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

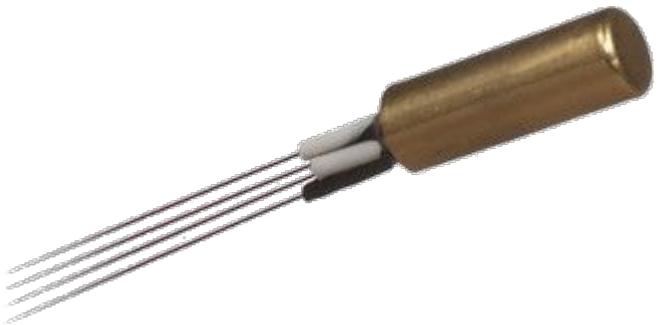
Optimized design process

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



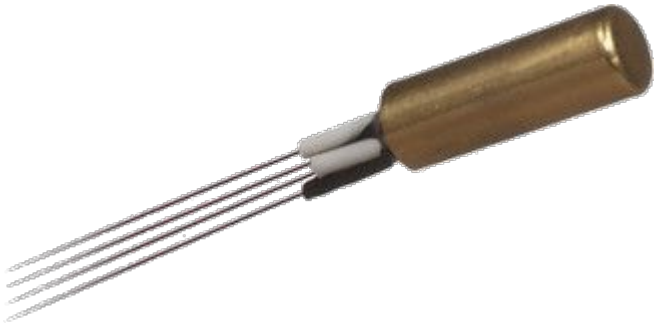
Case study: quantum material for thermometry

90% of the cost of a thermometer is for calibration

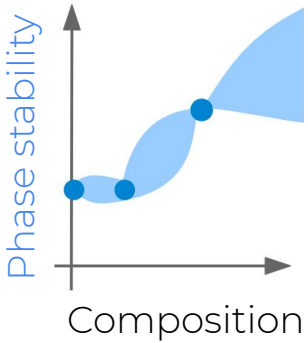
Require a simple resistance-temperature relationship over a wide temperature range

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

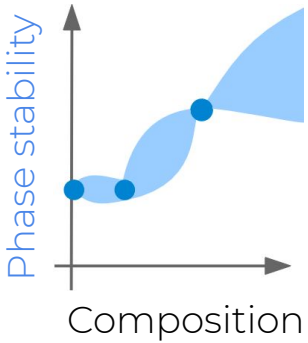
Thermometer must be stable

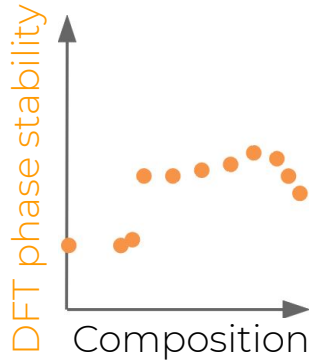


Lack of experimental data

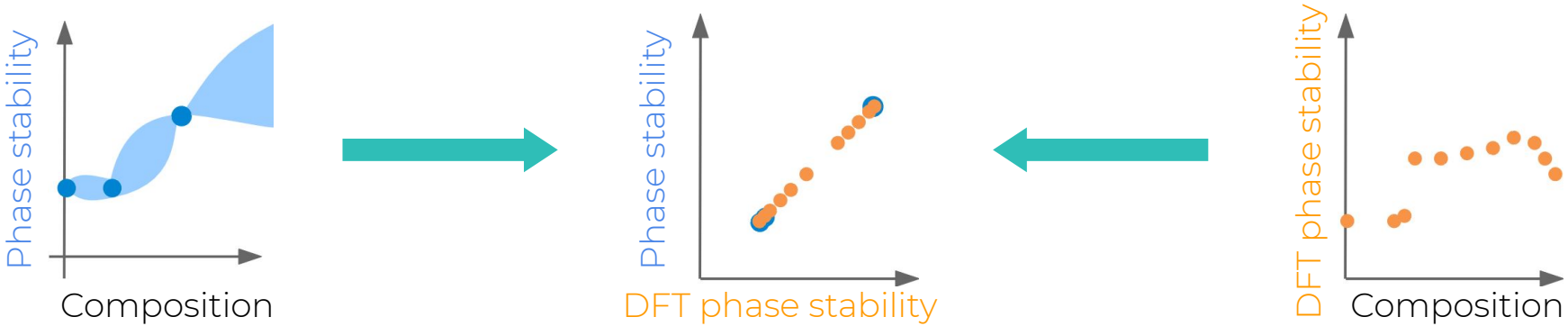


Large amount of computational data

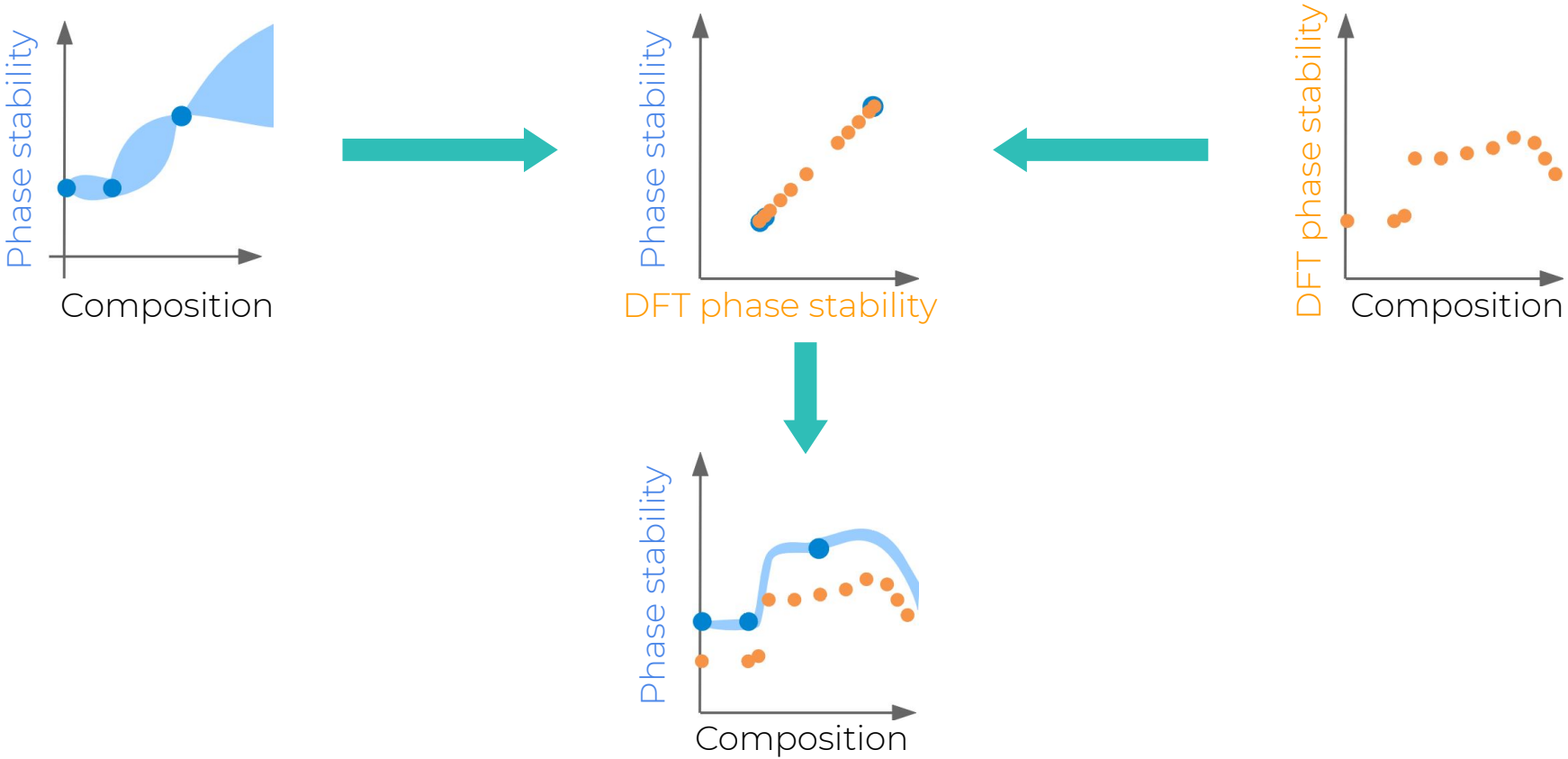




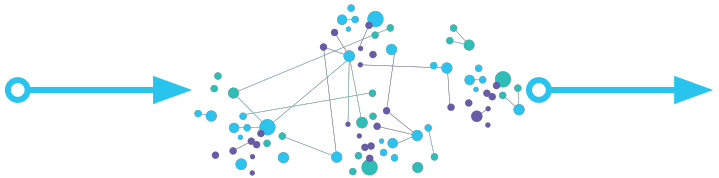
Simple experimental-computational relationship



Computational data guides extrapolation

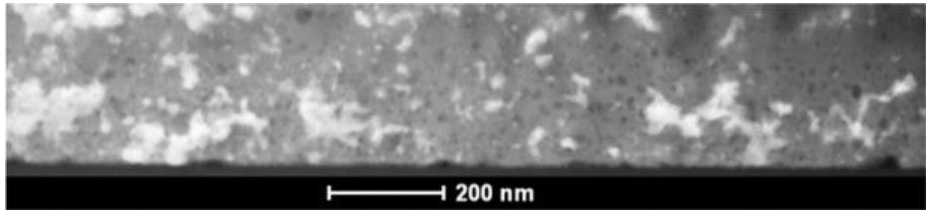


Alchemite machine learning



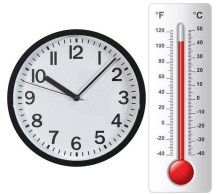
Temperature range
Sensitivity
Stability
Cost
Robust
Resistance
Contacts

Experimental validation



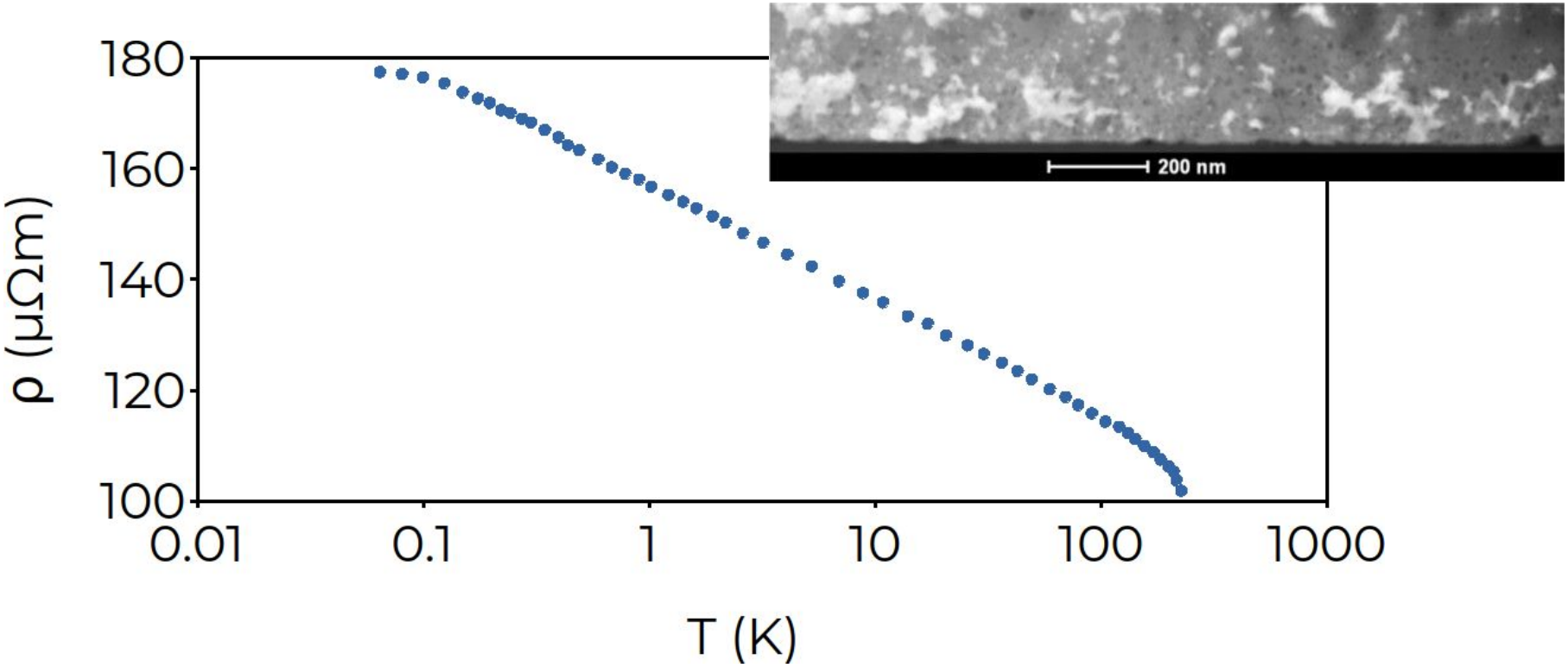
Ge 89%

Au 11%

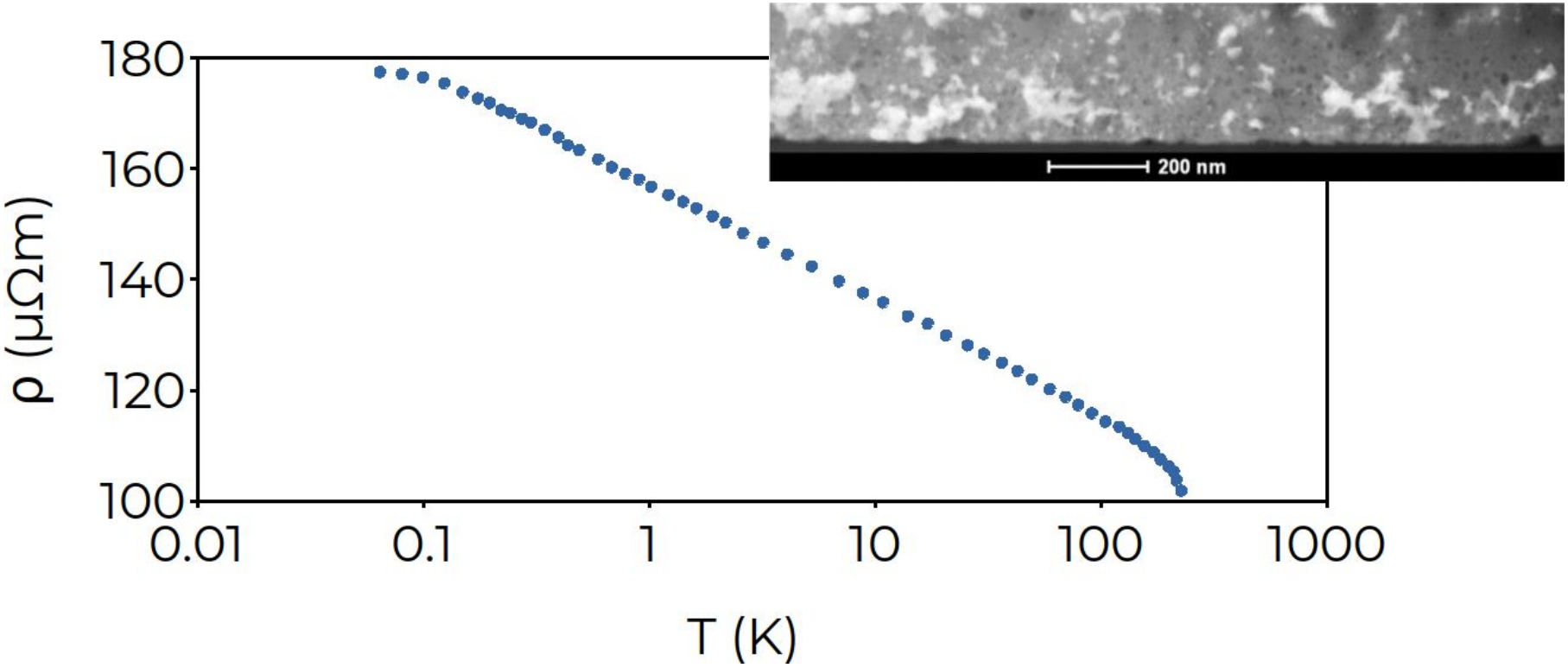


Quench

Experimental validation

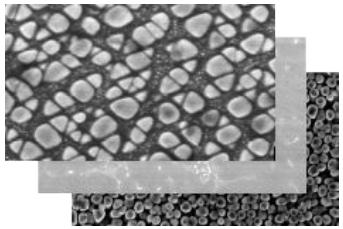


Experimental validation



Measurements stable over 25 cycles and 6 months

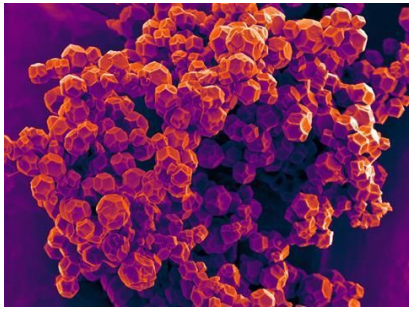
Further materials and drug design



Nickel & moly alloys

Batteries

Steels for welding



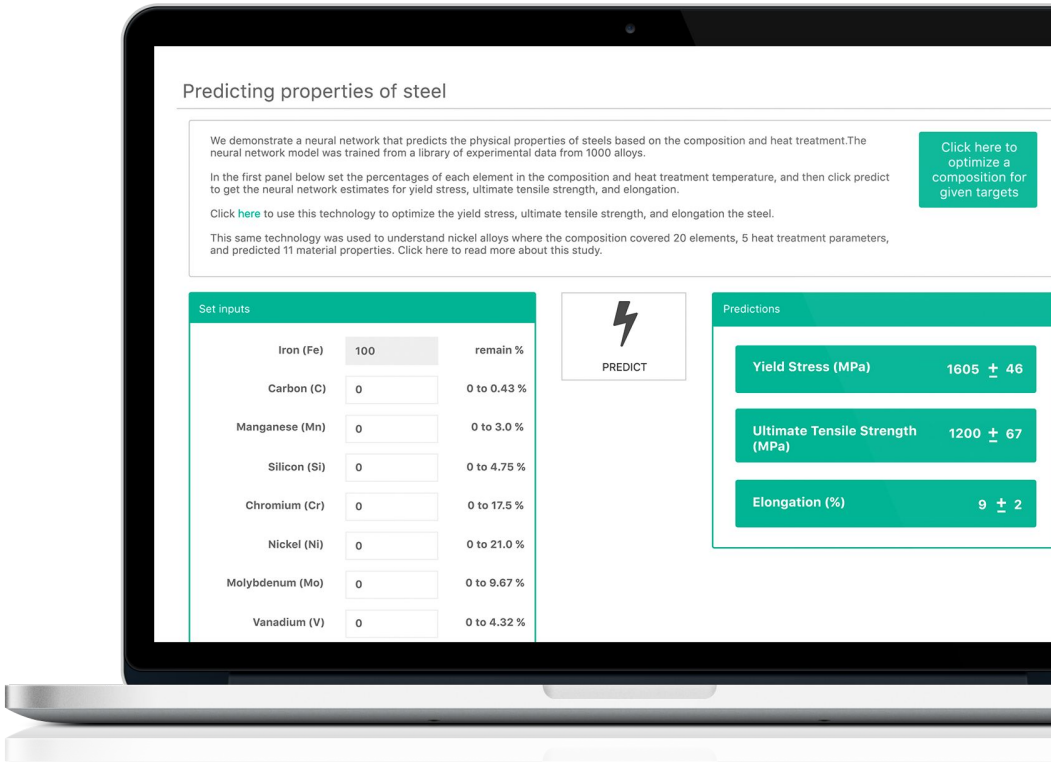
Metal-organic framework

Concrete

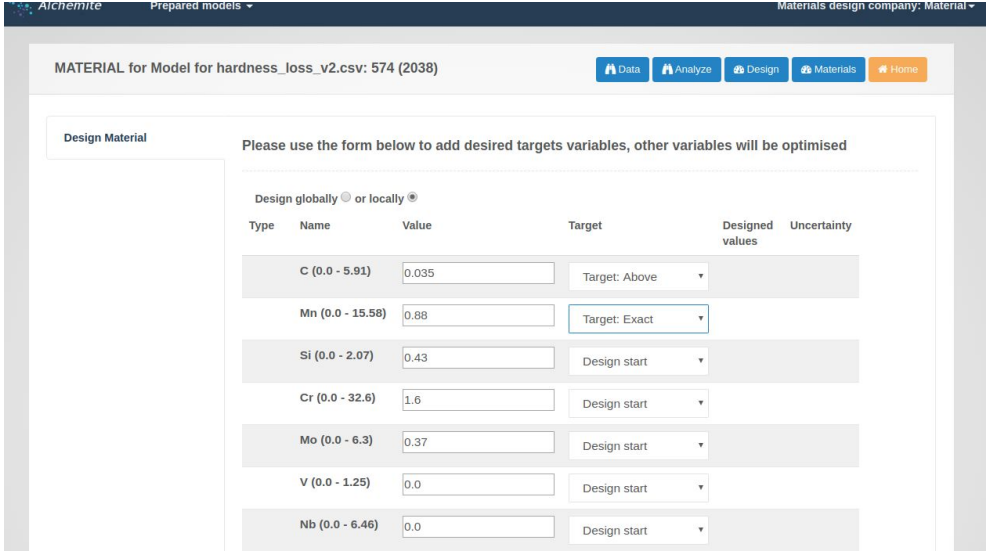
Drug design

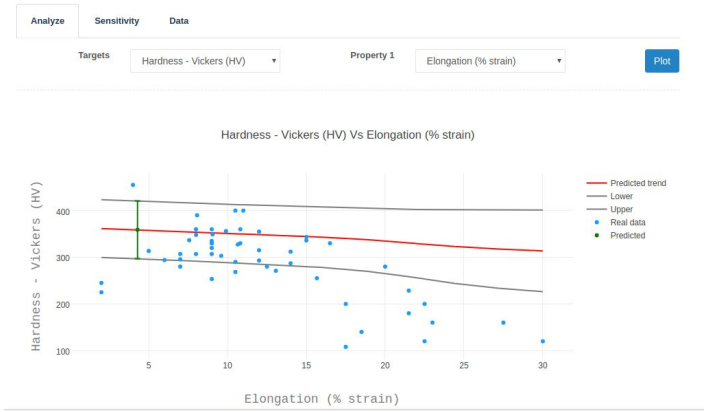
Future opportunities: Integrated software

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

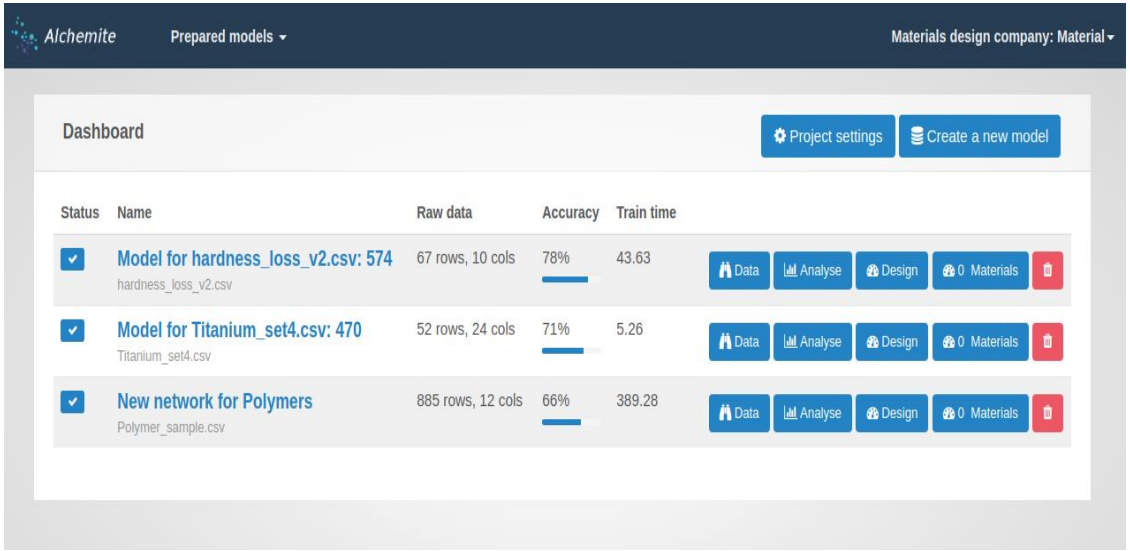


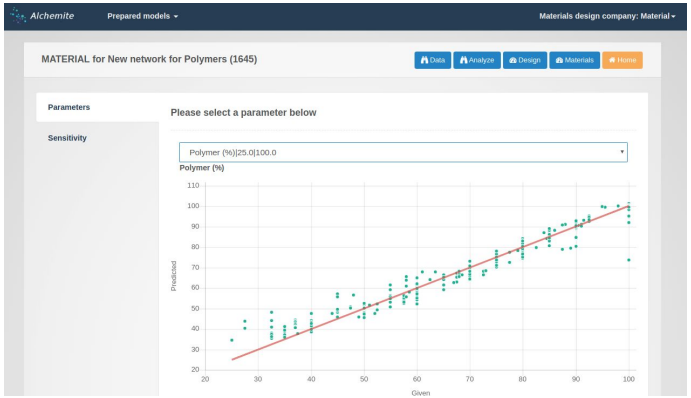
Design, analyse, and share new materials

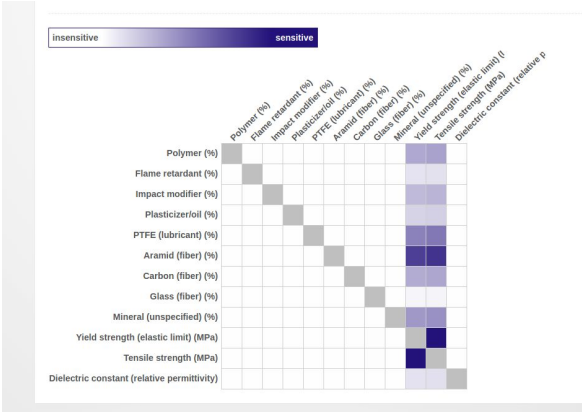




Manage models and analyse workflow







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
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