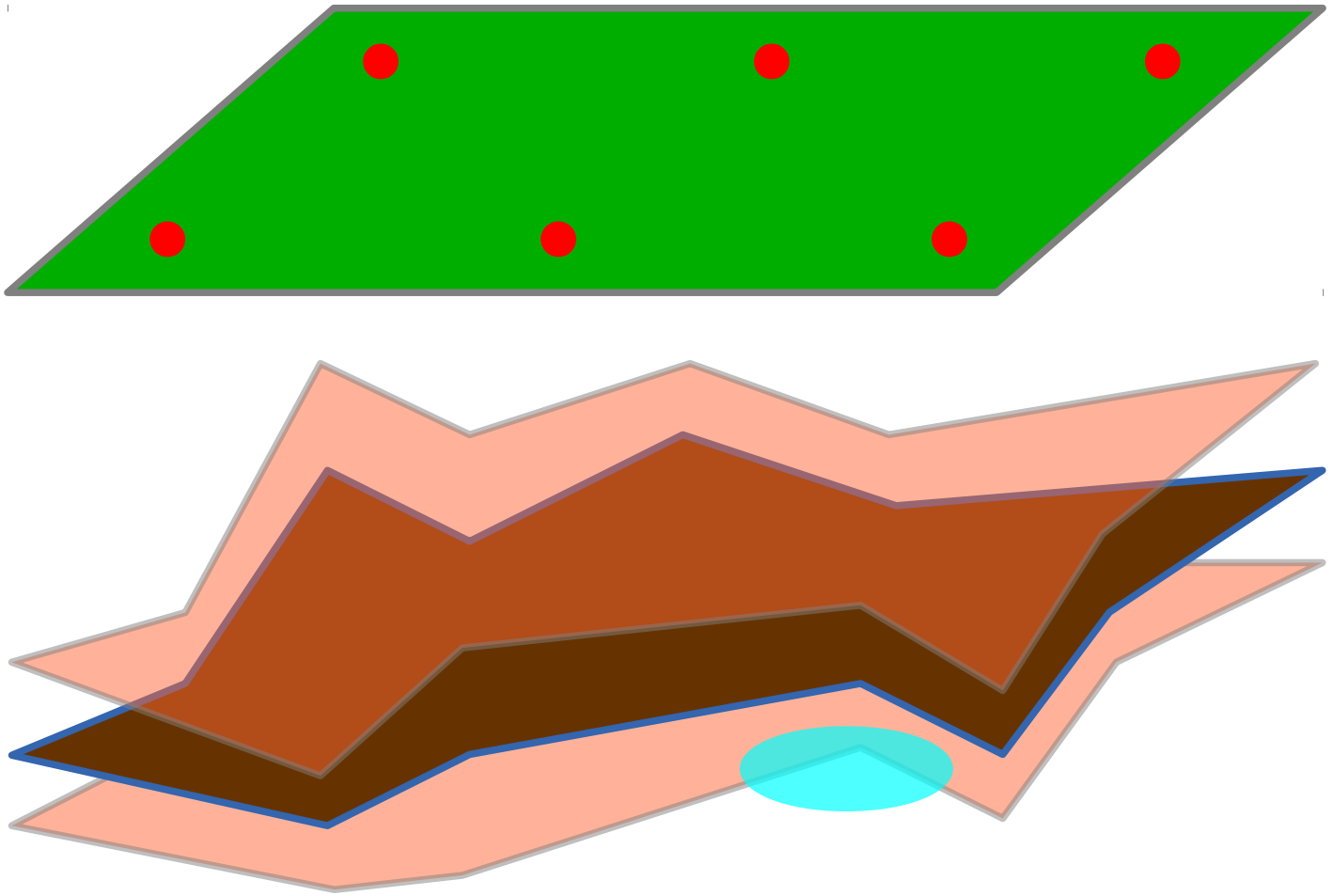




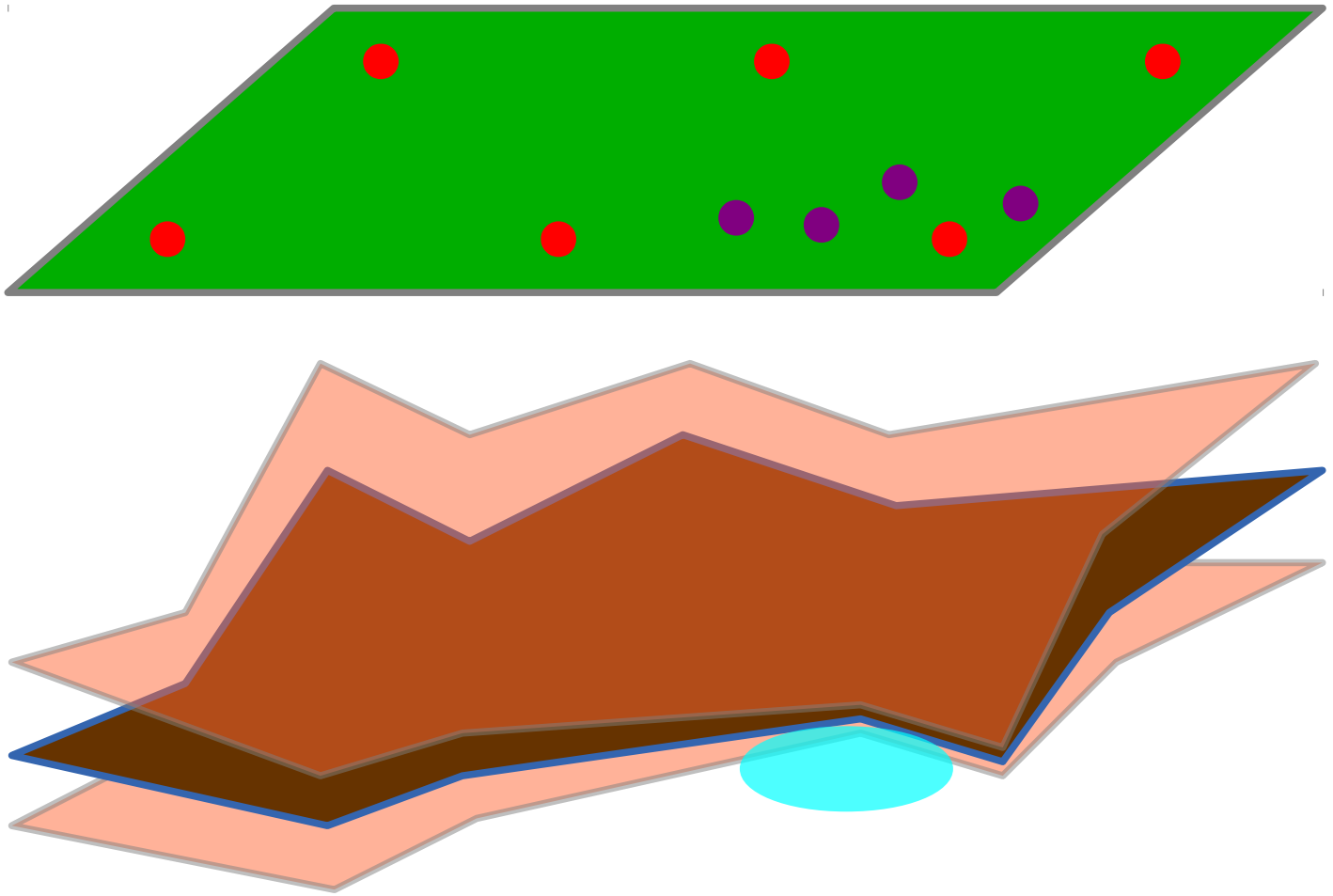
Seismic survey



Seismic survey



Seismic survey



Prospects in the future

Three tools in machine analysis to maximize information

- Maximum likelihood
- Correlations between properties
- Recursive learning

Concurrent materials design