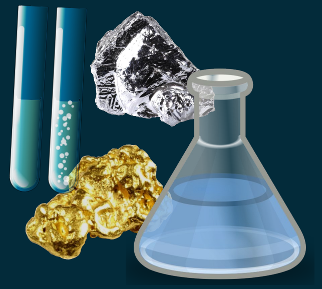
intellegens

DATA - DRIVEN DISCOVERY

Ingredients



Processes

Properties

Strength
Conductivity
Cost
Weight
Environmental impact

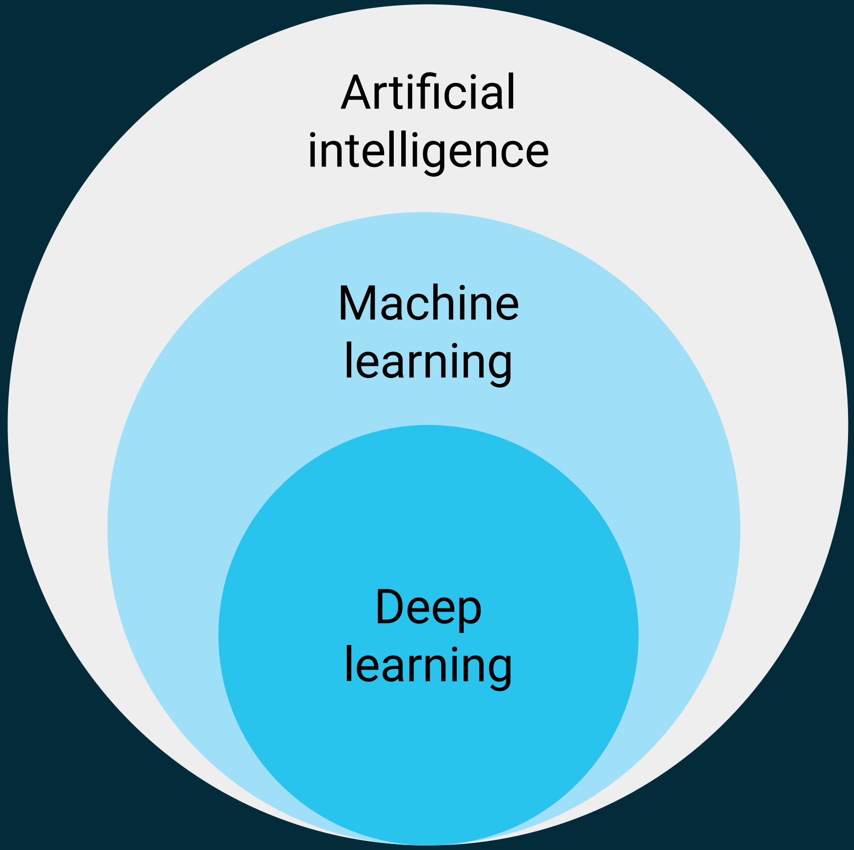
Chemicals, alloys, composites, plastics, batteries, glass, and ceramics

What approach do you currently follow to design materials or chemicals?

What approach do you currently follow to design materials or chemicals?

Trial and improvement
experimental development costs >$10m

Expert driven and subjective
does not always work toward optimal design



Artificial intelligence

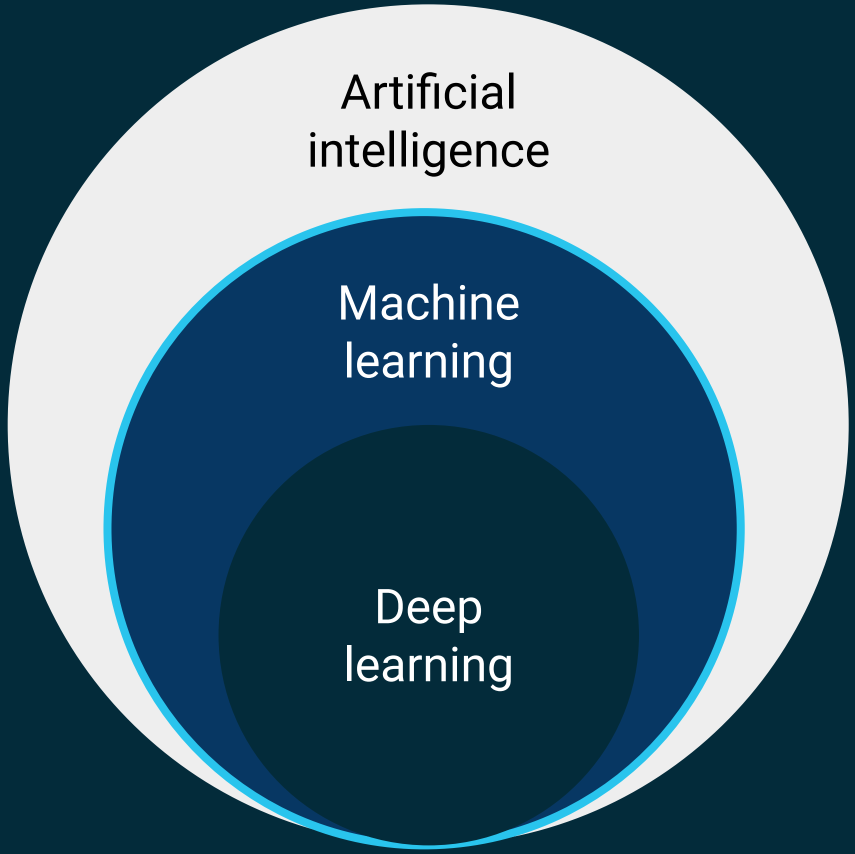
Machines that mimic human behaviour

Machine learning

Subset of artificial intelligence that uses statistical methods to enable machines to improve with experience

Deep learning

Subset of Machine Learning that makes the computation of multi-layer neural network feasible



Artificial intelligence

Machines that mimic human behaviour

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Subset of artificial intelligence that uses statistical methods to enable machines to improve with experience

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Subset of Machine Learning that makes the computation of multi-layer neural network feasible

Machine learning for materials and chemicals design

- **accelerates** research & development processes
- significantly reduces **costs**
- increases **productivity**

Difficulty with contemporary machine learning

Siloed data

Sparse data

Siloed data

Each silo may have different formats and measurements

Model not trained on all available information and data

Sparse data

Experimental data is sparse and noisy and disconnected from your simulation data

Only clean and complete data can be used by contemporary machine learning

Alchemite™

Deep learning for formulation and process optimization

Merge data silos

to exploit all streams of data

Impute missing values

to train from all available data

Reduce costs and accelerate discovery

through high quality predictive and reproducible models

Data

Fill in blanks in sparse data and merge together noisy data sets

Spot errors or potential outliers in your current data

Extract more knowledge from your data

Guide experiments

Use confidence levels to guide where you need to test further

Carry out the experiments that will add the greatest insights

Eliminate the scattergun approach, shorten time to market, and reduce prototype cost

Optimize formulations

Design a formulation based on multiple target requirements

Optimize the formulation of current material whilst maintaining its characteristics

EXAMPLE

For materials design

Historical materials data

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76		149
Steel 2	98.6		0.9			80	170
Steel 3		0.42		1100			179
Steel 4	98.4	0.55	0.8		118	70	241

Contemporary methods do properties separately

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76		~~149~~
Steel 2	~~98.6~~		~~0.9~~			~~80~~	~~170~~
Steel 3		~~0.42~~		~~1100~~			~~179~~
Steel 4	~~98.4~~	~~0.55~~	~~0.8~~		~~118~~	~~70~~	~~241~~

Exploit property-property correlations

TS ~ HBW/2

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76		149
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Alchemite™ trains and predicts all values

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76	**64**±2	149
Steel 2	98.6	**0.37**±0.1	0.9	**892**±17	**90**±5	80	170
Steel 3	**98.8**±0.8	0.42	**0.7**±0.1	1100	**91**±9	77±3	179
Steel 4	98.4	0.55	0.8	**980**±38	118	70	241

Set target material properties

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76	64±2	149
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Steel 3	98.8±0.8	0.42	0.7±0.1	1100	91±9	77±3	179
Steel 4	98.4	0.55	0.8	980±38	118	70	241
Steel 5			**0.8**		**93**	**80**	

Alchemite™ can design materials

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Steel 1	99.1	0.27	0.6	842	76	64±2	149
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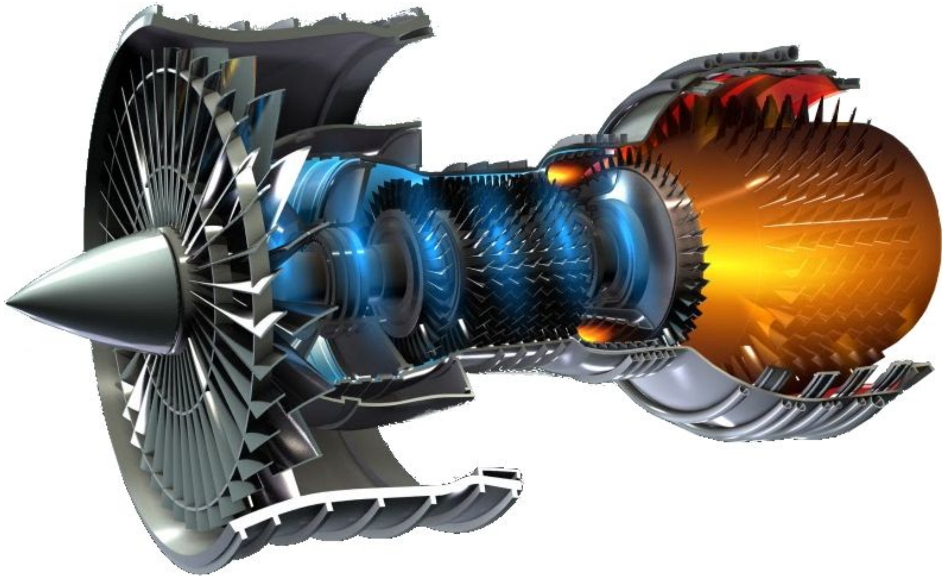
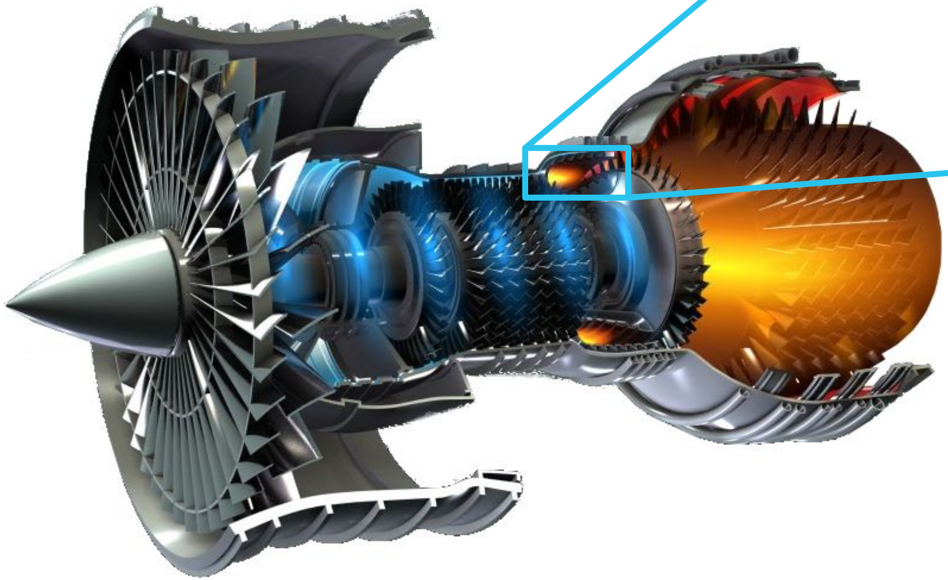
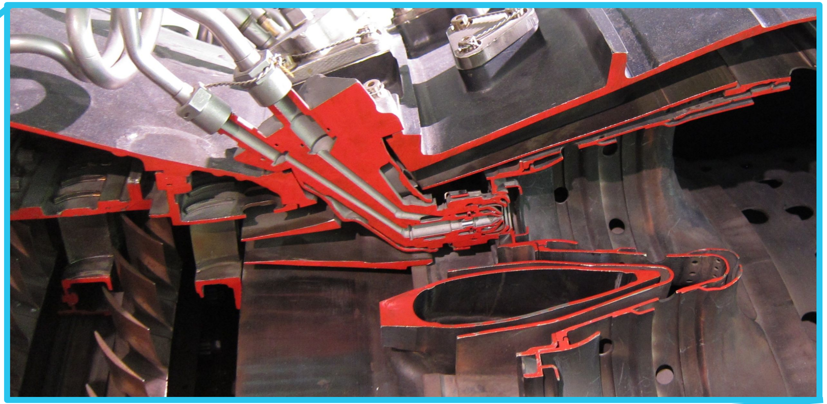
Steel 4	98.4	0.55	0.8	980±38	118	70	241
Steel 5	**98.9±0.3**	**0.49±0.1**	0.8	**990±20**	93	80	**201±12**

Schematic of a jet engine

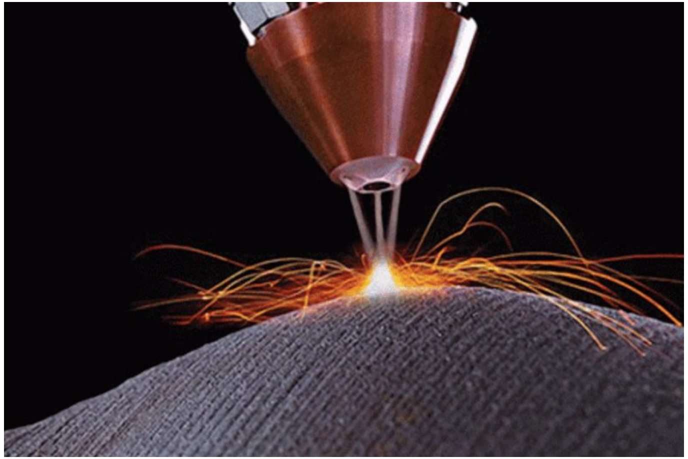


Combustor in a jet engine

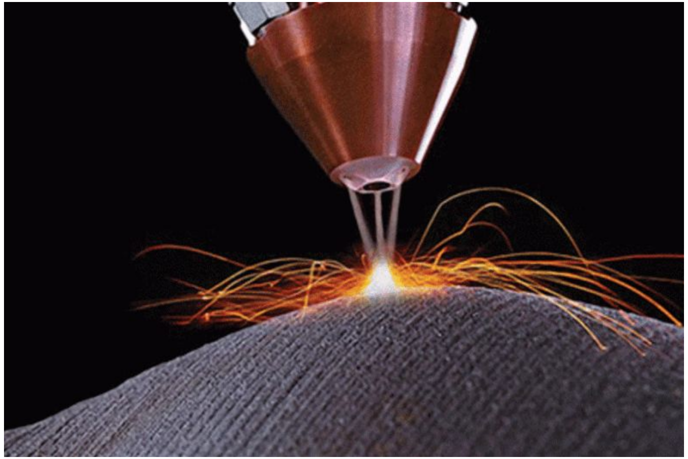




Direct laser deposition requires new alloys



Analogy between direct laser deposition and welding



Laser

Welding

Target properties

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 $K\Omega^{-1}m^{-3}$
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 and processing variables

Cr 19%

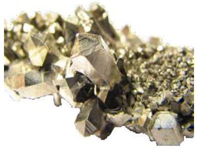
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



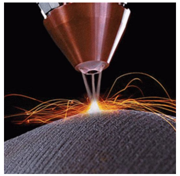
Al 2.9%

C 0.04%

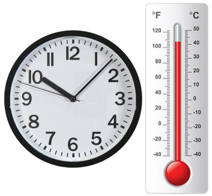
B 0.01%

Ni balance

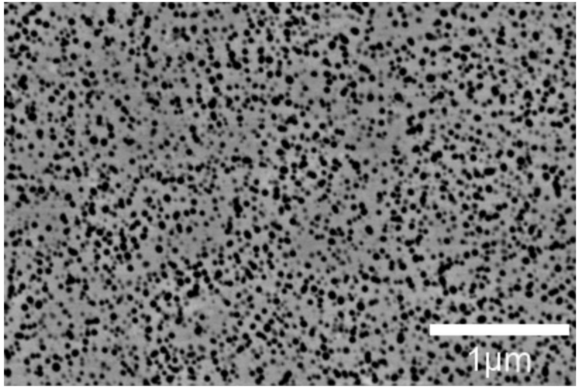
Exposure 0.8



T_{HT} 1230ºC



Experimental validation: microstructure



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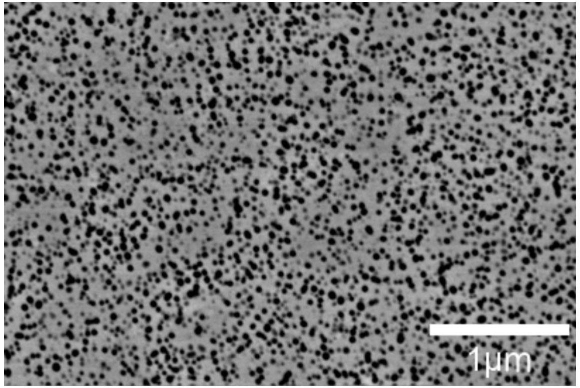
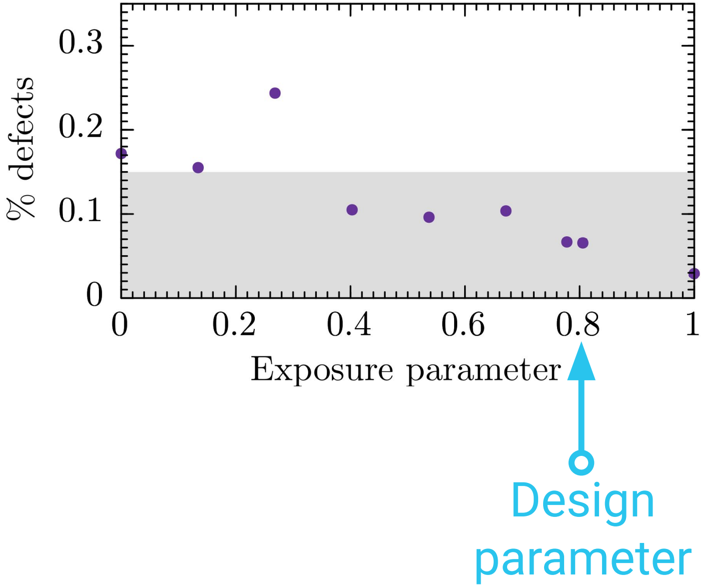
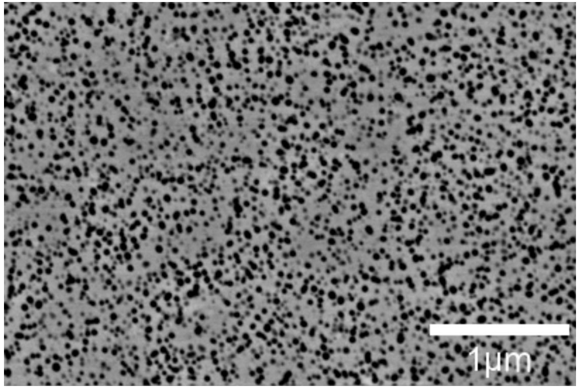
Experimental validation: defects

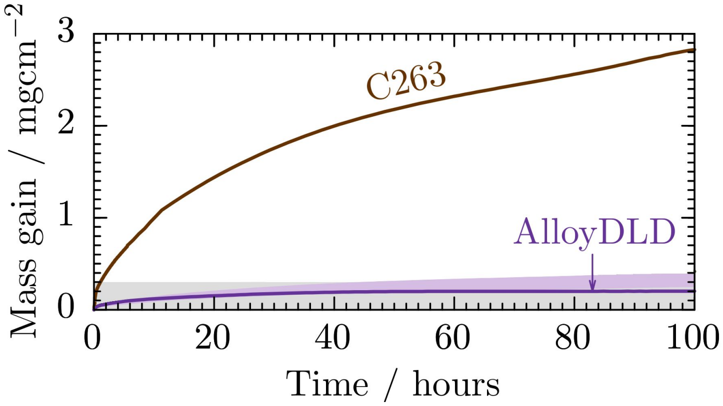




Materials & Design 168, 107644 (2019)

Experimental validation: oxidation resistance





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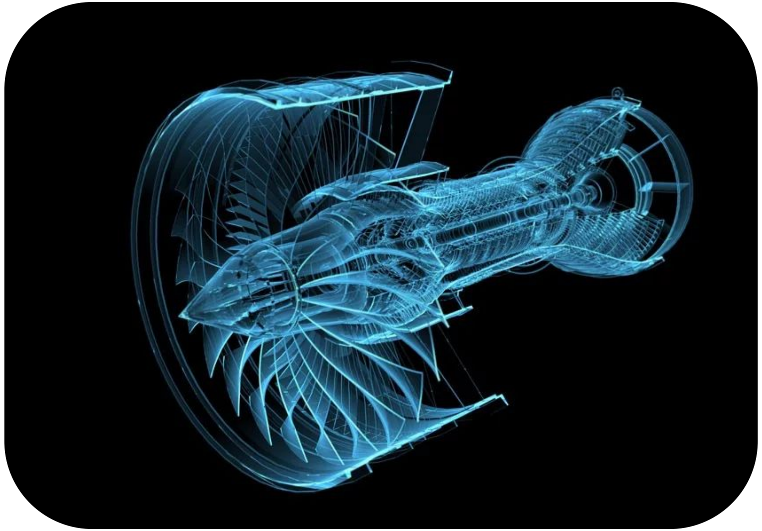
A better alloy cheaper and faster

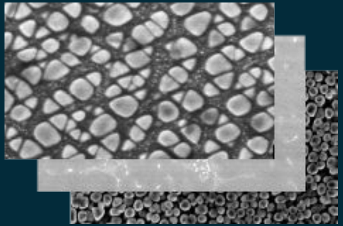


90% reduction in expensive experiments

Reduced costs by $10 million

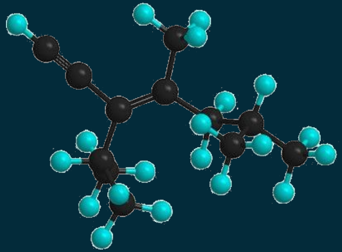
Accelerated discovery and validation from 20 to 2 years

Other applications



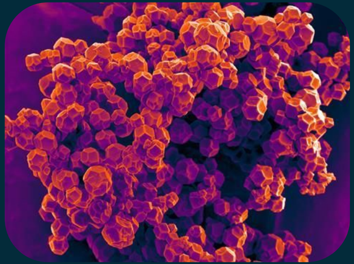
Nickel & moly alloys

Batteries



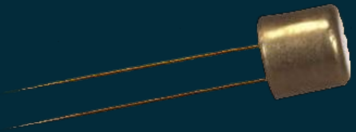
Lubricants

Steels for welding



Metal-organic framework

Concrete



Thermometry

Drug design

UNIVERSITY OF CAMBRIDGE

SKANSKA

GKN

ROLLS ROYCE

Rolls-Royce®

ghd

CARE fertility

optibrium

SAMSUNG

ATI Boeing Accelerator

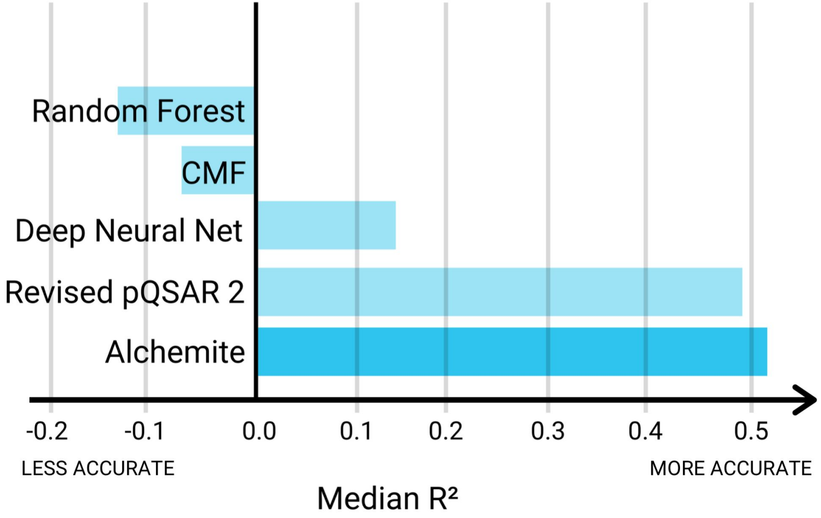
BASF

We create chemistry

Takeda

ANSYS® GRANTA

Predicting bioactivity from incomplete data



Alchemite™ accurately imputes assay activities

Significantly outperforms traditional QSAR models

Uses just 20% of computing resource

optibrium

ALCHEMITE™ ANALYTICS

The machine learning platform for materials and chemicals design

Consulting project

One-off project to design a formulation

Alchemite™ engine API

Deploy machine learning engine into existing software stack

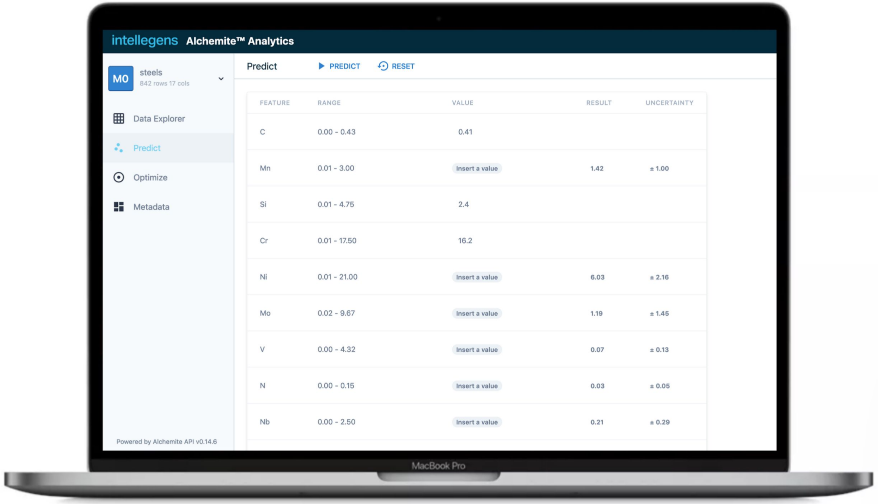
Alchemite™ Analytics platform

Software for use by engineers & scientists

Bespoke tool development

Front-end with underlying Alchemite™ engine

ALCHEMITE™ ANALYTICS



Accelerate R&D

Generate models to gain a better understanding of the landscape

Guide experiments

Choose the next best experiment to run in the optimal direction

Visualise and analyse

Verify data and visualise changing parameters intellegens

Upcoming online event

Alchemite™ Analytics platform demo

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