Intellegens

Advanced material design using deep learning

About Intellegens

Machine learning software to aid experimental design developed at University of Cambridge

Merge and aggregate data

Predictive models **reduce costs** and **accelerate discovery**

Traditional experimental design

Process is expert driven, subjective, and iterative through trial and improvement

Process takes ~20 years and specialist materials cost >$10m to develop, drugs cost >$1bn

Alchemite™ machine learning

Standard algorithms need all inputs to calculate outputs

Typical experimental data is 5% complete

Alchemite™ predicts from available inputs

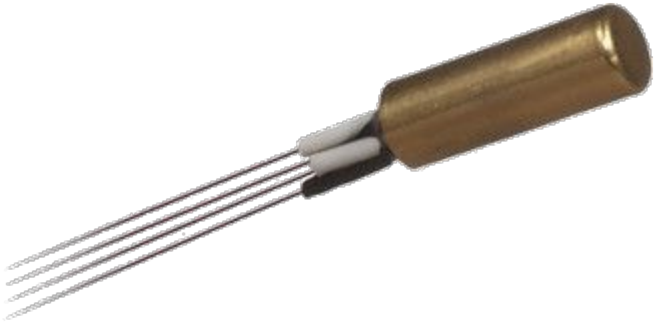
Optimized design process

Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

Case study: quantum material for thermometry

90% of the cost of a thermometer is for calibration



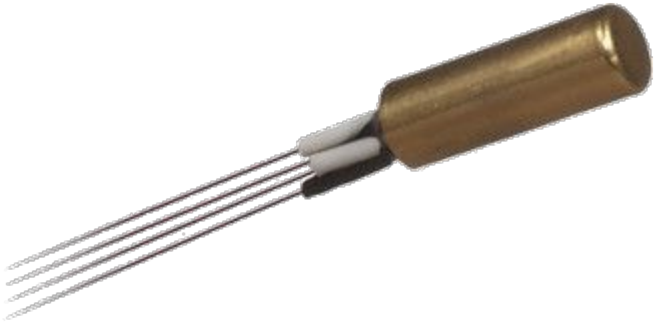
Case study: quantum material for thermometry

90% of the cost of a thermometer is for calibration

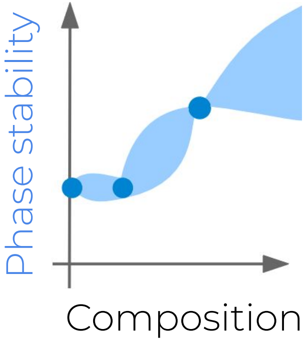
Require a simple resistance-temperature relationship over a wide temperature range

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

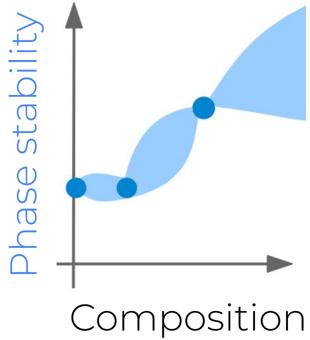
Thermometer must be stable

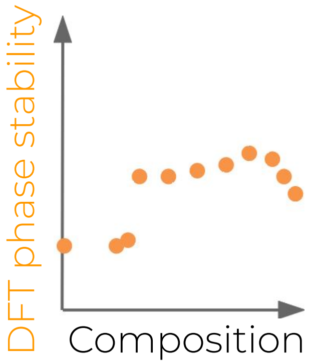


Lack of experimental data

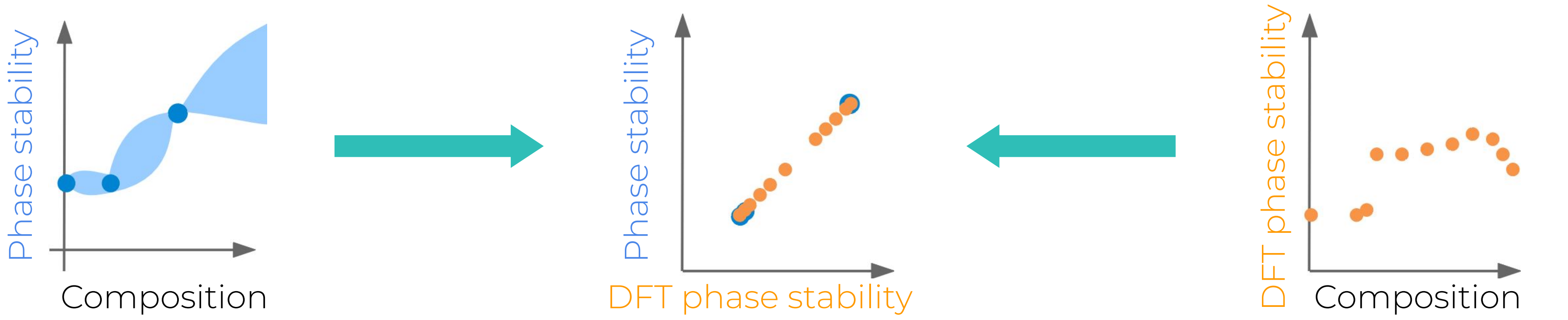


Large amount of computational data

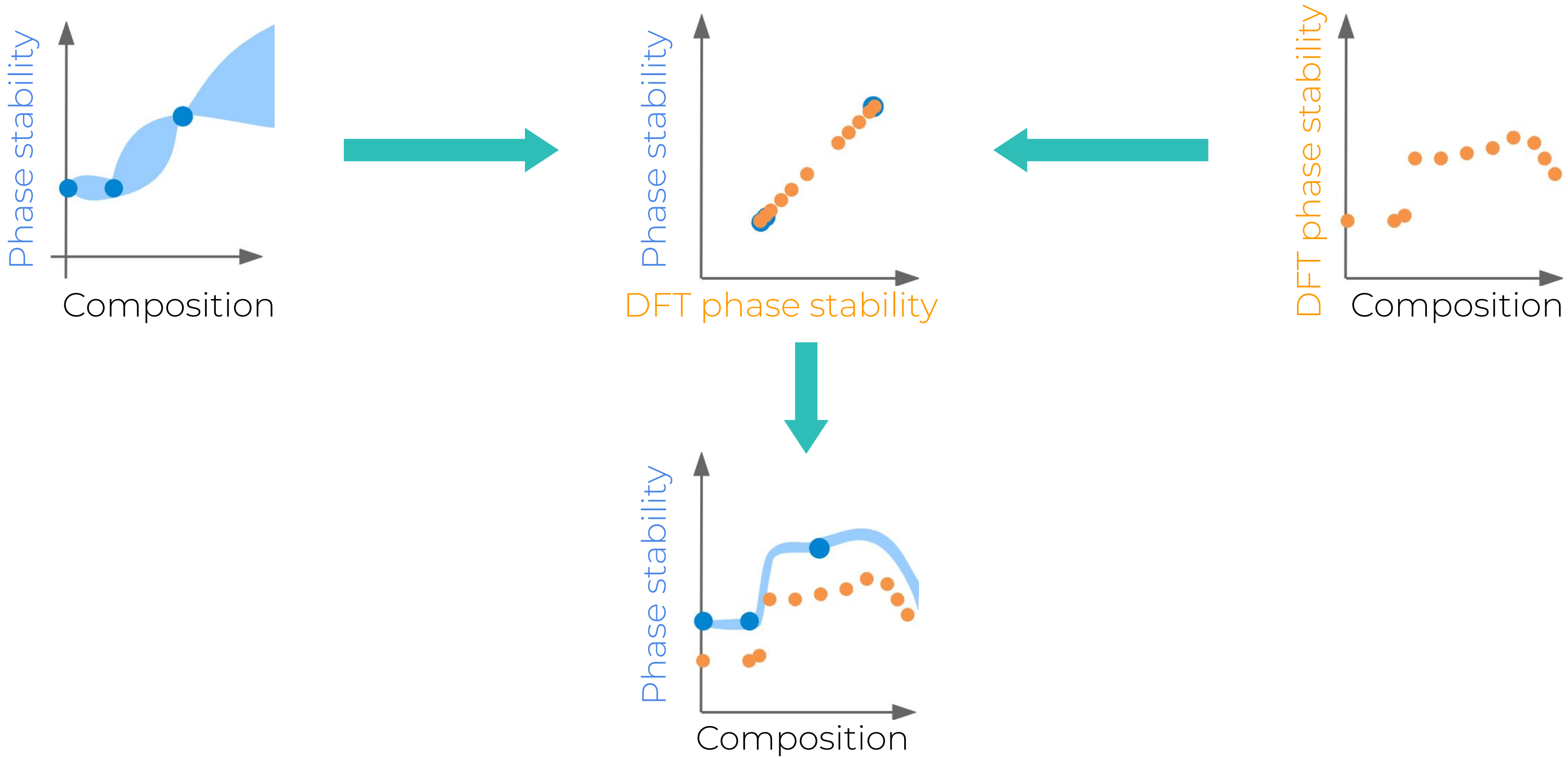




Simple experimental-computational relationship



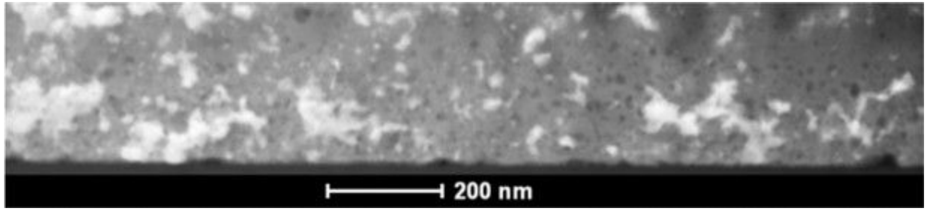
Computational data guides extrapolation



Alchemite machine learning

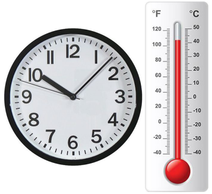
Temperature range
Sensitivity
Stability
Cost
Robust
Resistance
Contacts

Experimental validation



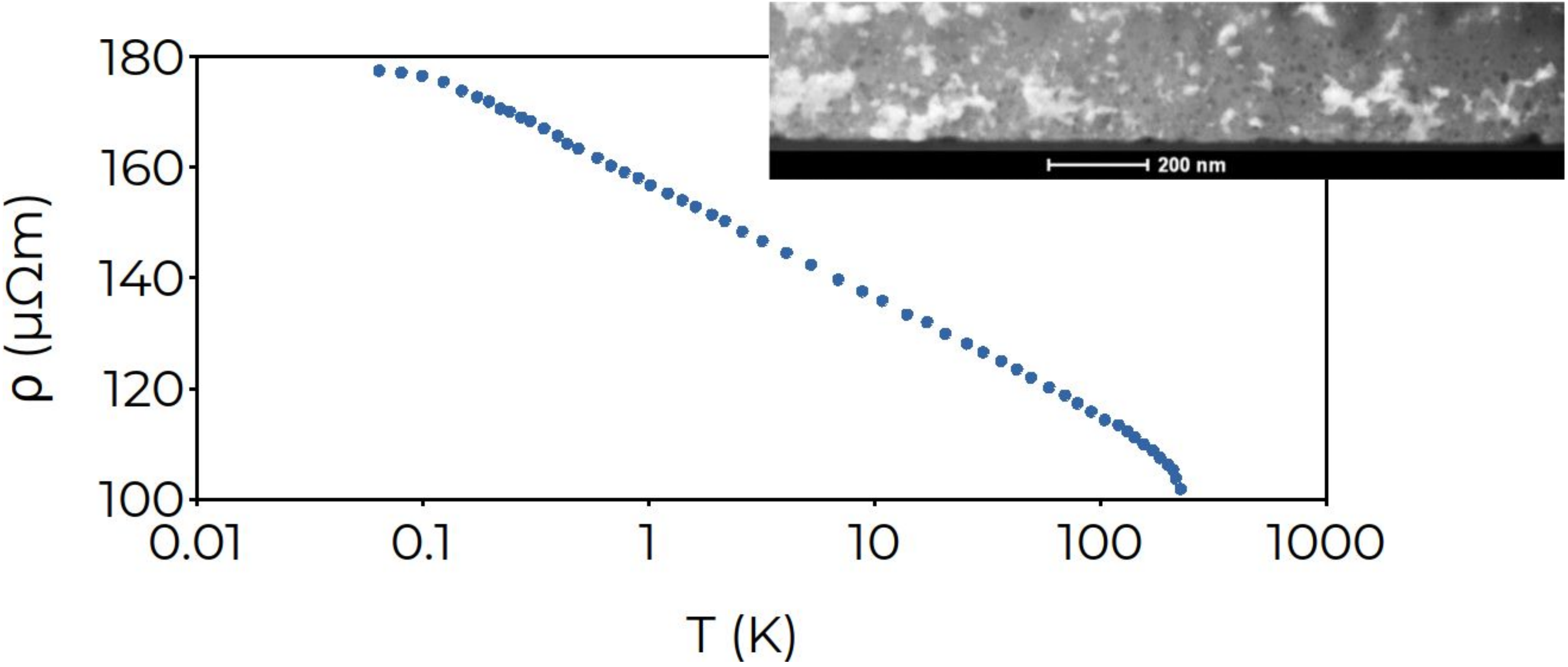
Ge 89%

Au 11%

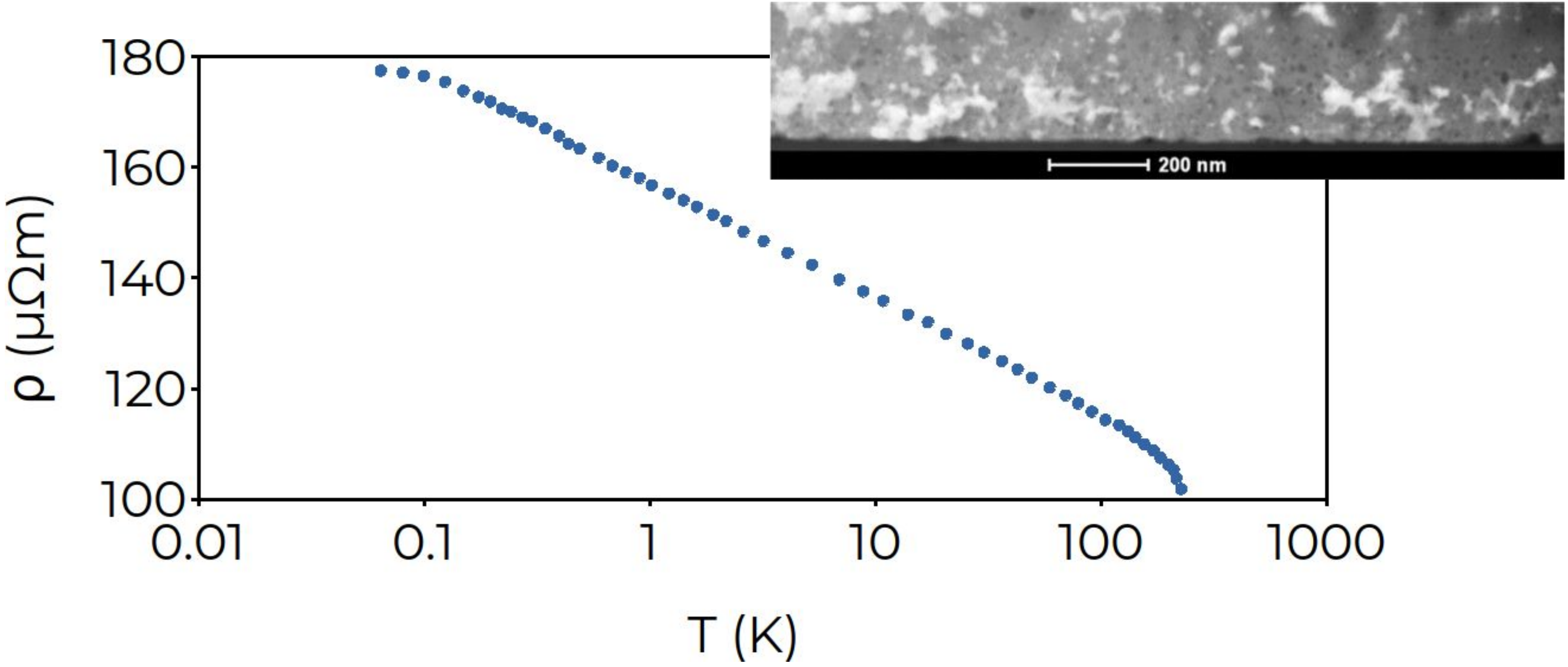


Quench

Experimental validation

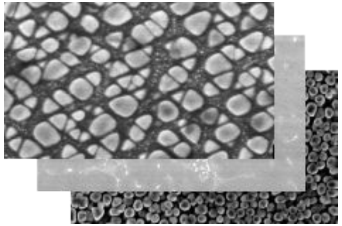


Experimental validation



Measurements stable over 25 cycles and 6 months intellegens.ai

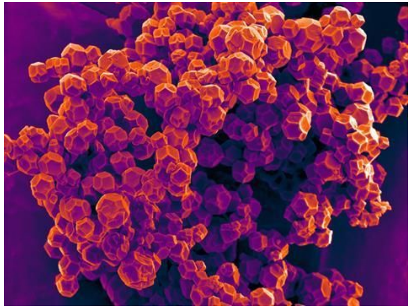
Further materials and drug design



Nickel & moly alloys

Batteries

Steels for welding



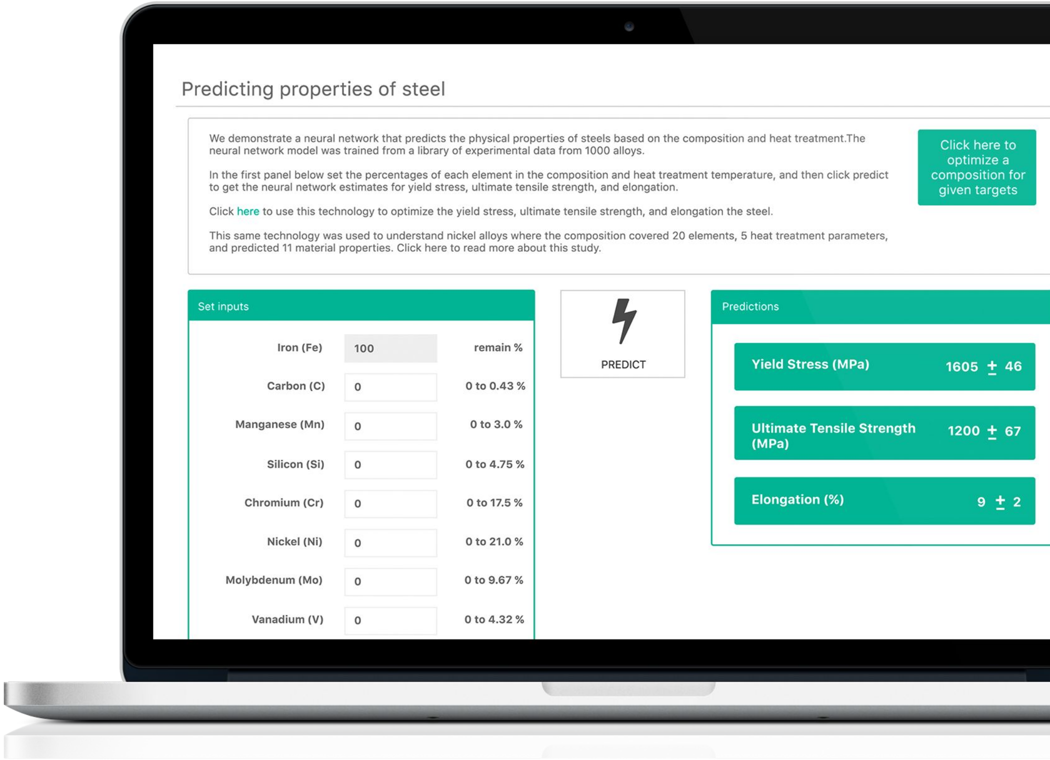
Metal-organic framework

Concrete

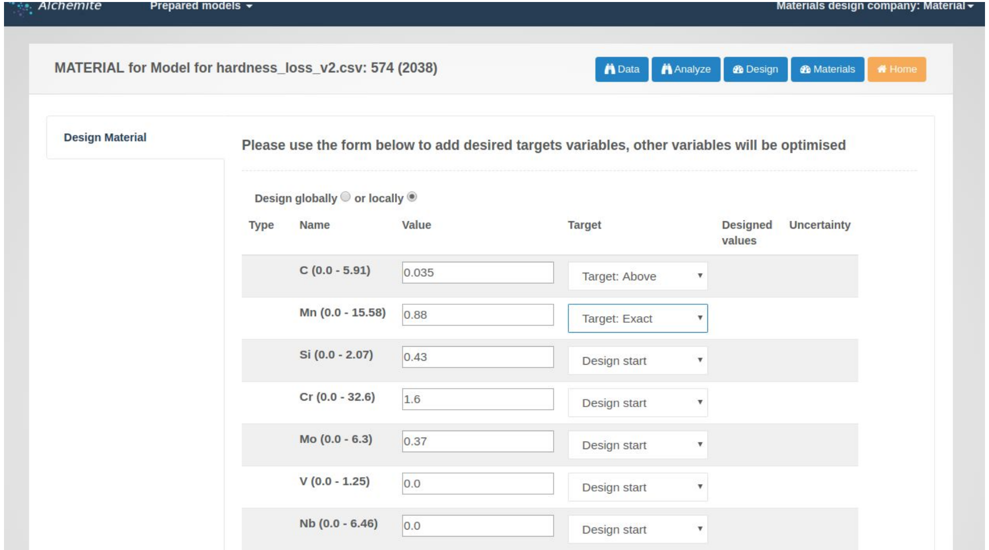
Drug design

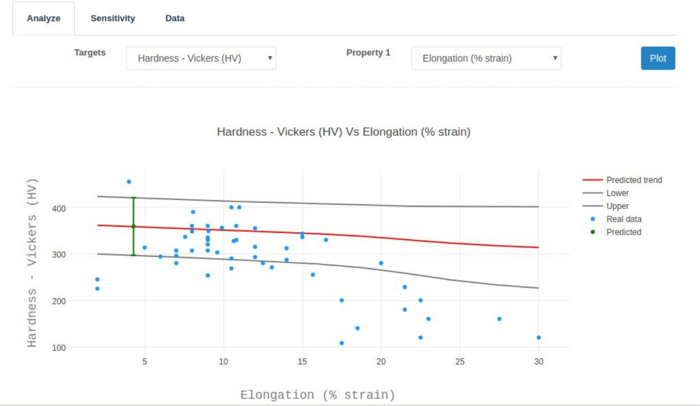
Future opportunities: Integrated software

1. Load data
2. Training
3. Predict & design

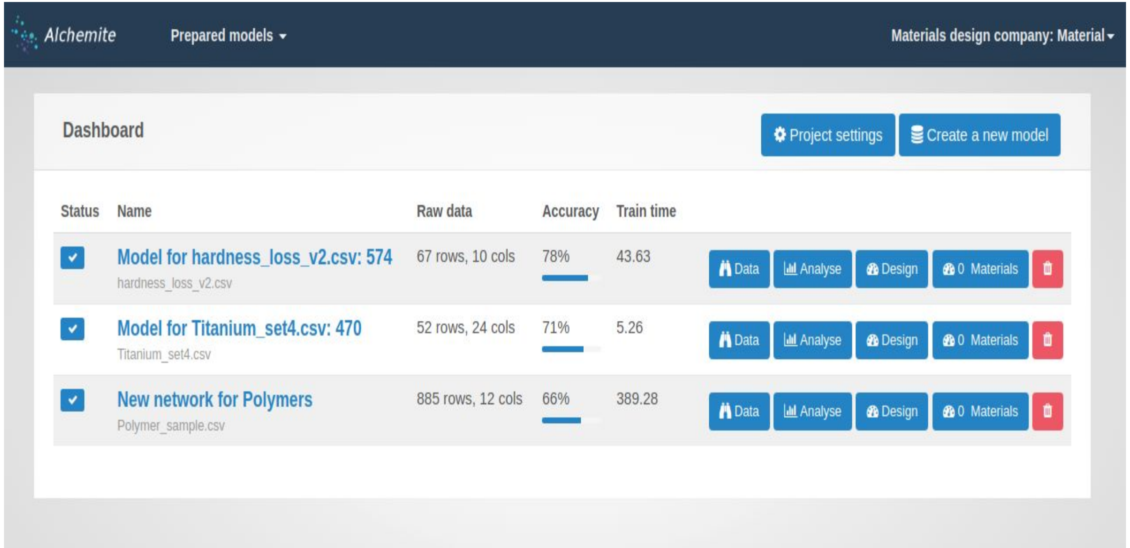


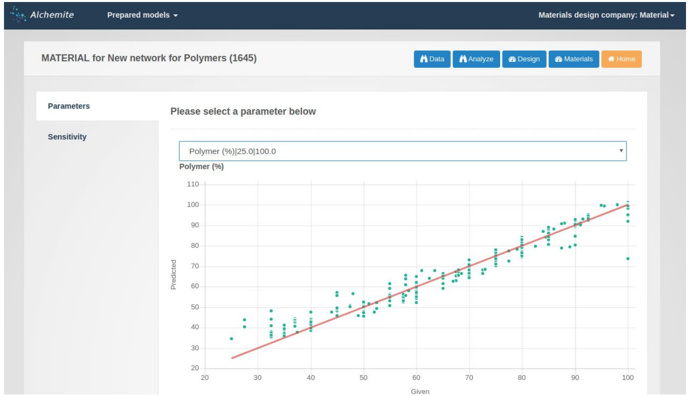
Design, analyse, and share new materials

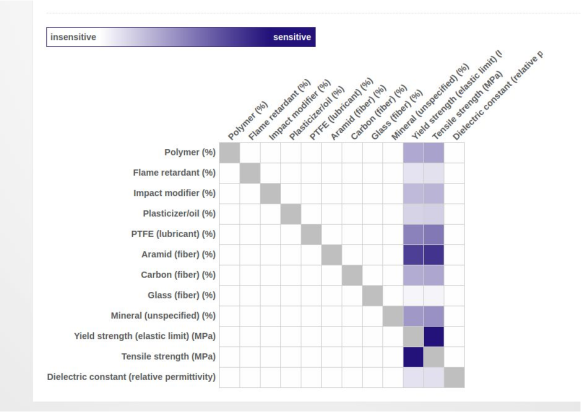




Manage models and analyse workflow







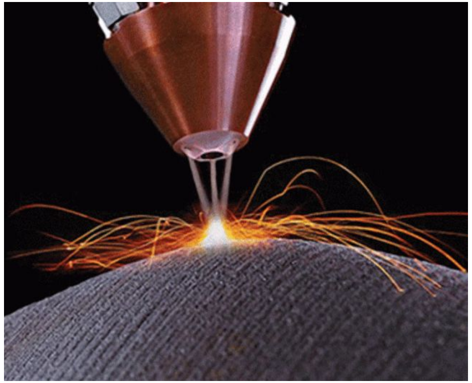
Summary of future opportunities of Alchemite™

Alchemite™, a full stack machine learning solution to merge sparse data

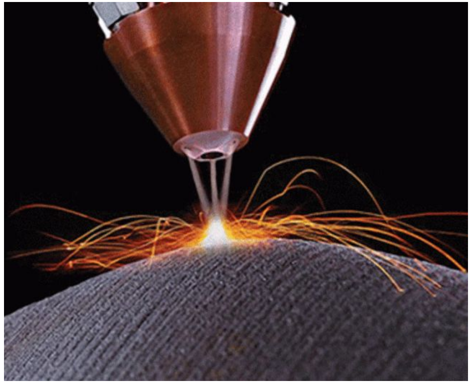
Designed and experimentally verified material for thermometry, and other alloys and drugs

Show	Stand 1311
Contact	ben@intellegens.ai
Website	https://intellegens.ai
Demo	https://app.intellegens.ai/steel_optimise
Papers	https://www.intellegens.ai/paper.html

Case study: alloy for direct laser deposition



Direct laser deposition is similar to welding



Direct laser deposition

Welding

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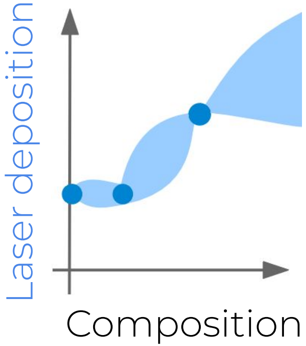
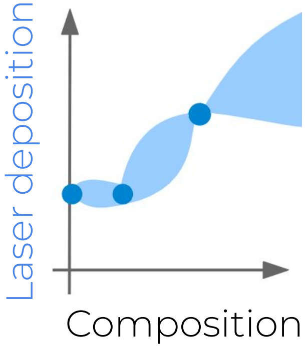
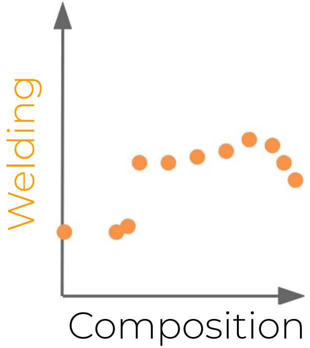
Lack of data for laser deposition

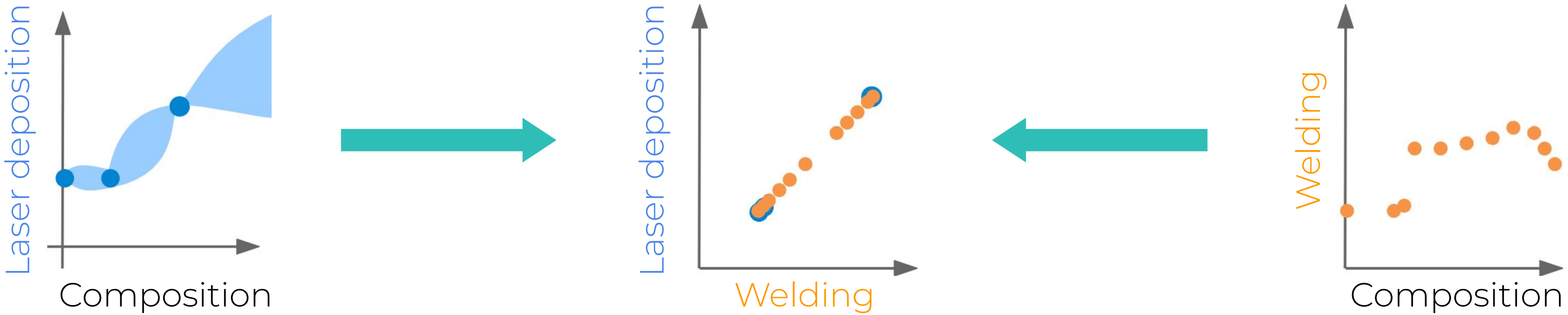


Large amount of welding data

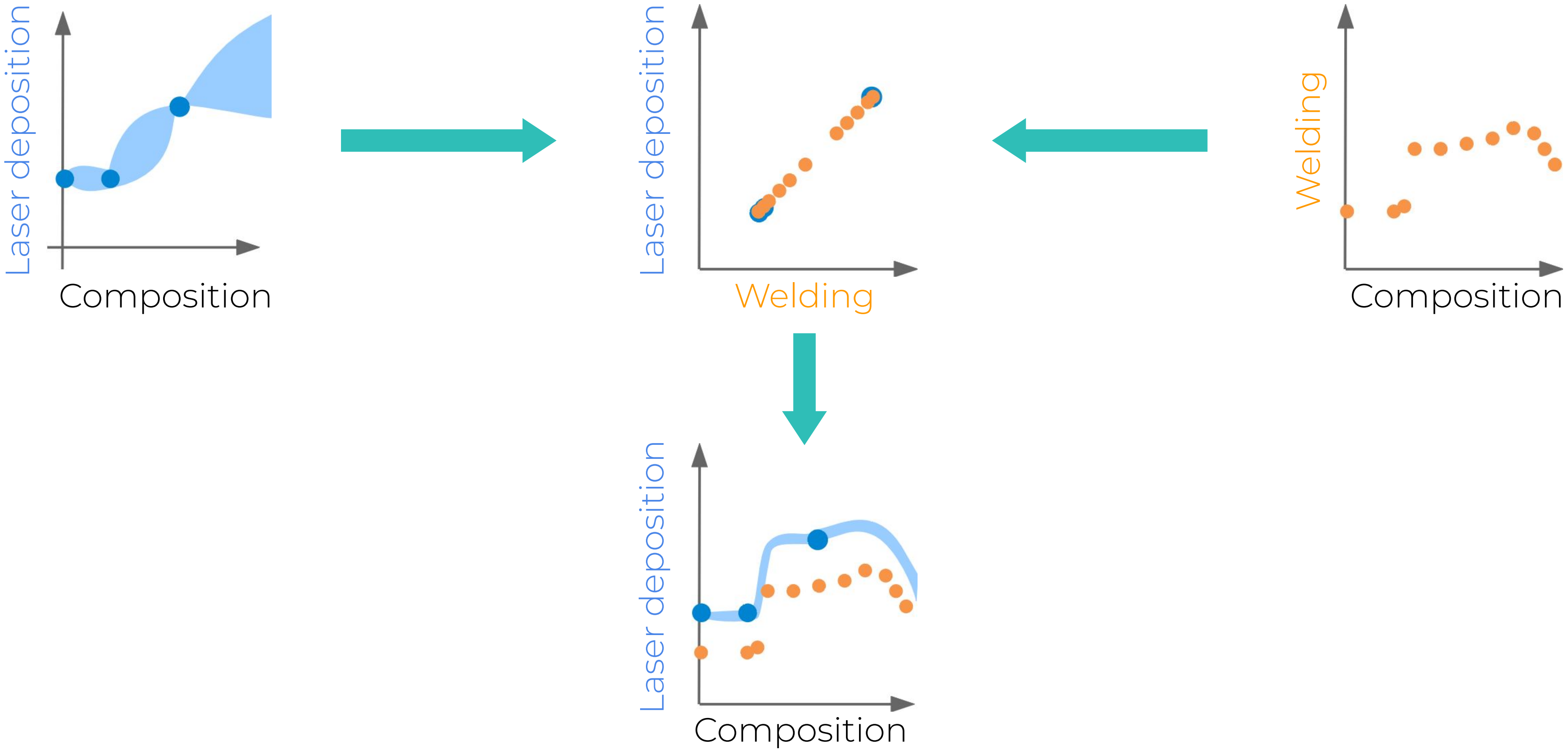




Simple welding-deposition relationship



Welding data guides extrapolation



Targets for direct laser deposition alloy

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	$> 1000^{\circ}C$
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 of alloy for direct laser deposition

Cr 19%

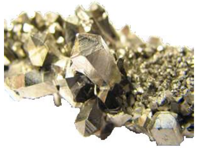
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



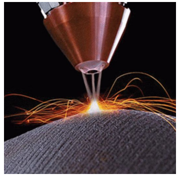
Al 2.9%

C 0.04%

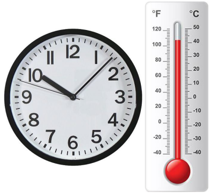
B 0.01%

Ni balance

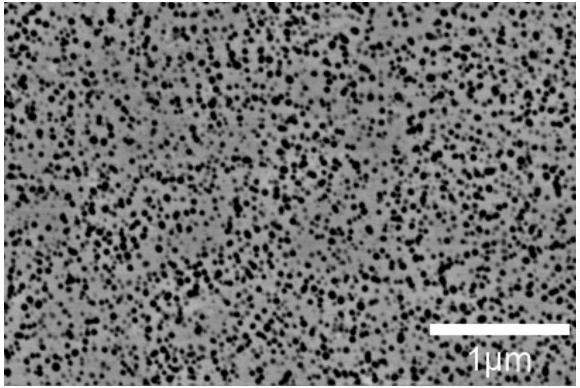
Exposure 0.8



T_{HT} 1230°C



Experimental validation



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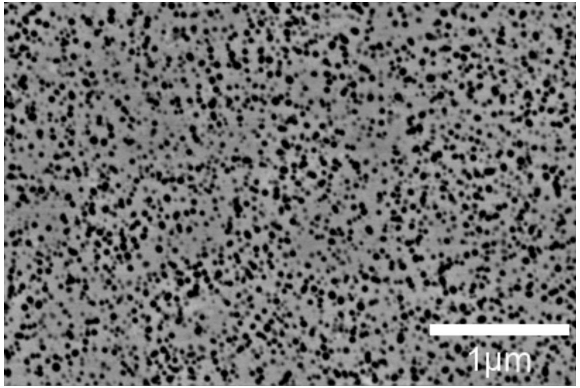
Experimental validation



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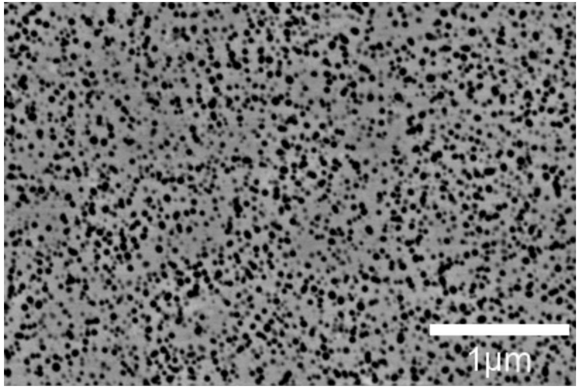

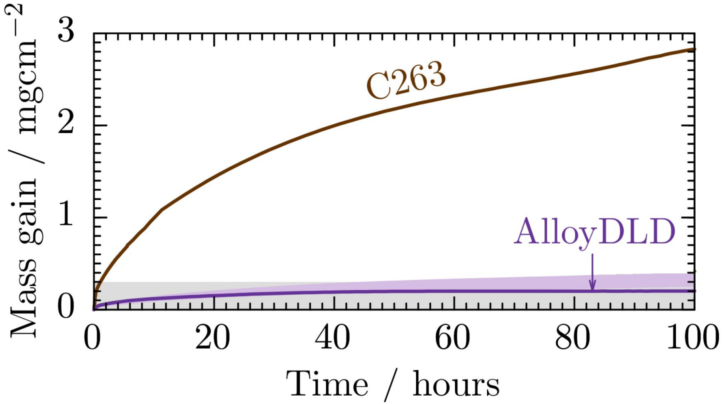

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