Intellegens

Probabilistic neural network identification of an alloy for direct laser deposition

Alchemite™ optimized design process

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

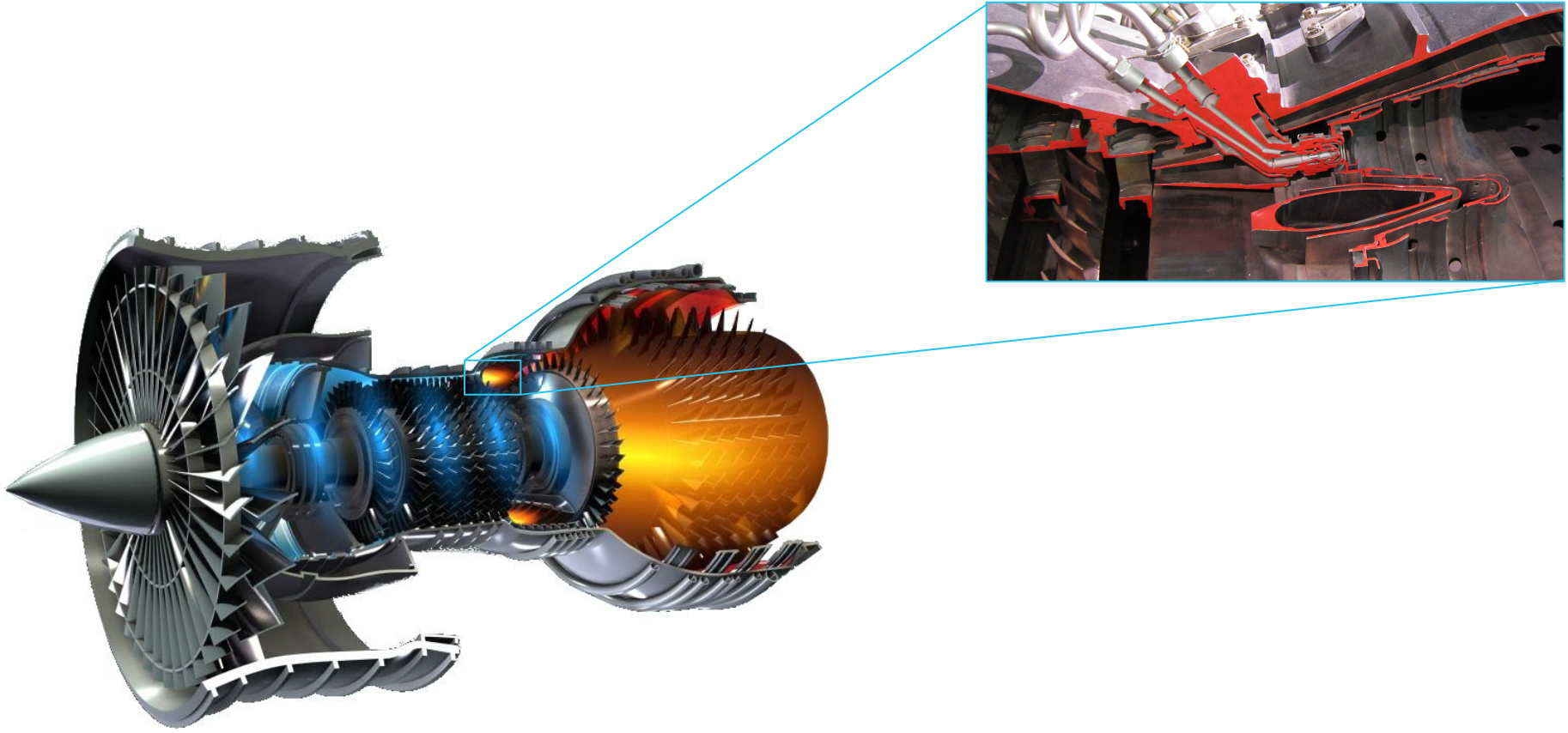Alchemite™ predicts from all available sparse data

Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities
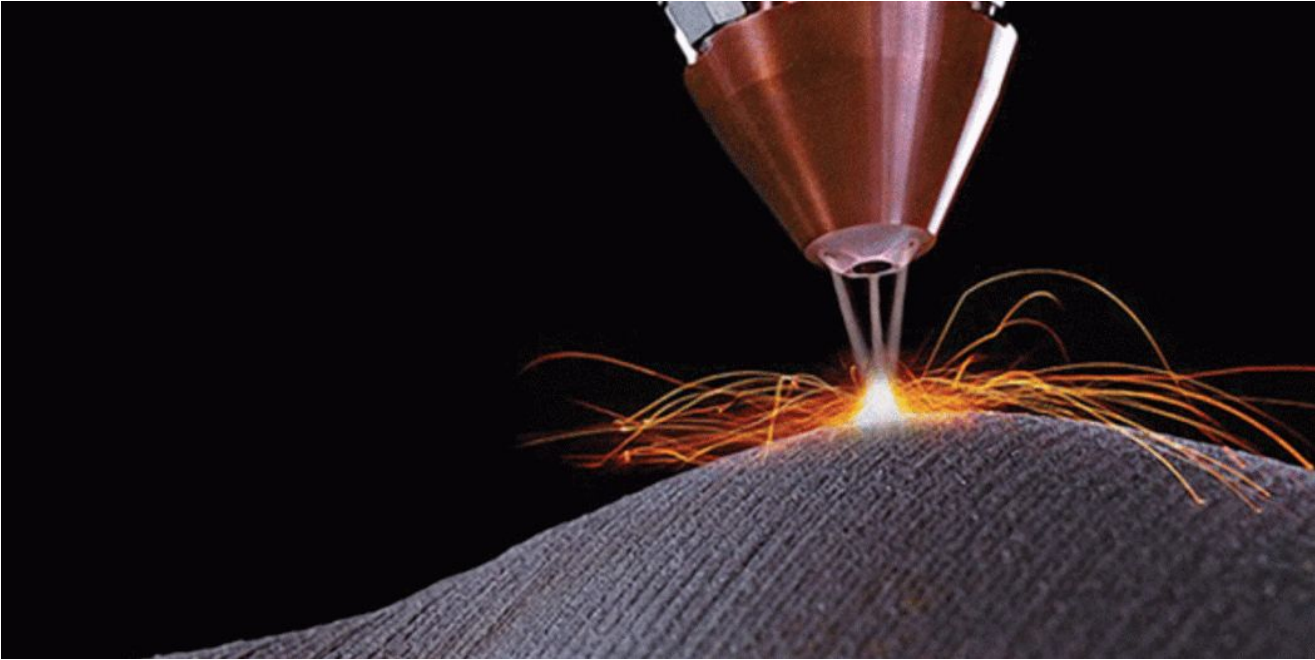
Accelerate discovery and validation to 1 year
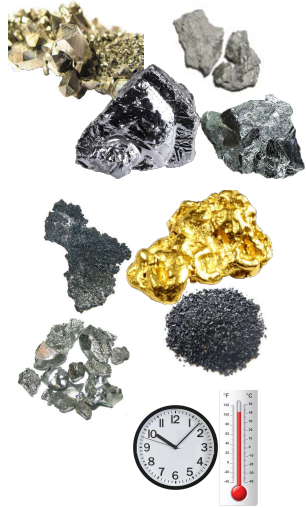
Case study: alloy for direct laser deposition
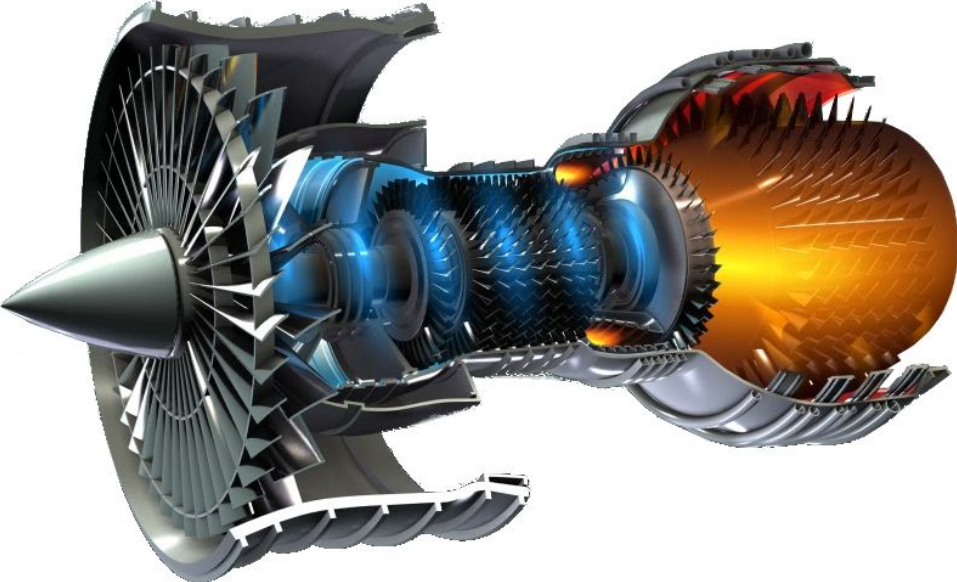
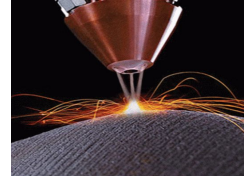# Case study: additive manufacturing

Additive manufacturing requires new alloys

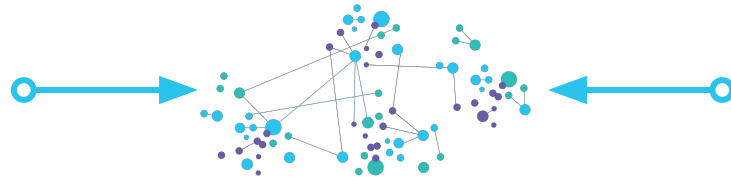# Machine learning
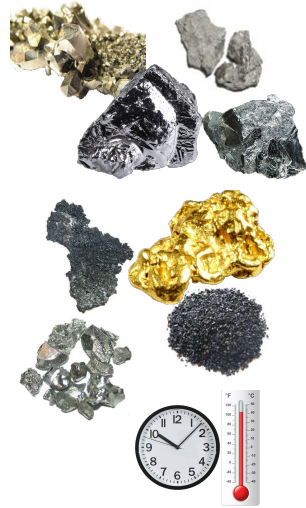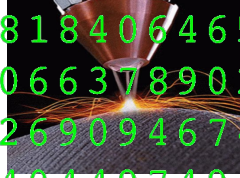
Processability

Fatigue life

Cost

Machine learning

Processability
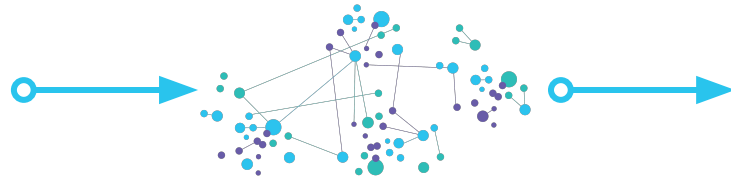
Fatigue life

Cost

Machine learning
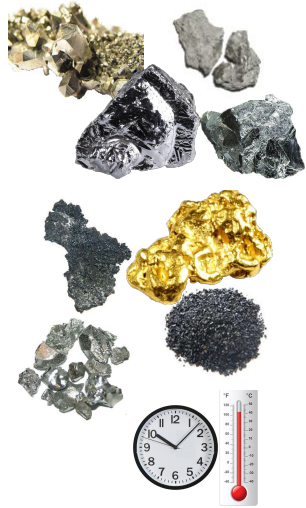
Processability
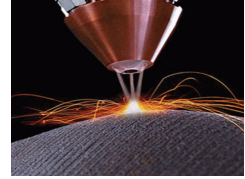
Fatigue life

Cost

Case study: alloy for direct laser deposition
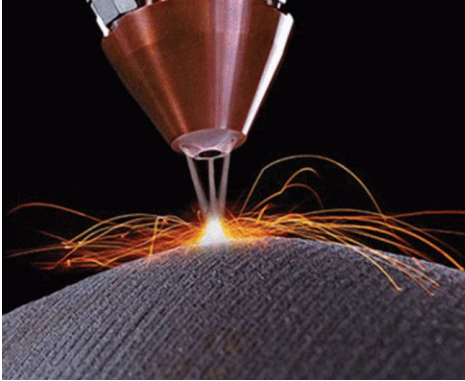
Direct laser deposition is similar to welding
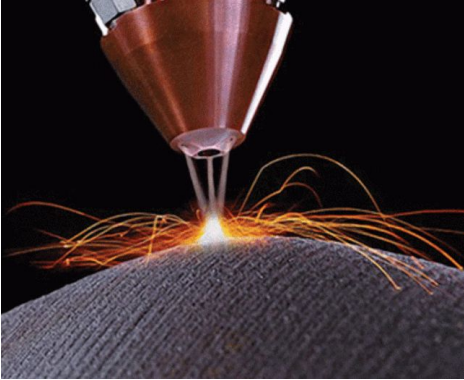
Direct laser
deposition

Welding

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°C
Thermal resistance	> 0.04 KΩ^{-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%
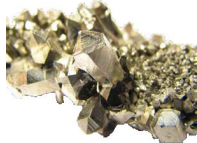
Al 2.9%

C 0.04%

B 0.01%

Ni balance

Exposure 0.8
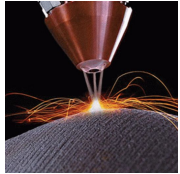
T_{HT} 1230°C

Experimental validation: microstructure
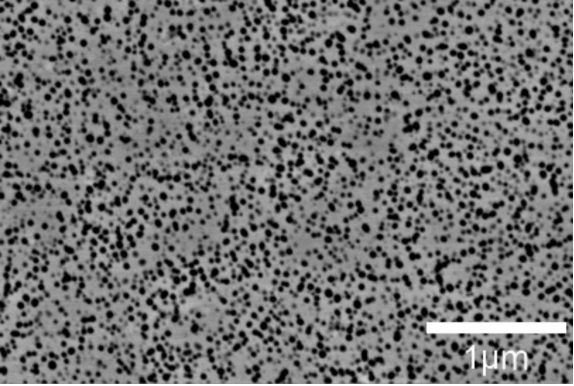
Experimental validation: defects

Design
parameter

Materials & Design 168, 107644 (2019)
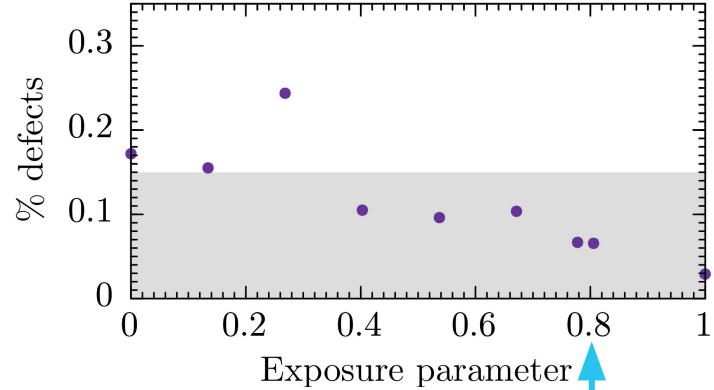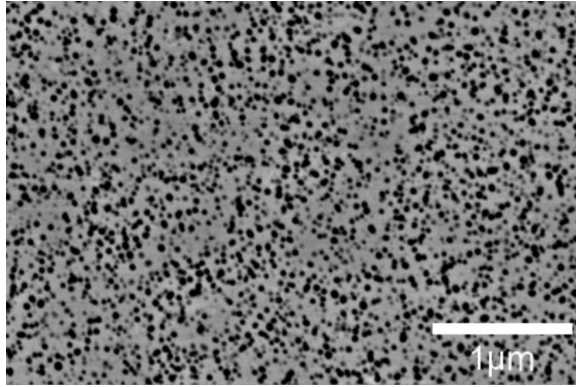
Experimental validation: oxidation resistance
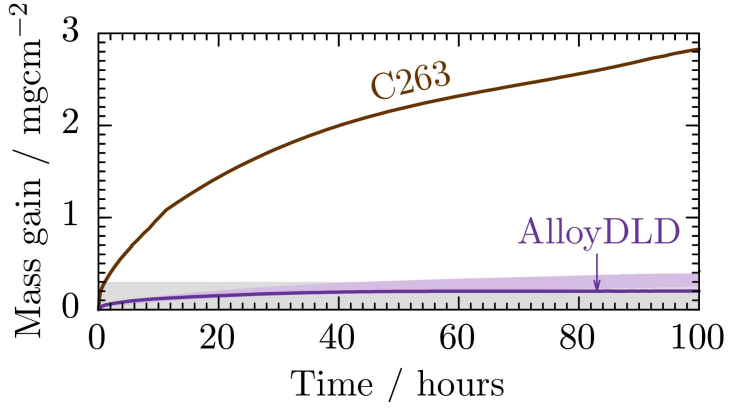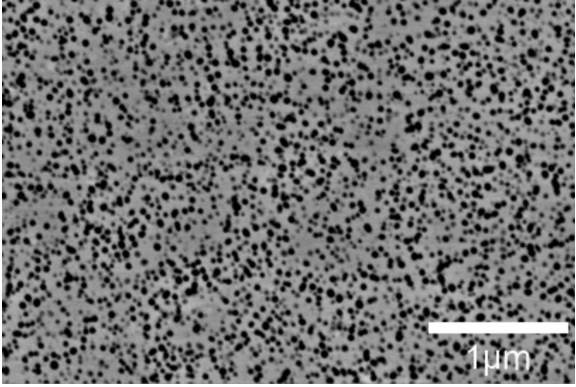
Further materials and drug design
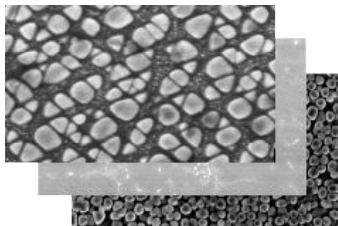
Nickel & moly alloys

Batteries

Steels for welding

Metal-organic framework

Concrete

Drug design

Future opportunities: Integrated software

1 Load data

2 Training

3 Predict & design

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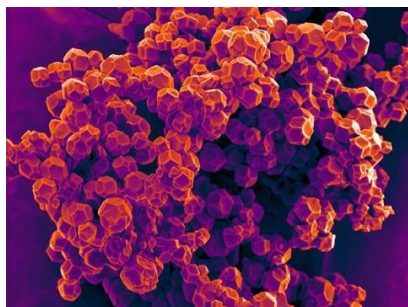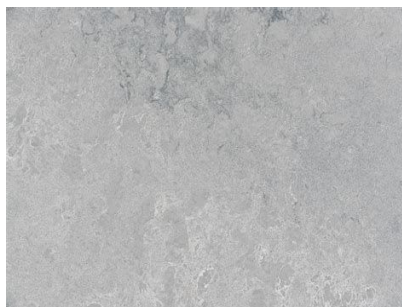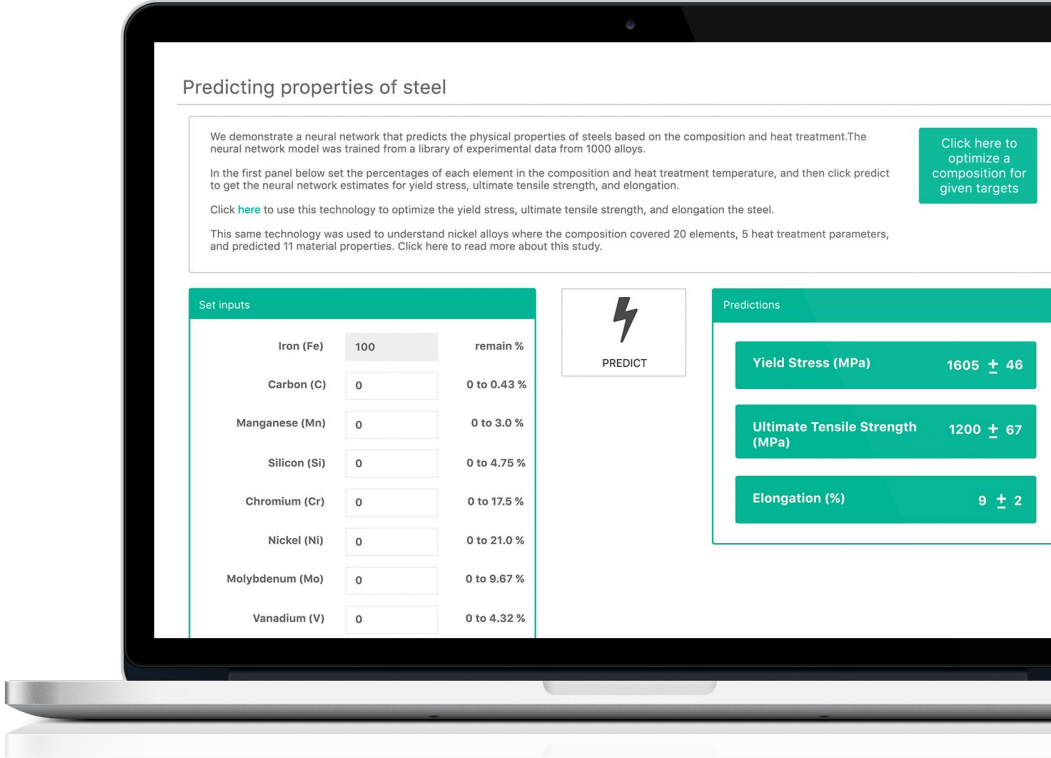
In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

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)	100	remain %
Carbon (C)	0	0 to 0.43 %
Manganese (Mn)	0	0 to 3.0 %
Silicon (Si)	0	0 to 4.75 %
Chromium (Cr)	0	0 to 17.5 %
Nickel (Ni)	0	0 to 21.0 %
Molybdenum (Mo)	0	0 to 9.67 %
Vanadium (V)	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 additive manufacture, other materials, and drugs

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Website   https://intellegens.ai
Demo   https://app.intellegens.ai/steel_optimise
Papers   https://www.intellegens.ai/paper.html