



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

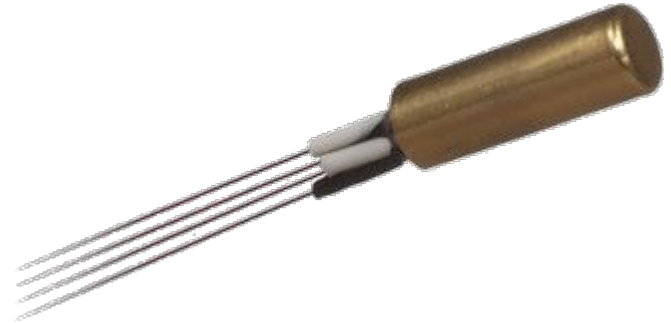
Optimized design process

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**



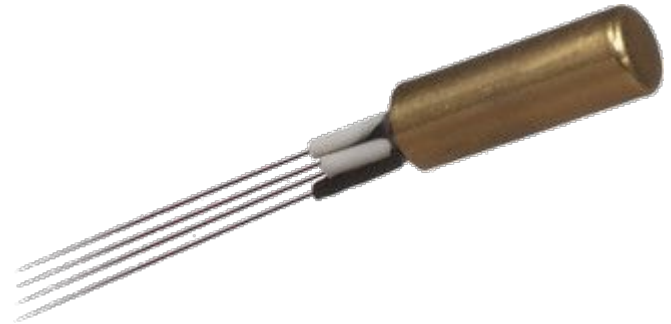
Case study: quantum material for thermometry

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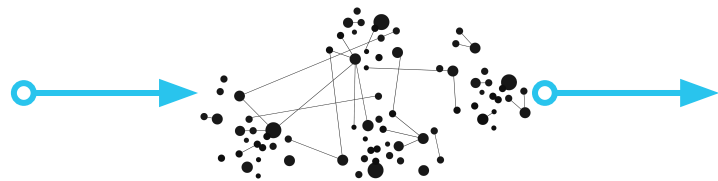
Require a simple resistance-temperature relationship over a **wide temperature range**

Want **constant sensitivity** $T/R \frac{dR}{dT}$ with temperature

Thermometer must be **stable**



Alchemite machine learning



Temp range
Sensitivity
Stability
Cost
Robust
Resistance
Contacts

Alchemite machine learning



293928764790904
 021364010360202
 686584970508185
 703818406465007
 501066378902902
 715269094674449
 011404497494802
 488685276110992
 207332721994995
 976579342243418
 394046703960392
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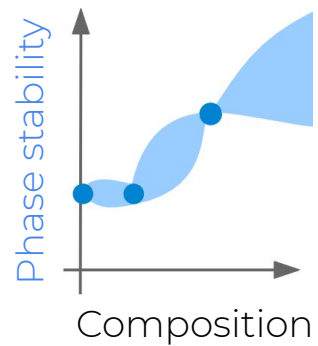
Temp range
 Sensitivity
 Stability
 Cost
 Robust
 Resistance
 Contacts

Alchemite machine learning

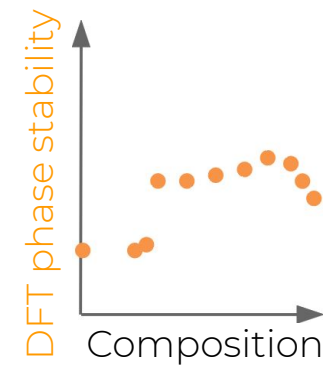
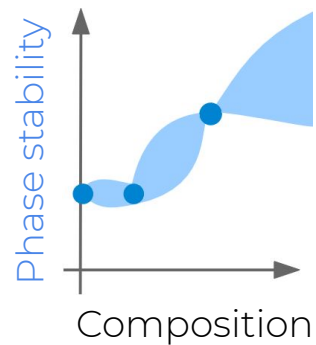


Temp range
Sensitivity
Stability
Cost
Robust
Resistance
Contacts

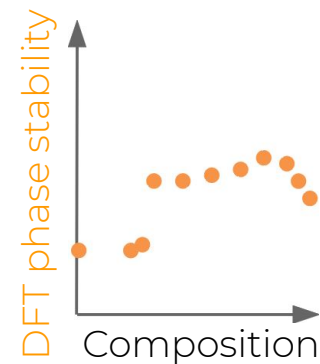
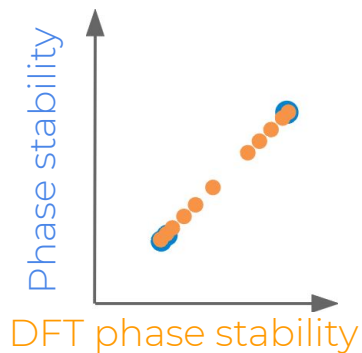
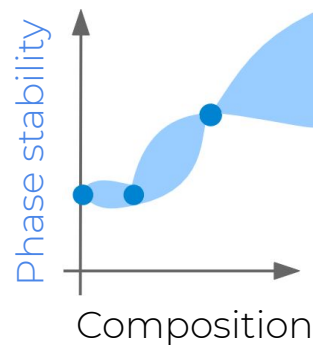
Lack of experimental data



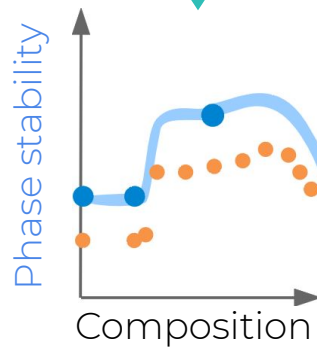
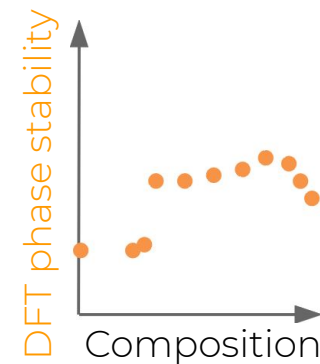
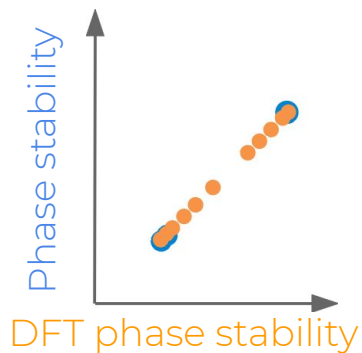
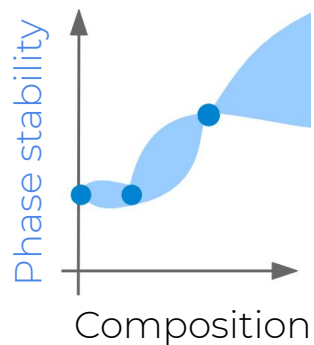
Large amount of computational data



Simple experimental-computational relationship

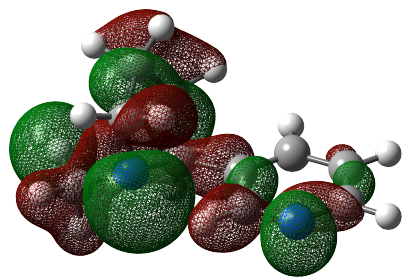


Computational data guides extrapolation



Flowchart to train

Computer
simulation

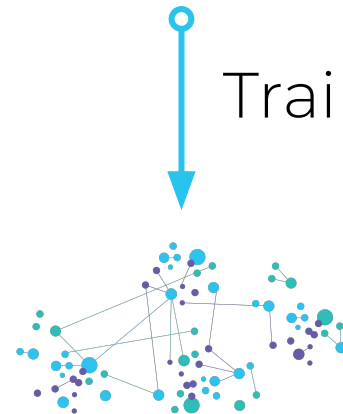


Properties



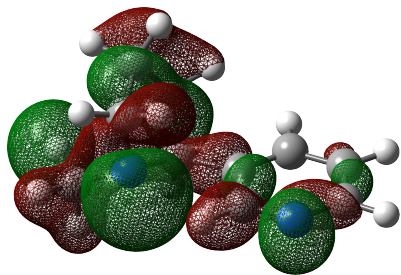
```
10001010  
00111010  
01011010
```

Train



Reinforcement learning

Computer
simulation

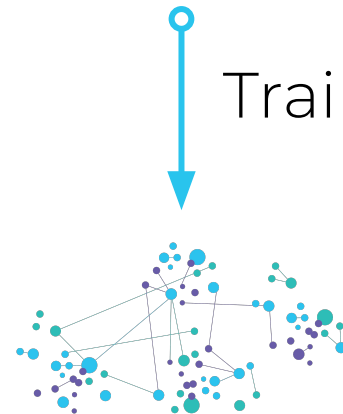


Properties



```
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00111010  
01011010
```

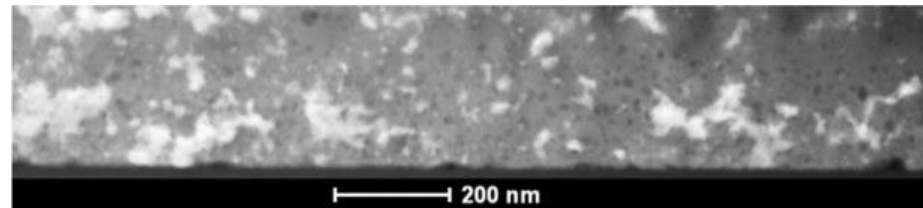
Train



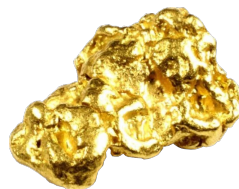
Request new result



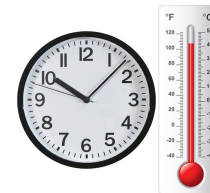
Experimental validation



Ge 89%

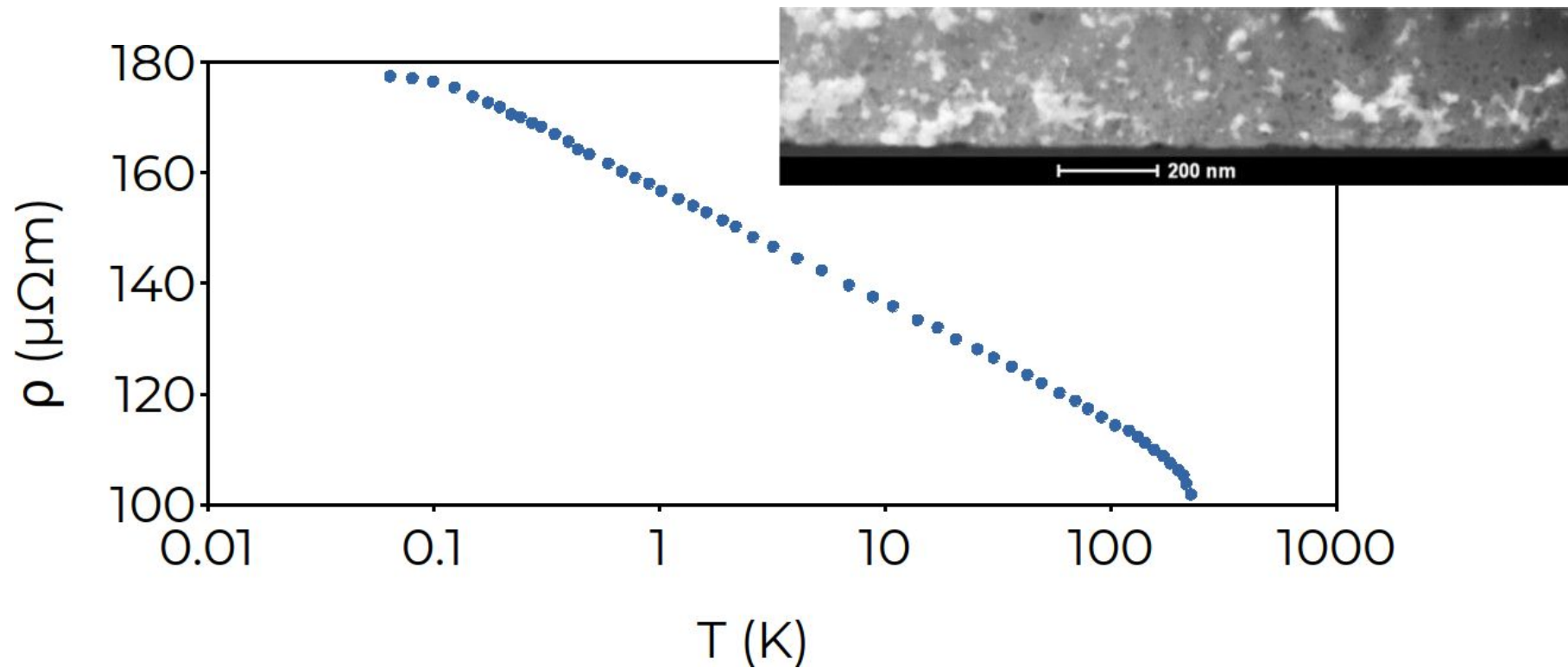


Au 11%

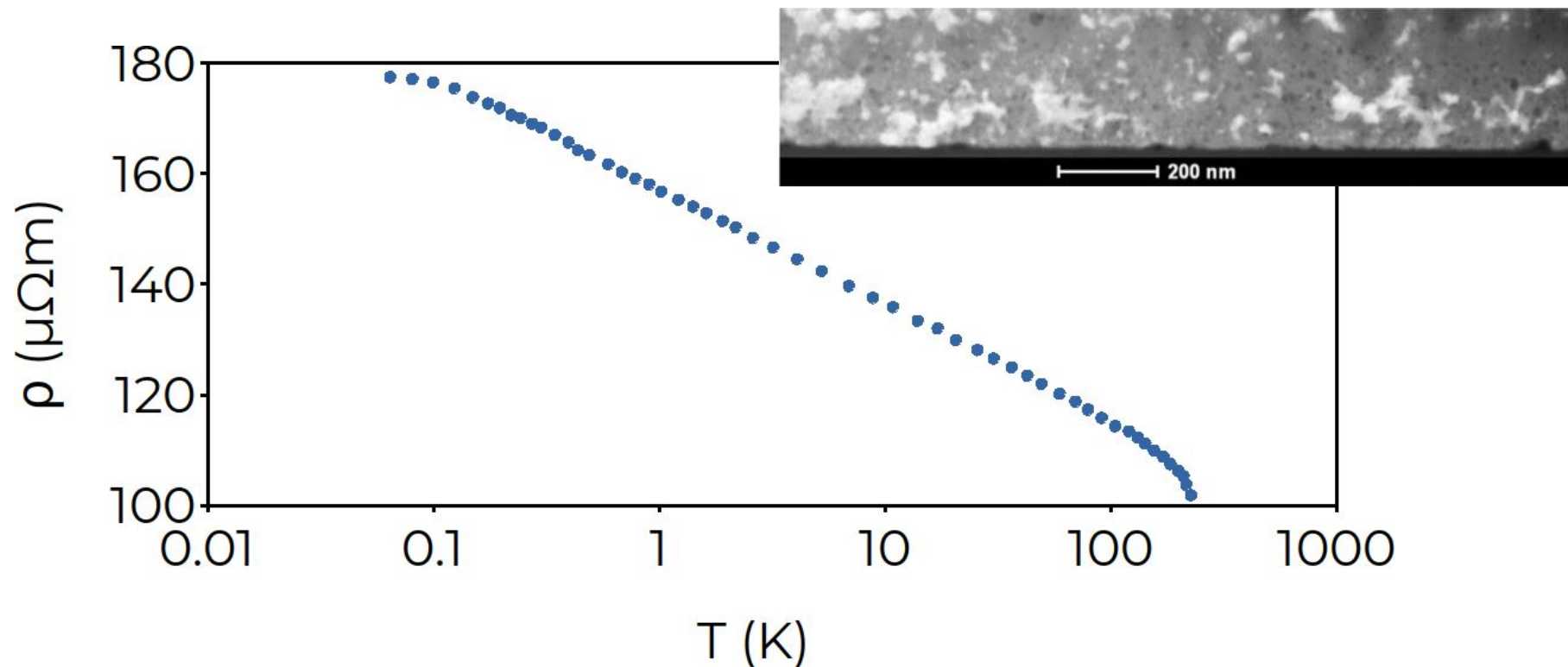


Quench

Experimental validation

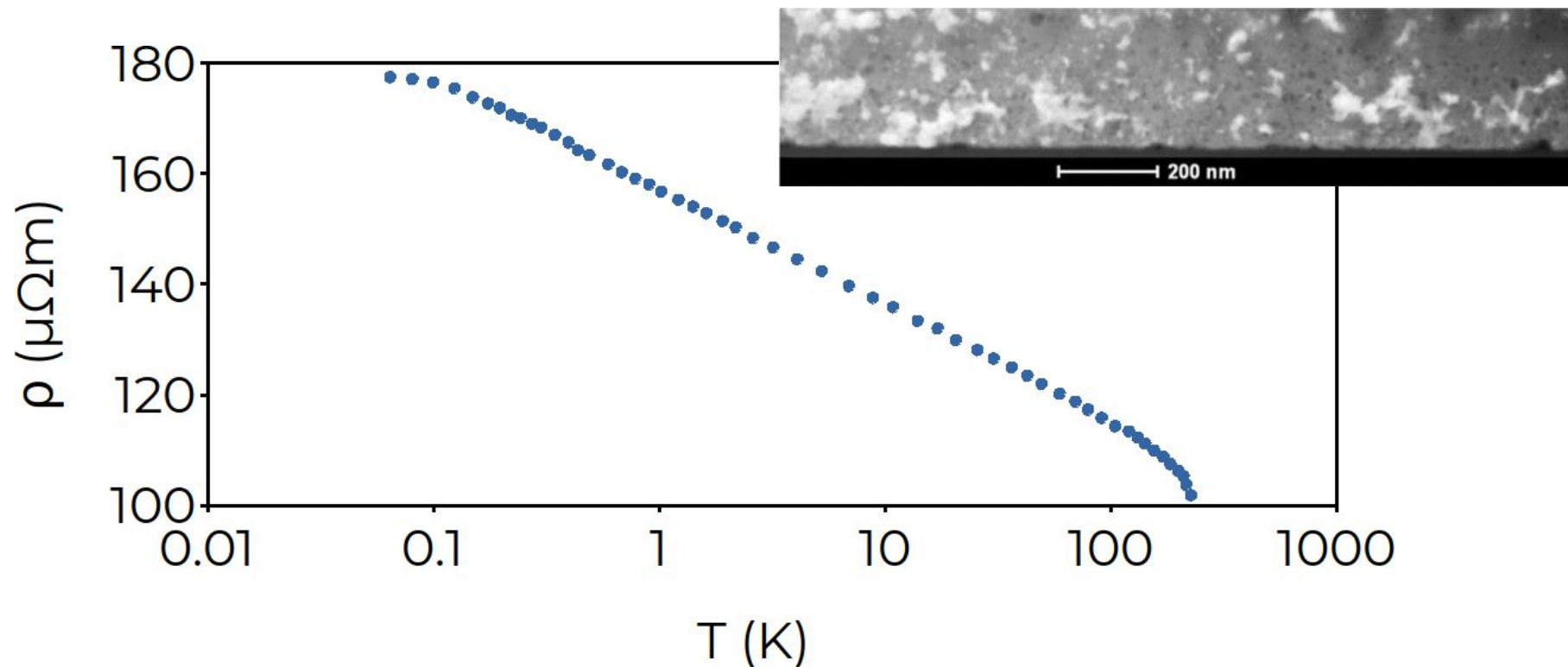


Experimental validation



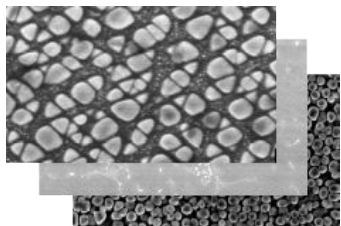
Measurements **stable** over 25 cycles and 6 months

Experimental validation



Physical Review Applied 12, 034024 (2019)

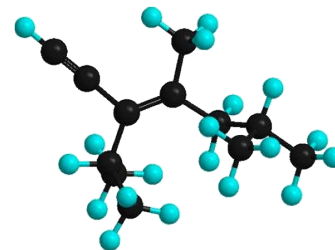
Further design of industrial formulations



Nickel & moly alloys



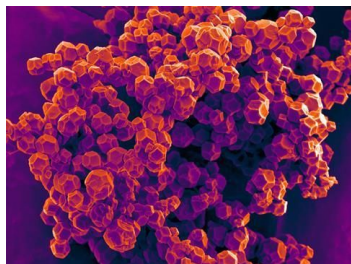
Batteries



Lubricants



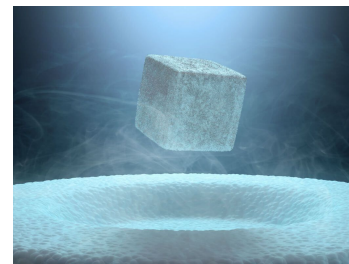
Steels for welding



Metal-organic framework



Concrete



Superconductor

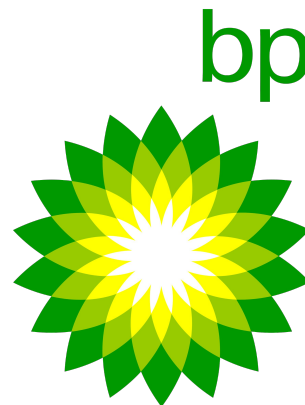


Drug design

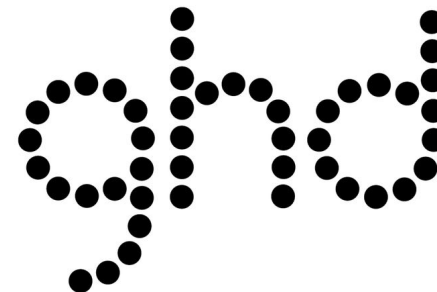
Who



Rolls-Royce®



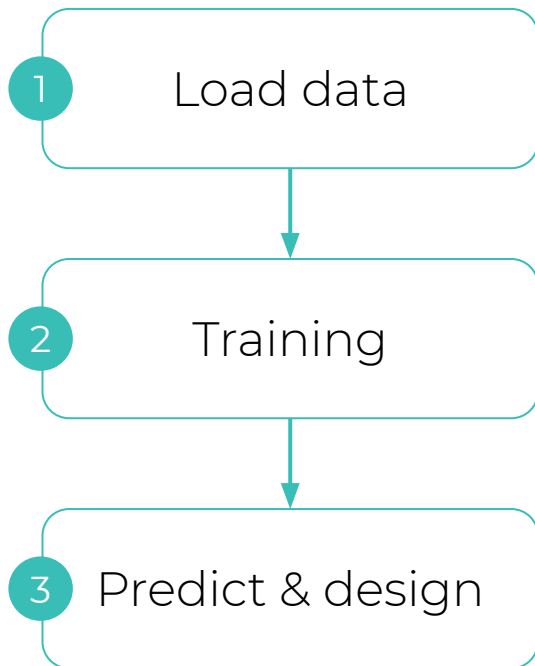
SKANSKA



GRANTA



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

Design, analyse, and share new materials

Alchemite Prepared models Materials design company: Material

MATERIAL for Model for hardness_loss_v2.csv: 574 (2038)

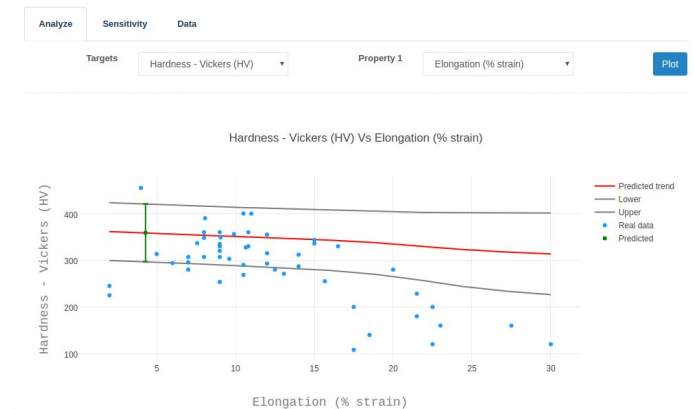
Data Analyze Design Materials Home

Design Material

Please use the form below to add desired targets variables, other variables will be optimised

Design globally or locally

Type	Name	Value	Target	Designed values	Uncertainty
	C (0.0 - 5.91)	<input type="text" value="0.035"/>	Target: Above		
	Mn (0.0 - 15.58)	<input type="text" value="0.88"/>	Target: Exact		
	Si (0.0 - 2.07)	<input type="text" value="0.43"/>	Design start		
	Cr (0.0 - 32.6)	<input type="text" value="1.6"/>	Design start		
	Mo (0.0 - 6.3)	<input type="text" value="0.37"/>	Design start		
	V (0.0 - 1.25)	<input type="text" value="0.0"/>	Design start		
	Nb (0.0 - 6.46)	<input type="text" value="0.0"/>	Design start		

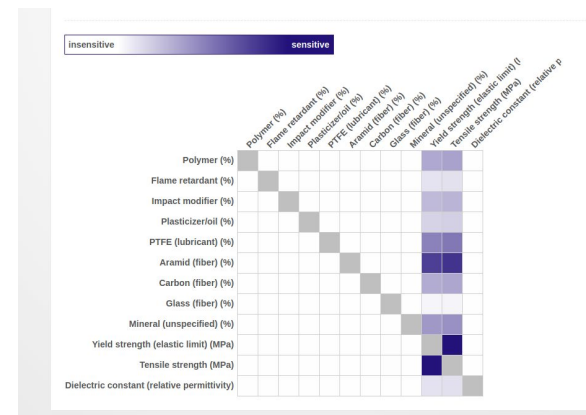
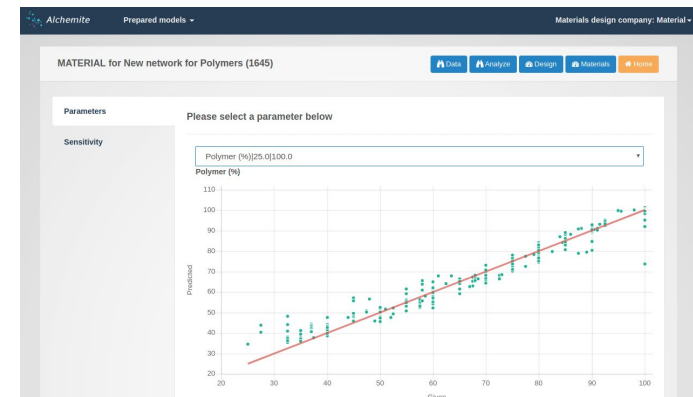


Manage models and analyse workflow

Alchemite Prepared models Materials design company: Material

Dashboard Project settings Create a new model

Status	Name	Raw data	Accuracy	Train time	
✓	Model for hardness_loss_v2.csv: 574 hardness_loss_v2.csv	67 rows, 10 cols	78% <div style="width: 78%;"></div>	43.63	Data Analyse Design Materials ⌵
✓	Model for Titanium_set4.csv: 470 Titanium_set4.csv	52 rows, 24 cols	71% <div style="width: 71%;"></div>	5.26	Data Analyse Design Materials ⌵
✓	New network for Polymers Polymer_sample.csv	885 rows, 12 cols	66% <div style="width: 66%;"></div>	389.28	Data Analyse Design Materials ⌵



Summary of future opportunities of Alchemite™

Alchemite™, a full stack machine learning solution to **merge** sparse computational and experimental data

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

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