UNIVERSITY OF CAMBRIDGE

The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

Neural network algorithm to

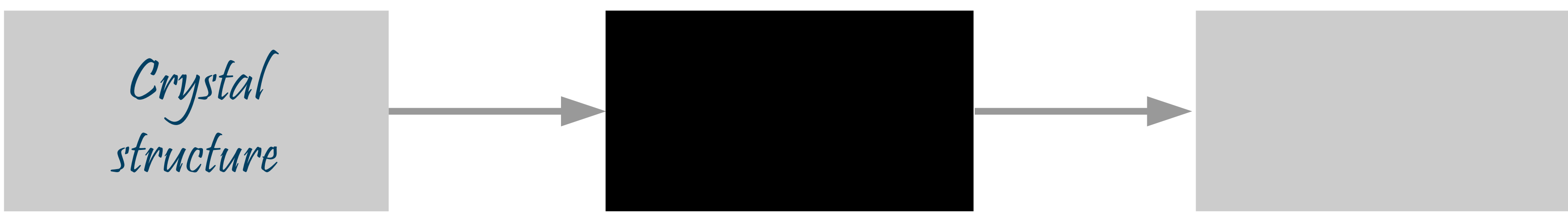
Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Merge simulations, physical laws, and experimental data

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

A black box



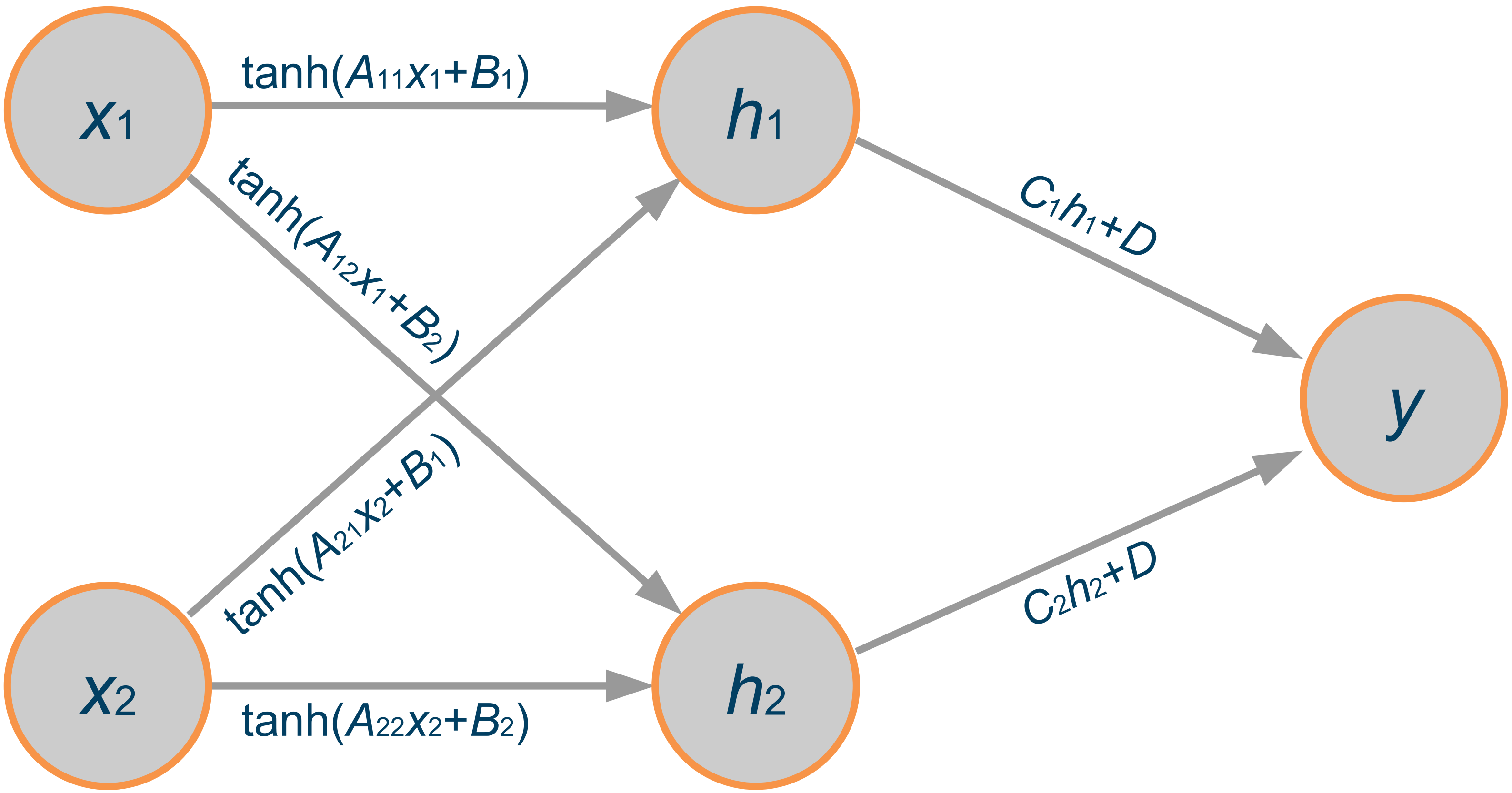
Train with complete data

Materials design

Materials design

Predict with complete data

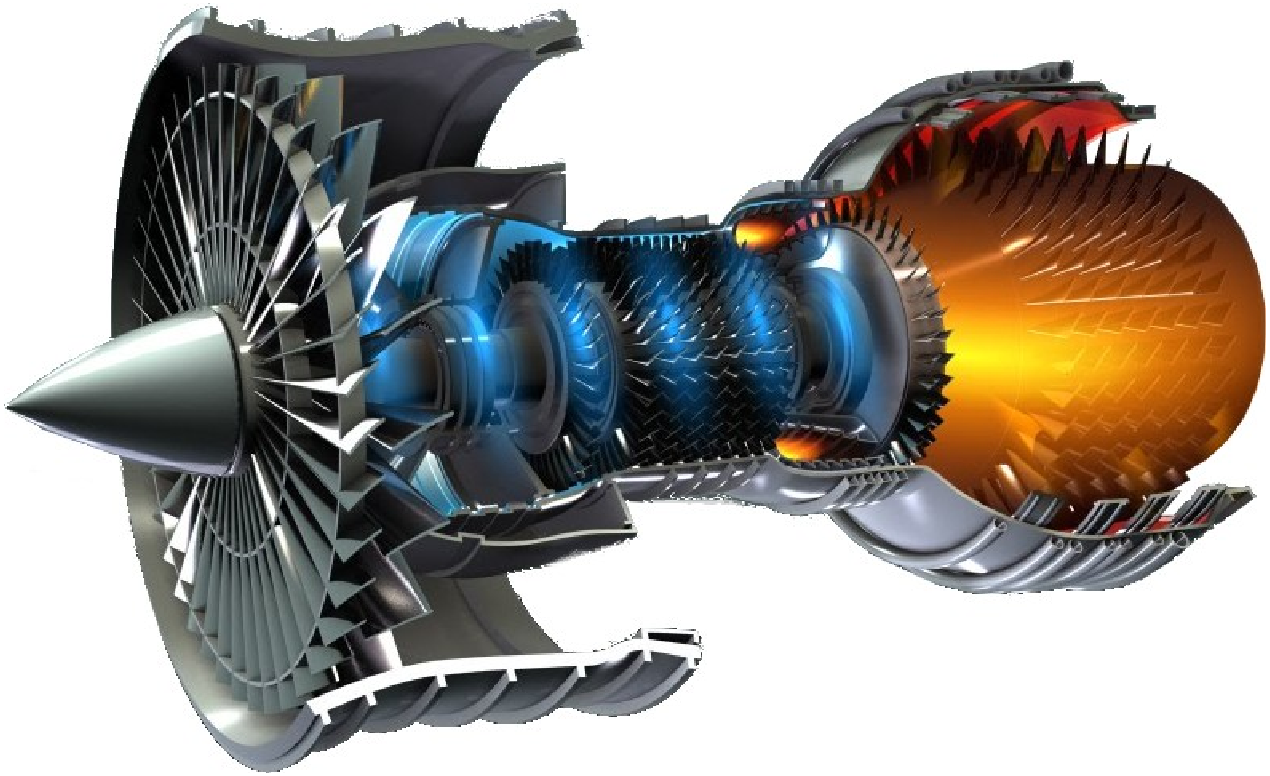
Architecture



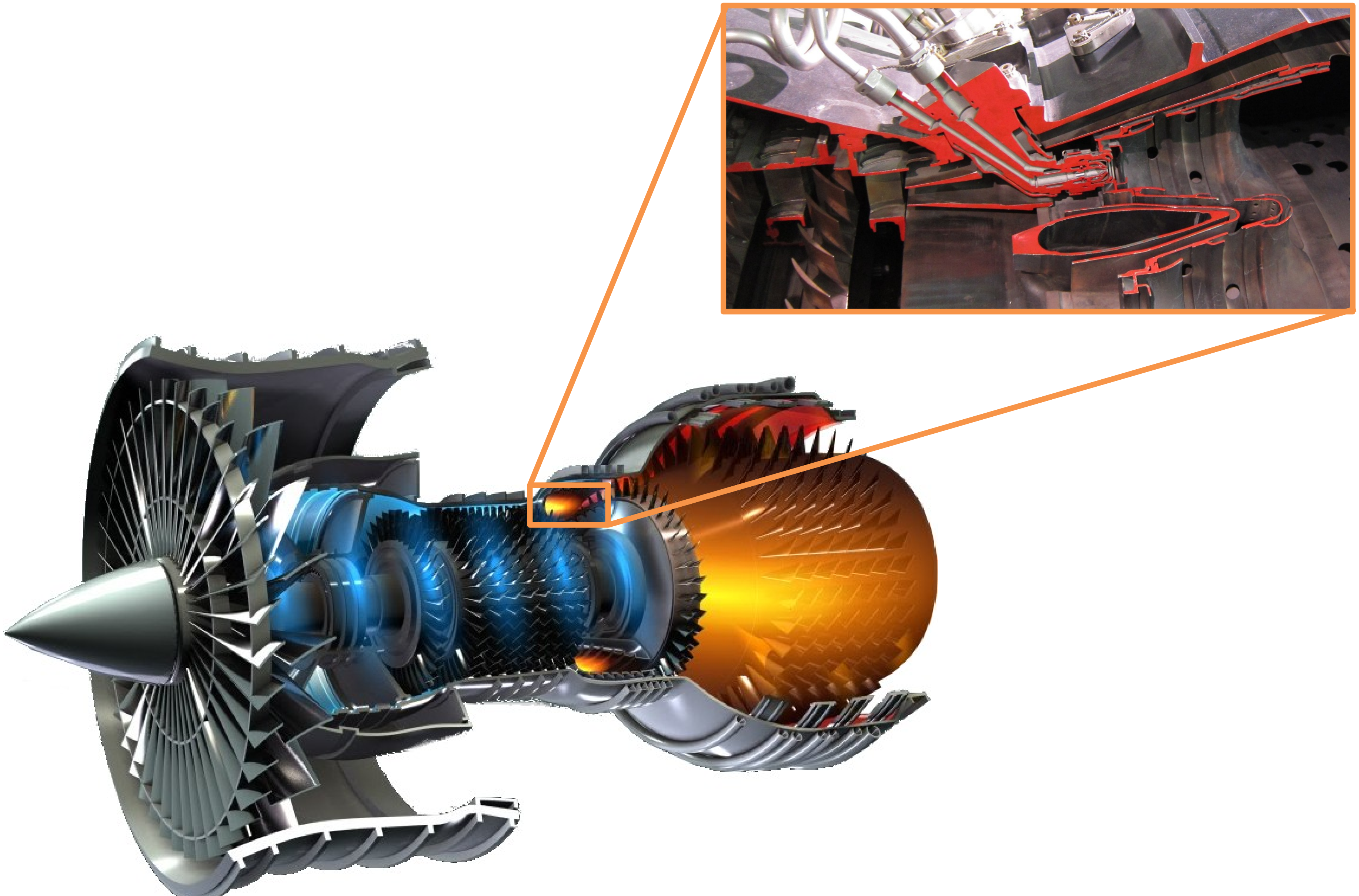
Train with fragmented data

Predict with fragmented data

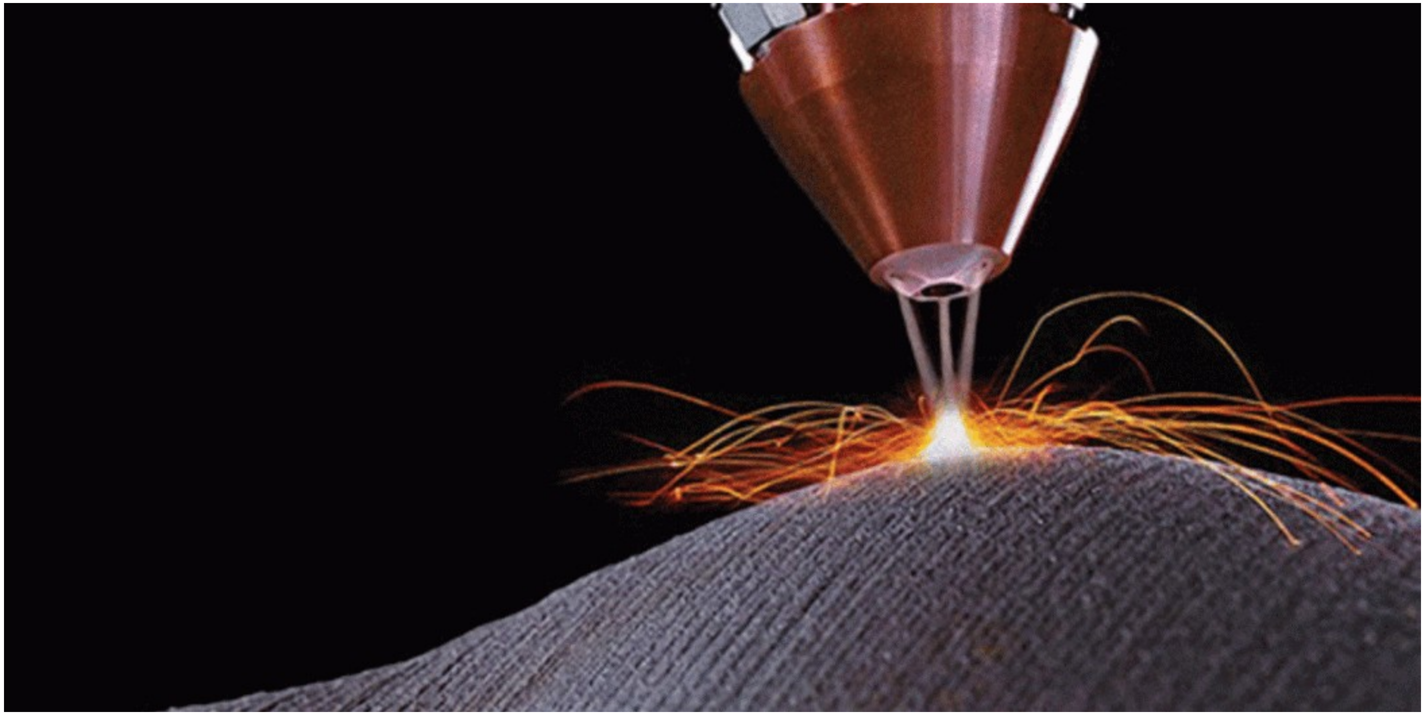
Schematic of a jet engine



Combustor in a jet engine



Direct laser deposition requires new alloys

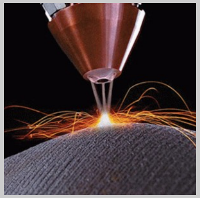


Neural networks for materials design

Composition

Properties

Process



Fatigue

Welding

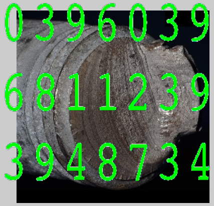
Neural networks for materials design

Composition

Properties

Process

Fatigue



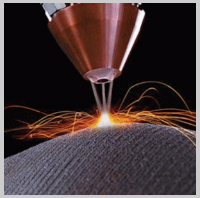
Welding

Neural networks for materials design

Composition

Properties

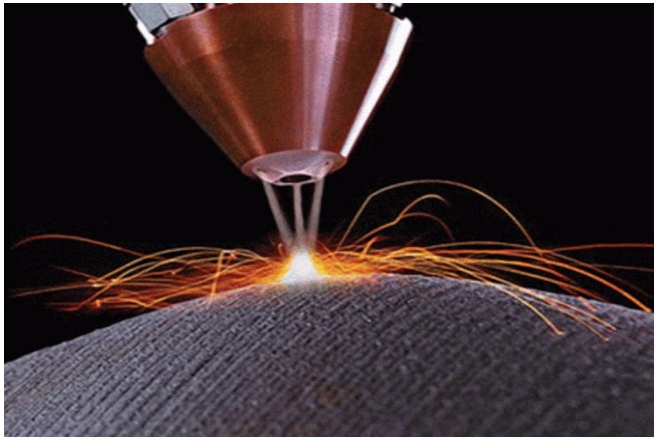
Process



Fatigue

Welding

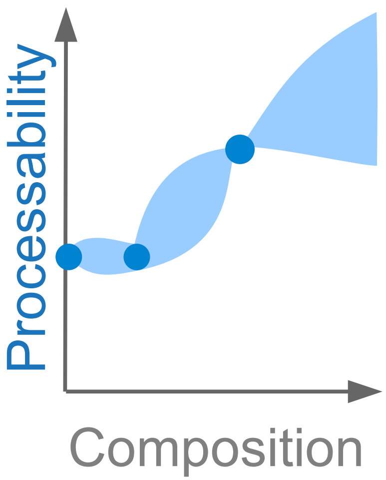
Neural networks for materials design



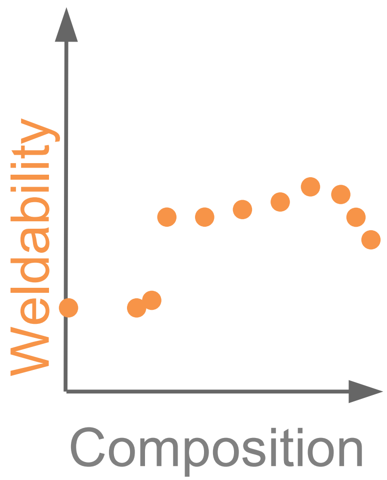
Laser

Electricity

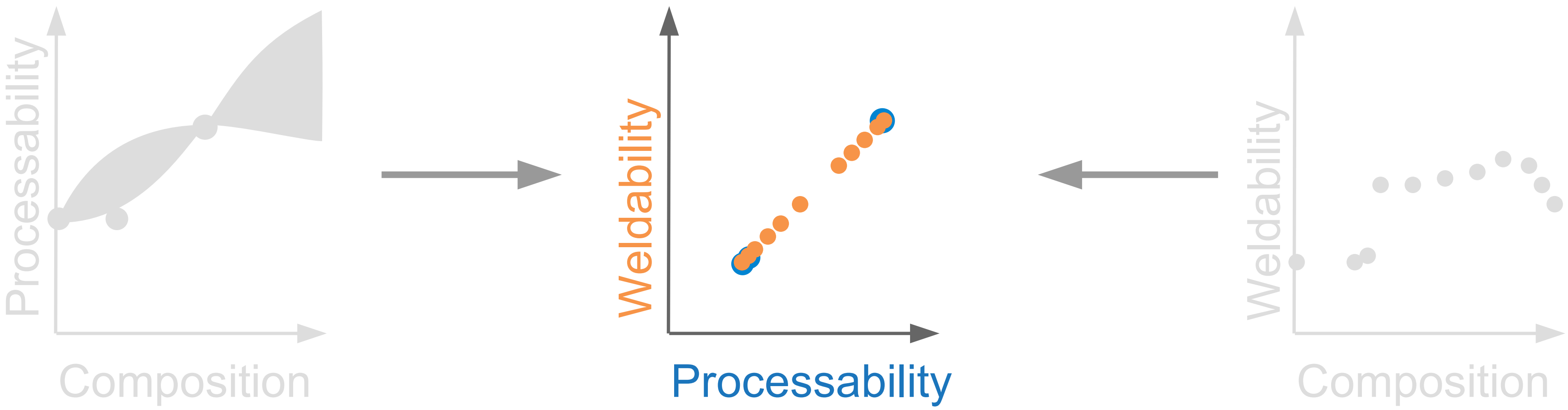
Insufficient data for processability



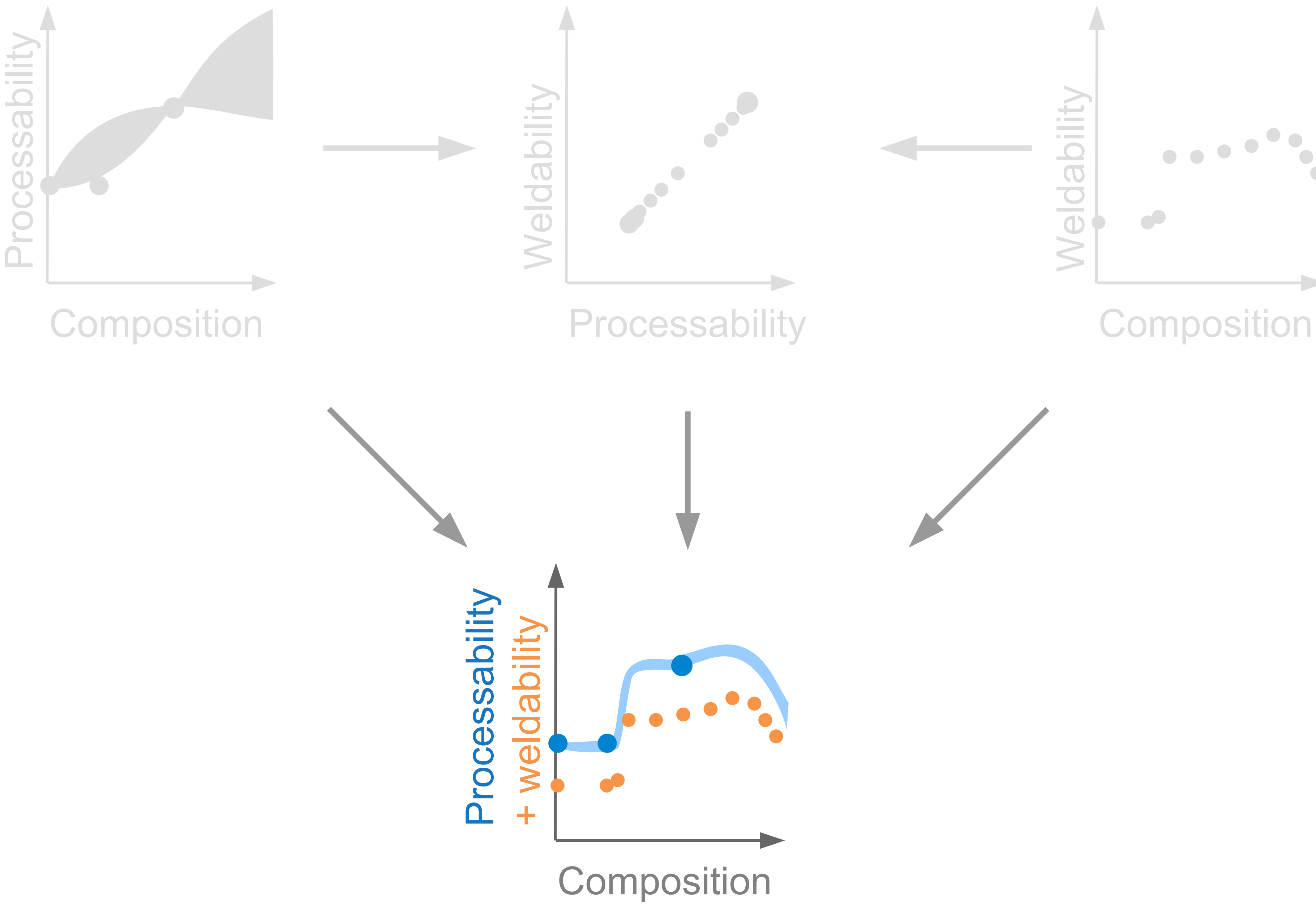
Welding is analogous to direct laser deposition



Simple processability-welding relationship



Merging properties with the neural network

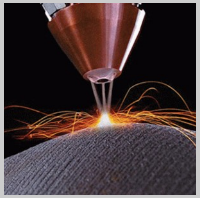


Neural networks for materials design

Composition

Properties

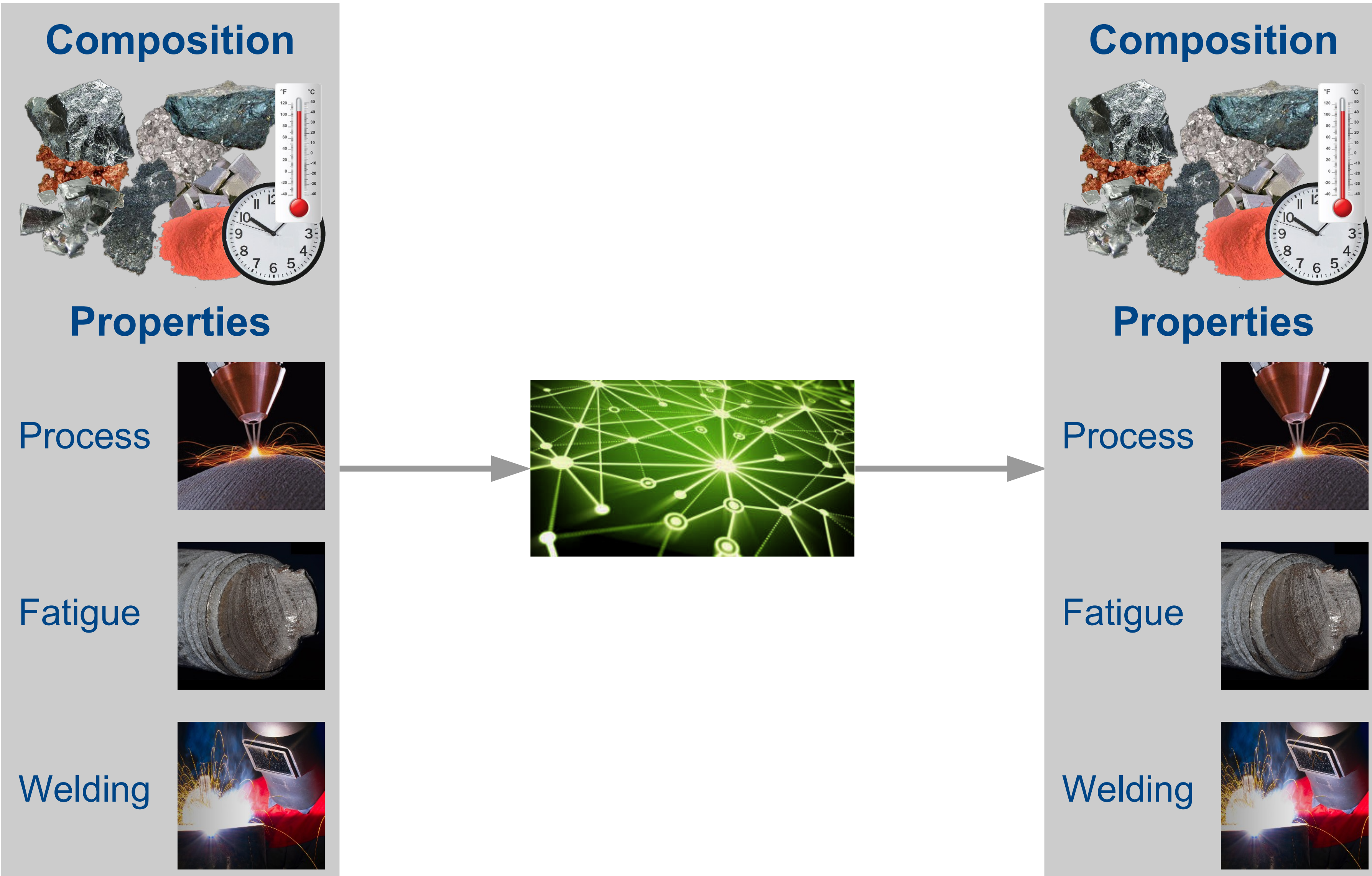
Process



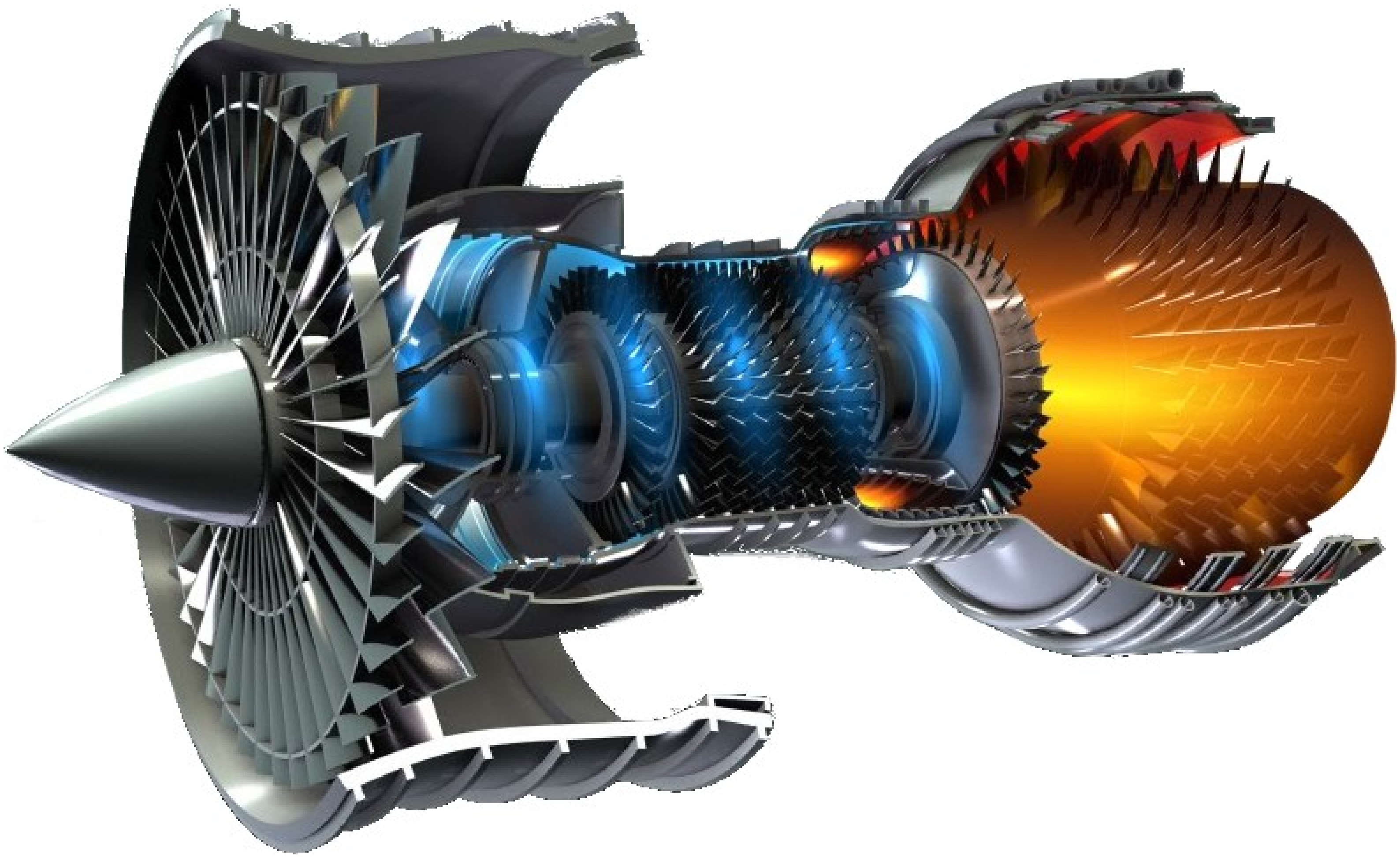
Fatigue

Welding

Neural networks for materials design



Schematic of a jet engine



Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Composition

Cr: 19%

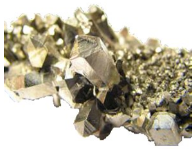
Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%



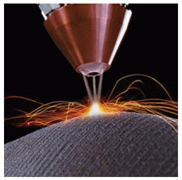
Al: 2.9%

C: 0.04%

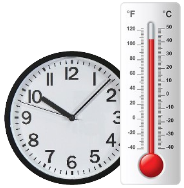
B: 0.01%

Ni

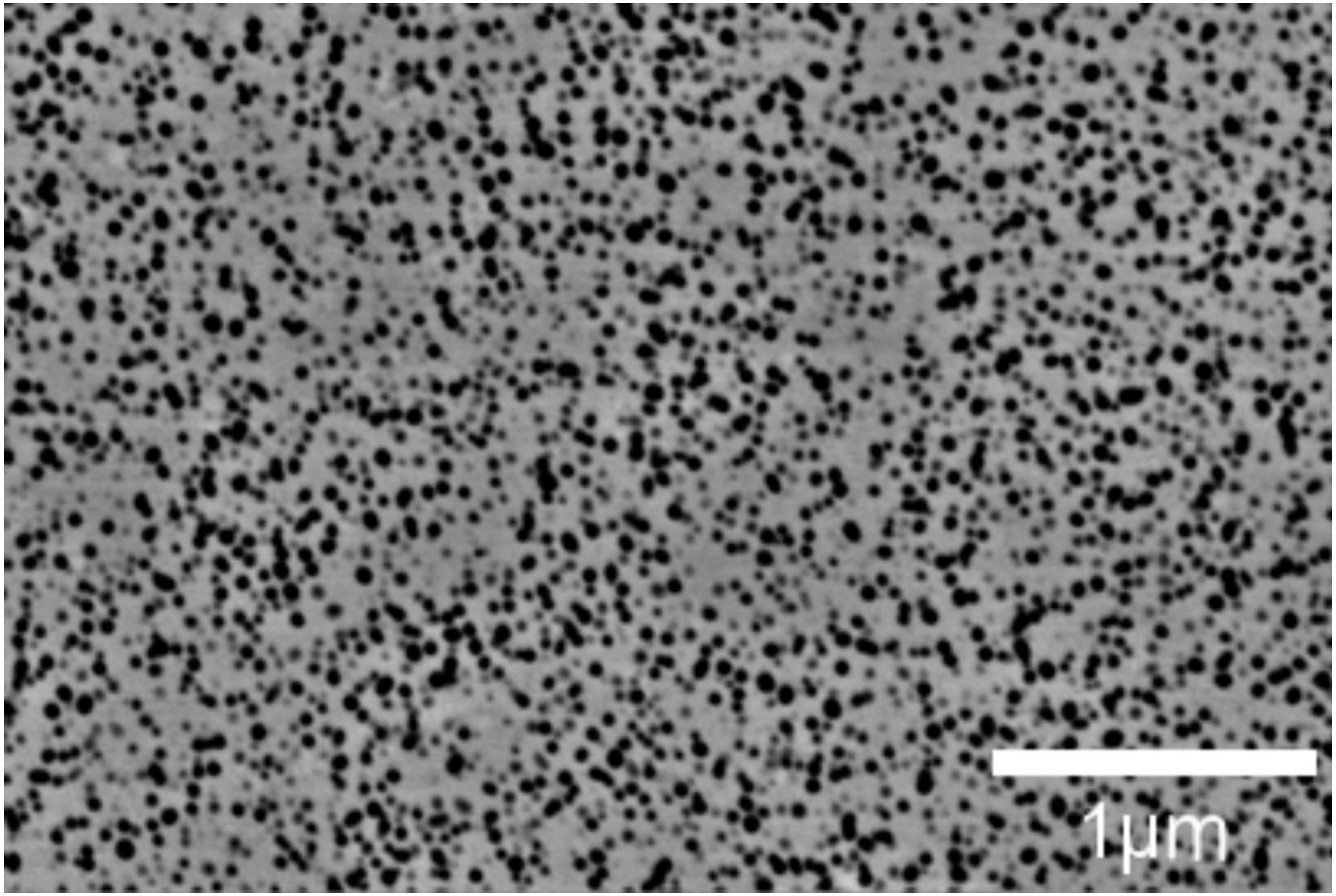
Expose 0.8



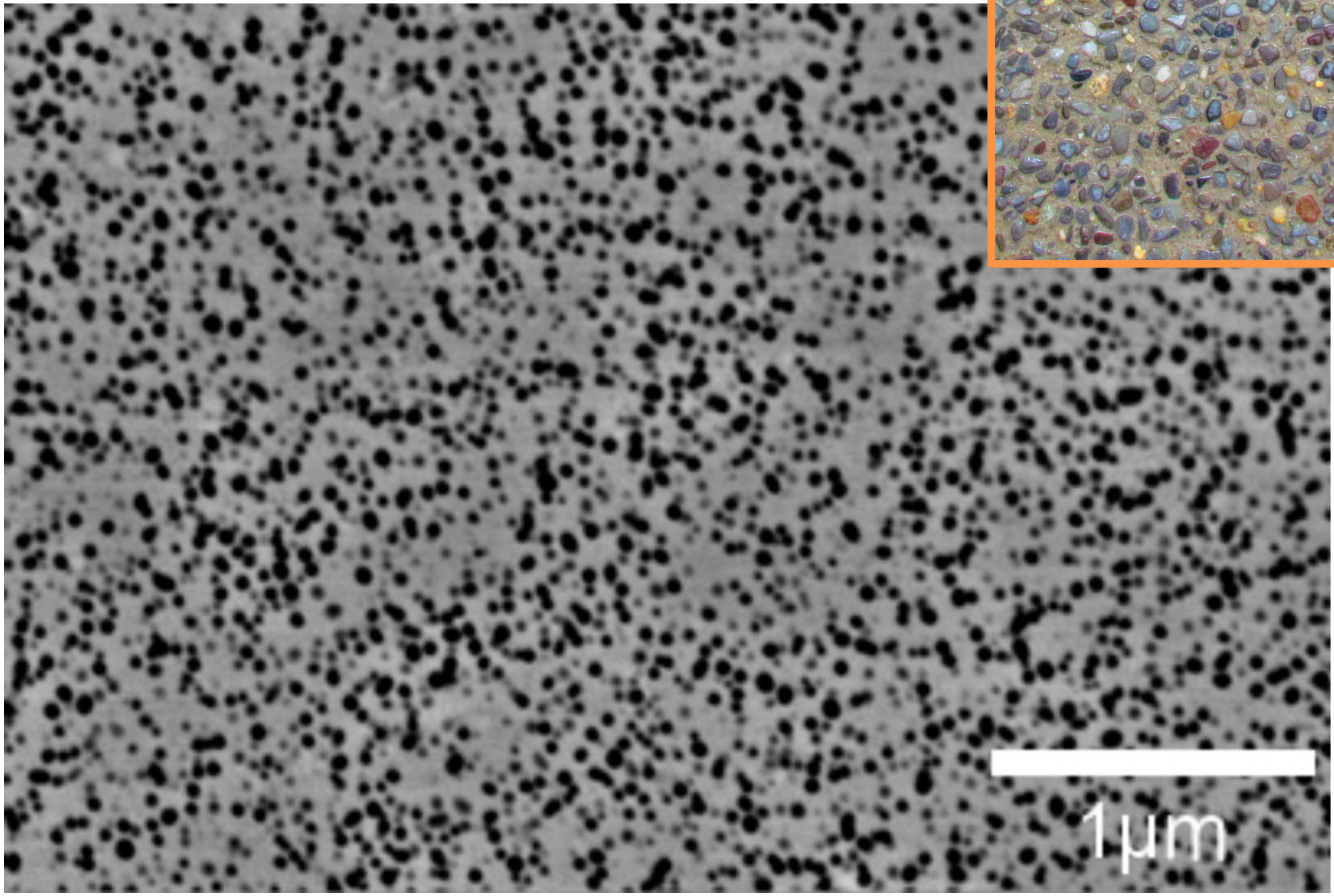
T_{HT} 1300ºC



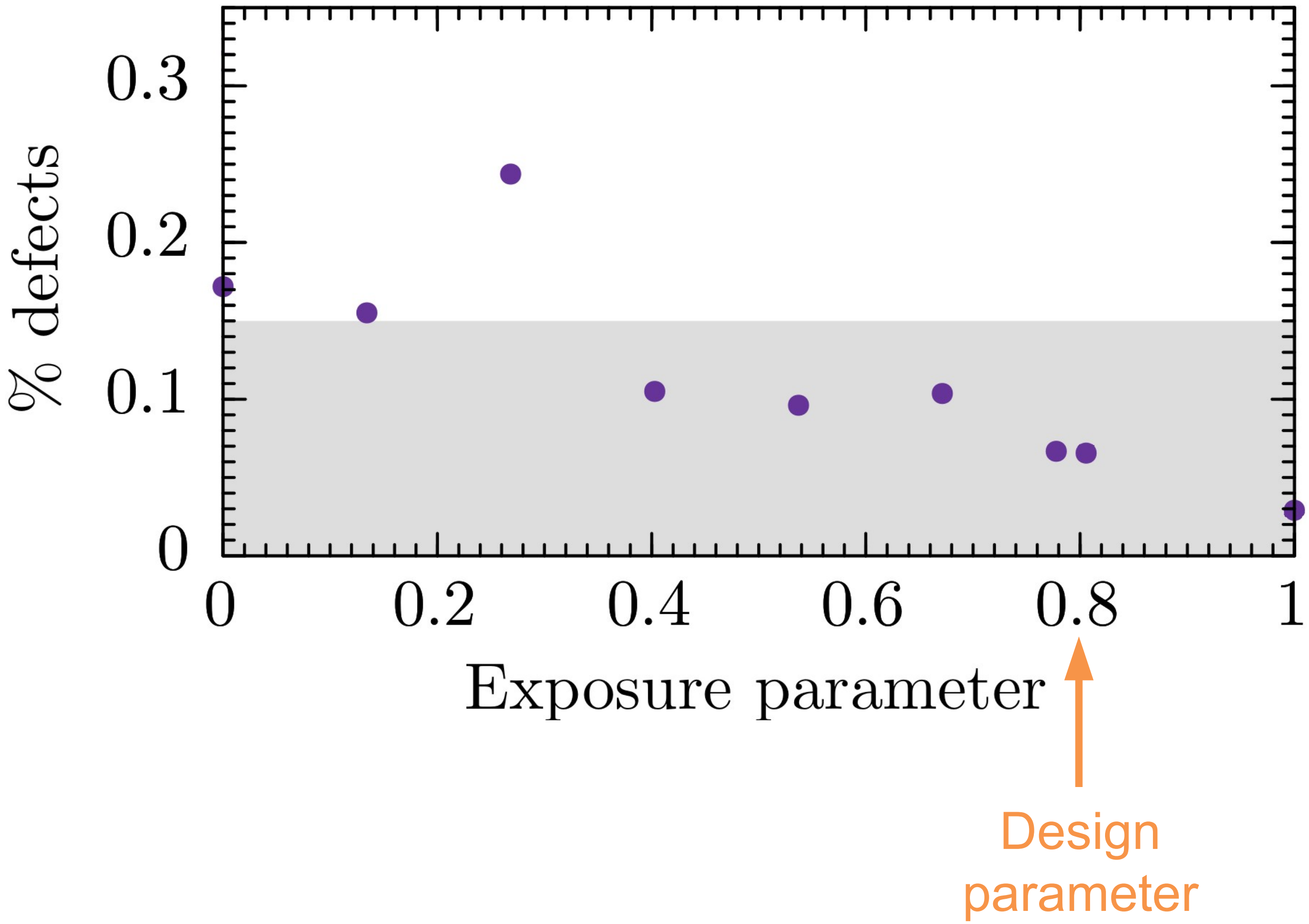
Microstructure



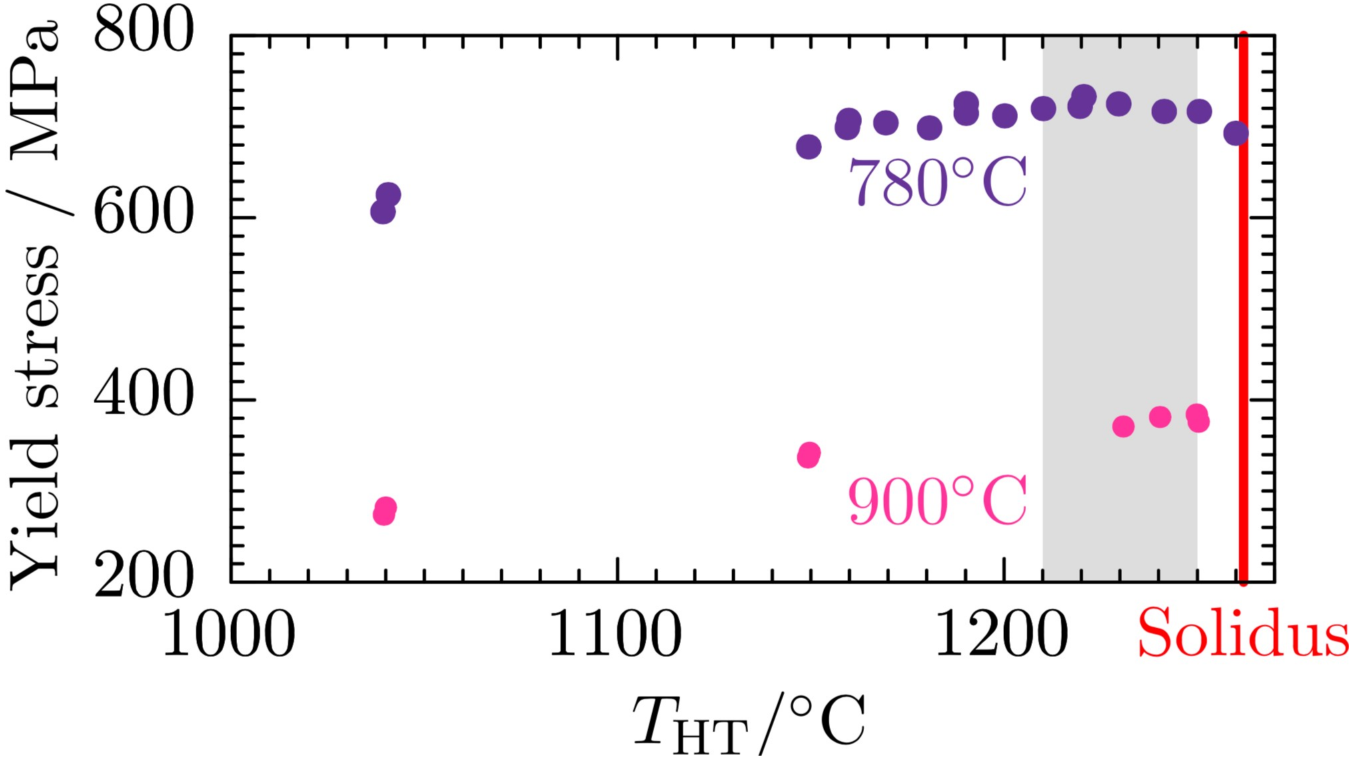
Microstructure analogous to concrete



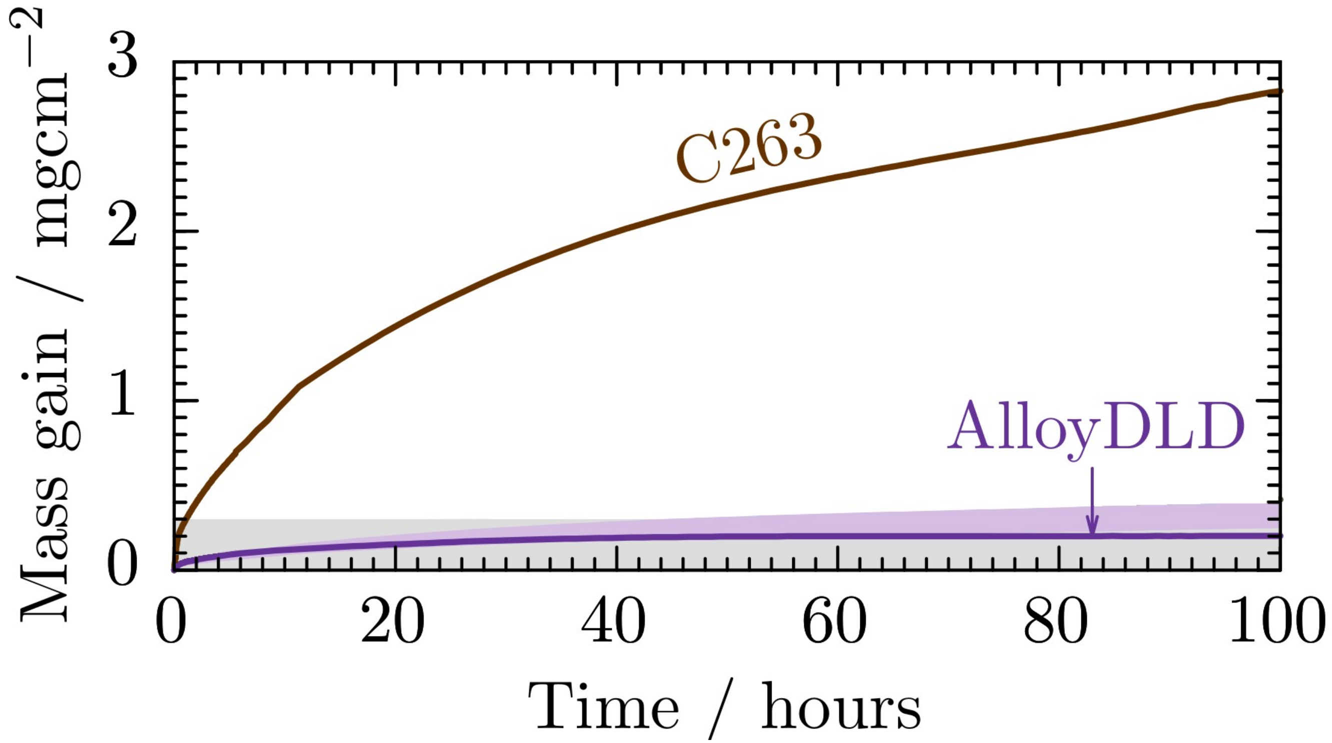
Testing the processability: horizontal printing



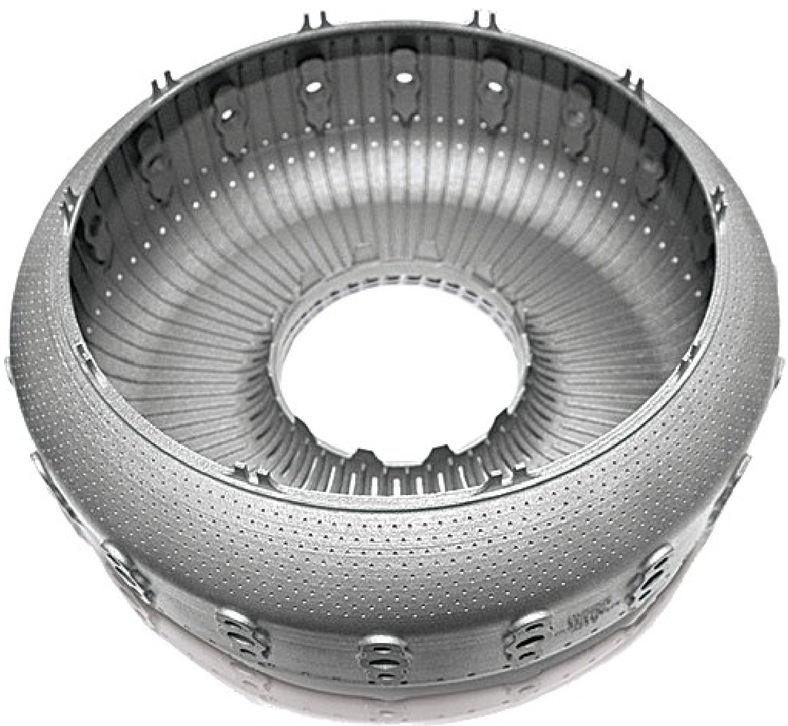
Testing the processability: horizontal printing



Testing the oxidation resistance



Printing components for an engine



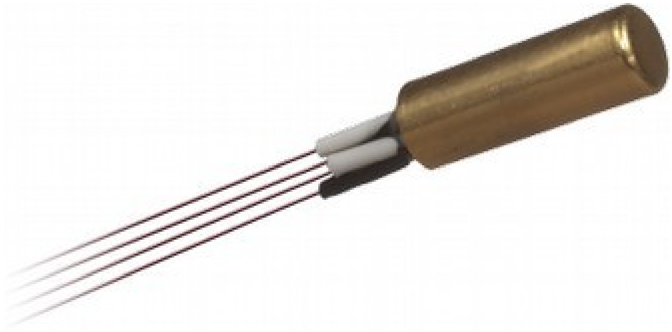
Materials Solutions

ROLLS ROYCE

Low temperature physics

Specification for a thermometer

90% of the cost of a thermometer is for calibration



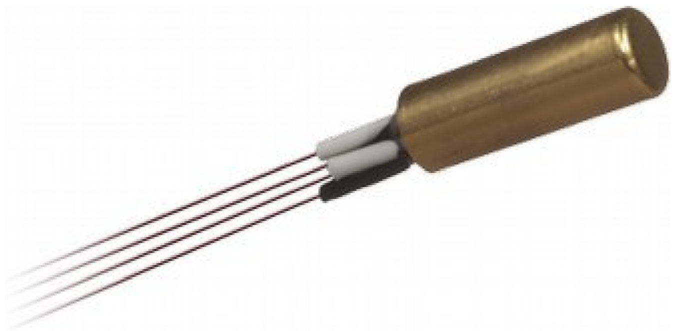
Specification for a thermometer

90% of the cost of a thermometer is for calibration

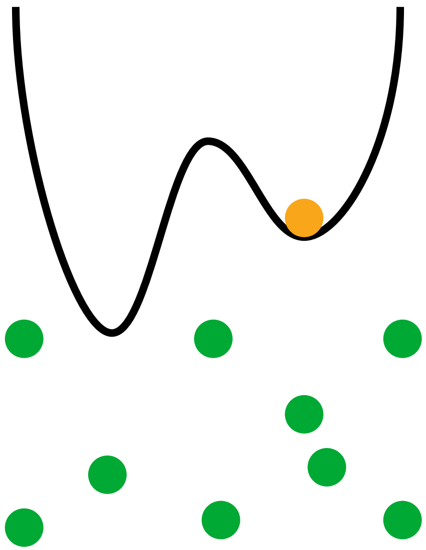
Require a simple resistance-temperature relationship over a wide temperature range

Want constant sensitivity $T/R\, \mathrm{d}R/\mathrm{d}T$ with temperature

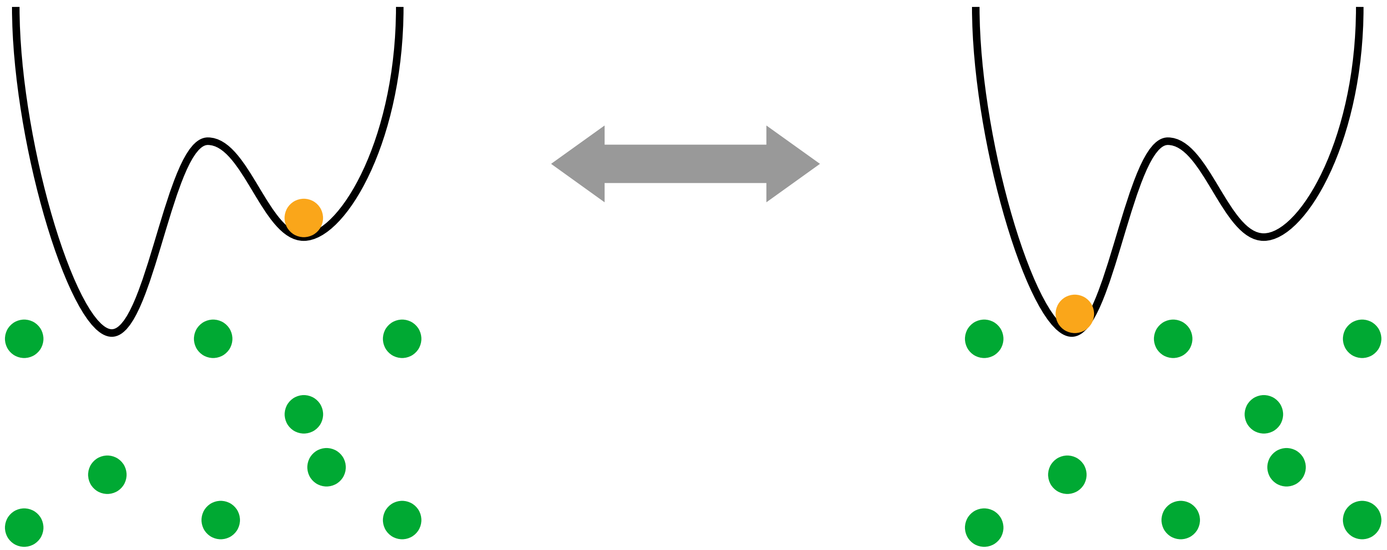
Thermometer must be stable with time and temperature



Mechanism: atom in lattice potential

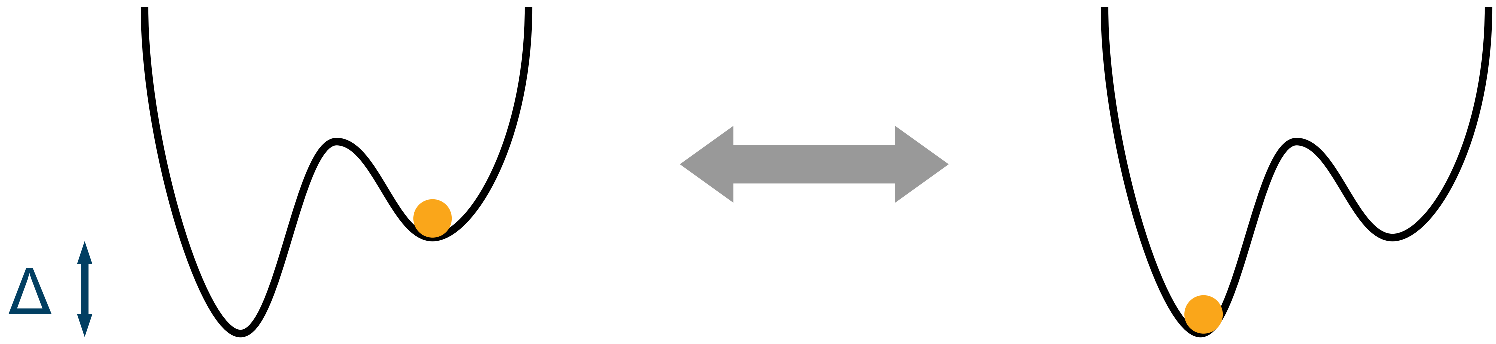


Mechanism: atom hops into second state



Mechanism: analogy to Kondo effect

Atom hopping between sites analogous to Kondo effect

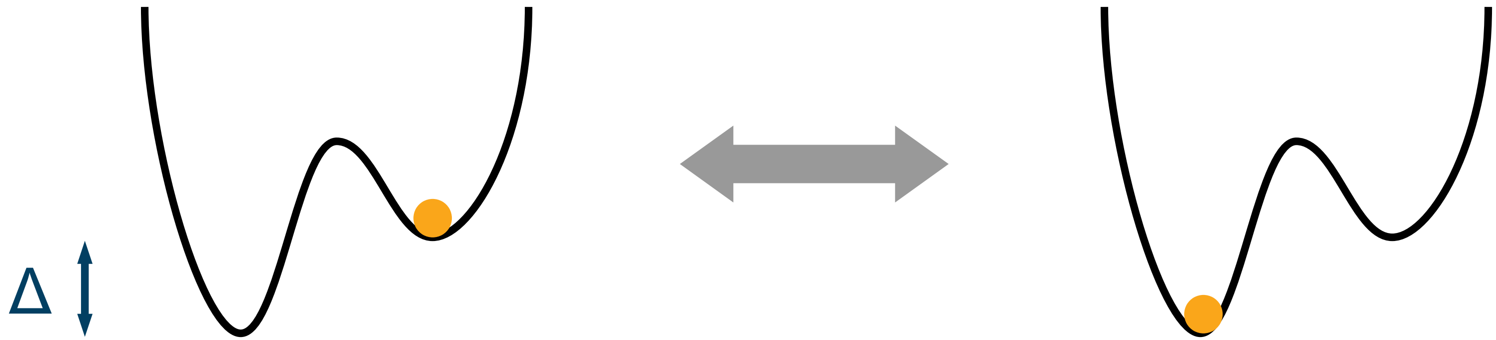


$R \sim \log(\Delta^2 + T^2)$

Cochrane *et al.*, PRL **35**, 676 (1975)

Mechanism: integrate over disorder

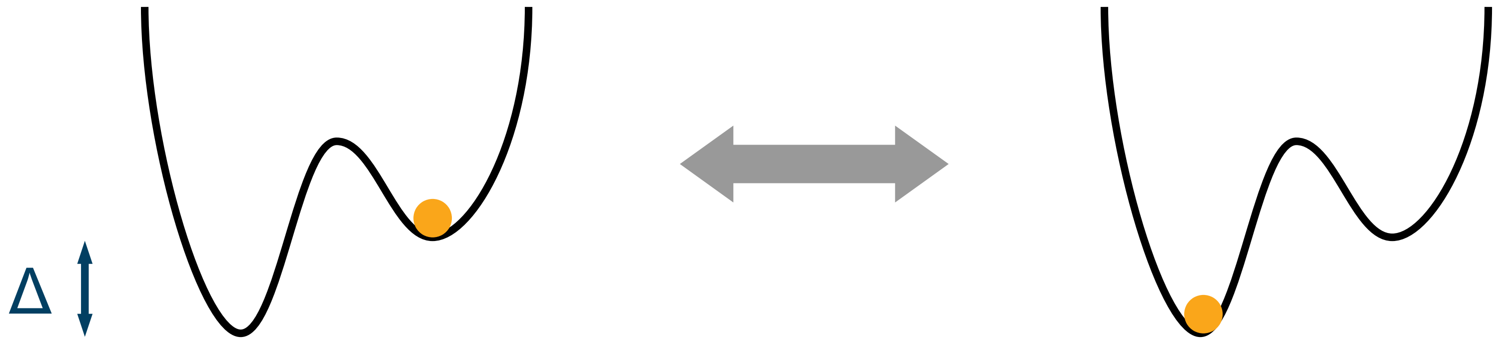
Atom hopping between sites analogous to Kondo effect



$$R \sim \int_{\Delta_{min}}^{\Delta_{max}} \log\left(\Delta^2 + T^2\right) \frac{1}{\Delta} d\Delta$$

Mechanism: simple logarithmic dependence on T

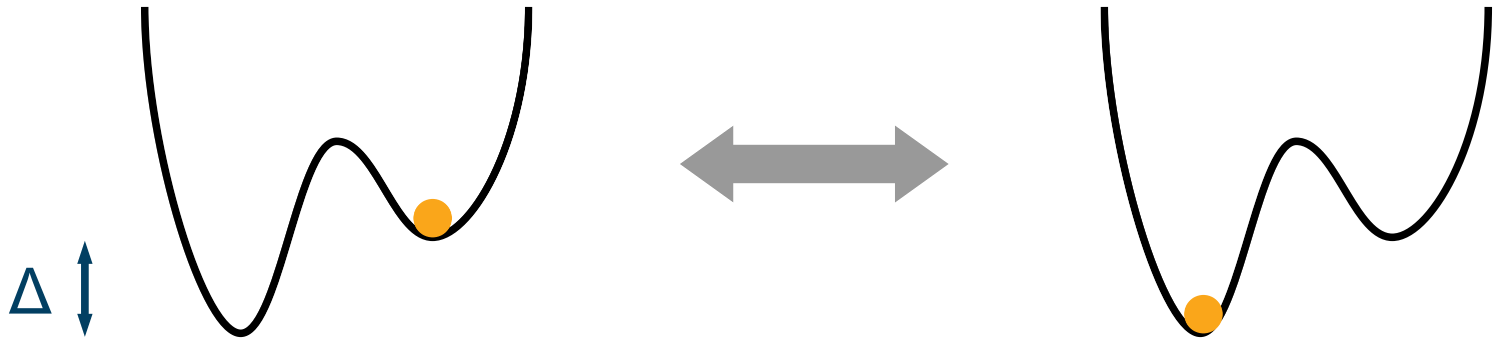
Atom hopping between sites analogous to Kondo effect



$$R \sim \int_{\Delta_{\mathrm{min}}}^{\Delta_{\mathrm{max}}} \log\left(\Delta^2 + T^2\right) \frac{1}{\Delta} d\Delta \sim \log(T) \quad \text{for} \quad \Delta_{\mathrm{min}} < T < \Delta_{\mathrm{max}}$$

Mechanism: data sources

Atom hopping between sites analogous to Kondo effect

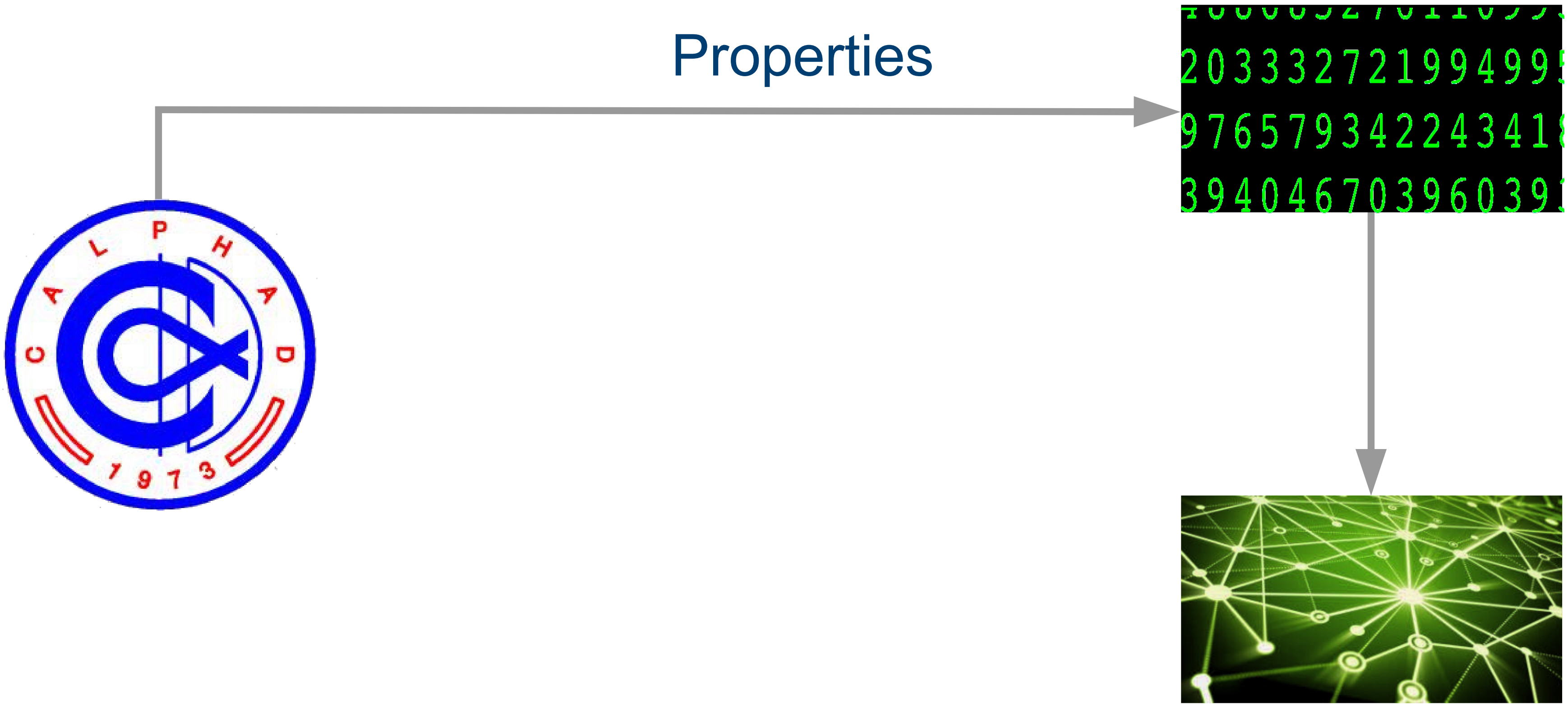


$$R \sim \int_{\Delta_{min}}^{\Delta_{max}} \log(\Delta^2 + T^2) \frac{1}{\Delta} d\Delta \sim \log(T) \quad \text{for} \quad \Delta_{min} < T < \Delta_{max}$$

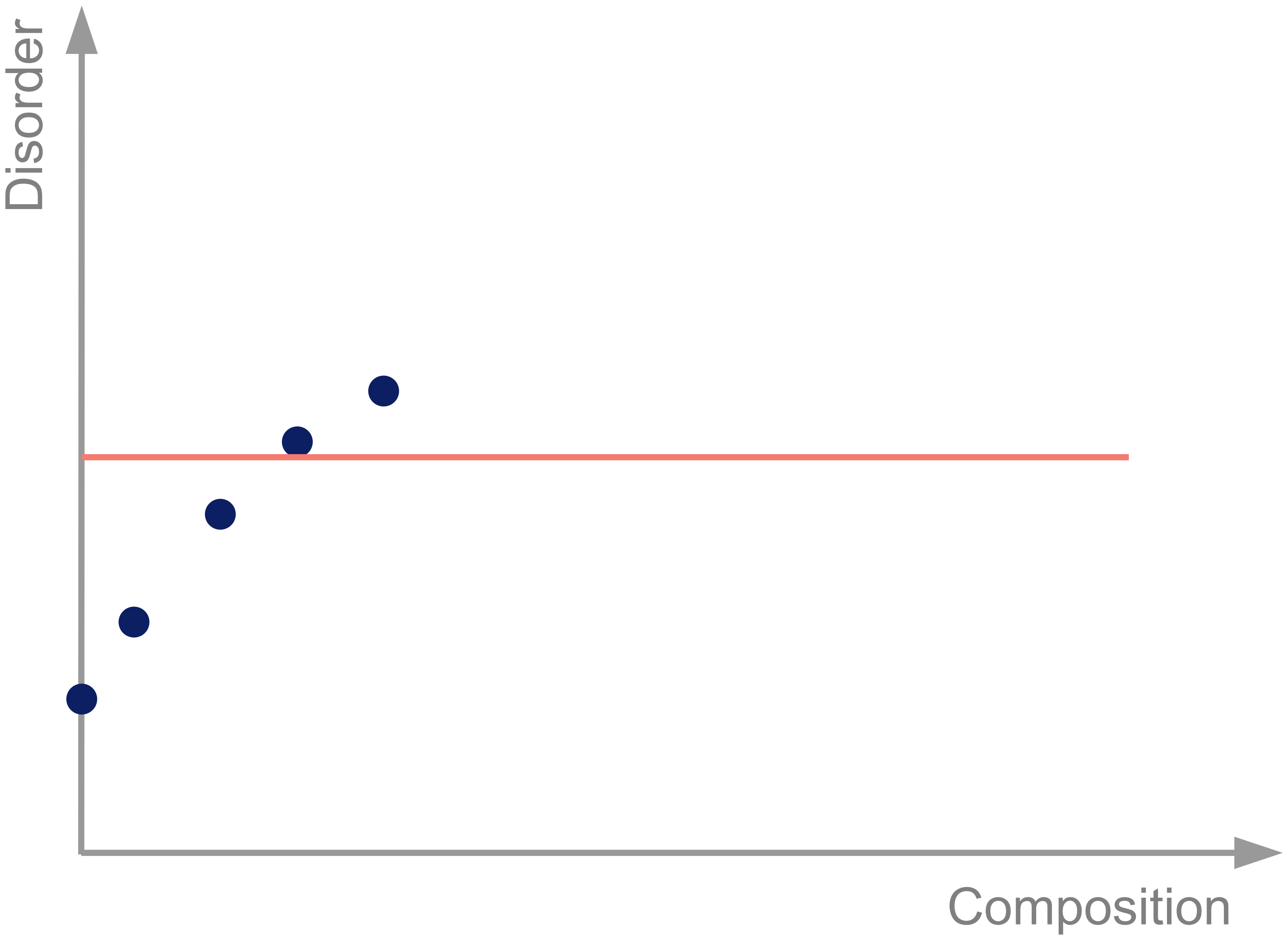
1000 DFT simulations probe the energy landscape and 10000 CALPHAD for phase equilibrium

Merge properties together with deep learning

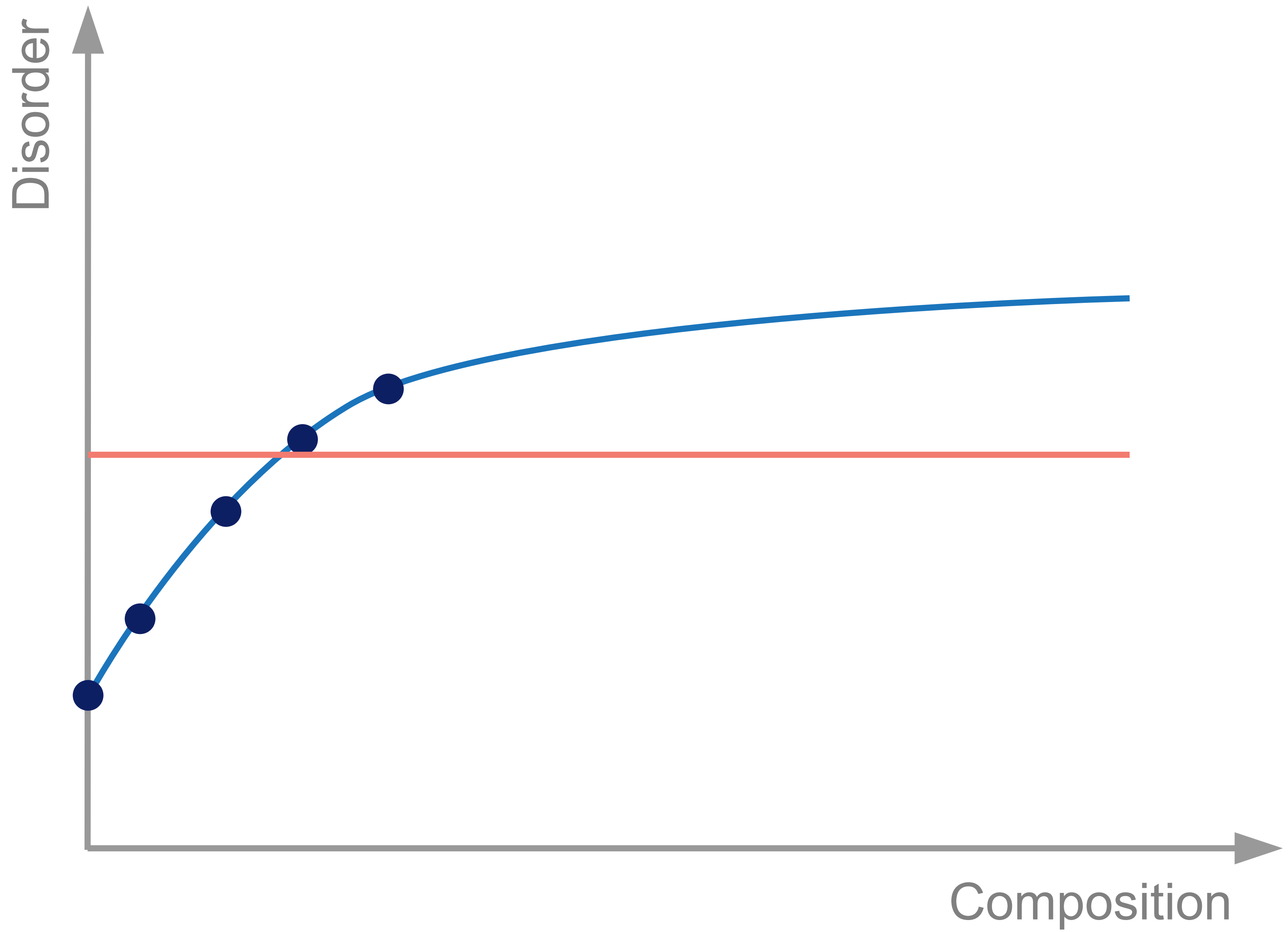
Flowchart to train neural network



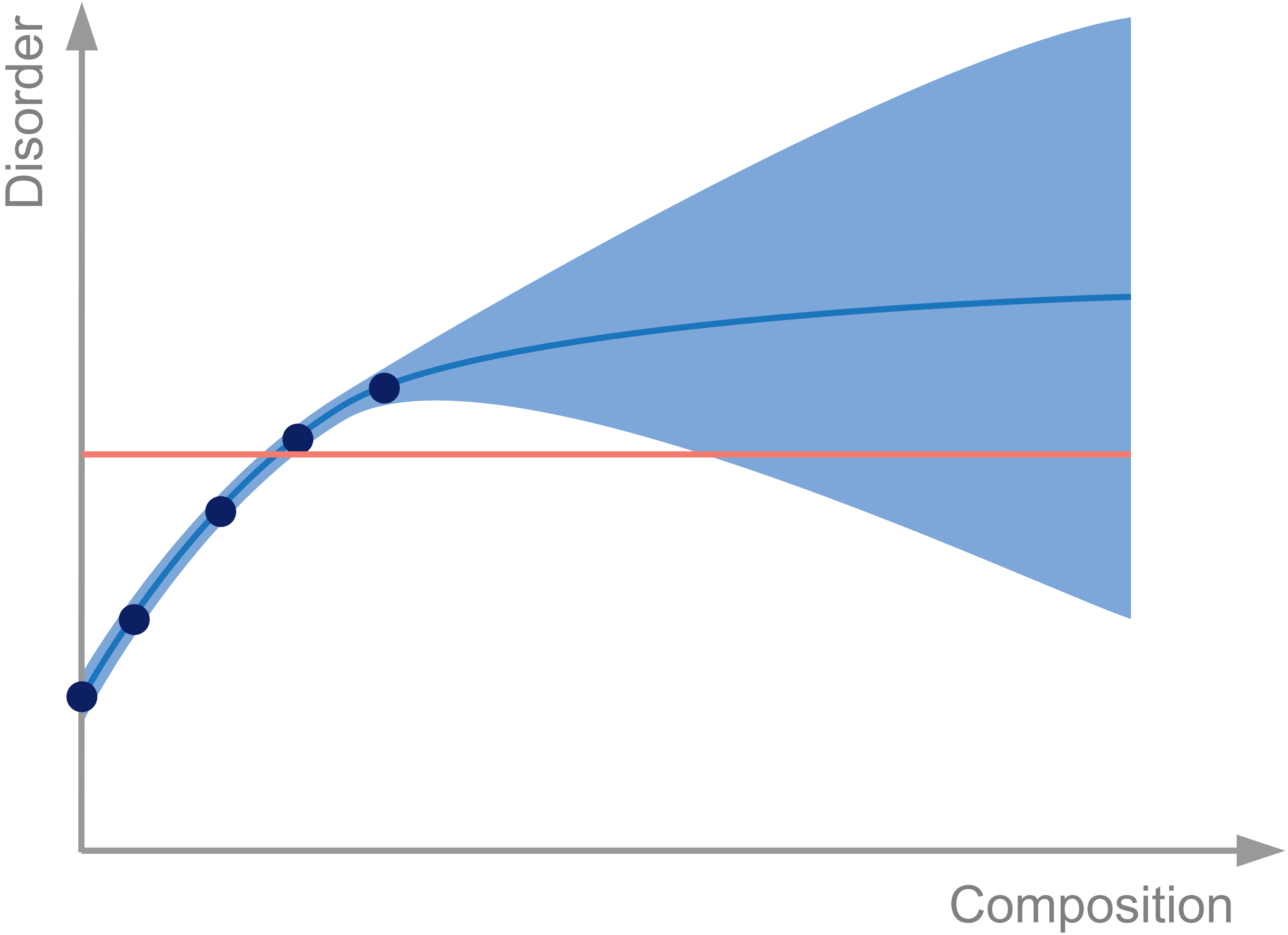
Prediction of disorder



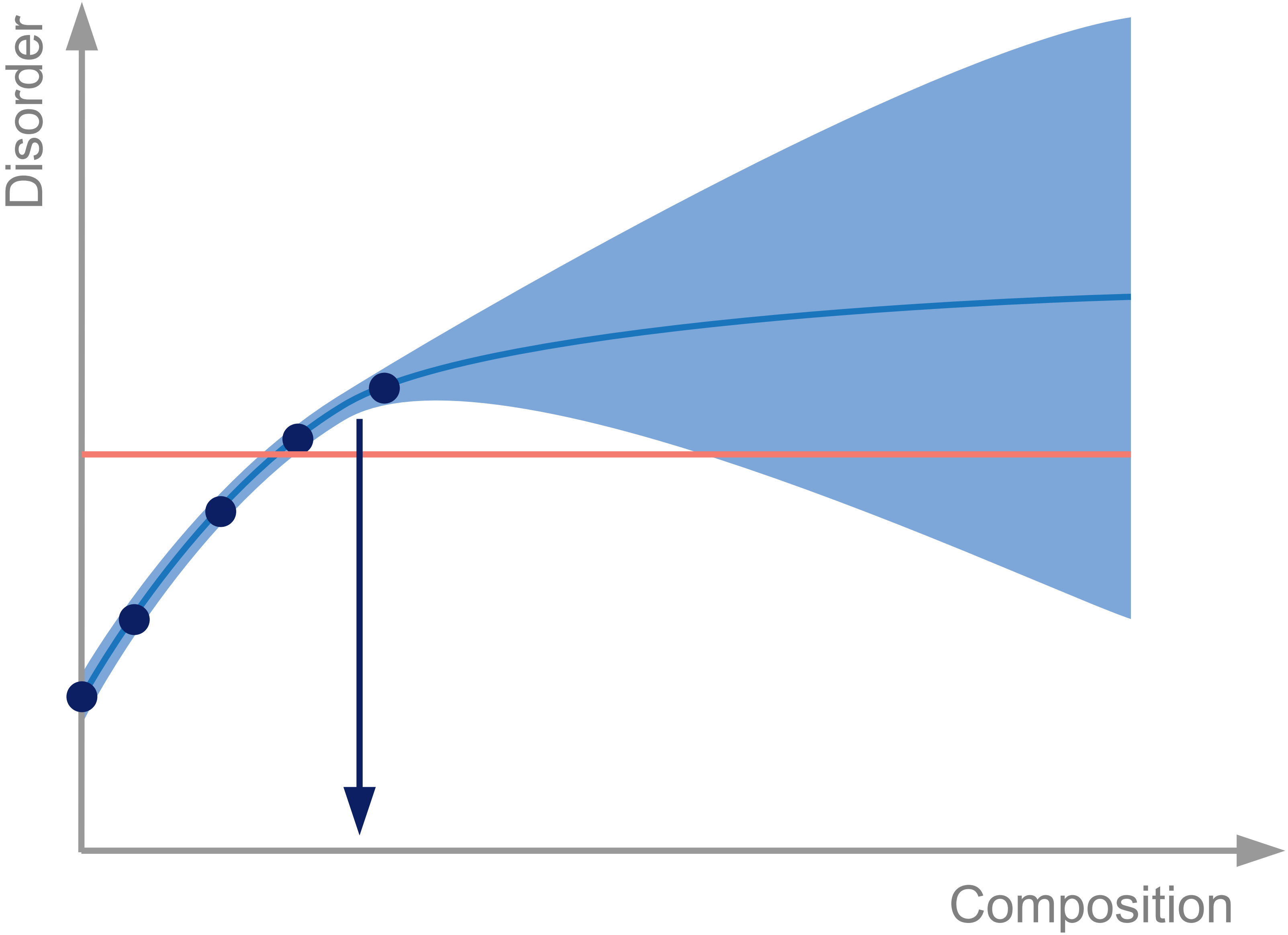
Prediction of disorder



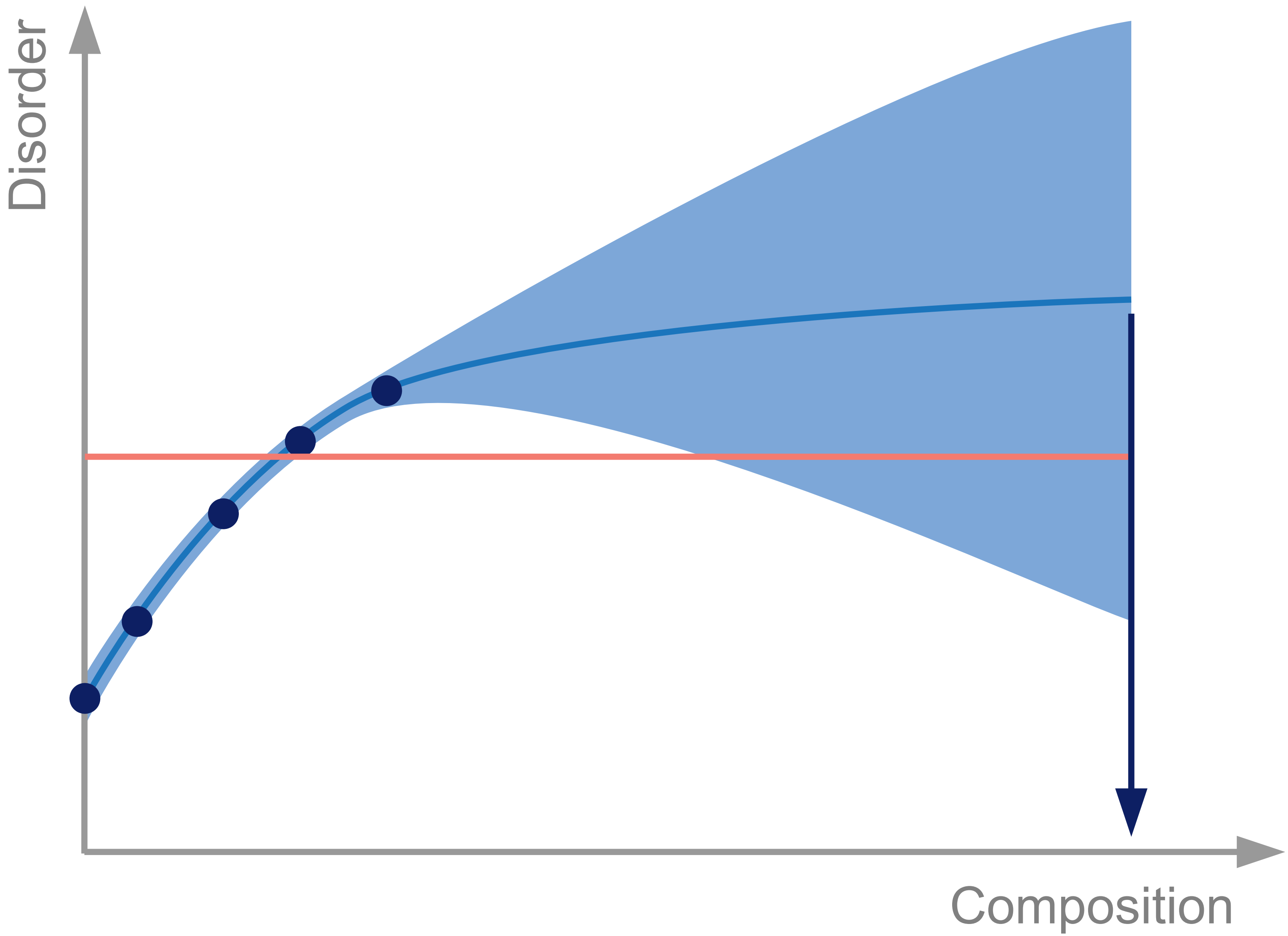
Uncertainty in neural network prediction



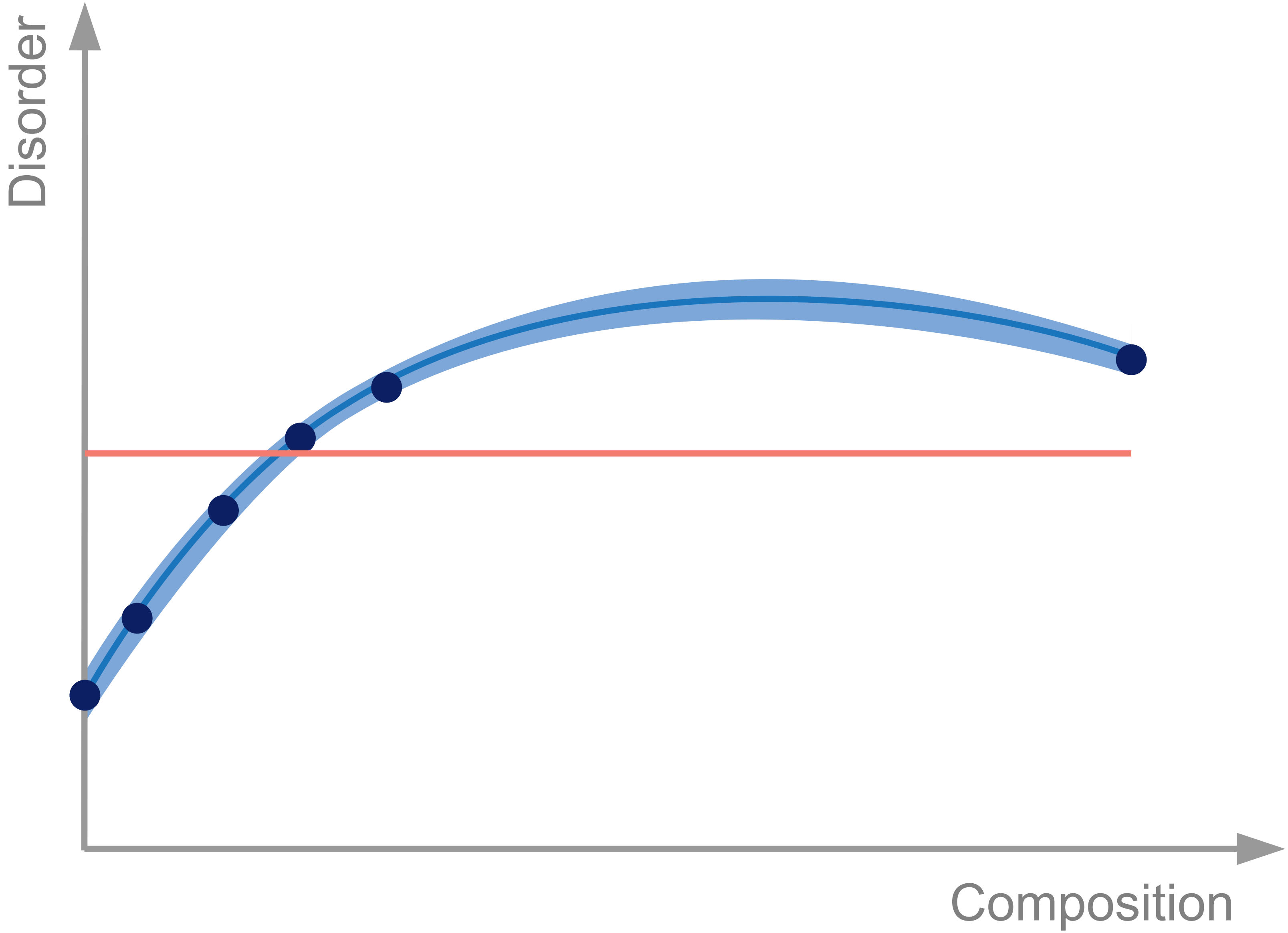
Material most likely to work



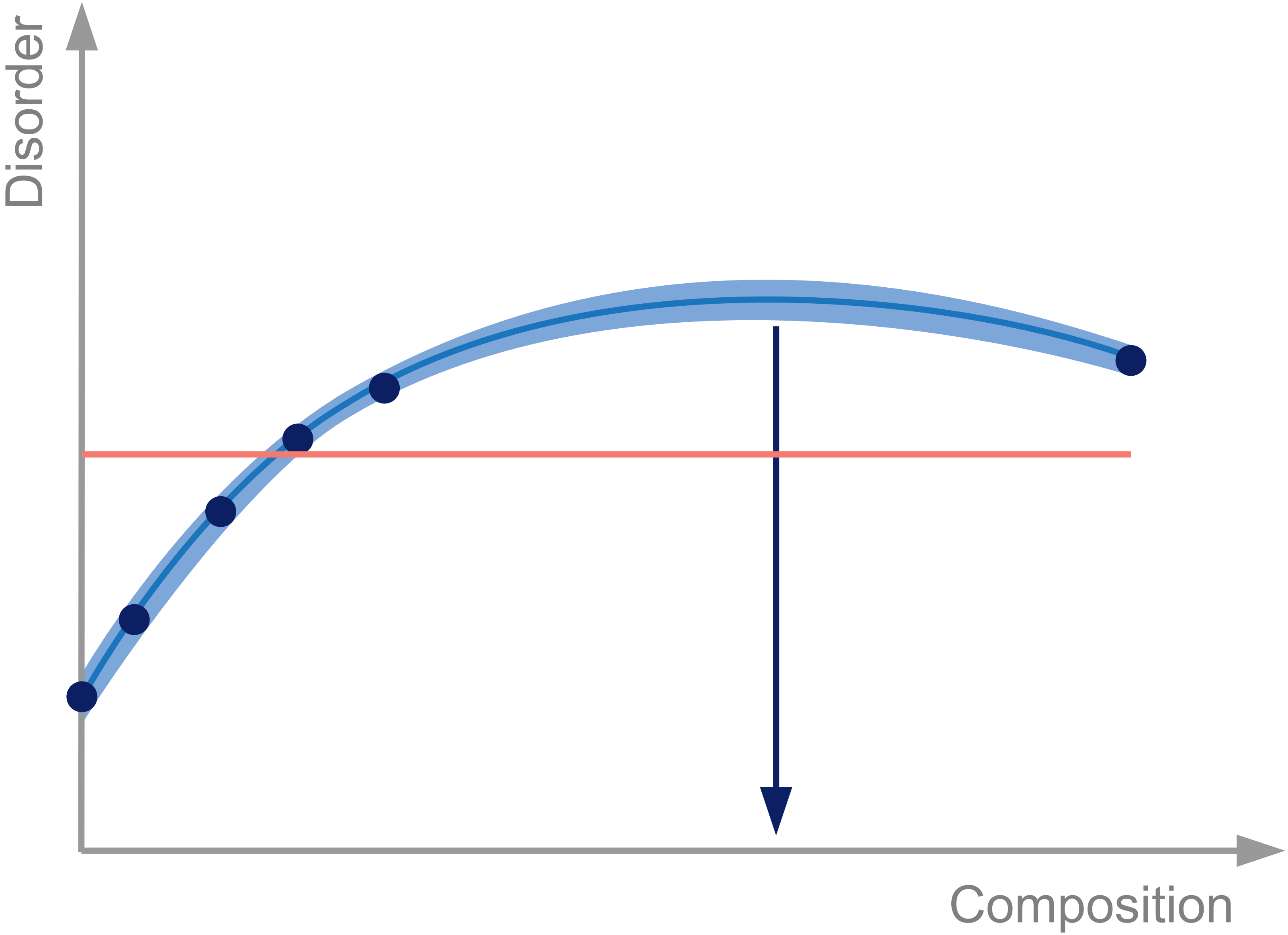
Most useful simulation



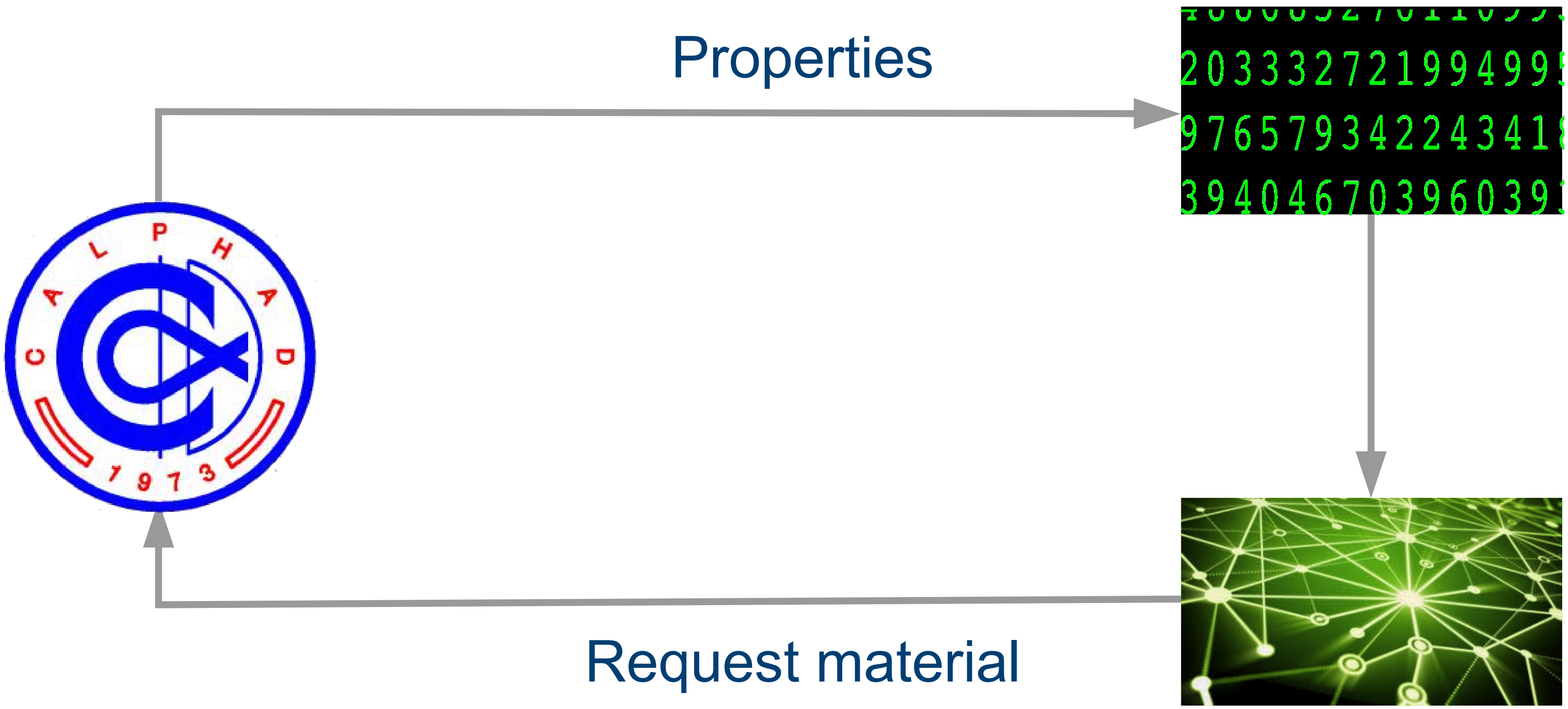
Improved neural network model



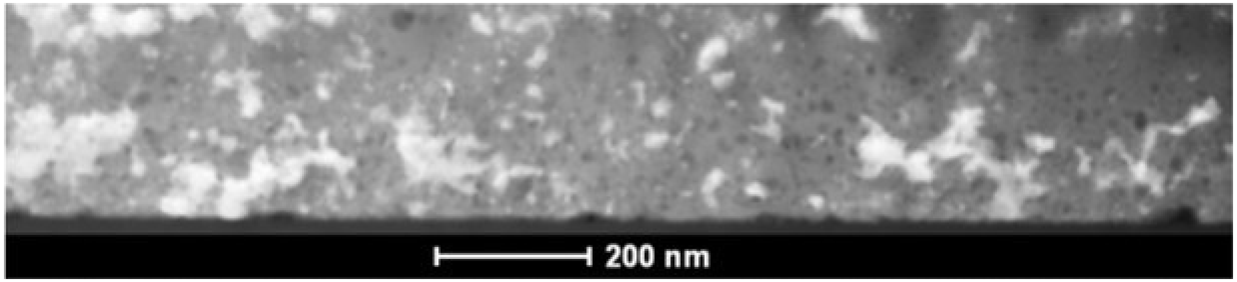
New material most likely to work



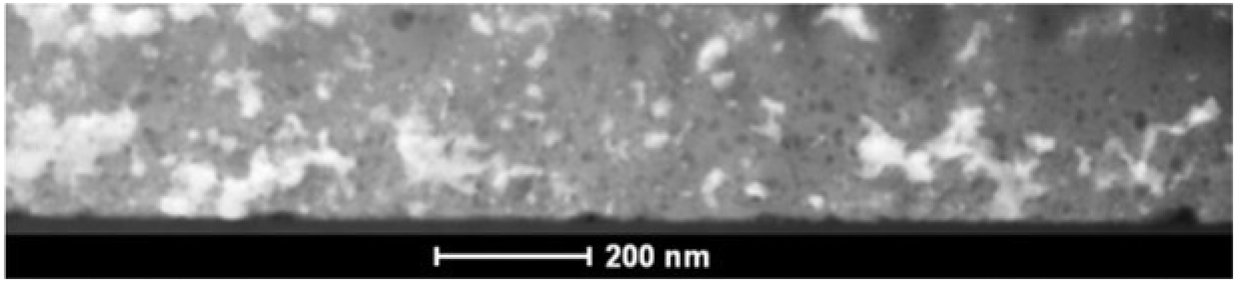
Flowchart with reinforcement learning

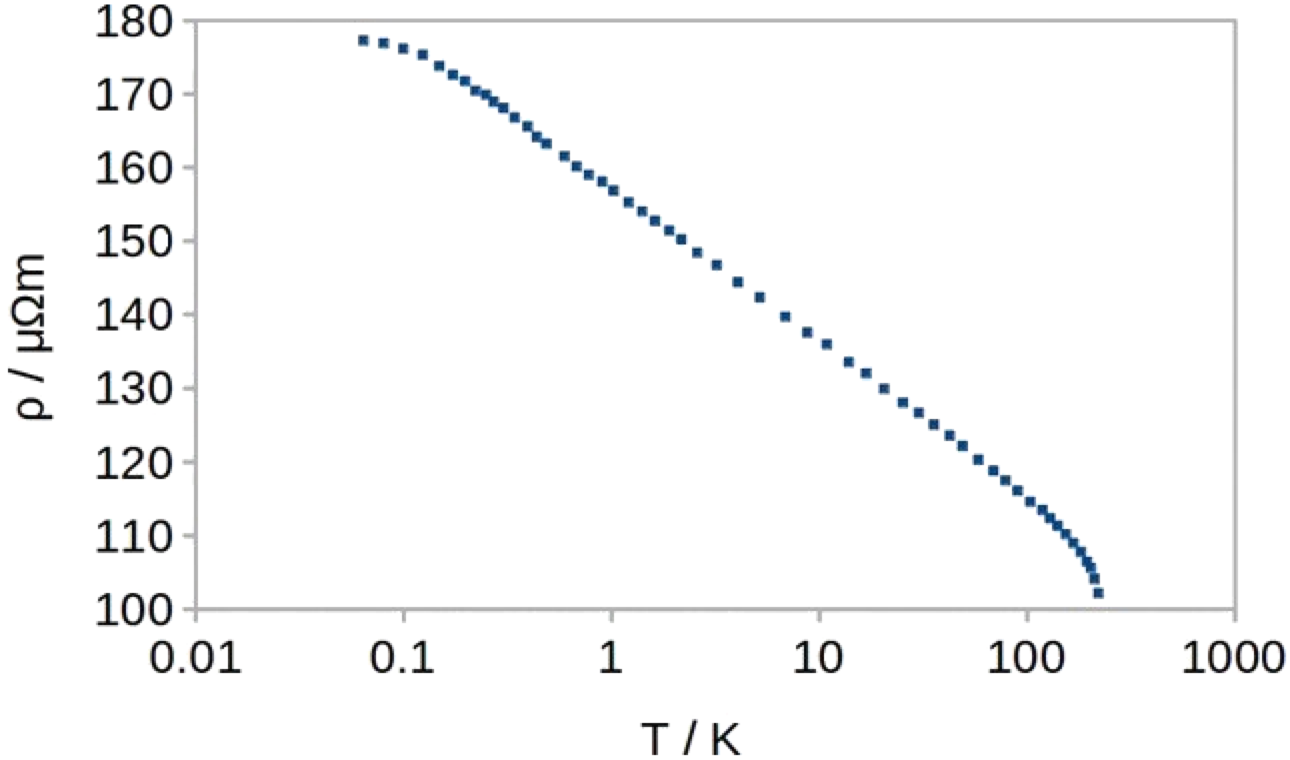


Thermometer under the microscope

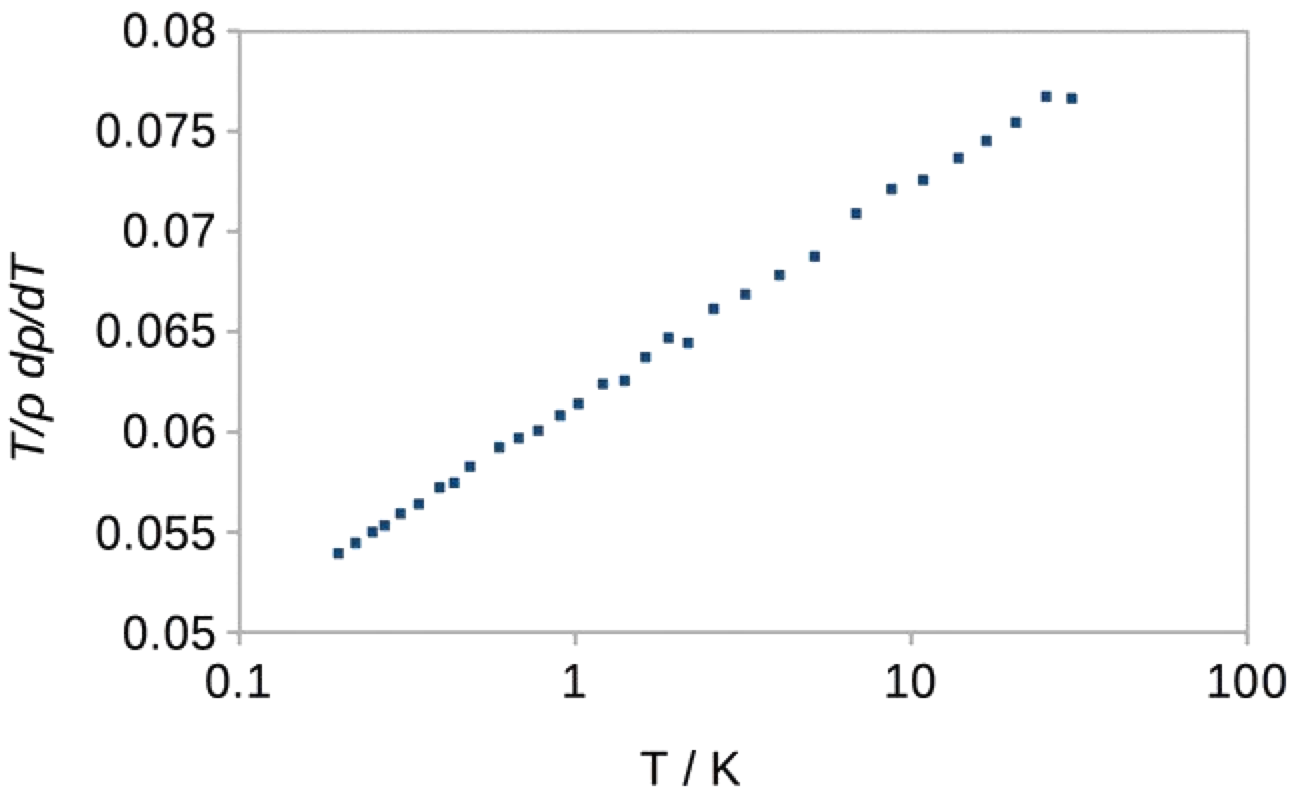


Experimental verification of the thermometer





Sensitivity and stability of the thermometer



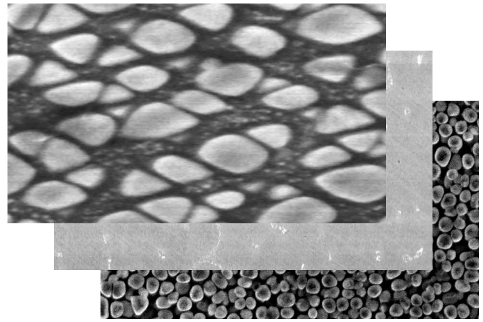
Sensitivity increases by a factor of 2 over the temperature range

Measurements stable over 25 cycles and 6 months

Thermometer being sold by Cambridge Cryogenics

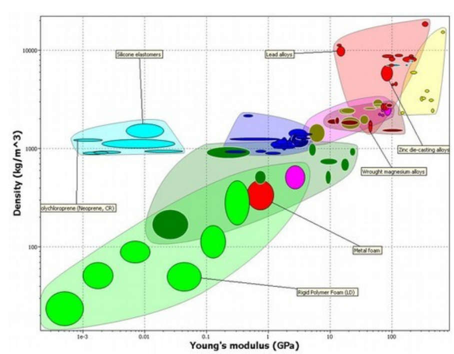
Materials designed

Nickel and molybdenum



Experiment and DFT for batteries

Identified and corrected errors in materials database

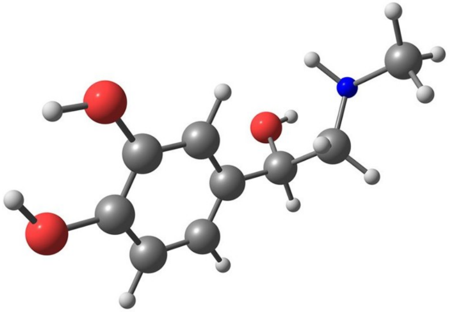


Beyond materials

Lubricants with molecular dynamics and experiments

bp

Assay activity



e-therapeutics

Drug design

optibrium

Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Thermometer that works over 1000x temperature range

Further experimentally proven materials, founded start-up intellegens.ai

https://app.intellegens.ai/steel_search