

# Machine learning in materials design, oil exploration, and beyond

G. Conduit, H. Stone, B. Conduit, B. Monserrat, D. Oliveira Sanchez,  
N. Jones

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, Rolls-Royce UTC, Centre for Scientific Computing

# 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



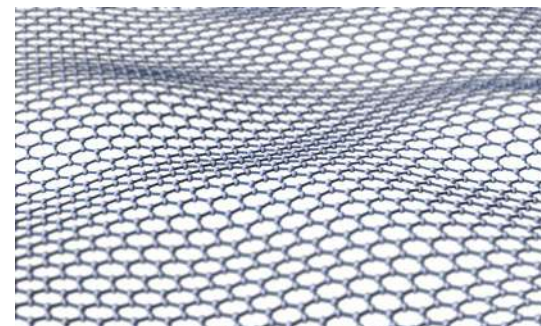
1930s  
Plastics



1940s  
Semiconductors

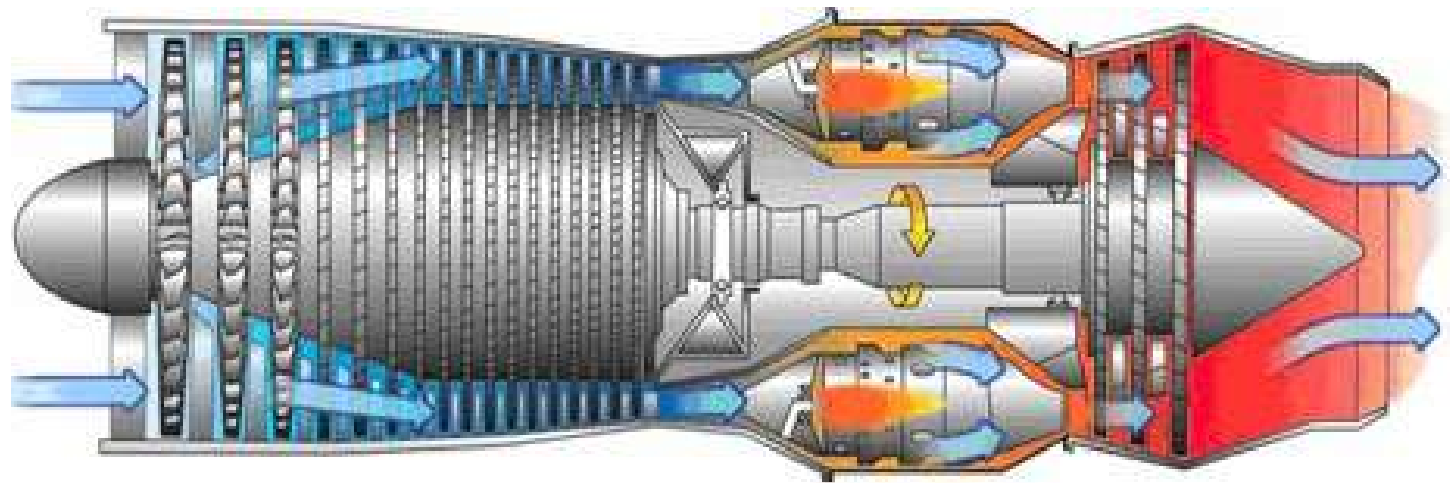


1990s  
High temperature  
superconductors



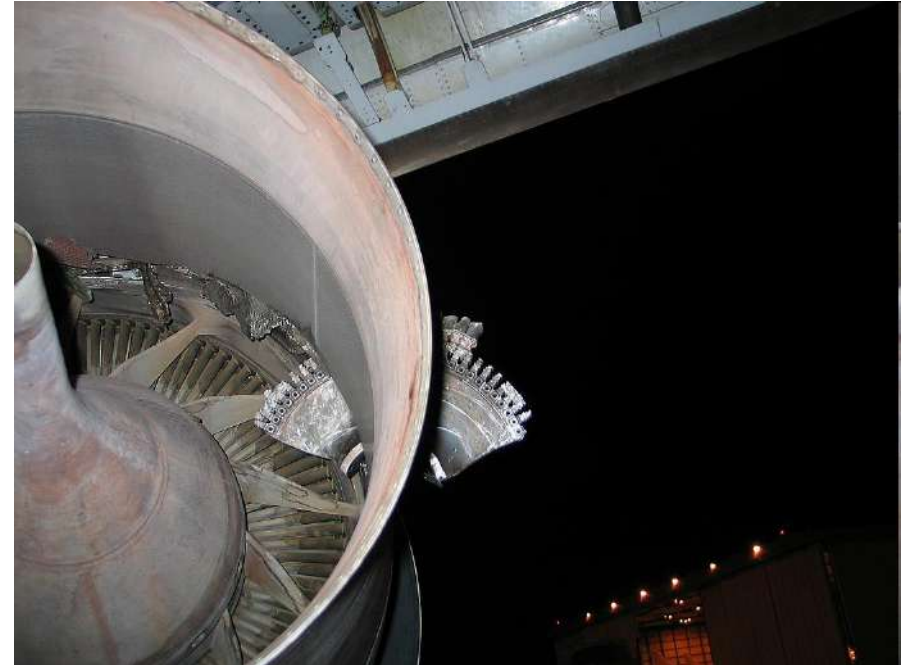
2000s  
Graphene

# Jet engine

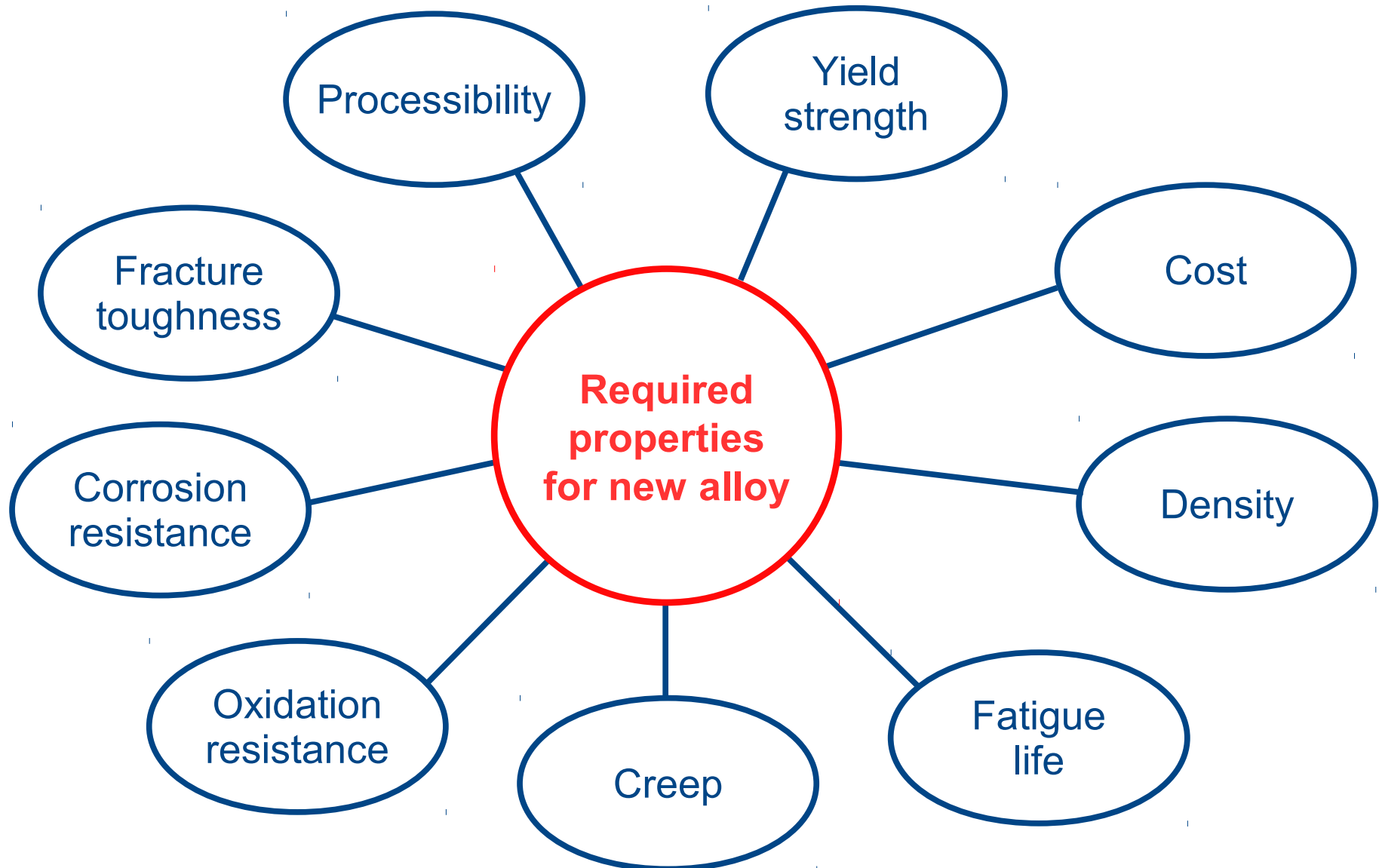




# Jet engine



# 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

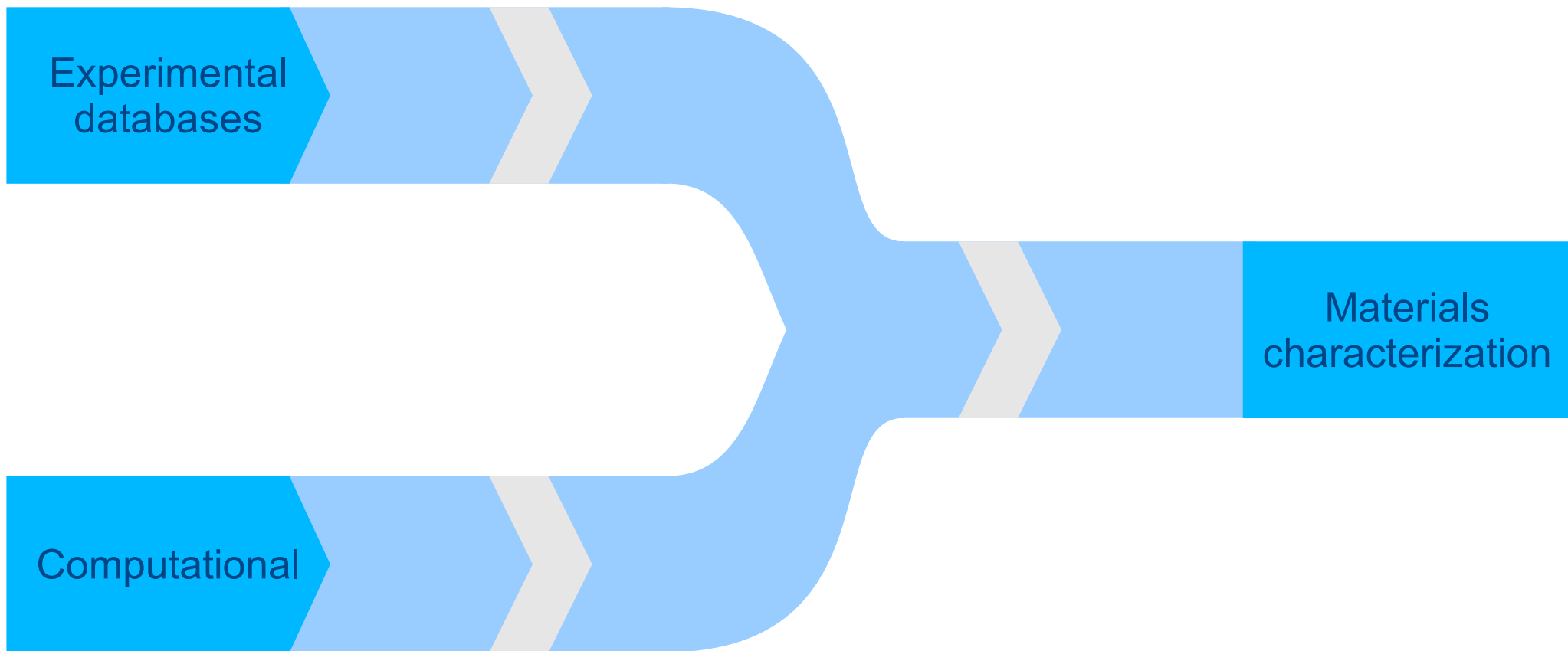


Ni



and 4 different manufacturing processes

# Materials pipeline

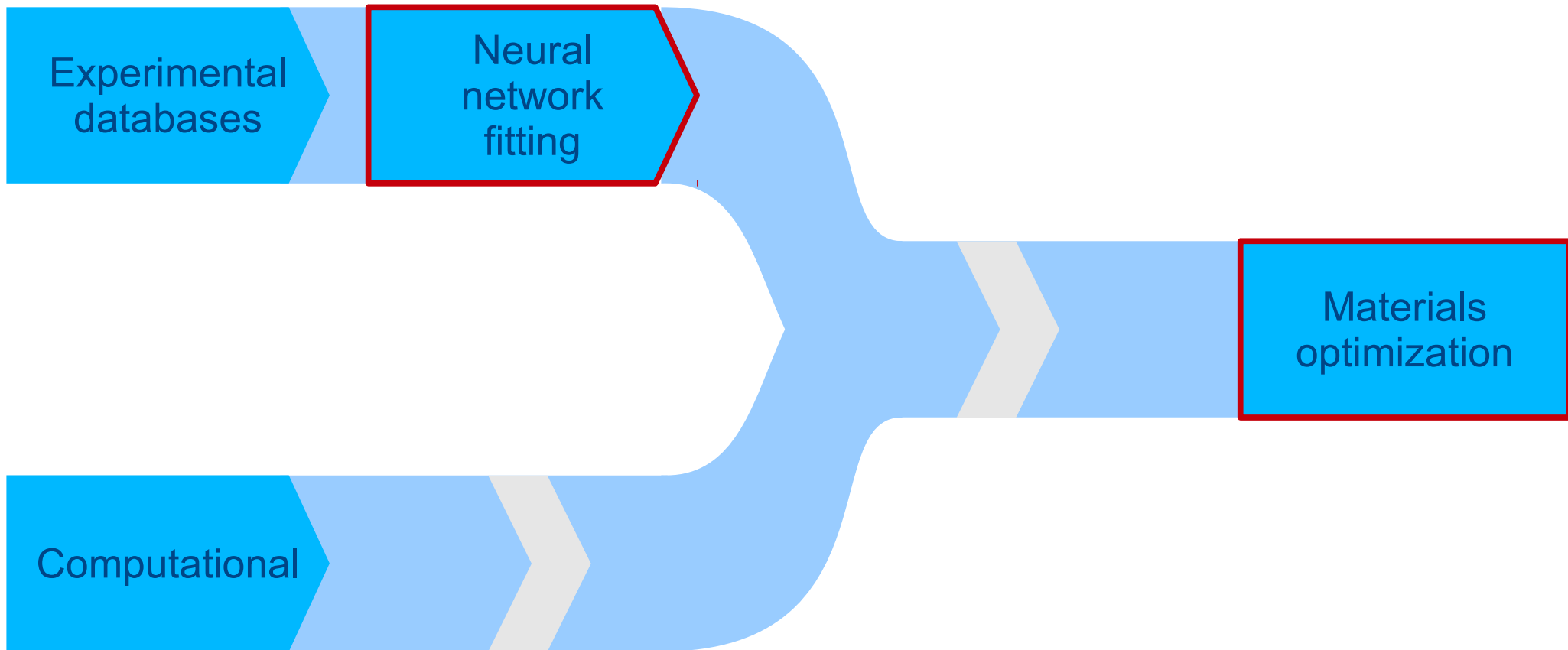


Experimental  
databases

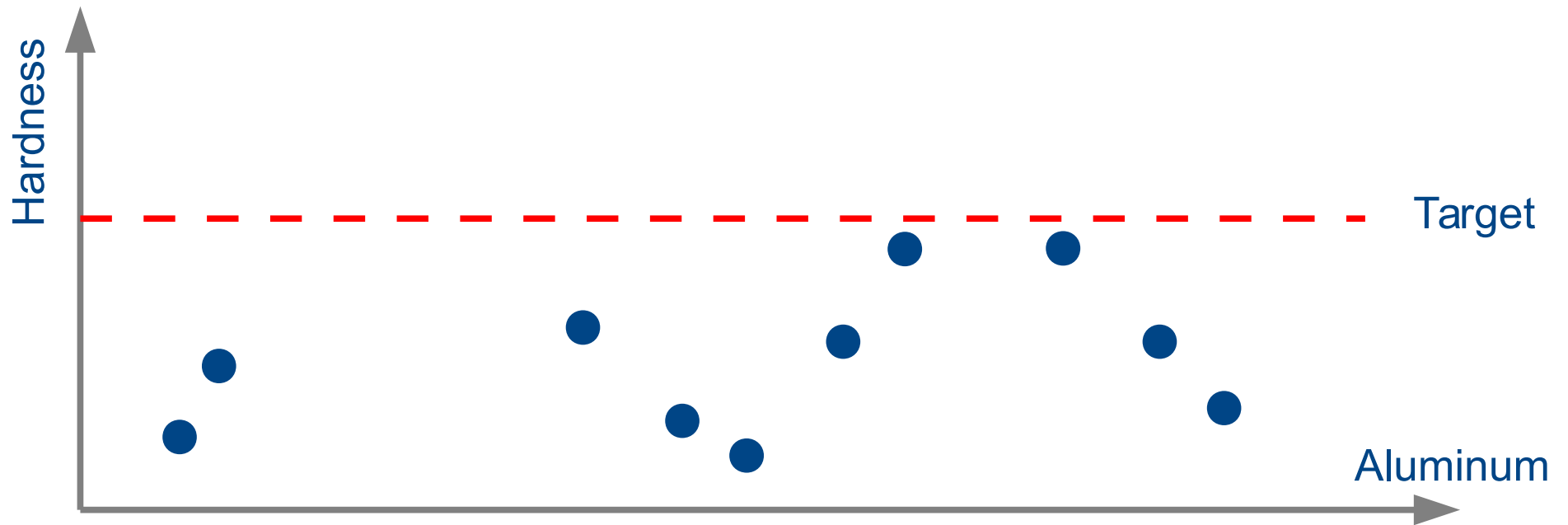
Computational

Materials  
characterization

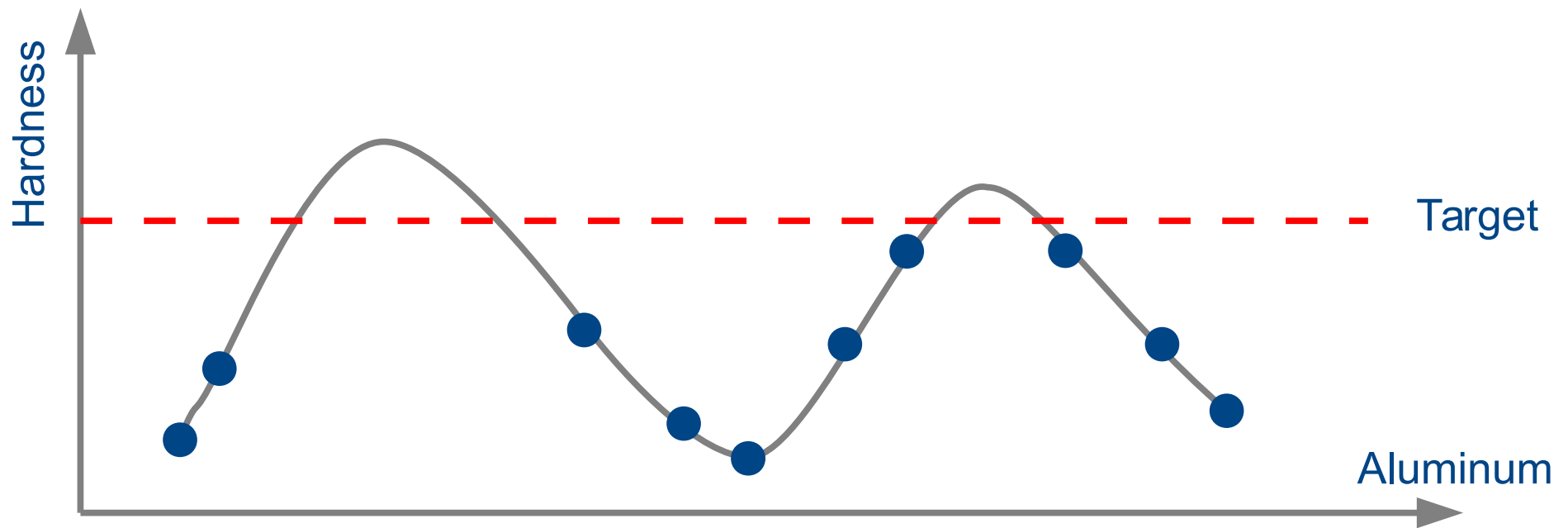
# Two new tools



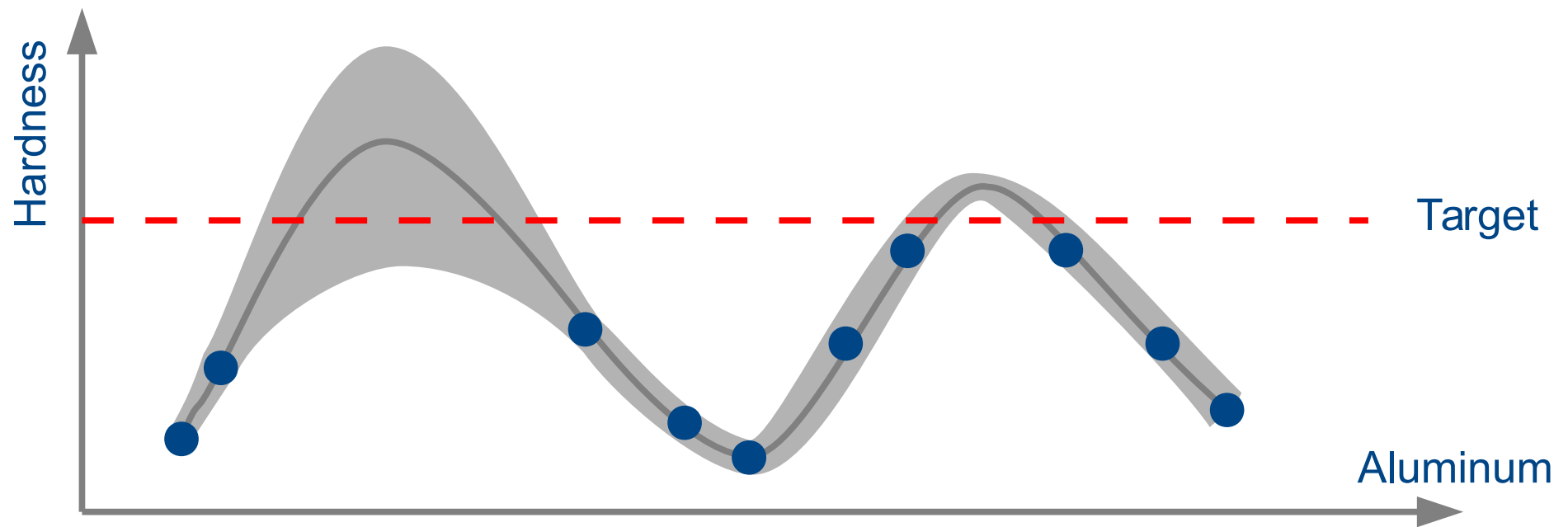
# Neural network fitting & optimization



# Neural network fitting & optimization

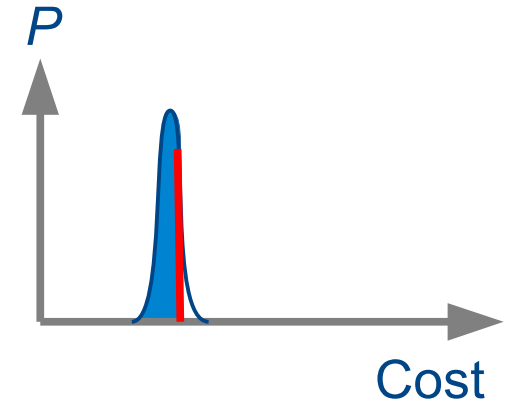
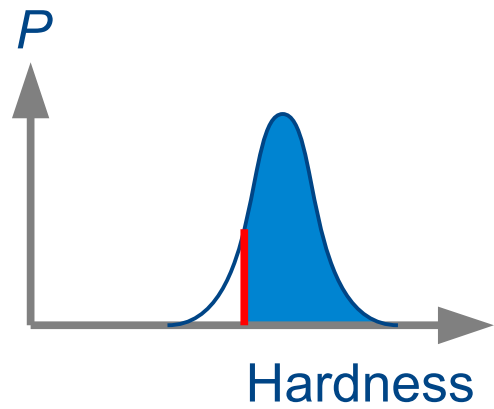


# Neural network fitting & optimization

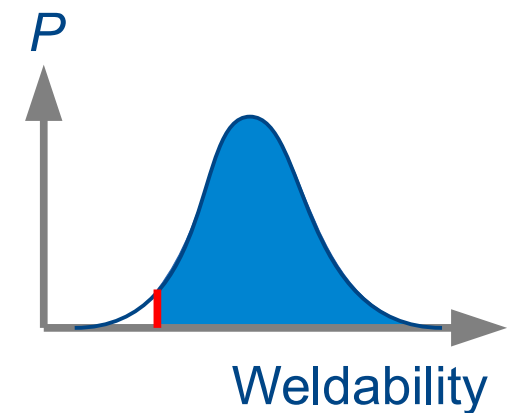
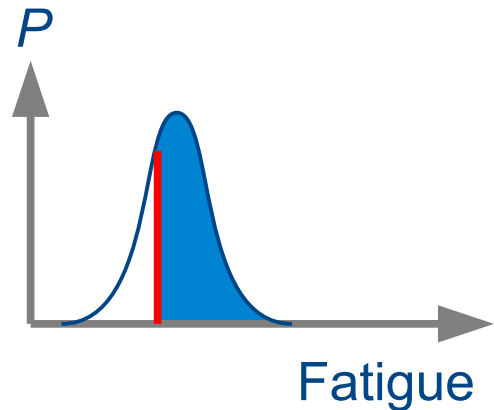




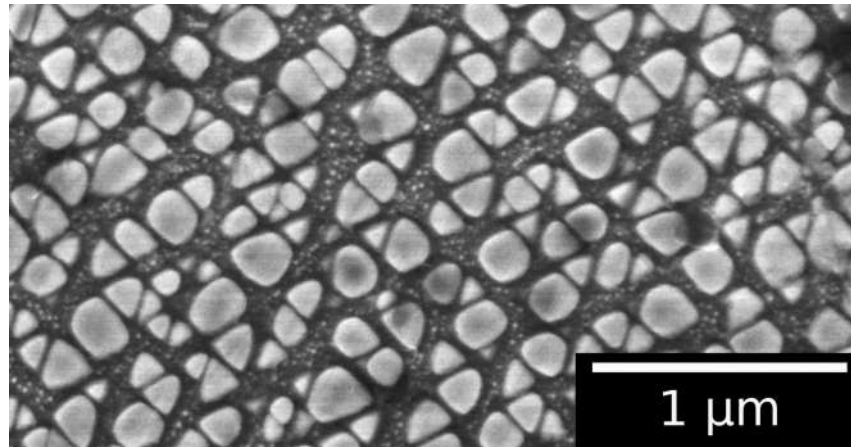
# Optimizing the likelihood



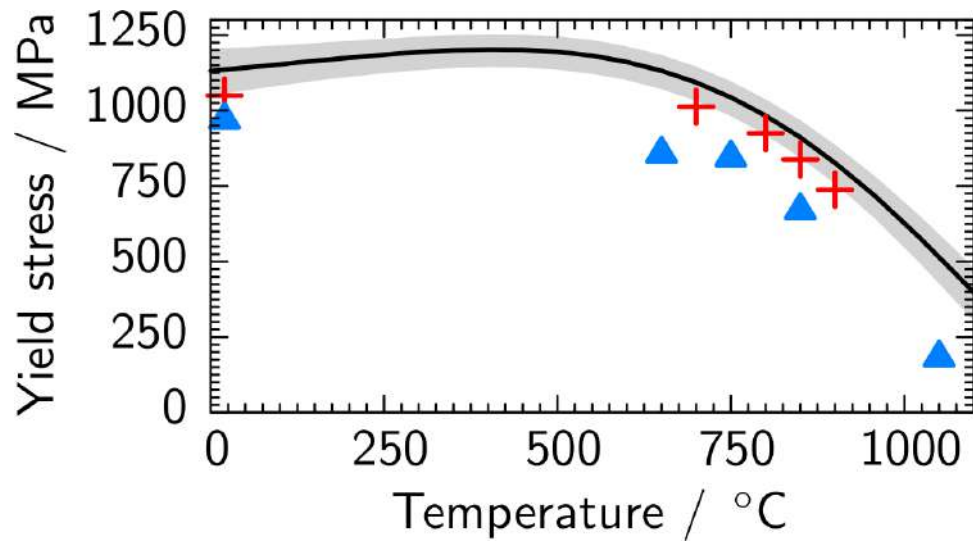
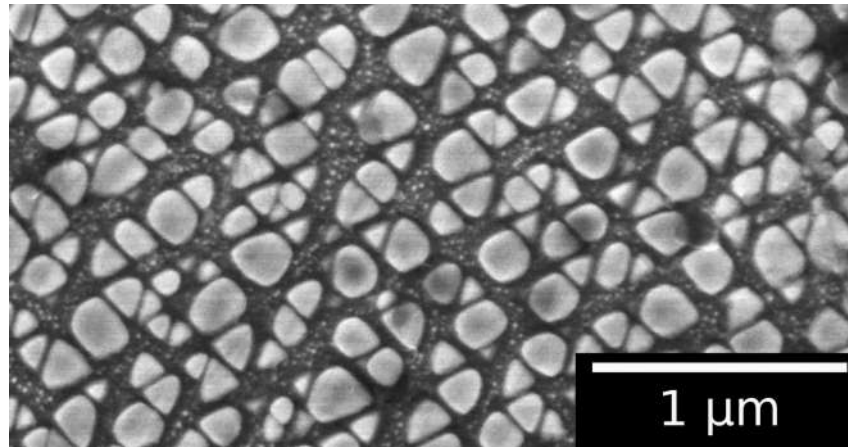
Likelihood of alloy satisfying all targets



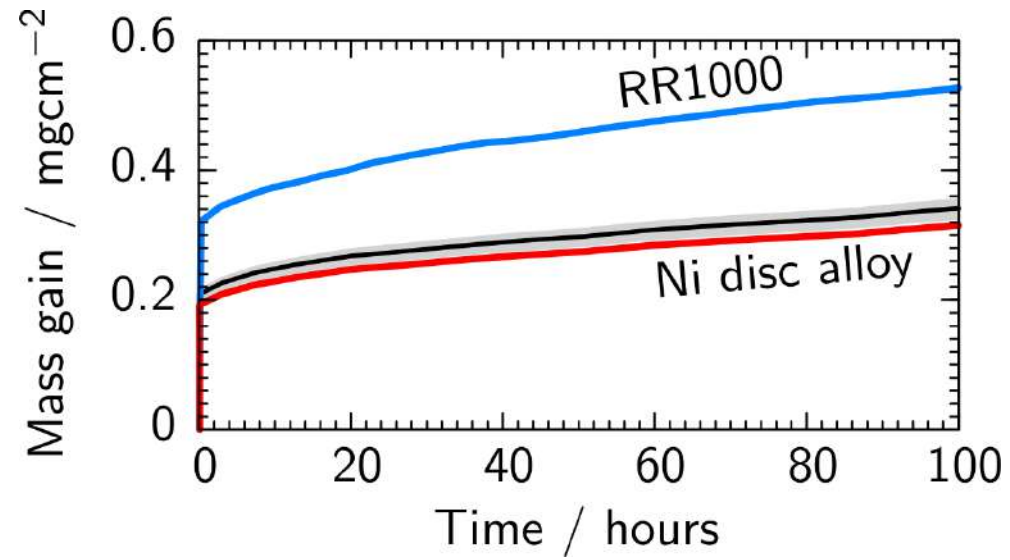
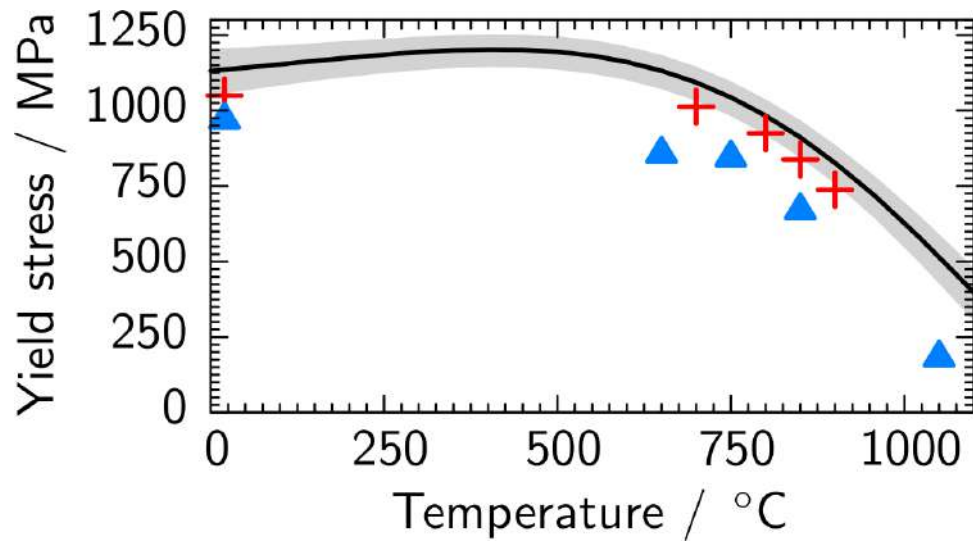
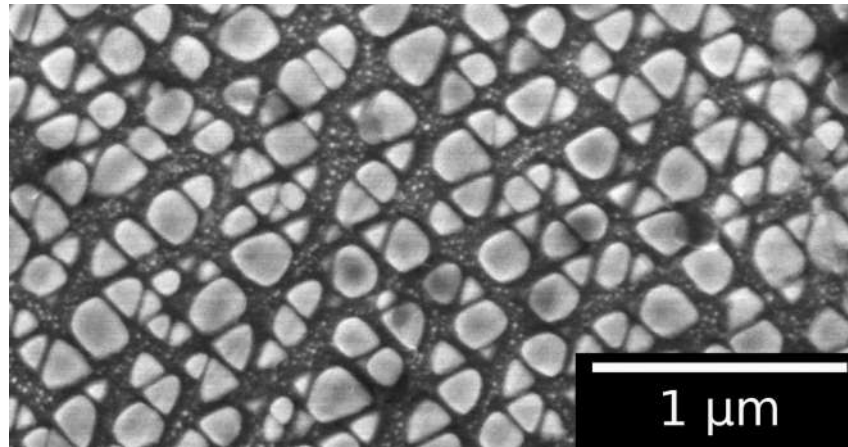
# Ni-base superalloy



# Ni-base superalloy



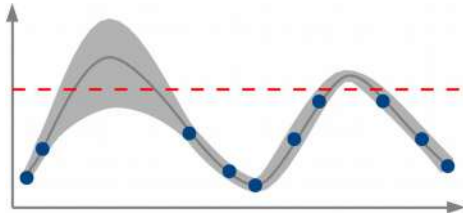
# Ni-base superalloy



# Alloys discovered

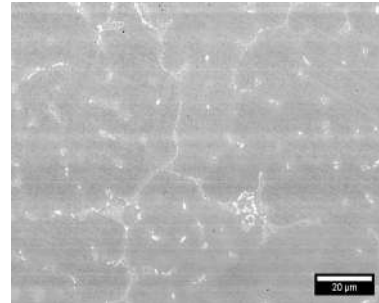
## Discovery algorithm

EP14153898.3  
US 2014/177578  
GB1302743.8



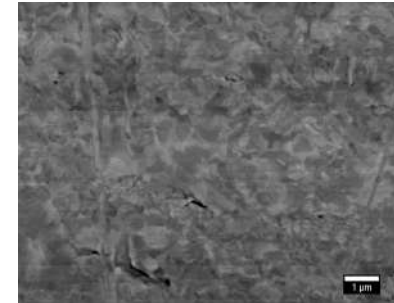
## Mo-Hf forging alloy

EP14161255.6  
US 2014/223465  
GB1307533.8



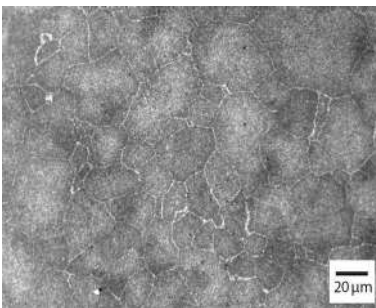
## Mo-Nb forging alloy

EP14161529.4  
US 2014/224885  
GB1307535.3



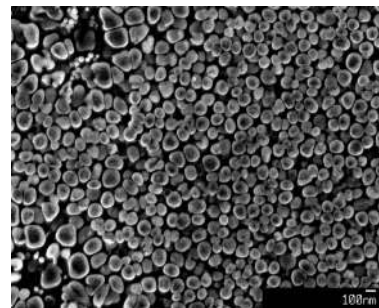
## RR1000 grain growth

Acta Materialia, 61, 3378



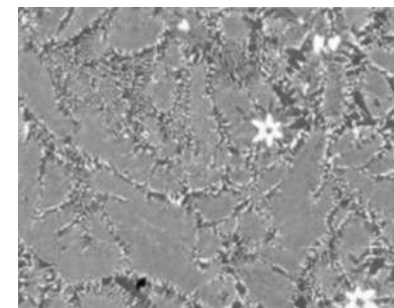
## Ni disc alloy

EP14157622.3  
US 2013/0052077 A2  
GB1408536.9

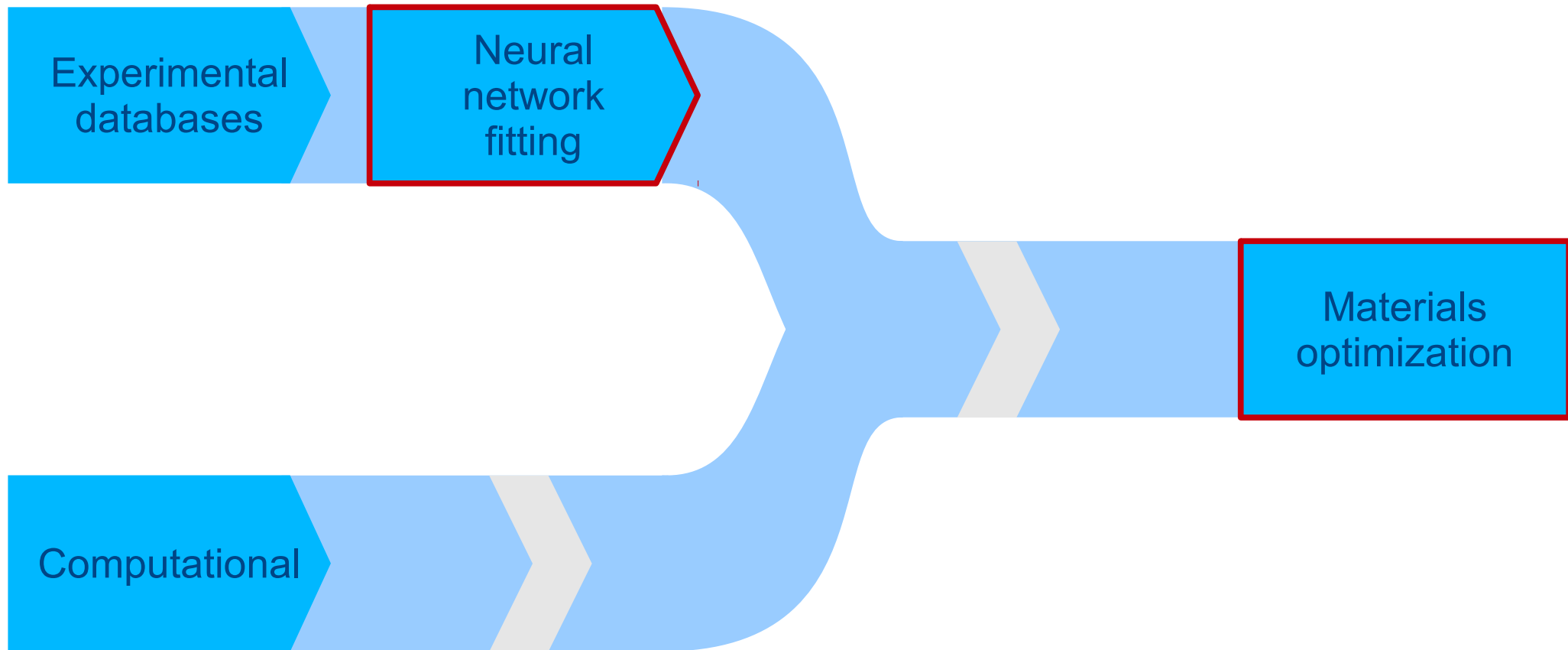


## Cr-Cr2Ta alloys

Intermetallics 48, 62



# Two new tools



# Light emitting diodes

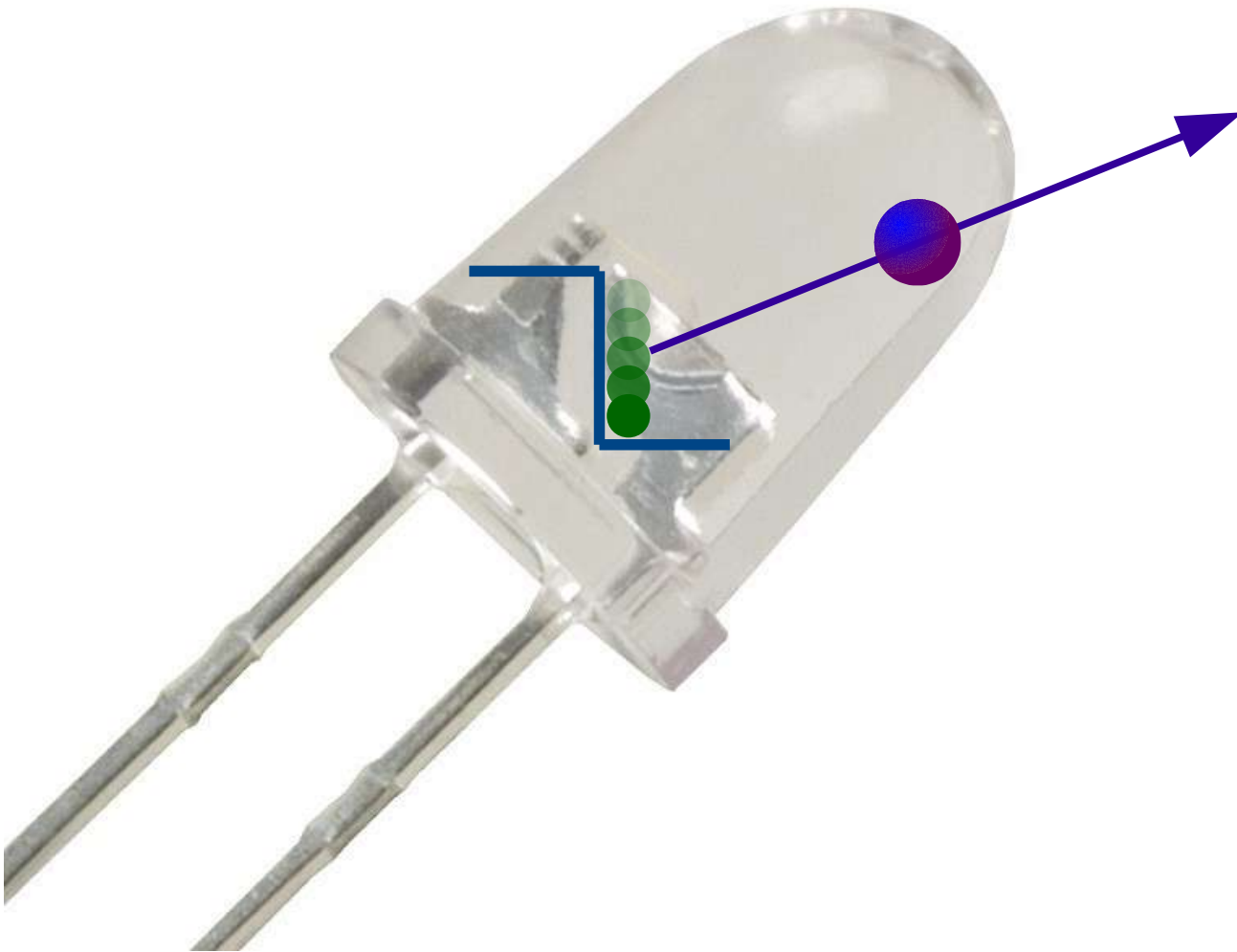


Cost

Efficiency

Color

# Light emitting diodes



Cost

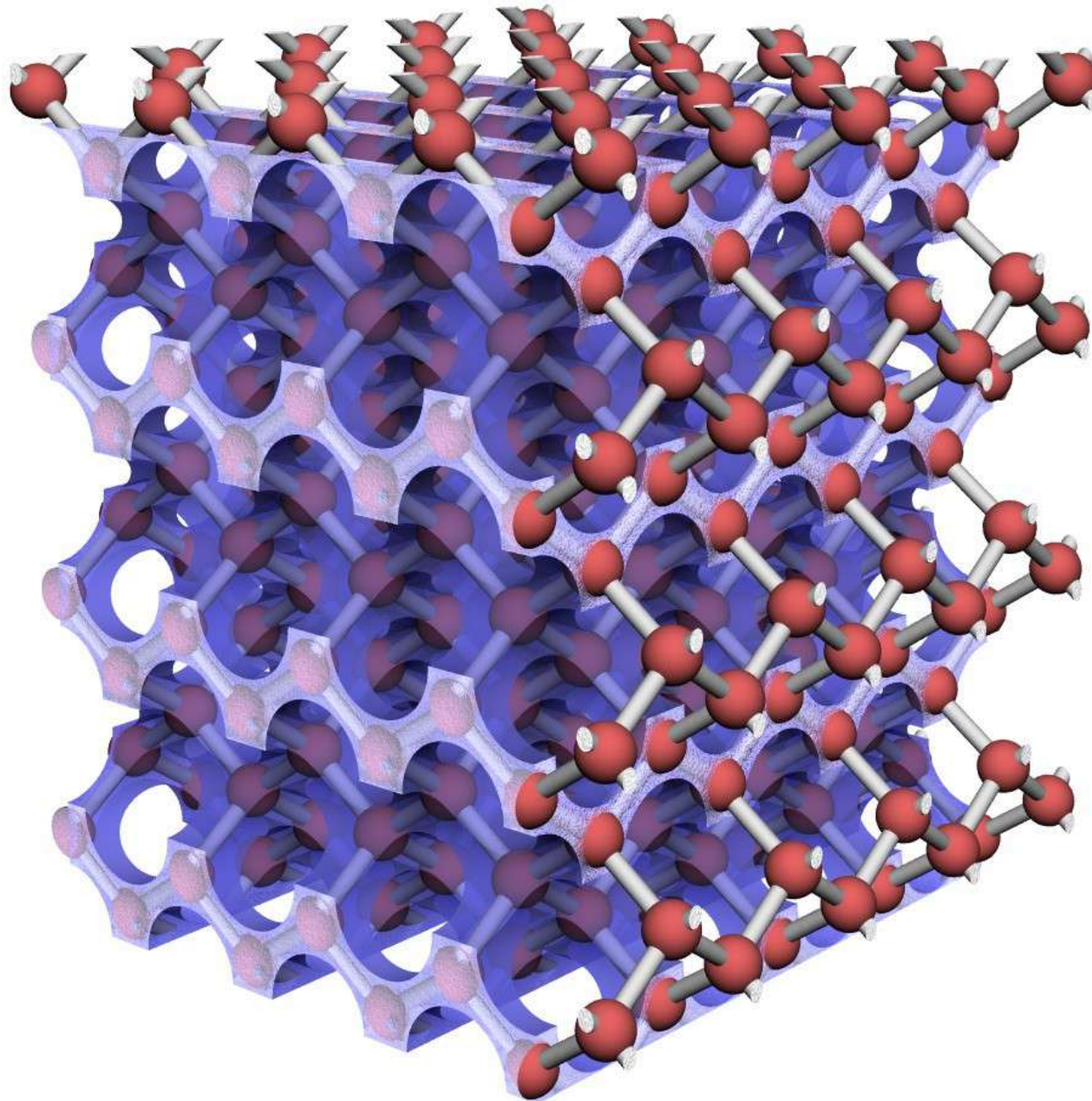
Efficiency

Color

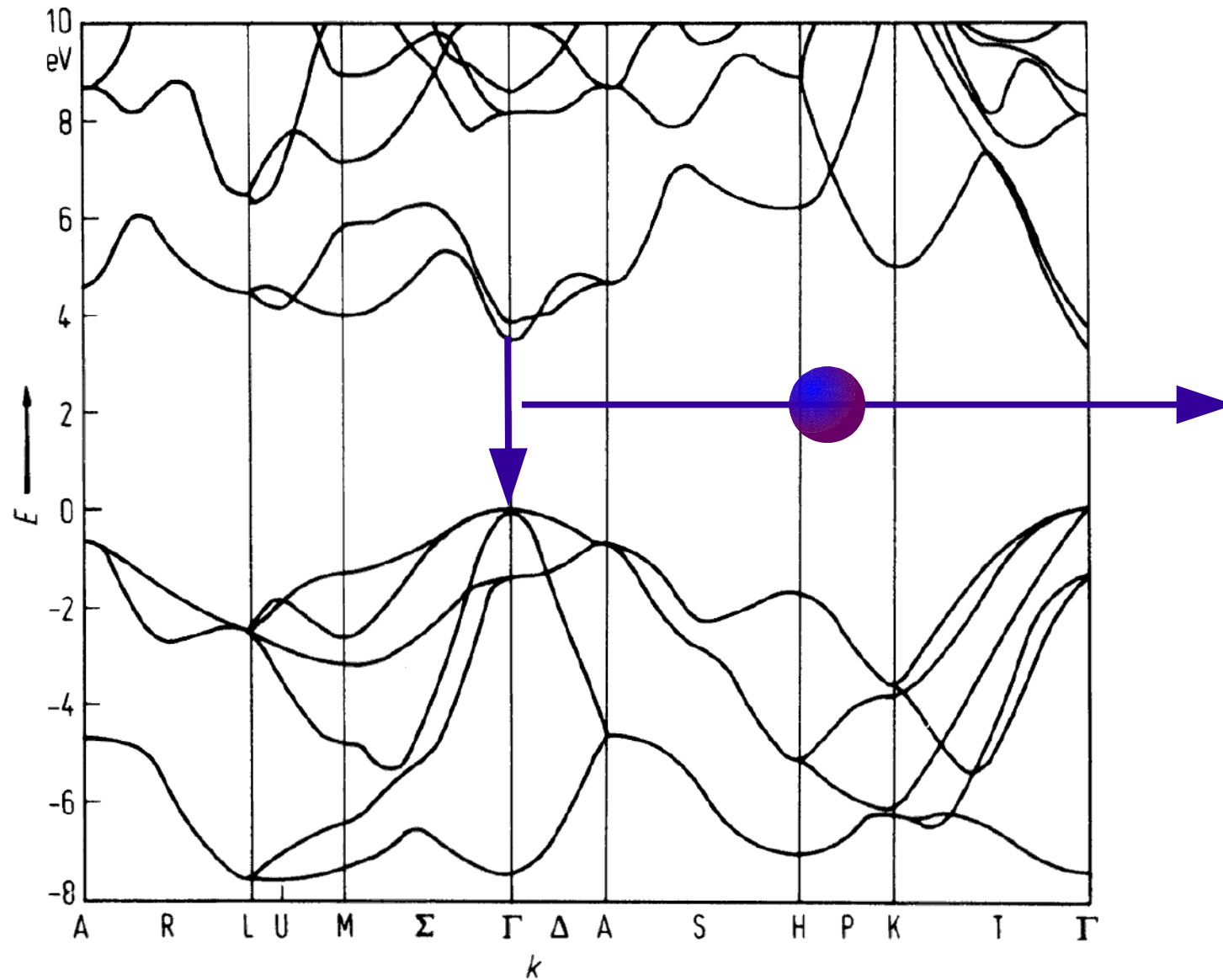
Band gap



# Computer simulations



# Band gap

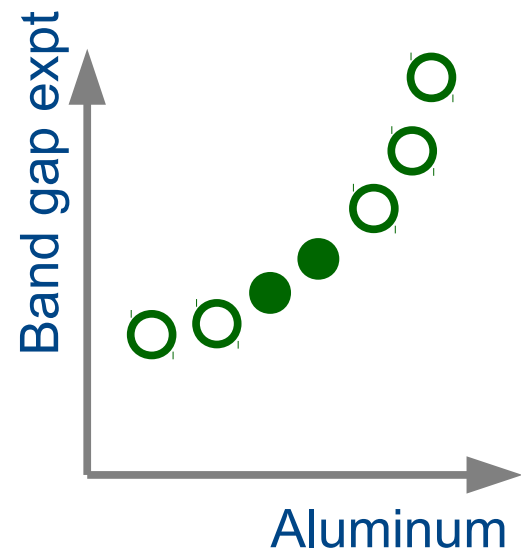


# Computational challenges

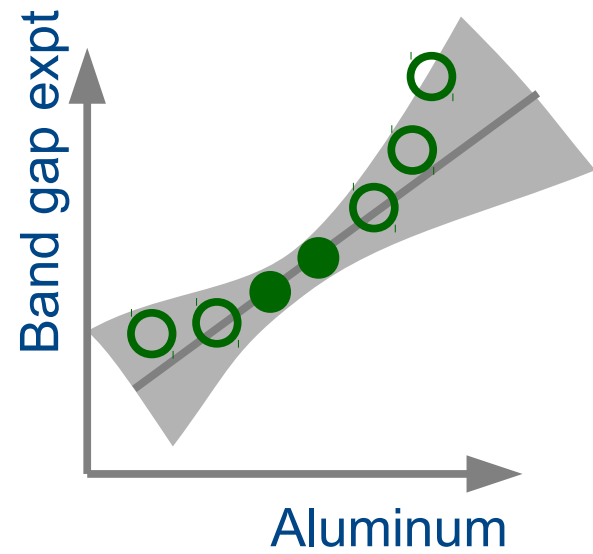
Inevitable approximations behind first principles simulations

Reducing number of simulations performed

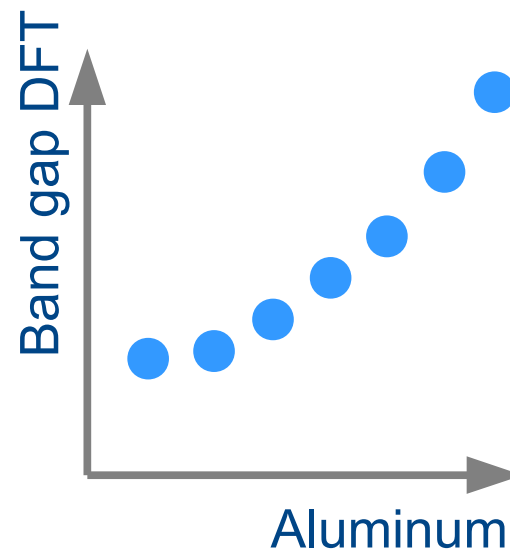
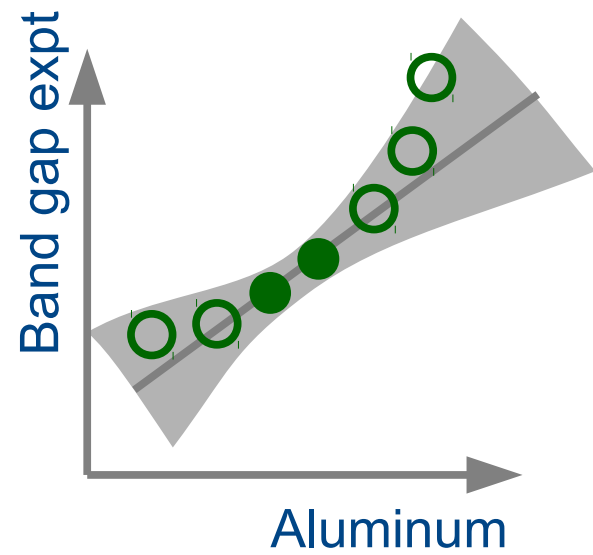
# Correlations between properties



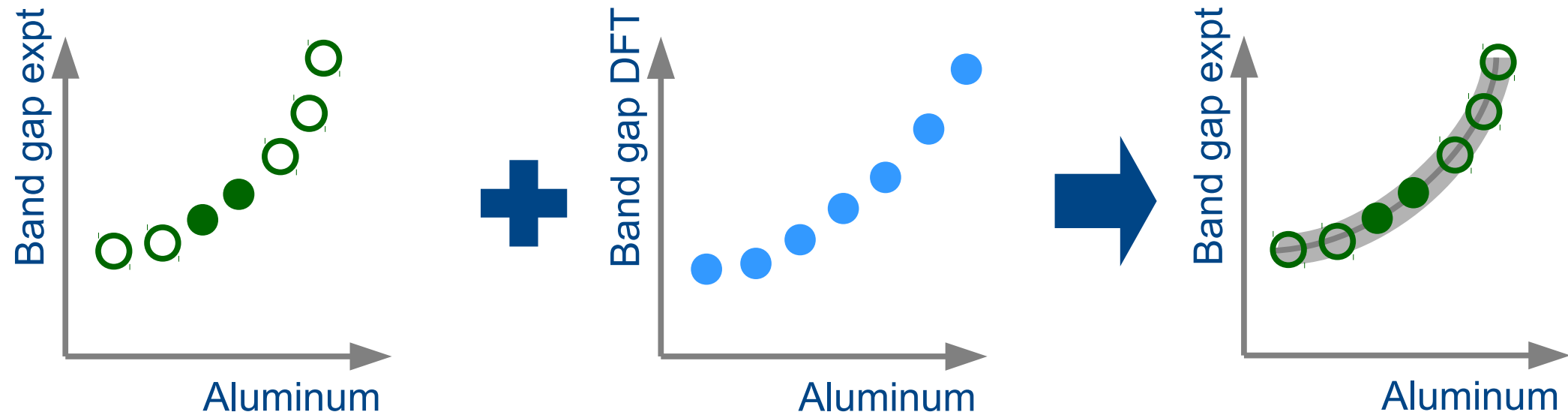
# Correlations between properties



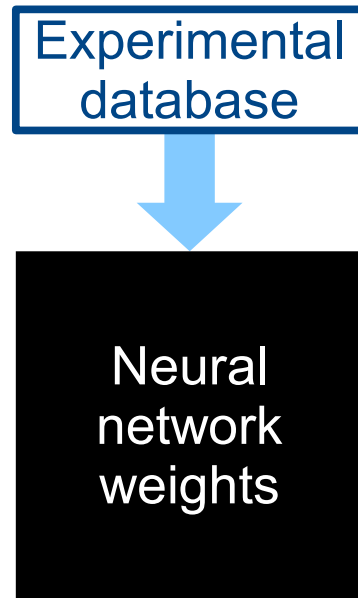
# Correlations between properties



# Correlations between properties

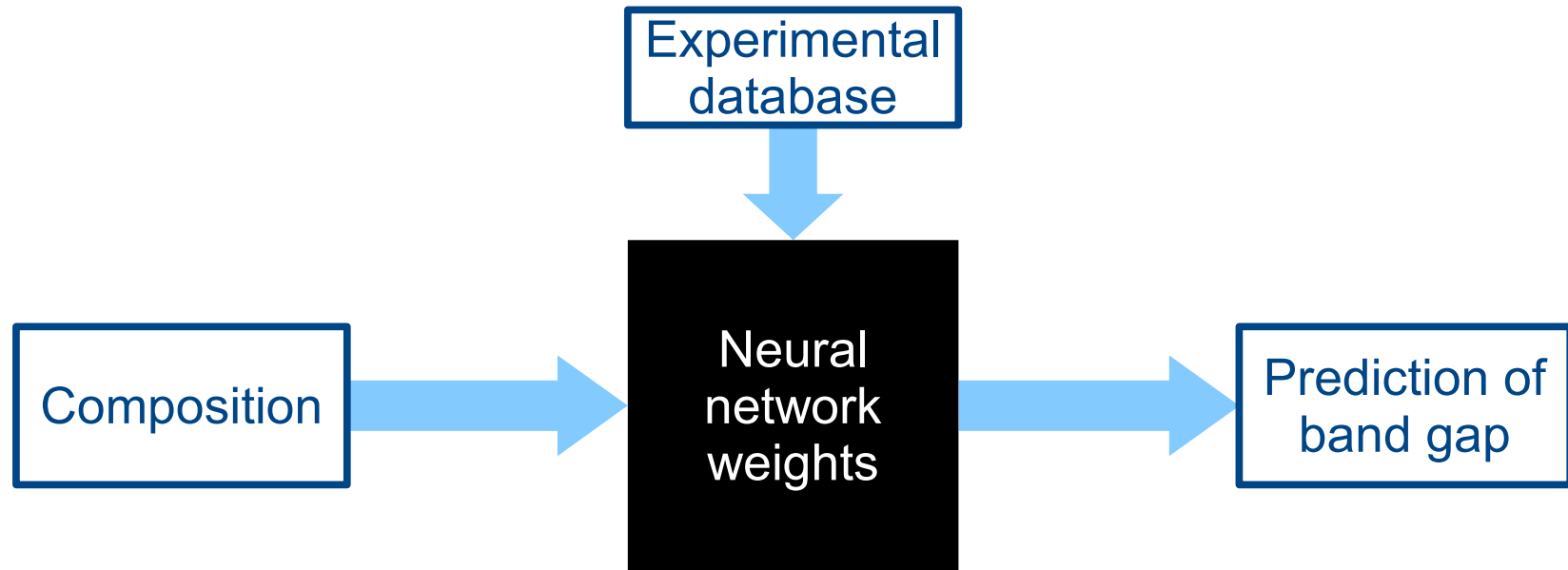


# Correlations between properties

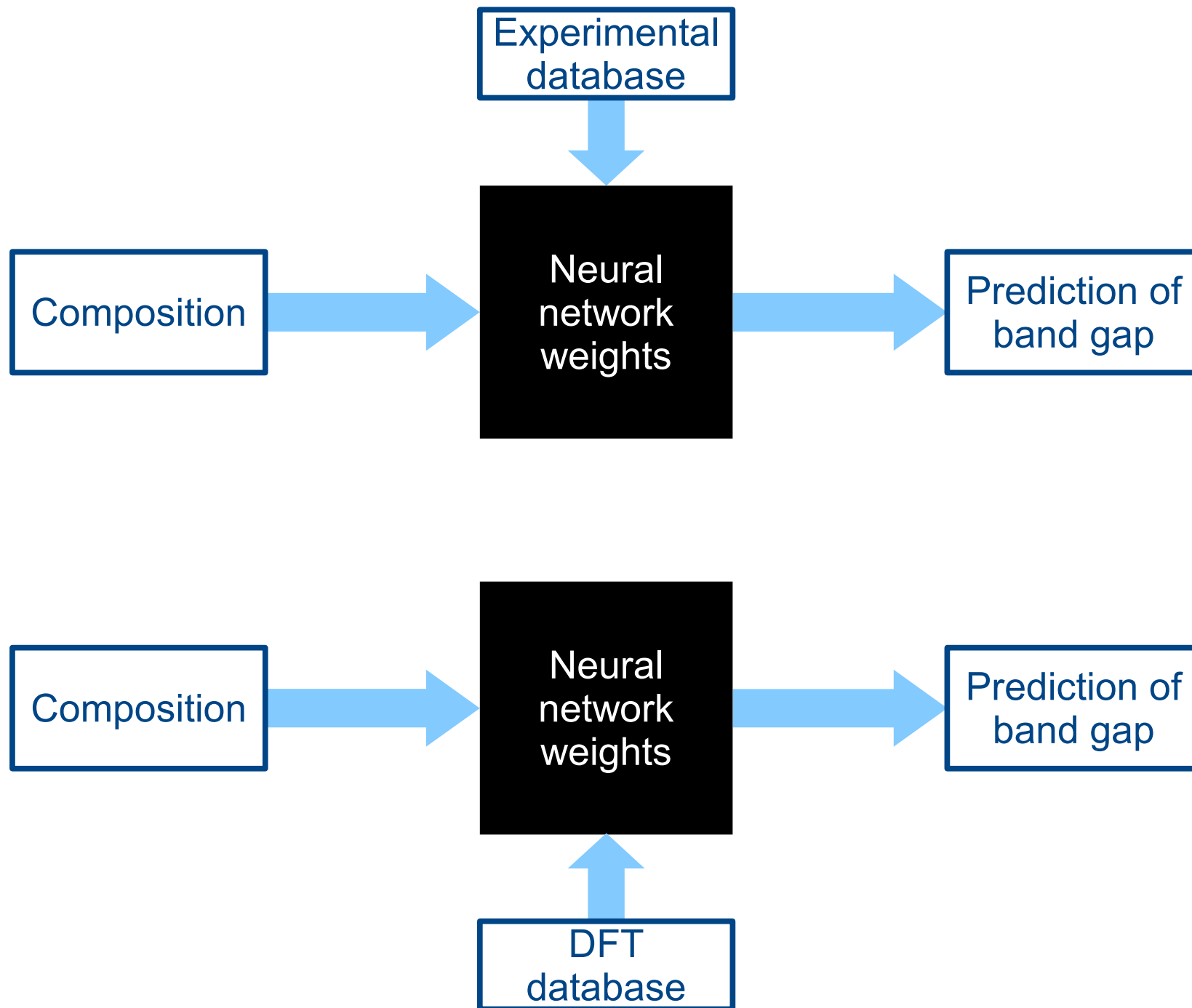




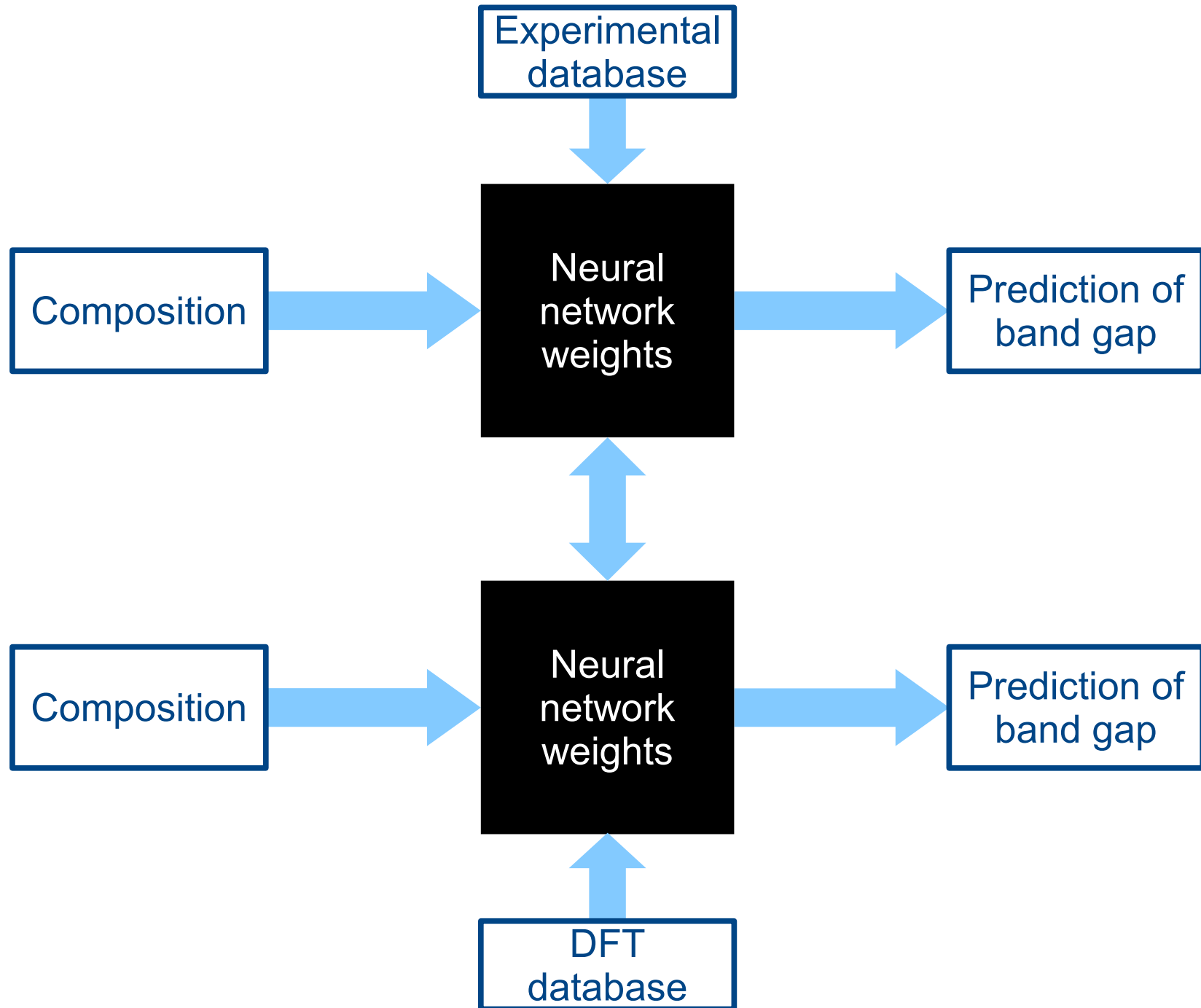
# Correlations between properties



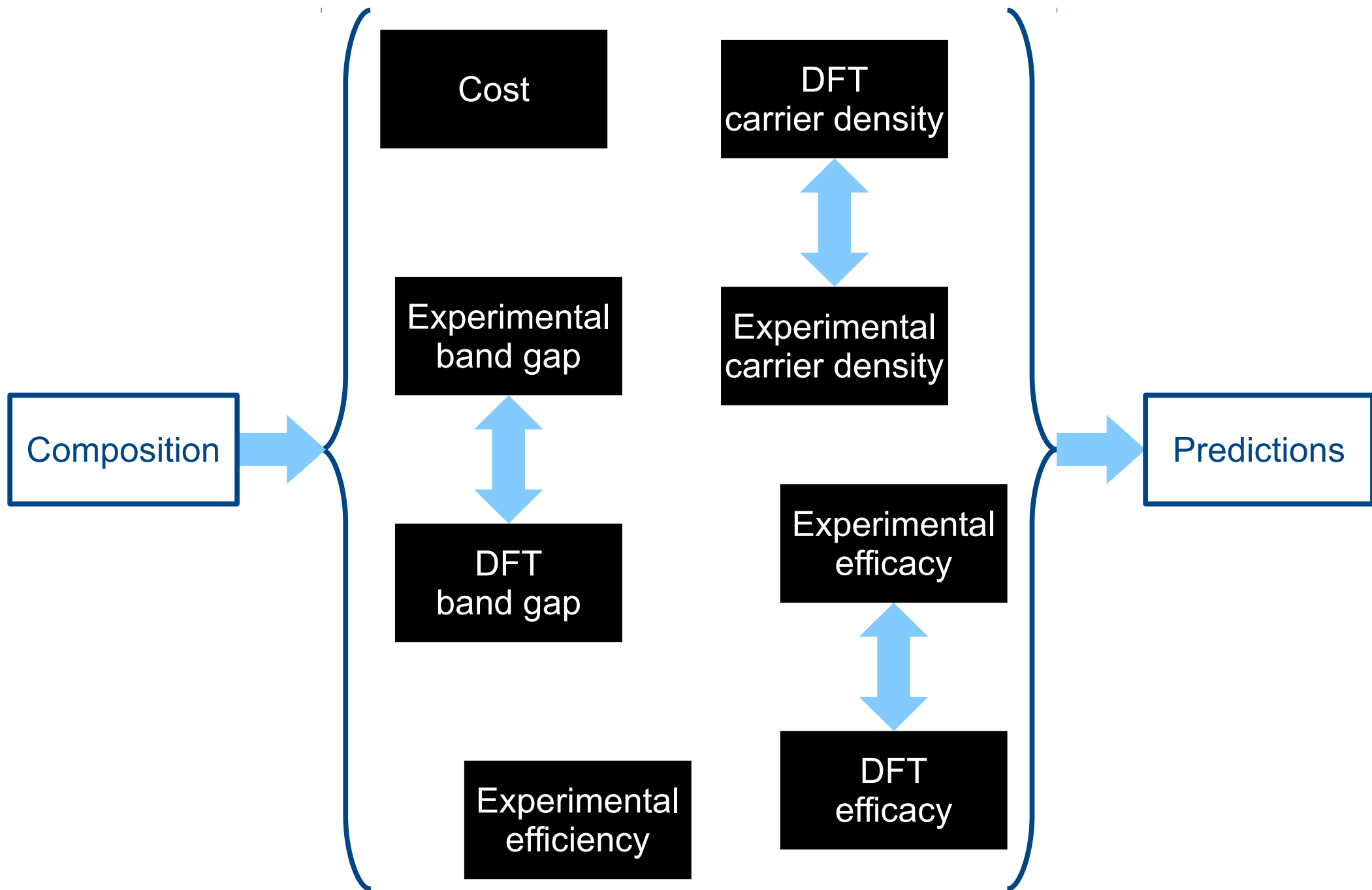
# Correlations between properties



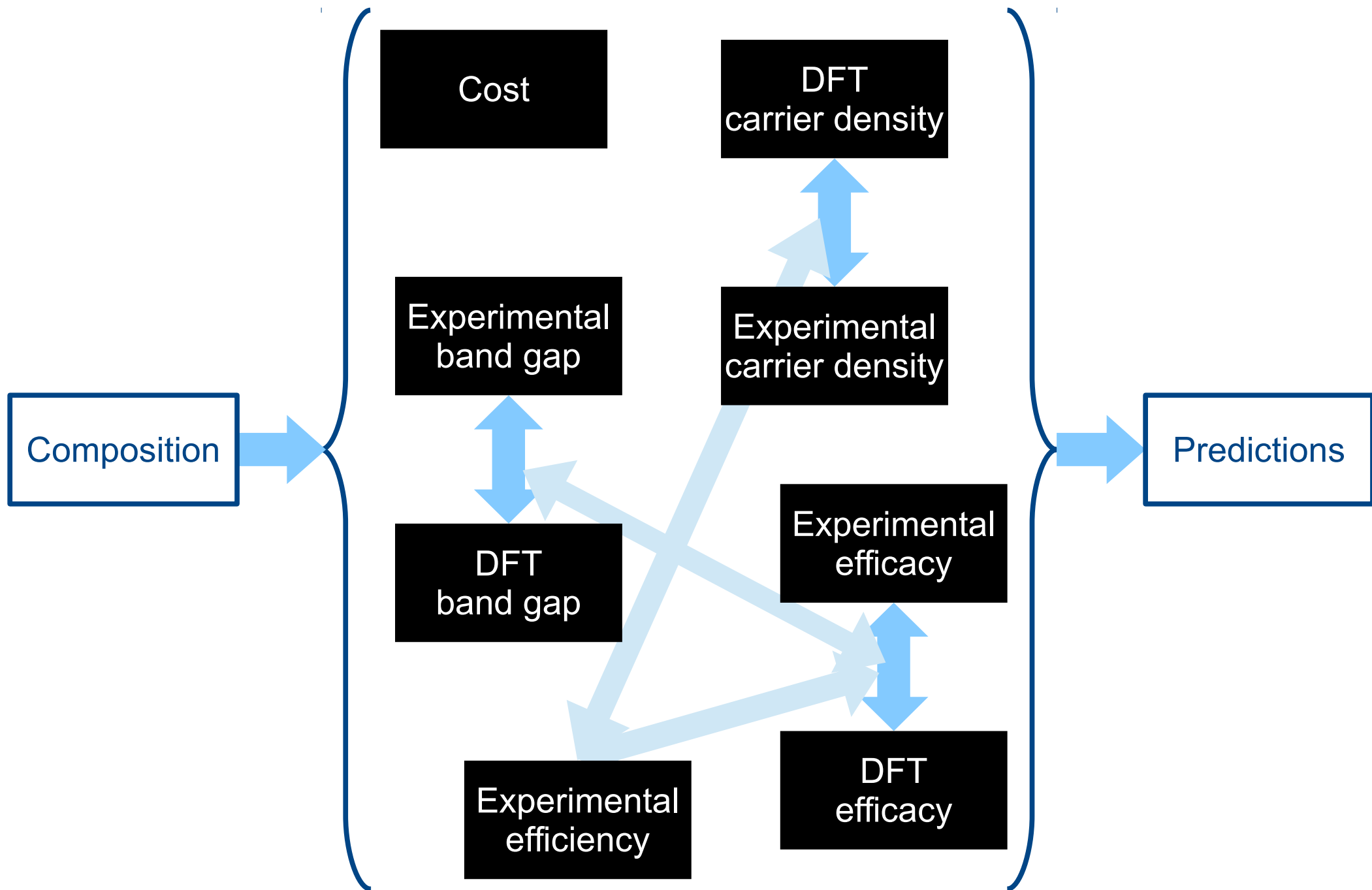
# Correlations between properties



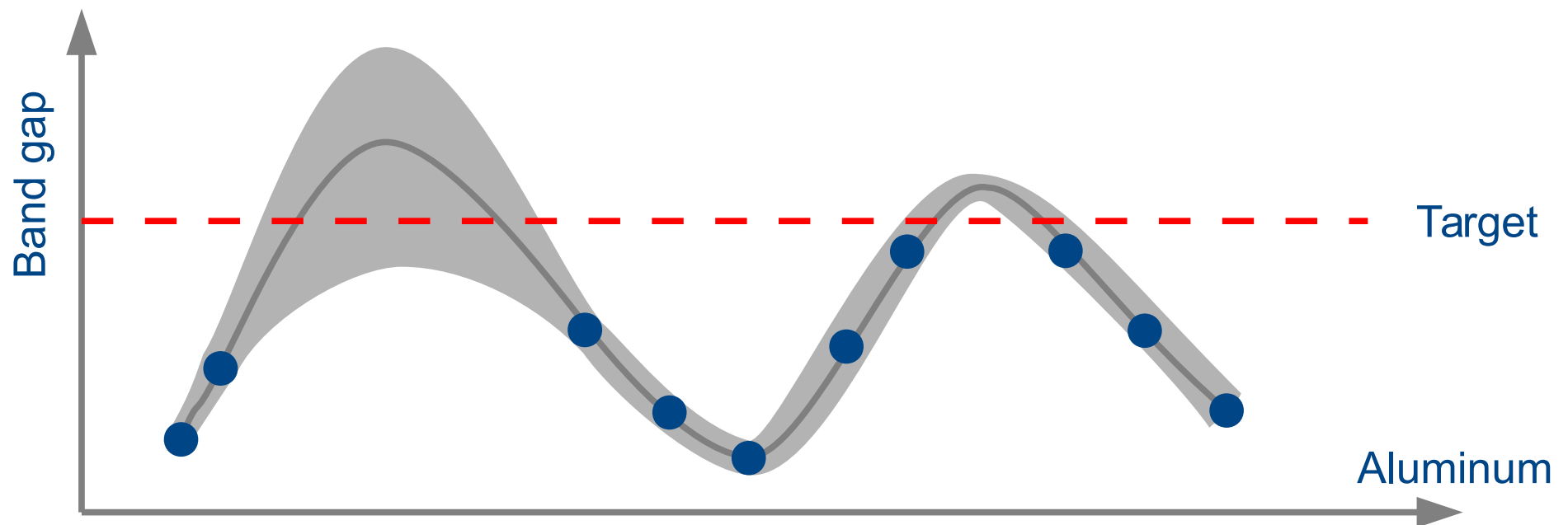
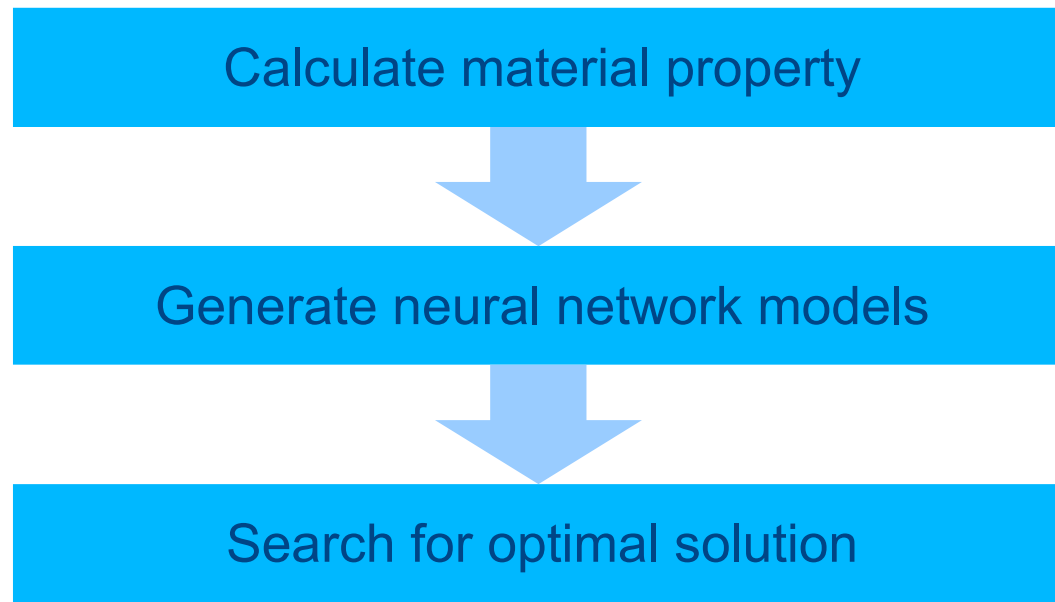
# Correlations between properties



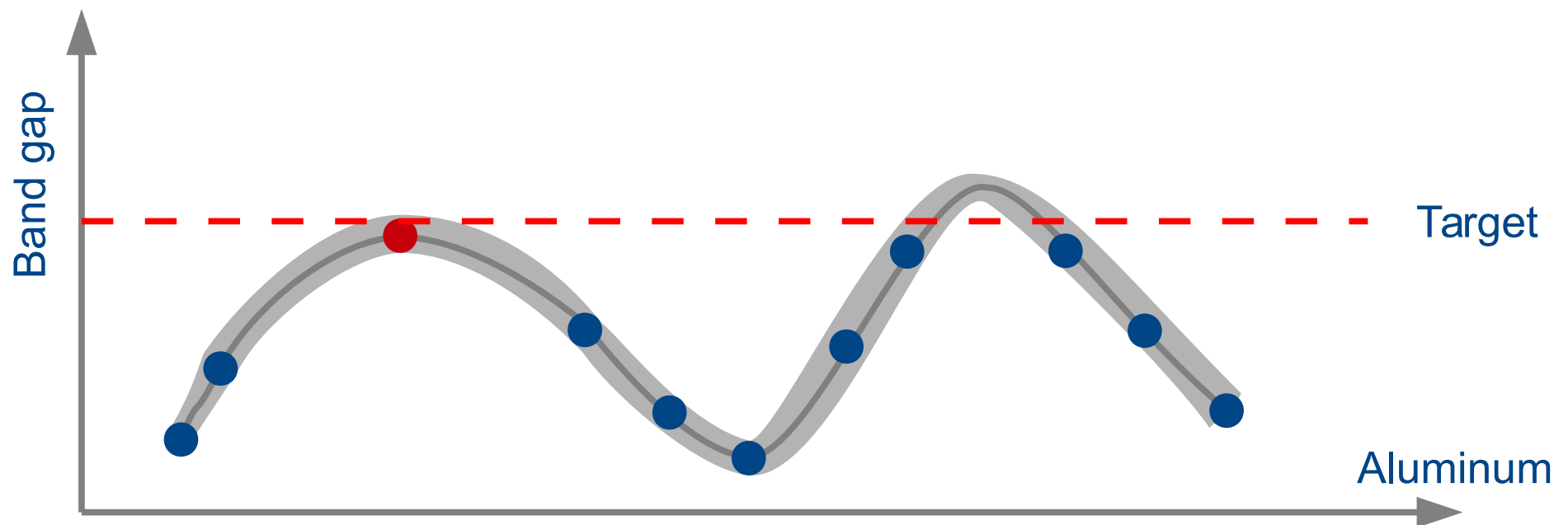
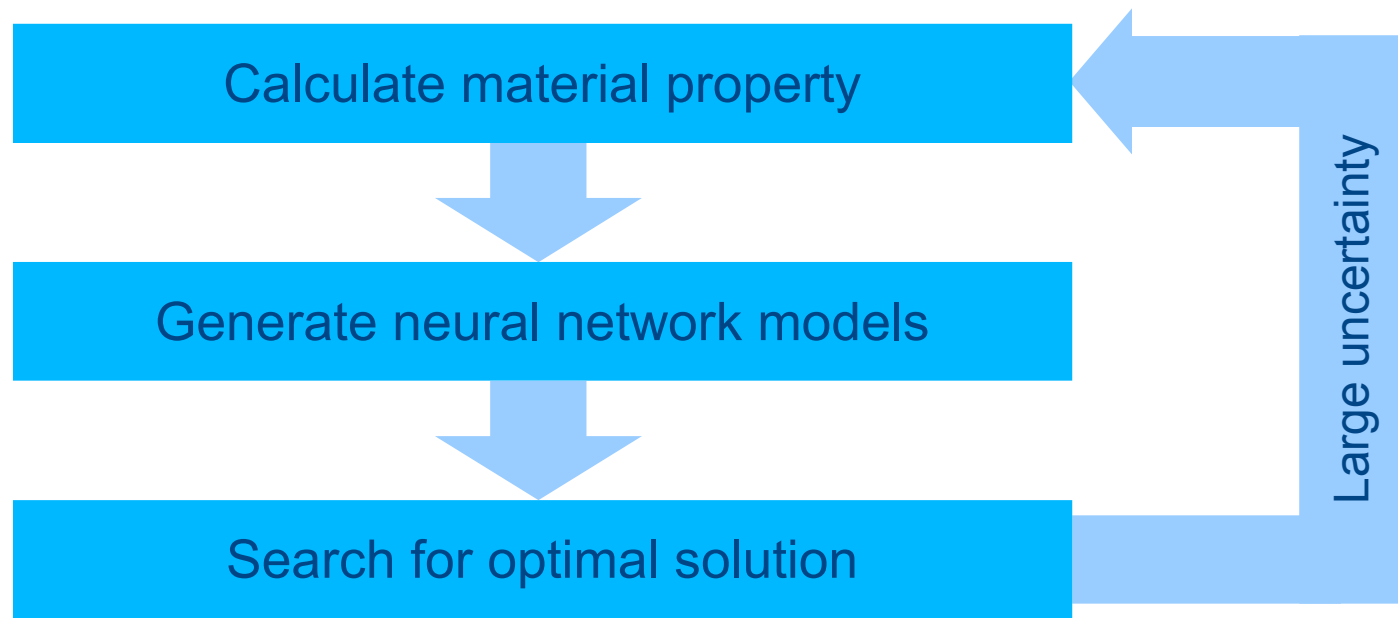
# Correlations between properties



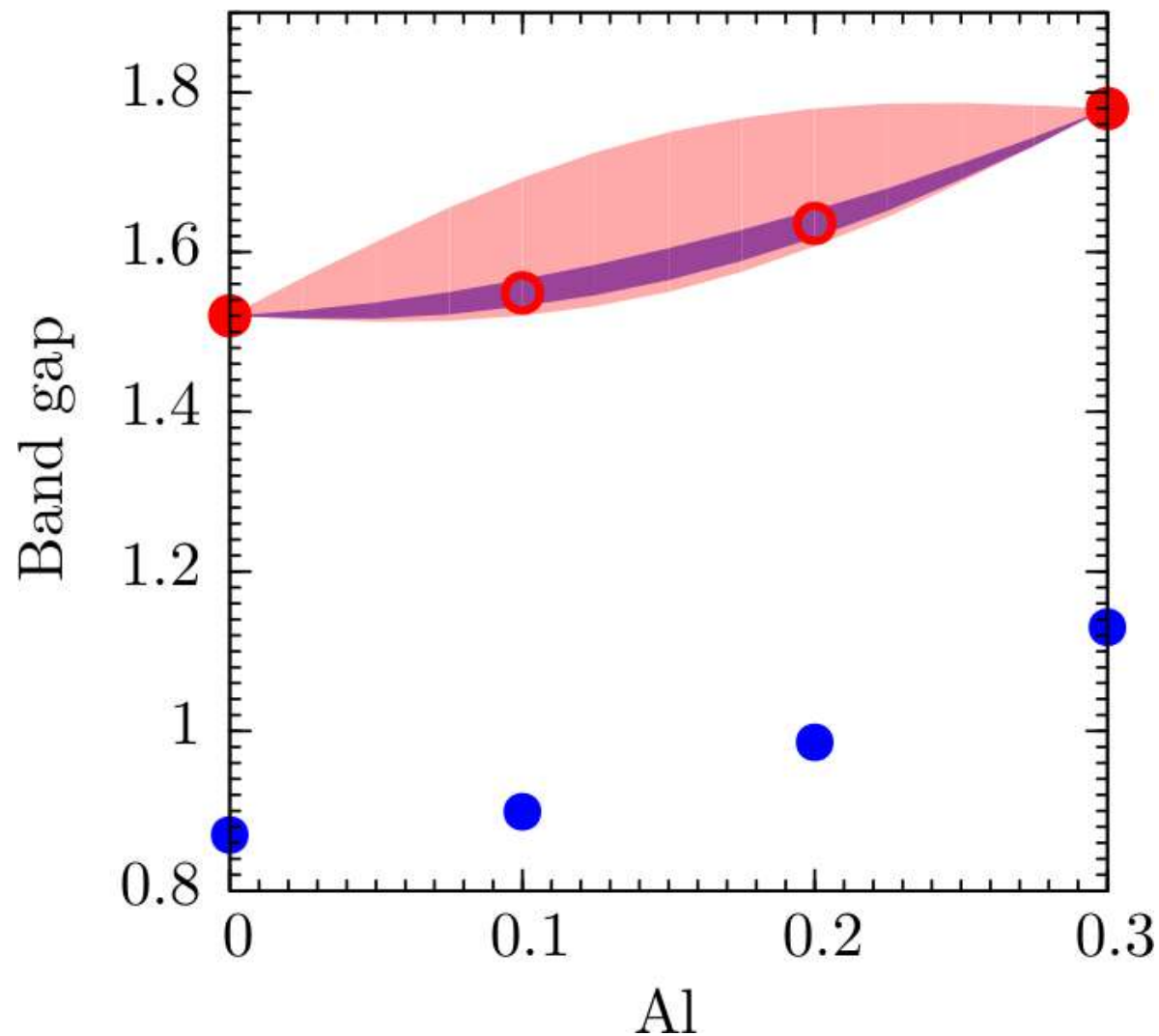
# Recursive learning



# Recursive learning

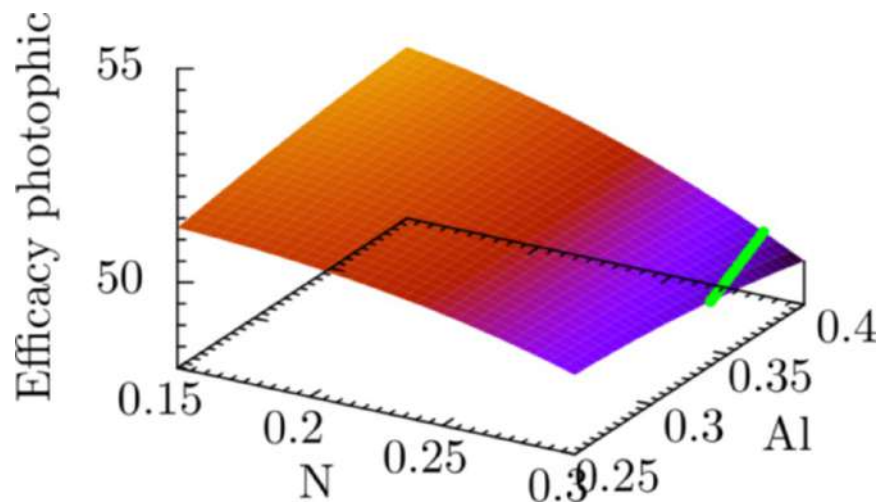


# Case study: III-V InGaN-base semiconductors

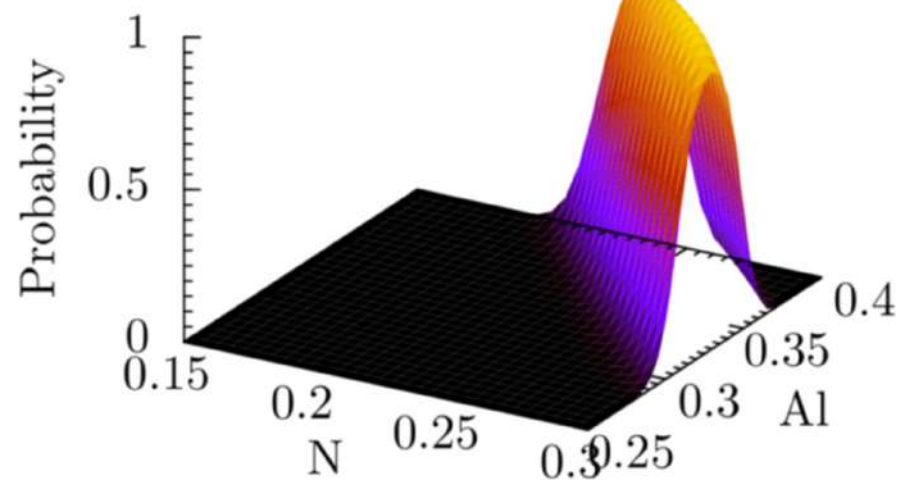
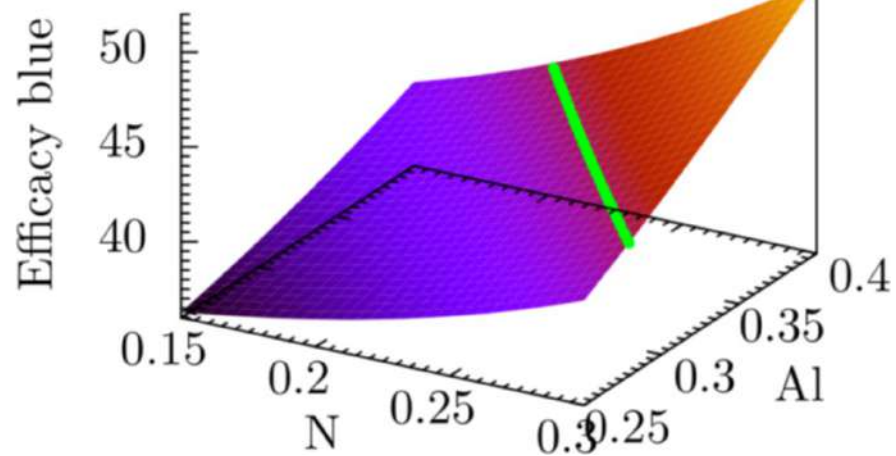




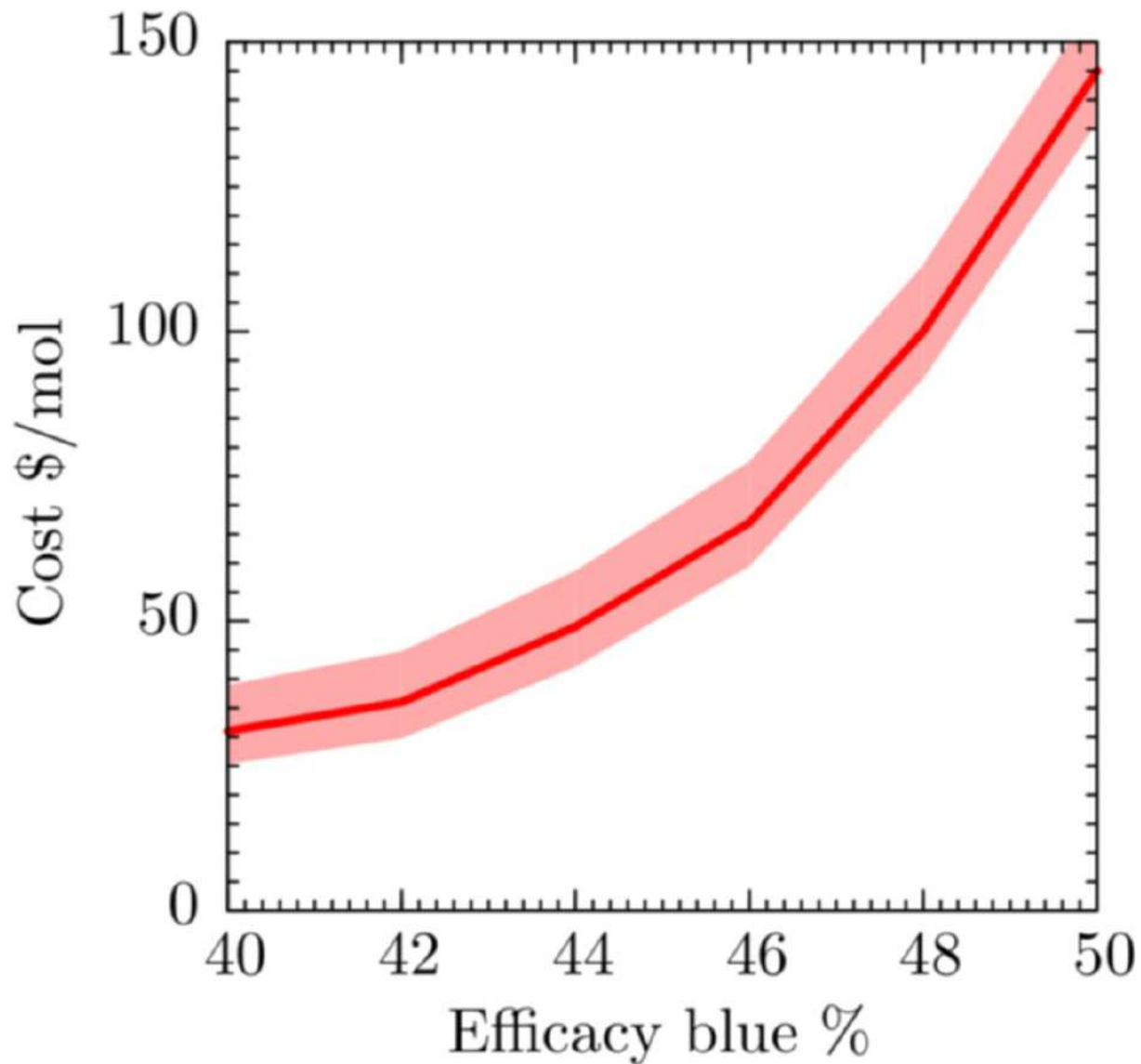
# Case study: III-V InGaN-base semiconductors



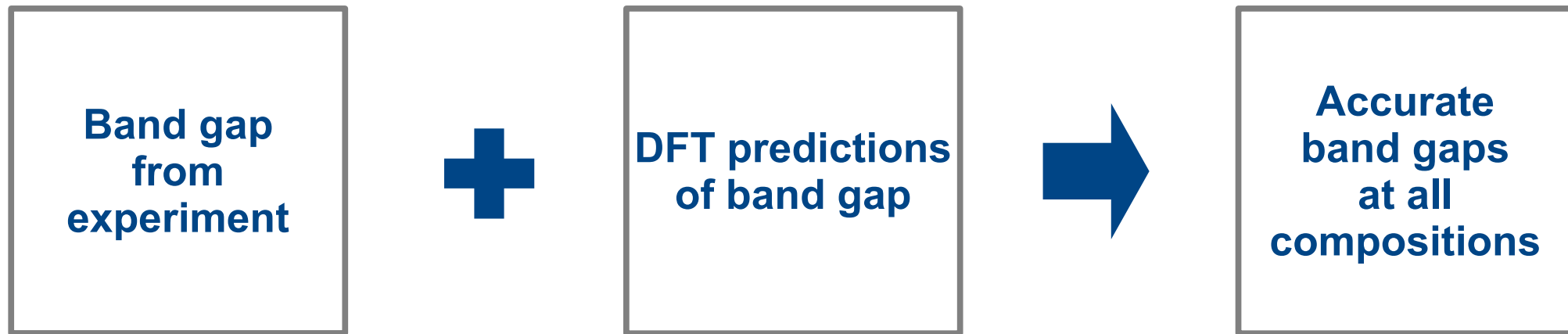
Combine



# Case study: III-V InGaN-base semiconductors



# Exploiting correlations: LEDs

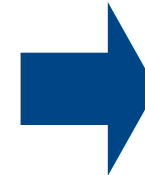


# Exploiting correlations: 3D printing

**7 points for  
3D printability**



**Weldability  
Heat capacity  
Conductivity  
Precipitates**



**Accurate  
predictions for  
3D printability**

# Three new tools

Experimental  
databases

Neural  
network  
fitting

Property  
correlations

Computational

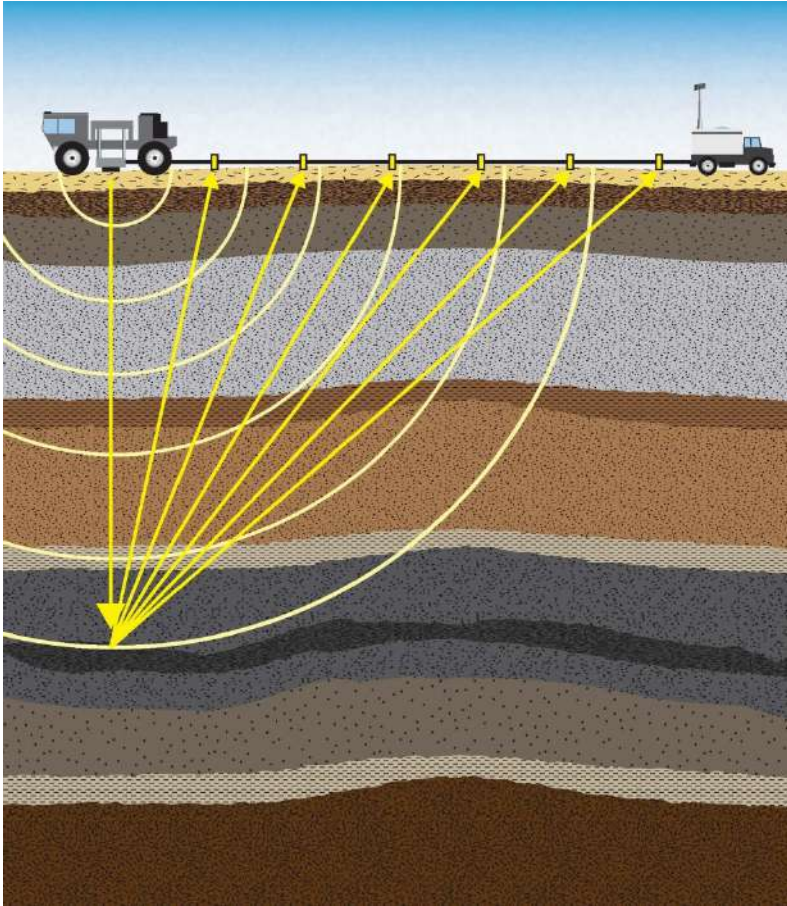
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2013/0052077 A1  
GB1408536.9

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

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

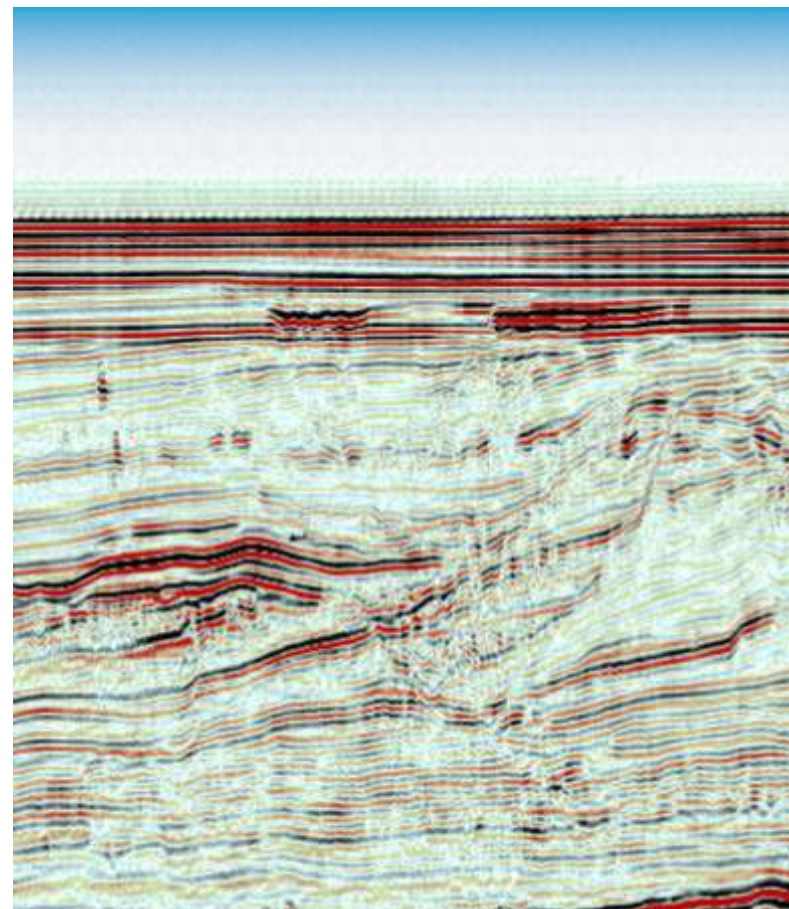
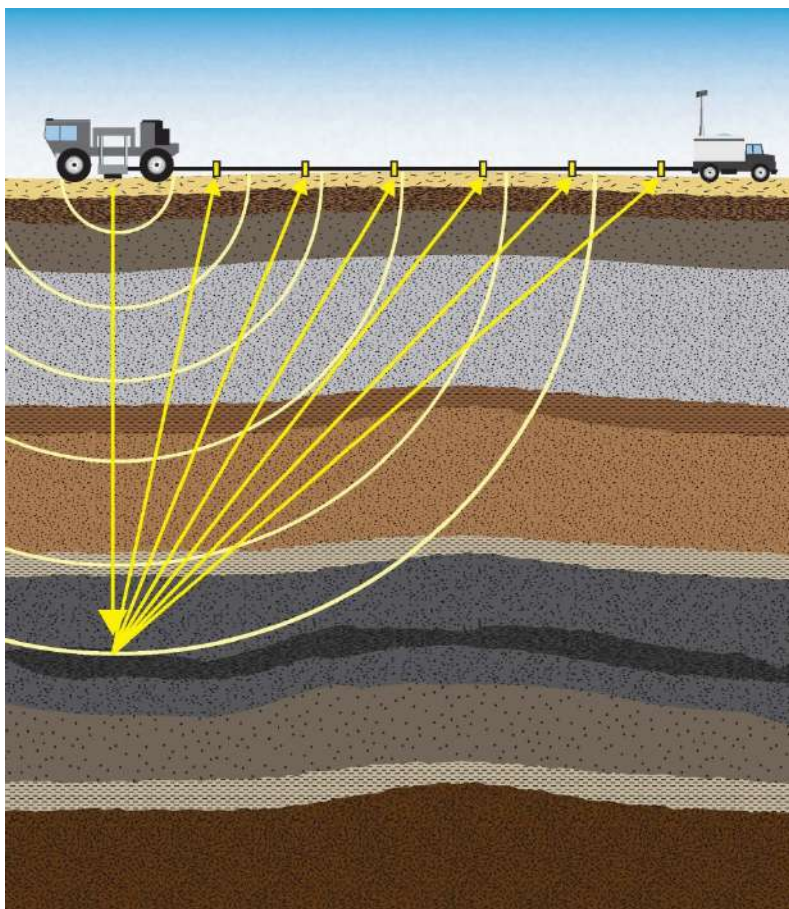
InGaN-based LED

# Search for oil

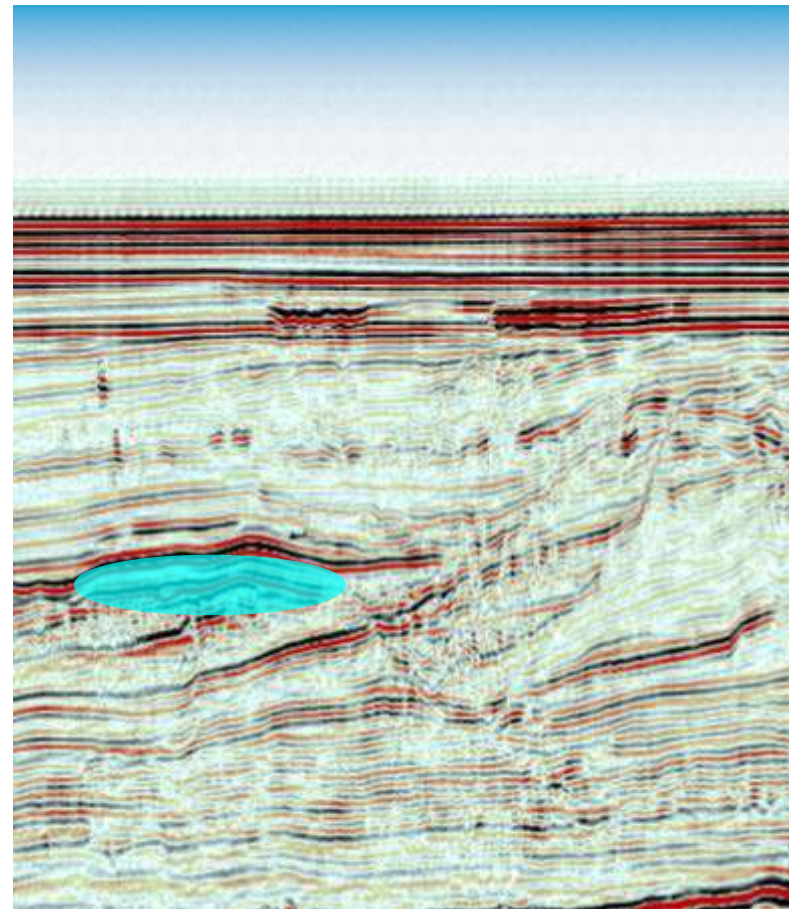
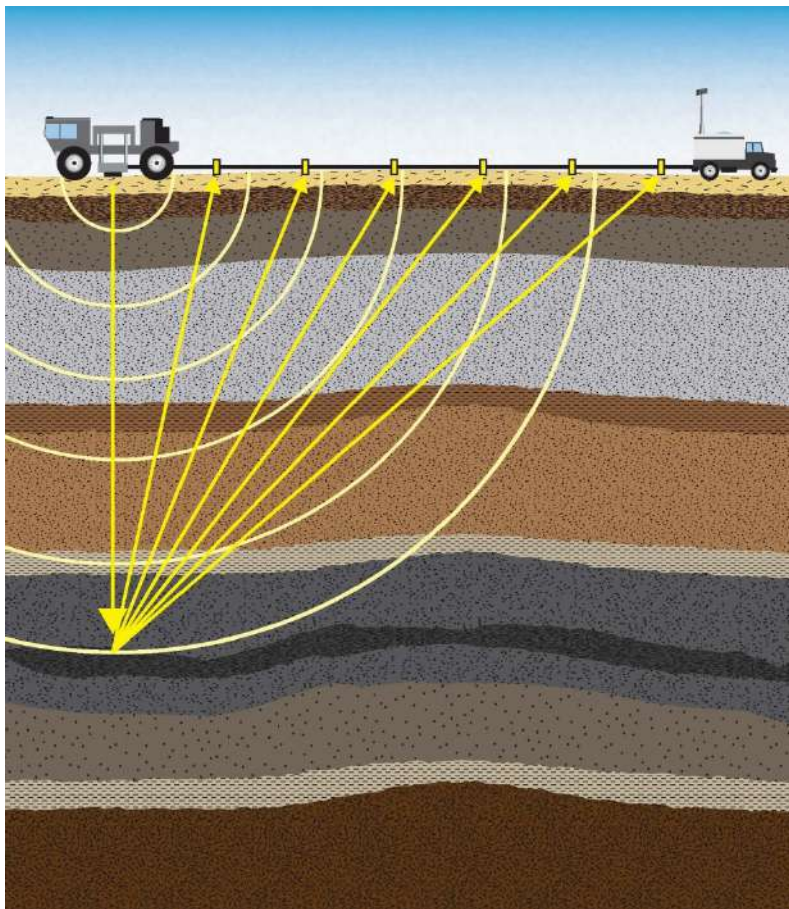




# Search for oil

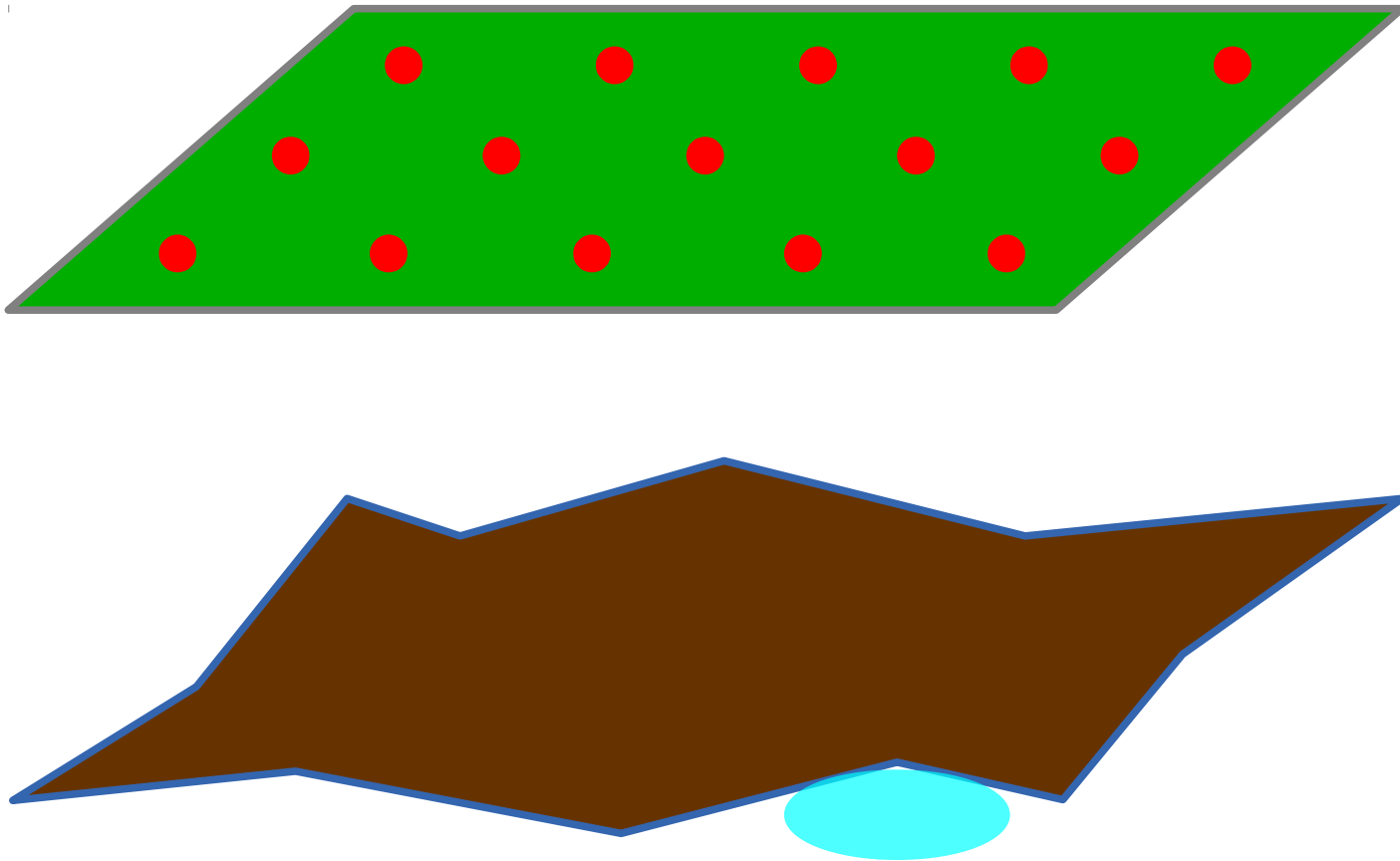


# Search for oil

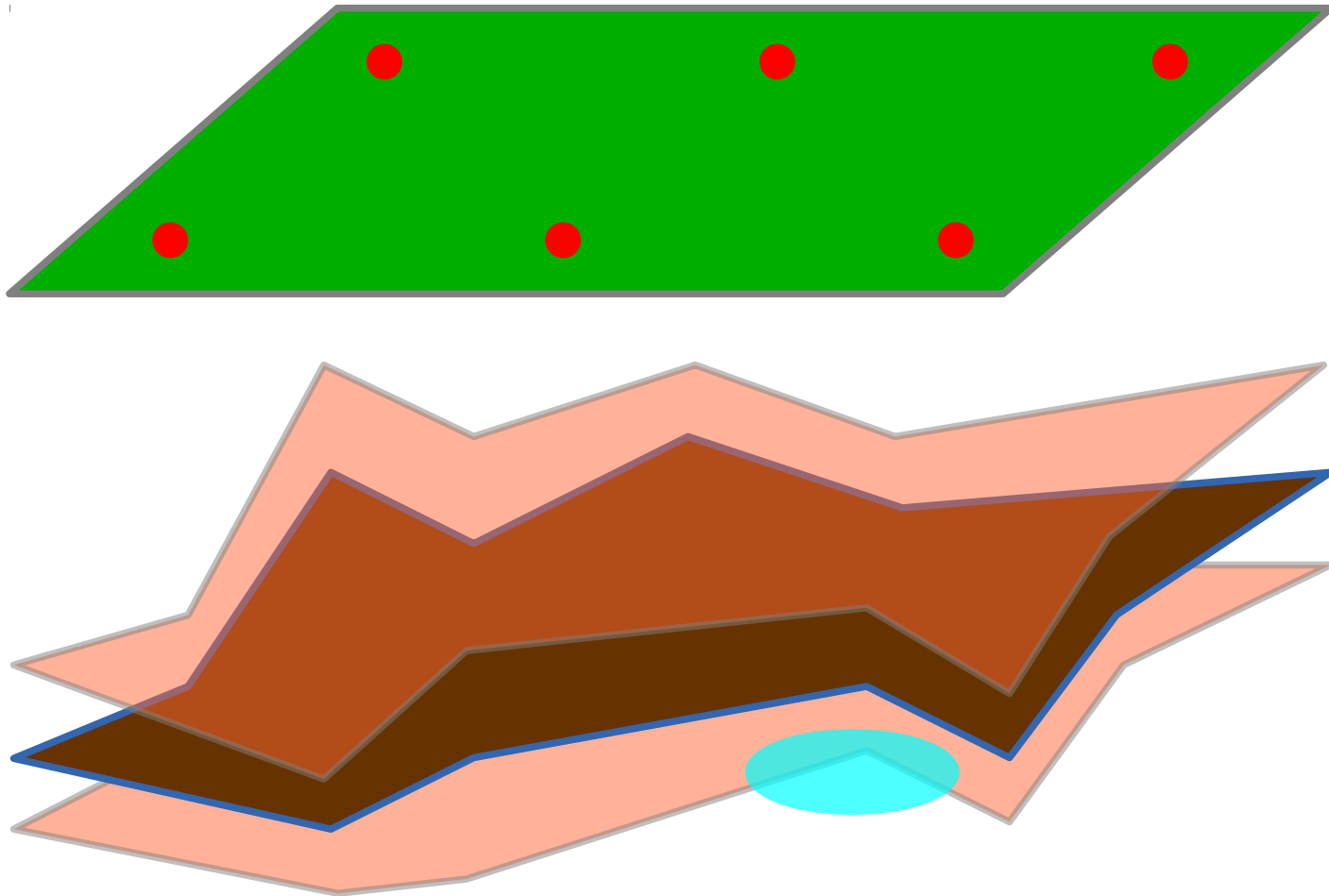




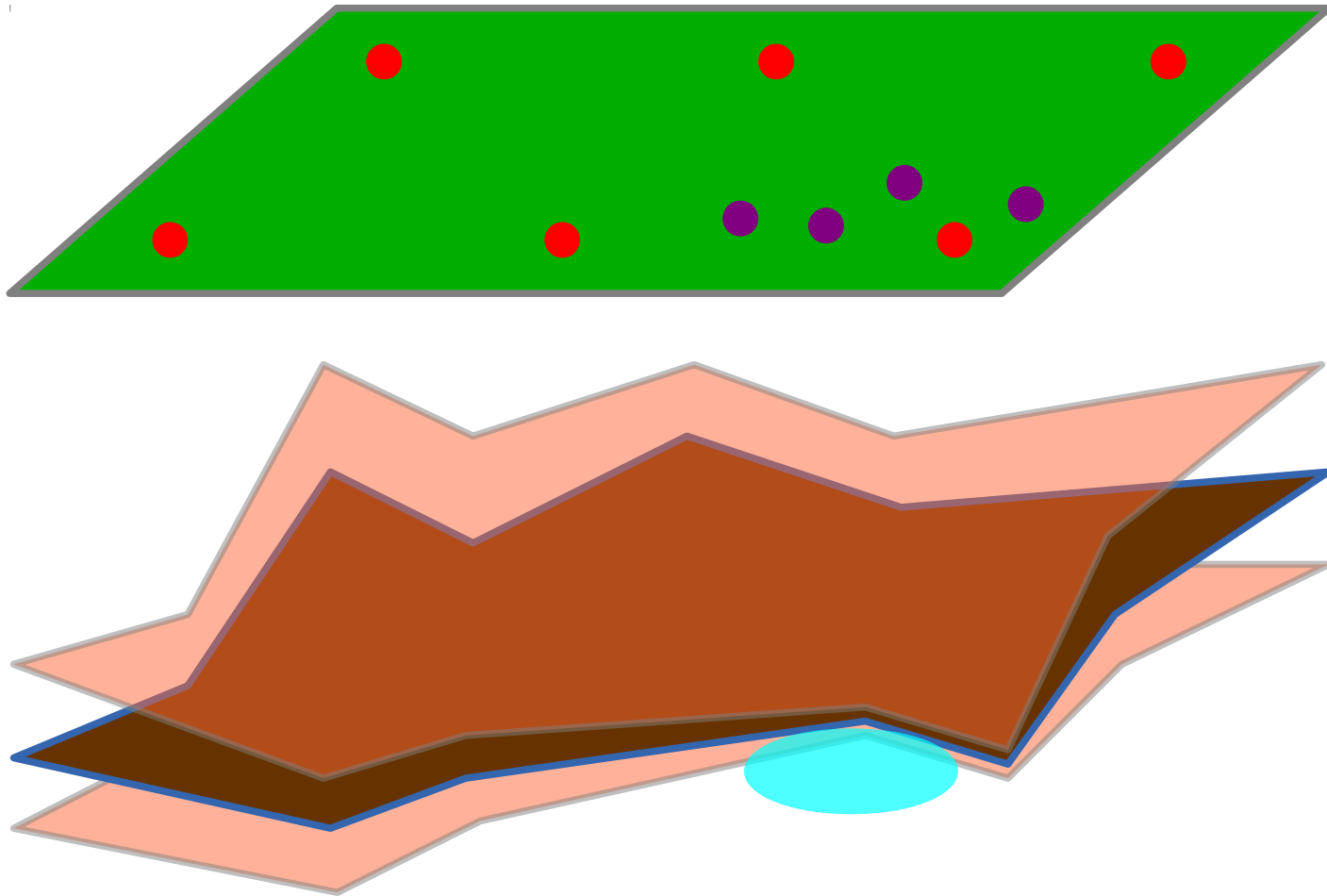
# Seismic survey



# 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