



Advanced material design  
using deep learning

## Alchemite™ optimized design process

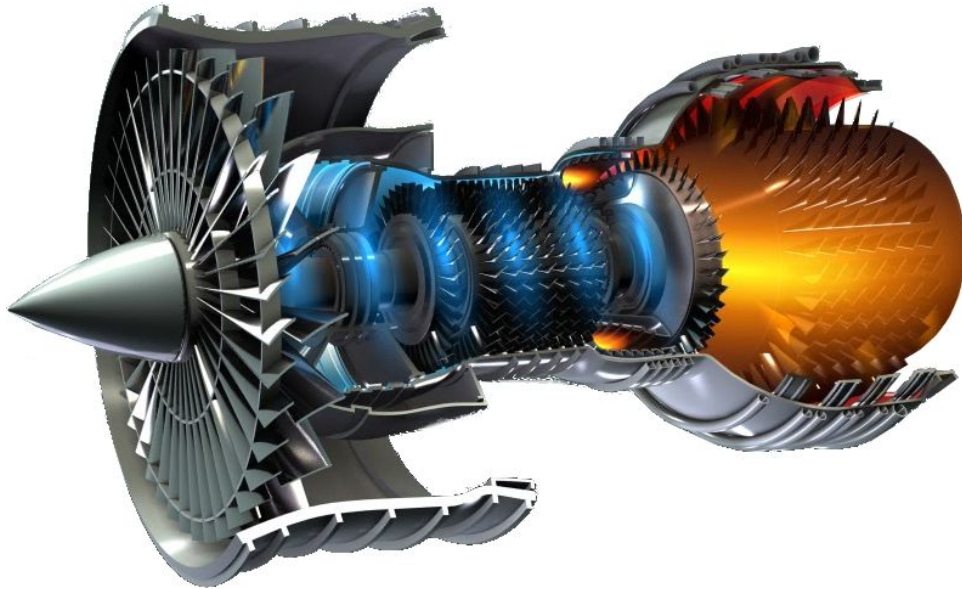
Machine learning software to aid experimental design  
developed at University of Cambridge

Alchemite™ predicts from **available** inputs

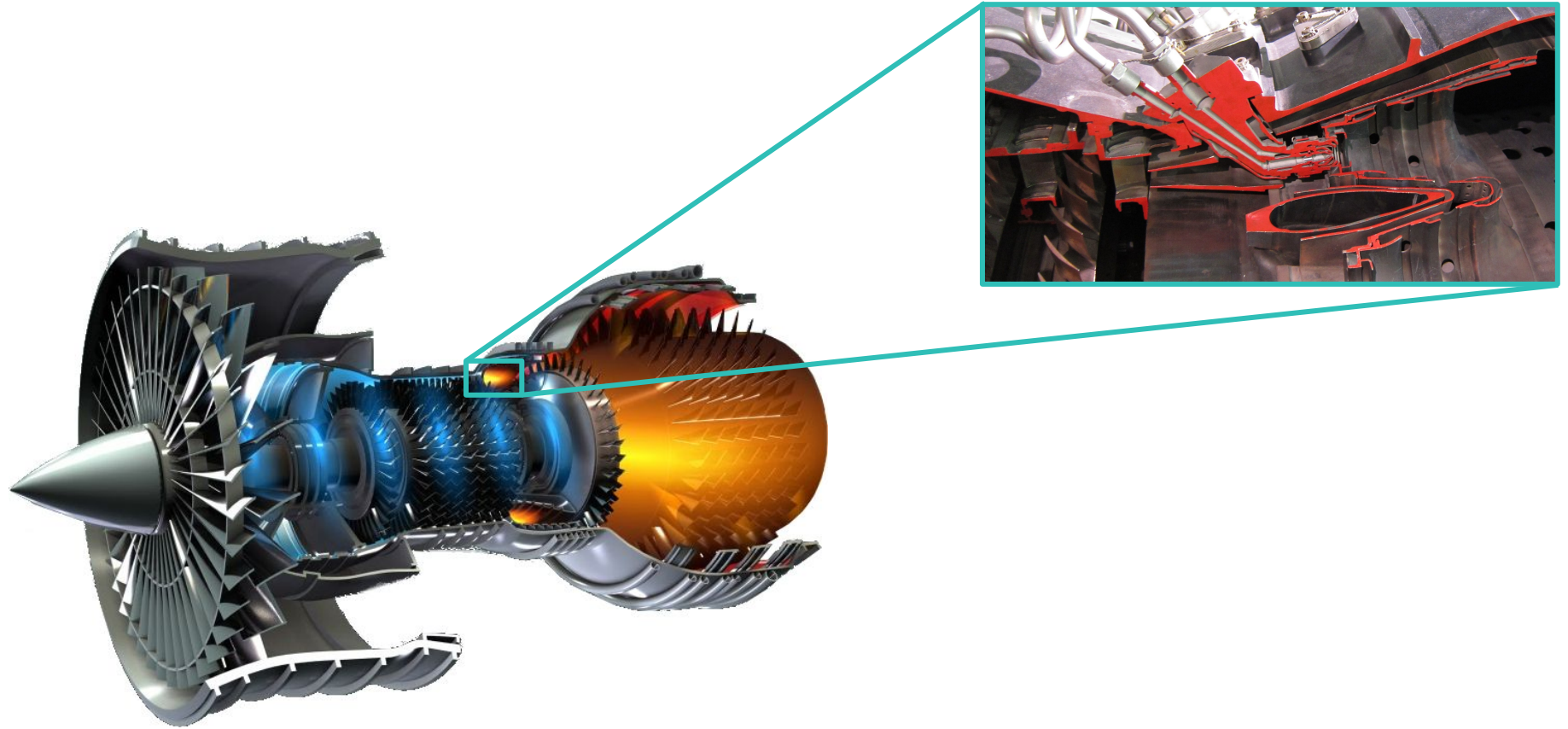
**Reduce costs** - 90% reduction in experiments and fewer  
measurements for expensive quantities

**Accelerate** discovery and validation to 2 years

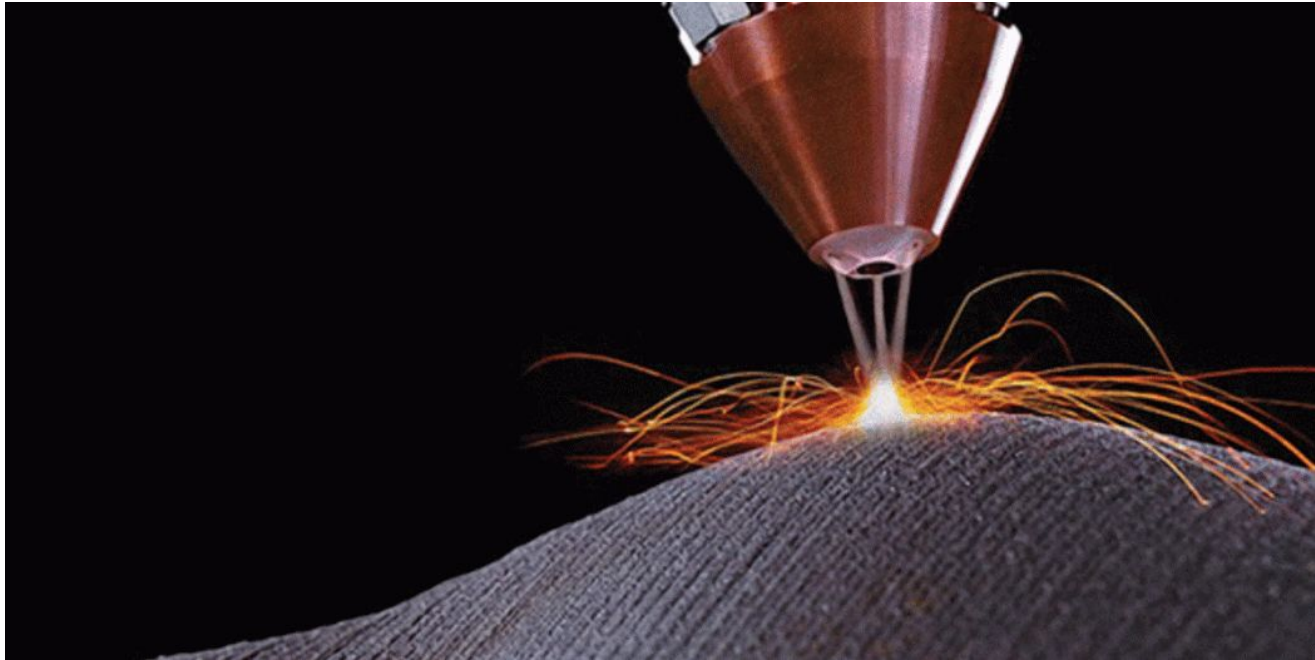
# Case study: alloy for direct laser deposition



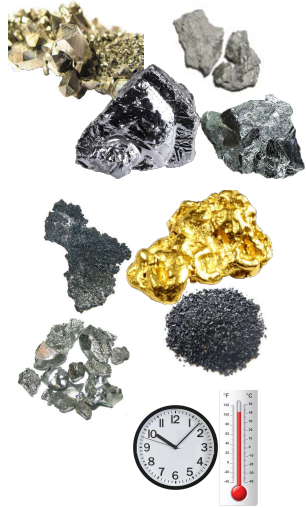
# Case study: additive manufacturing



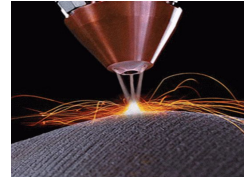
# Additive manufacturing requires new alloys



# Machine learning



Processability



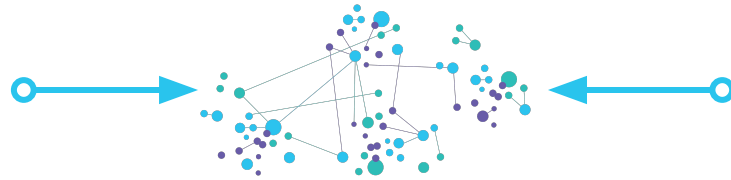
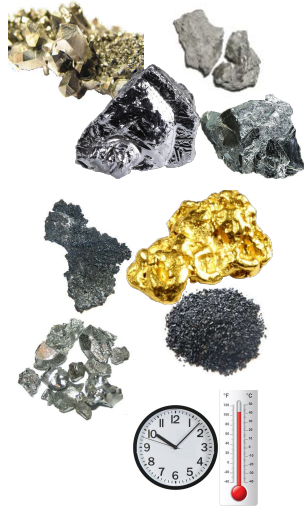
Fatigue life



Cost



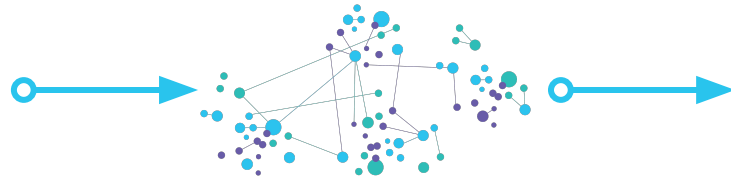
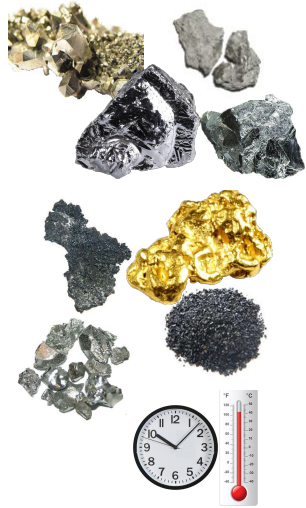
# Machine learning



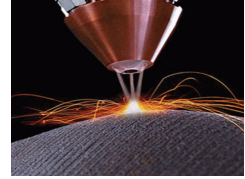
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Fatigue life  
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Cost  
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# Machine learning



Processability



Fatigue life

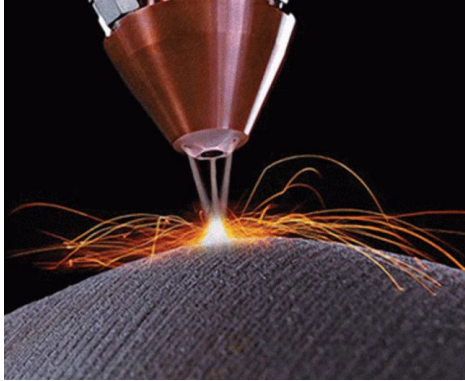


Cost

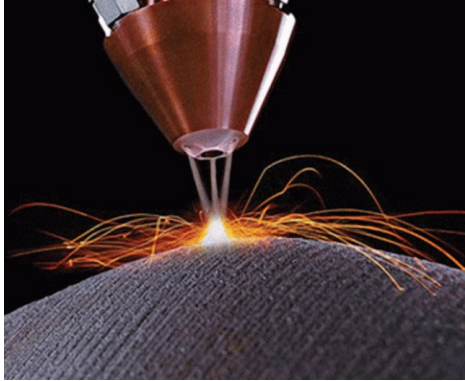




# Case study: alloy for direct laser deposition



# Direct laser deposition is similar to welding

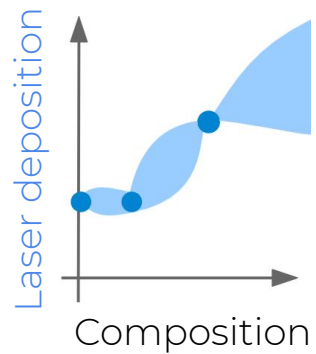


Direct laser  
deposition

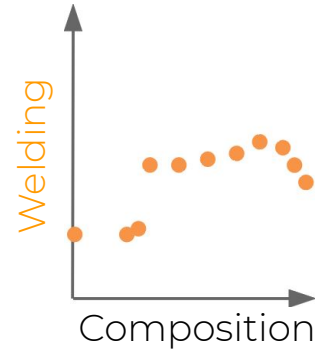
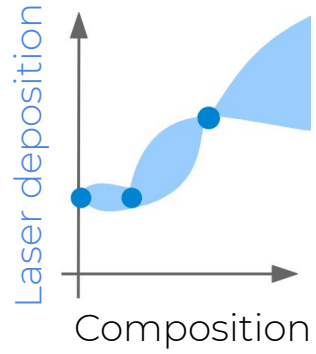


Welding

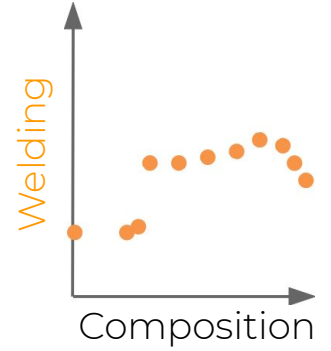
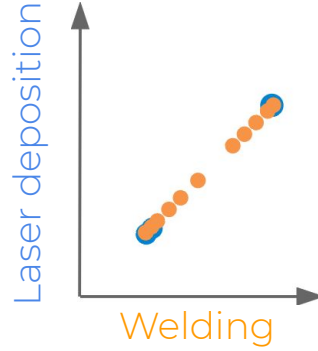
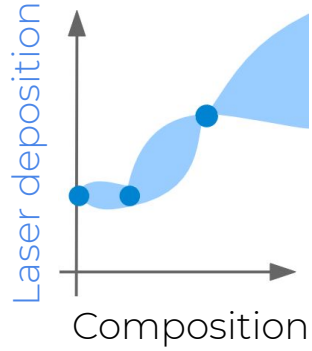
# Lack of data for laser deposition



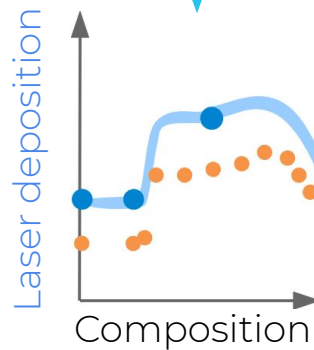
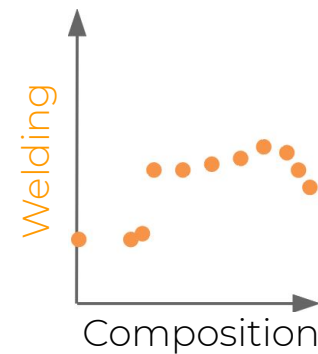
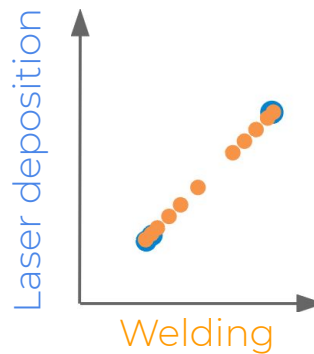
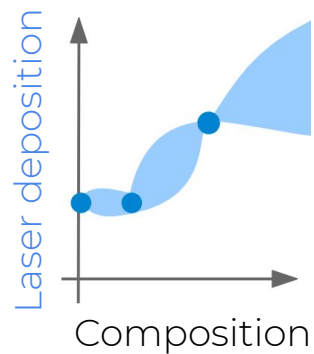
# Large amount of welding data



# Simple welding-deposition relationship



# Welding data guides extrapolation



# Targets for direct laser deposition alloy

Elemental cost	< 25 \$kg <sup>-1</sup>
Density	< 8500 kgm <sup>-3</sup>
$\gamma'$ content	< 25 wt%
Oxidation resistance	< 0.3 mgcm <sup>-2</sup>
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
$\gamma'$ solvus	> 1000 °C
Thermal resistance	> 0.04 K $\Omega^{-1}$ m <sup>-3</sup>
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 <sup>5</sup> cycles

# Composition of alloy for direct laser deposition

Cr 19%



Co 4%



Mo 4.9%



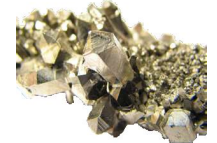
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



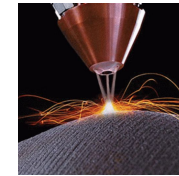
B 0.01%



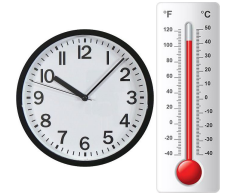
Ni balance



Exposure 0.8

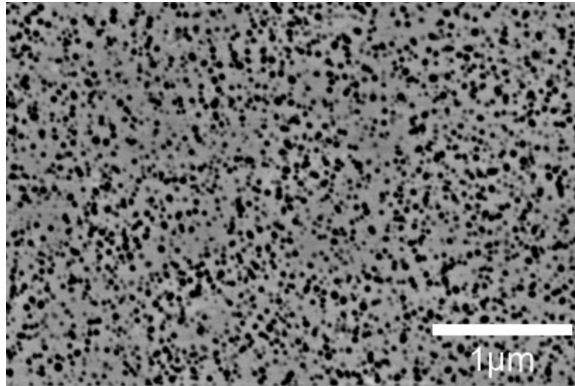


T<sub>HT</sub> 1230°C

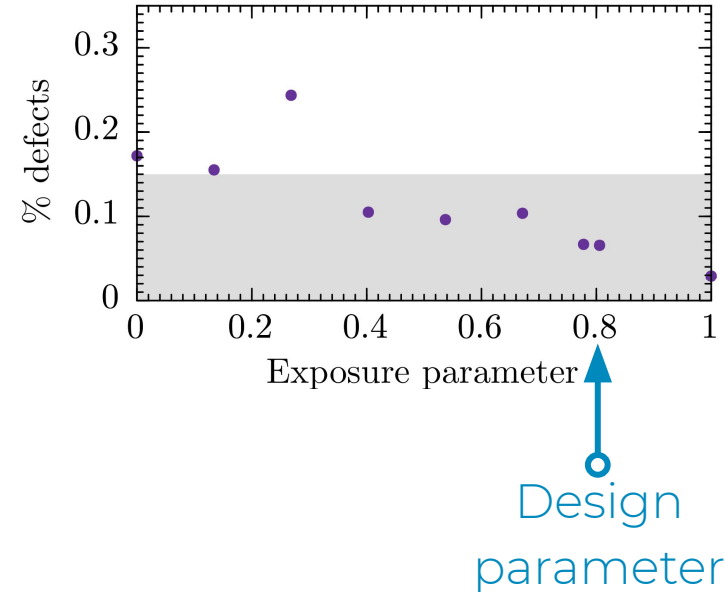
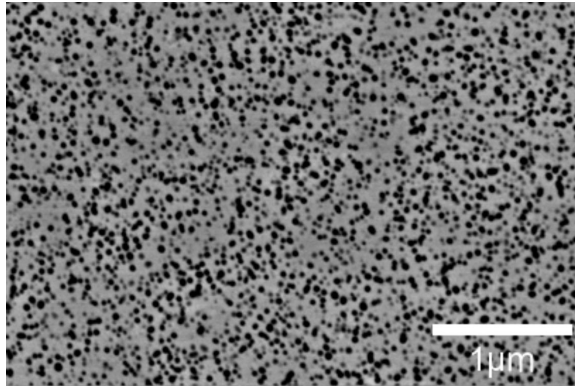




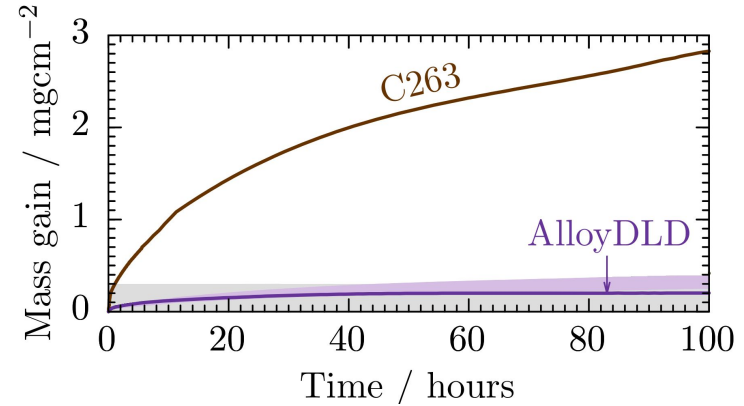
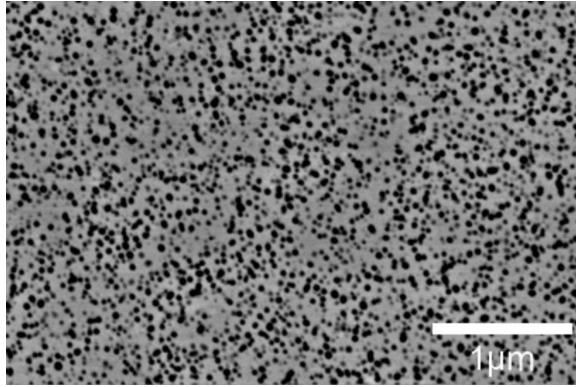
# Experimental validation: microstructure



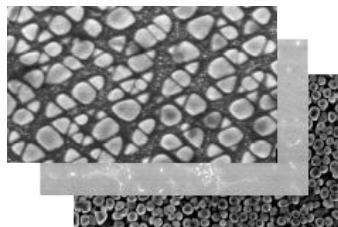
# Experimental validation: defects



# Experimental validation: oxidation resistance



# Further materials and drug design



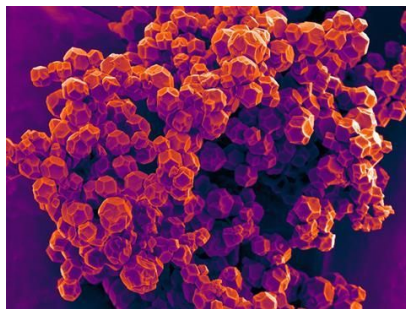
Nickel & moly alloys



Batteries



Steels for welding



Metal-organic framework

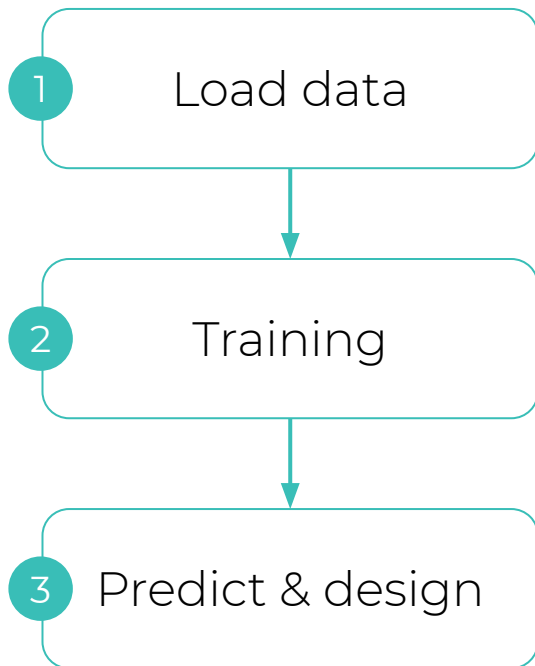


Concrete



Drug design

# Future opportunities: Integrated software



### Predicting properties of steel

We demonstrate a neural network that predicts the physical properties of steels based on the composition and heat treatment. The neural network model was trained from a library of experimental data from 1000 alloys.


In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

Click [here](#) to use this technology to optimize the yield stress, ultimate tensile strength, and elongation the steel.

This same technology was used to understand nickel alloys where the composition covered 20 elements, 5 heat treatment parameters, and predicted 11 material properties. Click here to read more about this study.

Click here to optimize a composition for given targets

Set inputs		
Iron (Fe)	<input type="text" value="100"/>	remain %
Carbon (C)	<input type="text" value="0"/>	0 to 0.43 %
Manganese (Mn)	<input type="text" value="0"/>	0 to 3.0 %
Silicon (Si)	<input type="text" value="0"/>	0 to 4.75 %
Chromium (Cr)	<input type="text" value="0"/>	0 to 17.5 %
Nickel (Ni)	<input type="text" value="0"/>	0 to 21.0 %
Molybdenum (Mo)	<input type="text" value="0"/>	0 to 9.67 %
Vanadium (V)	<input type="text" value="0"/>	0 to 4.32 %

 PREDICT

Predictions	
Yield Stress (MPa)	1605 ± 46
Ultimate Tensile Strength (MPa)	1200 ± 67
Elongation (%)	9 ± 2

# 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

Contact	<a href="mailto:gareth@intellegens.ai">gareth@intellegens.ai</a>
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Demo	<a href="https://app.intellegens.ai/steel_optimise">https://app.intellegens.ai/steel_optimise</a>
Papers	<a href="https://www.intellegens.ai/paper.html">https://www.intellegens.ai/paper.html</a>