intellegens

Innovative machine learning for simulations, experiments, and beyond

Ansys 2021

Alchemite™ machine learning

Alchemite™ developed at University of Cambridge and Intellegens

Design formulations for multiple target properties

Merge simulations, physical laws, and experimental data to exploit all available information

Exploit uncertainties to deliver most robust predictions to customers

Accelerate formulation design at reduced cost

Handling sparse data

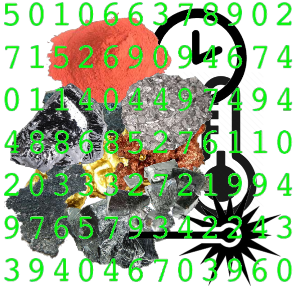
Approach problems with a black box

Formulation | **Black box** | **Properties**

Defects
Strength
Cost
Weight
Fatigue
Environment

Train the machine learning

Formulation



Black box

Properties

Defects

Strength

Cost

Weight

Fatigue

Environment

Use the machine learning

Formulation

Black box

Properties

Defects
Strength
Cost
Weight
Fatigue
Environment

Sparse data

Formulation

Black box

Properties

Defects

Strength

Cost

Weight

Fatigue

Environment

Exploit imputed first principles simulations

Formulation

Black box

Properties

Defects
Strength
Cost
Weight
Fatigue
Environment

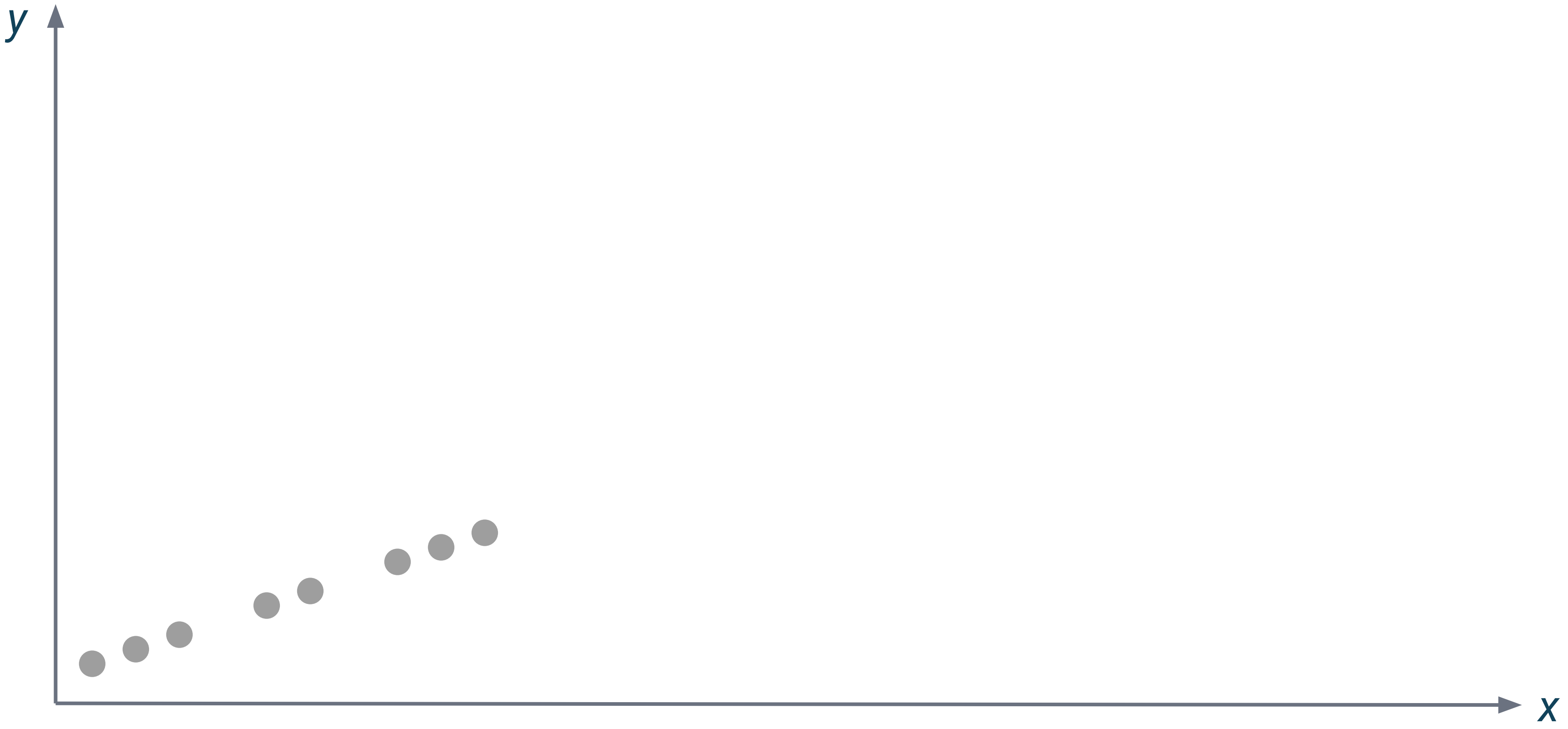
Black box

Properties

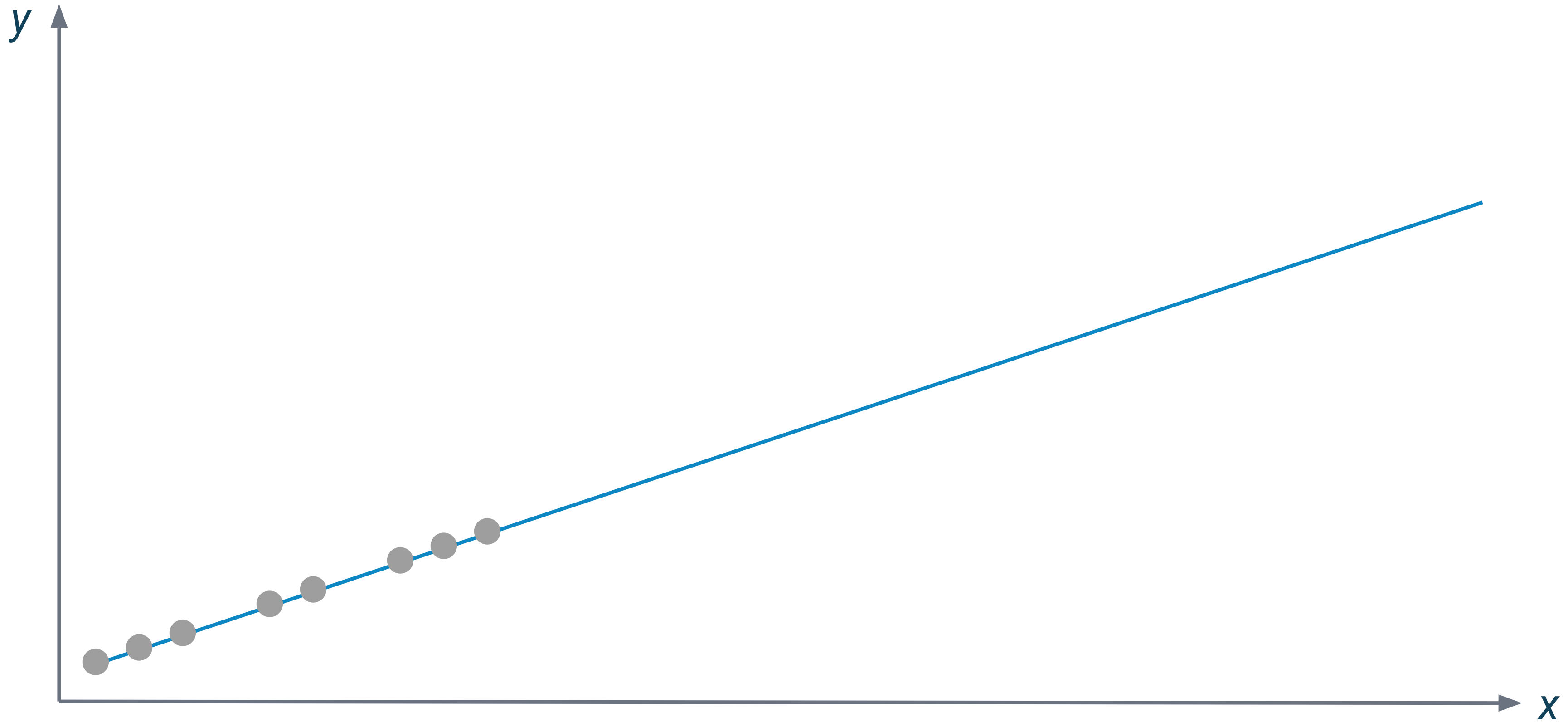
Defects
Strength
Cost
Weight
Fatigue
Environment

Use of uncertainty

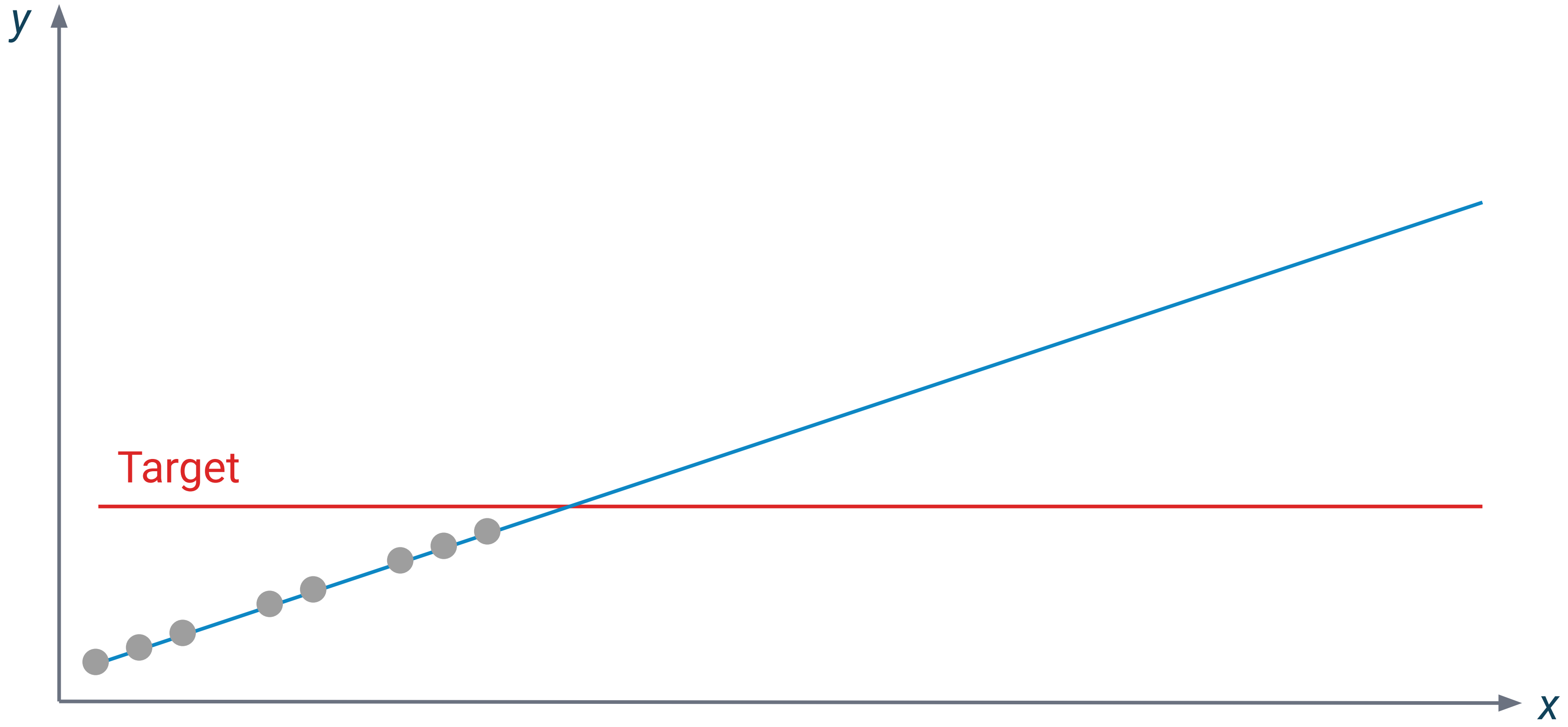
Training data



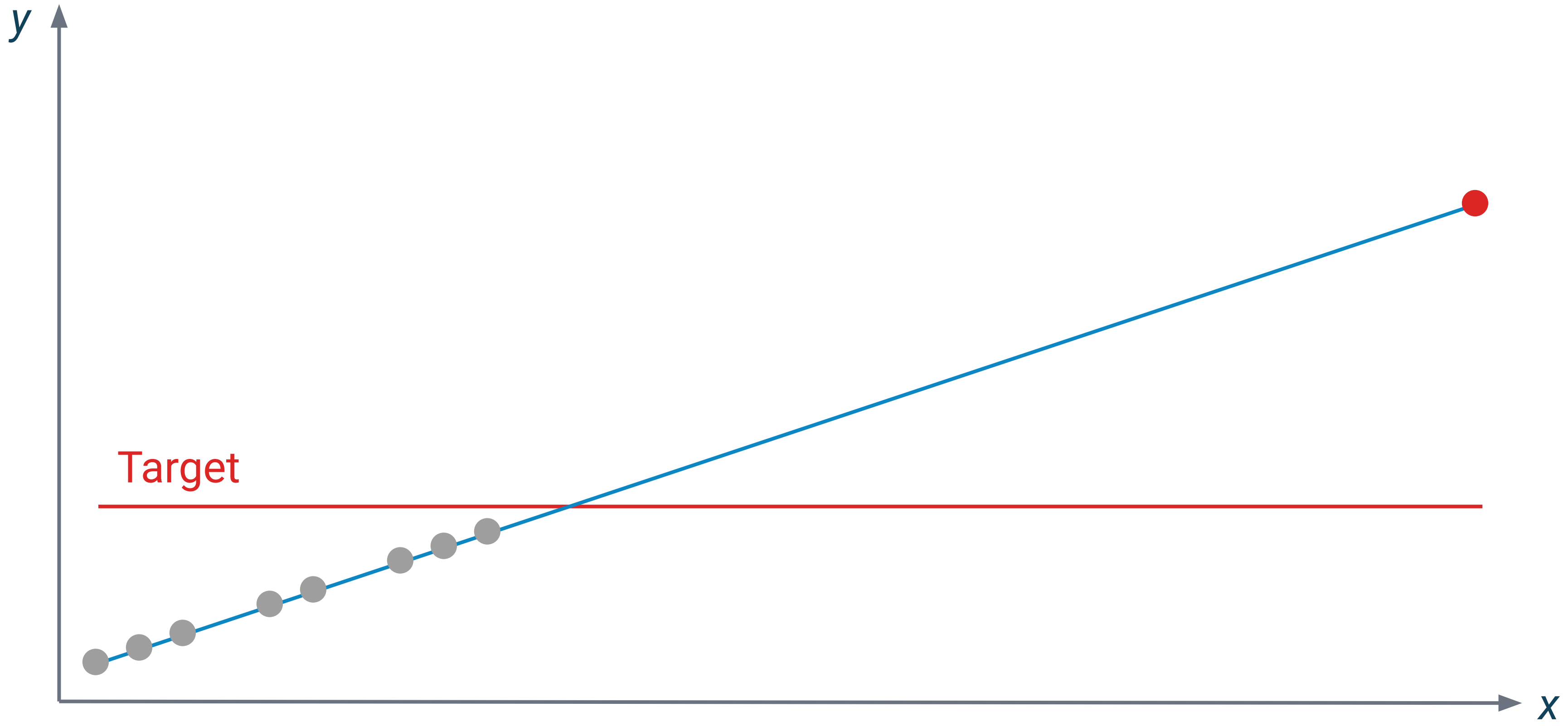
Machine learning model



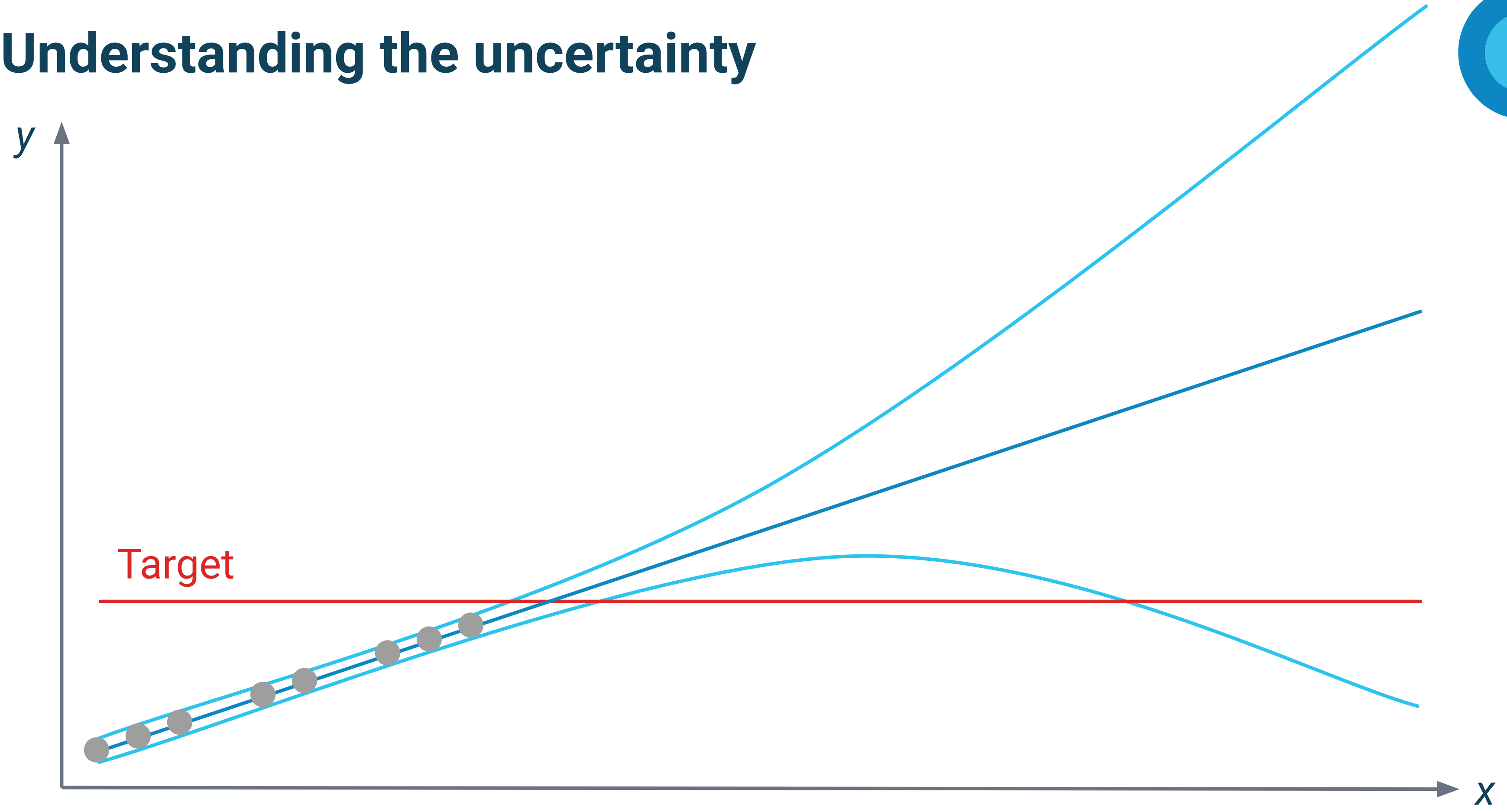
Target for the design



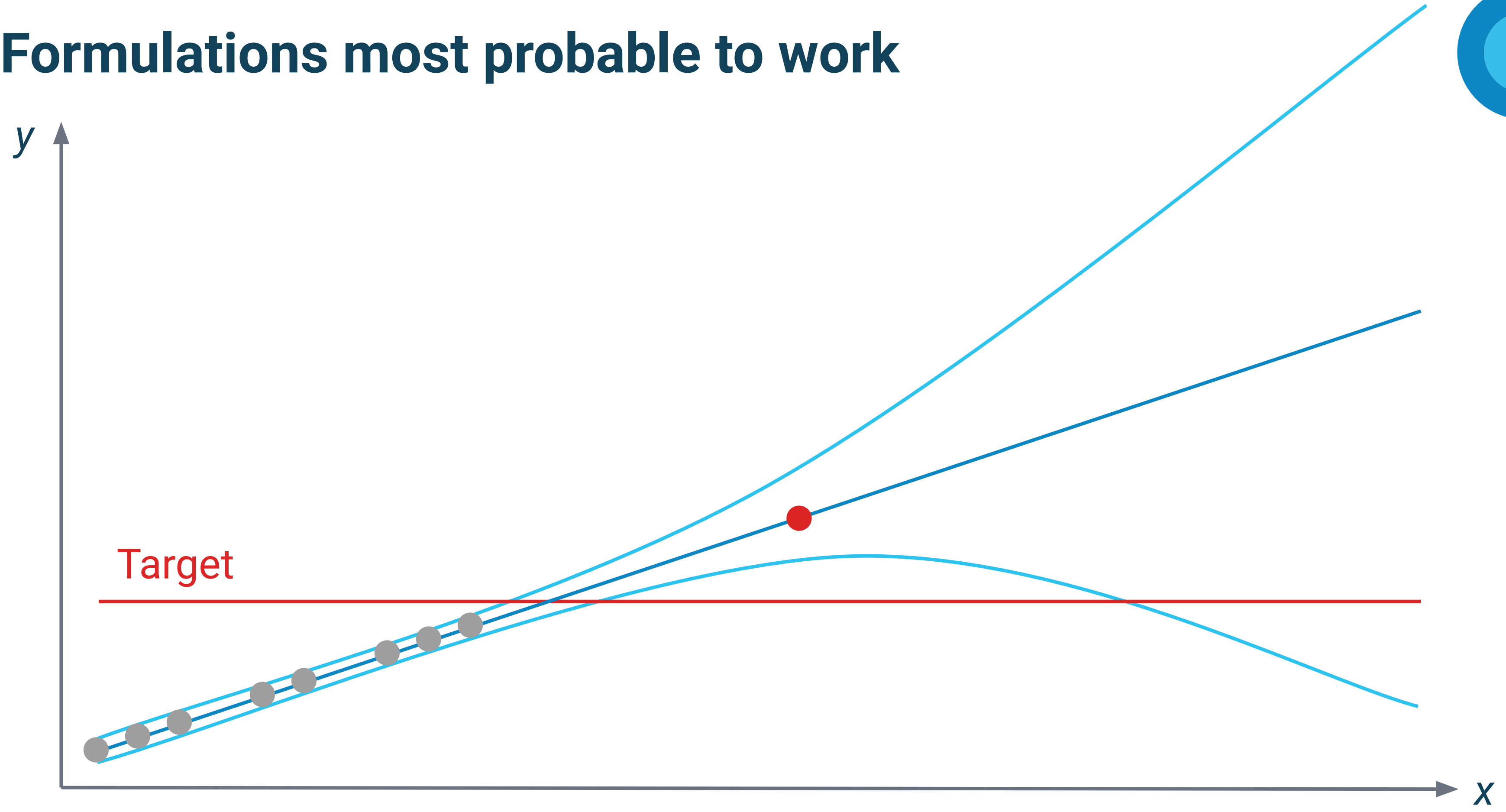
Choose the formulation with best expected property



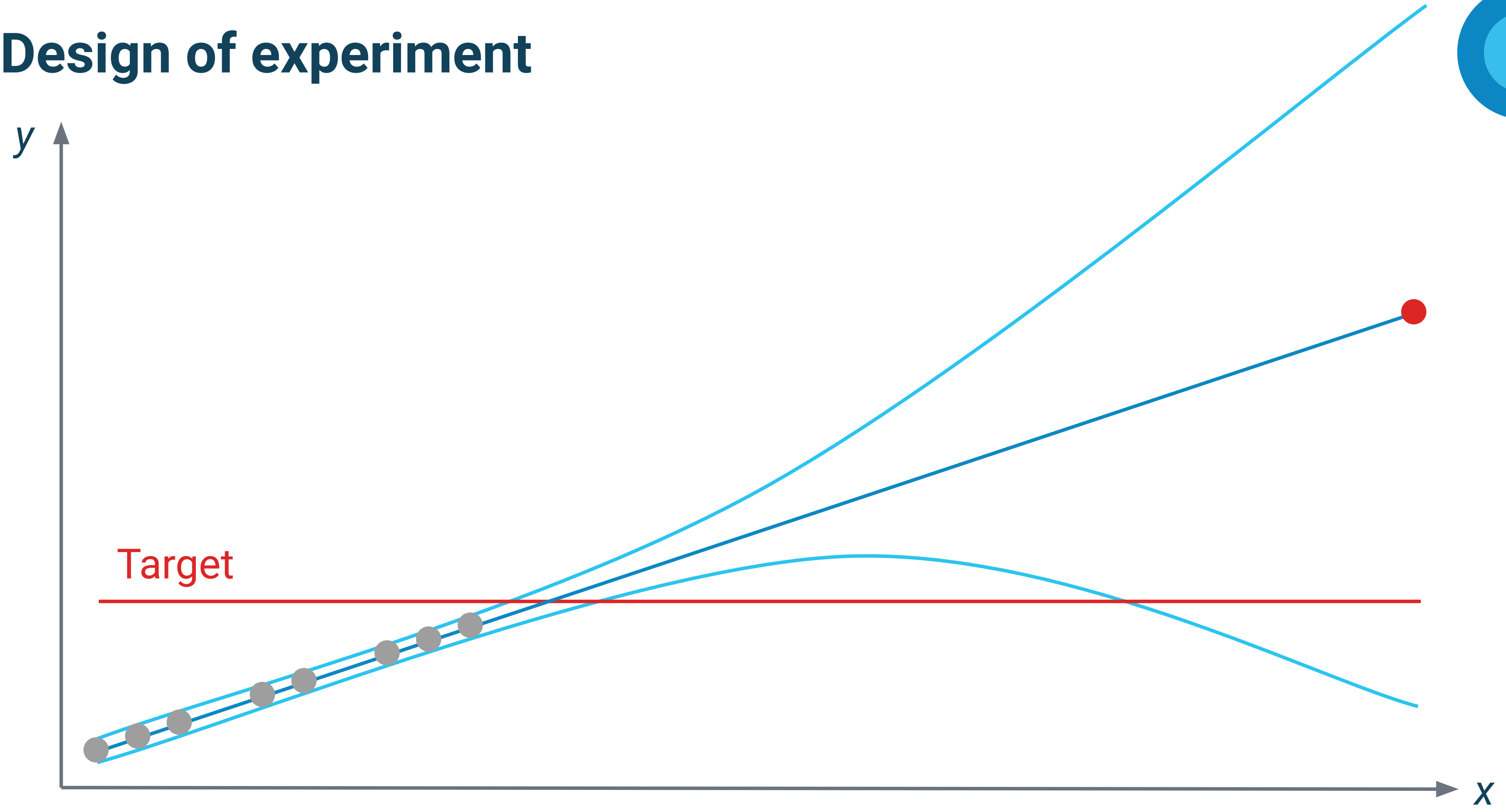
Understanding the uncertainty



Formulations most probable to work



Design of experiment



Alchemite™ technology offers a unique combination

Value from sparse, noisy data

Unique self-consistent, iterative algorithm imputes sparse data

Quantify uncertainty to enable rational decisions

Accurate method (nonparametric probability distributions)

Optimise against multiple targets

Solves high-dimensional problems that were intractable

Make a fast start

Auto-generates models, requiring minimal assumptions

Speed and scalability

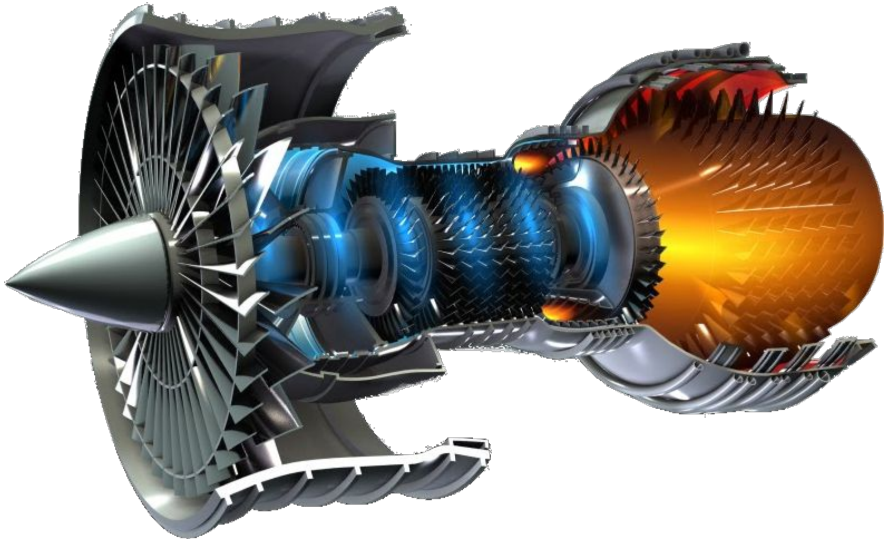
Light CPU / memory footprint: replace first principles simulations and handle huge datasets

A global view

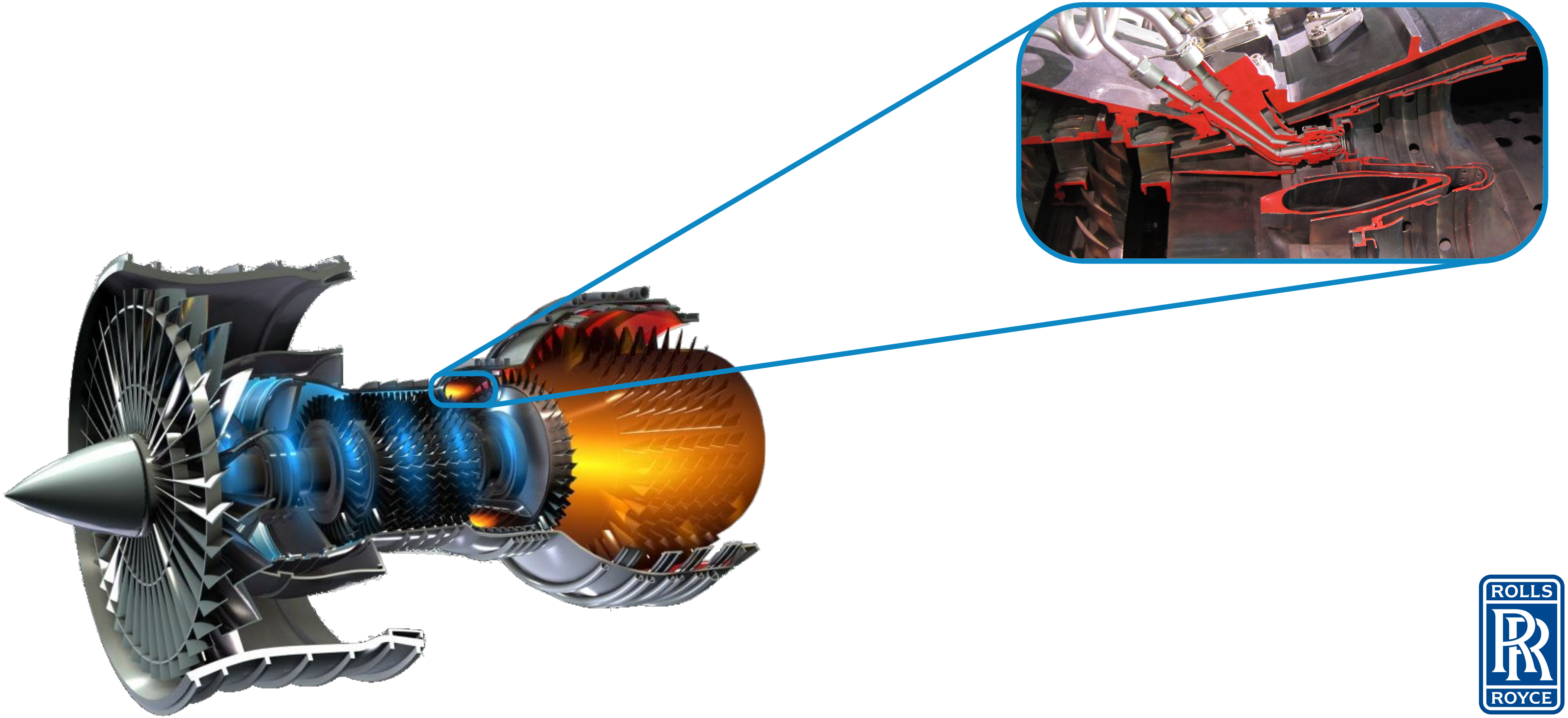
e.g., ingredients *and* processing parameters in a combined study

Case studies

Schematic of a gas turbine engine



Combustor in a gas turbine engine



Target properties

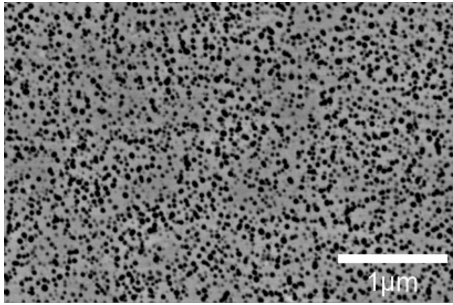
Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ' content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 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

Processability had just 8 entries available

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

Properties from first principles methods

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 design parameters

Cr 19%

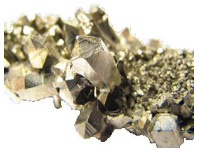
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



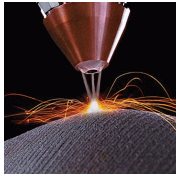
Al 2.9%

C 0.04%

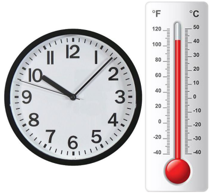
B 0.01%

Ni balance

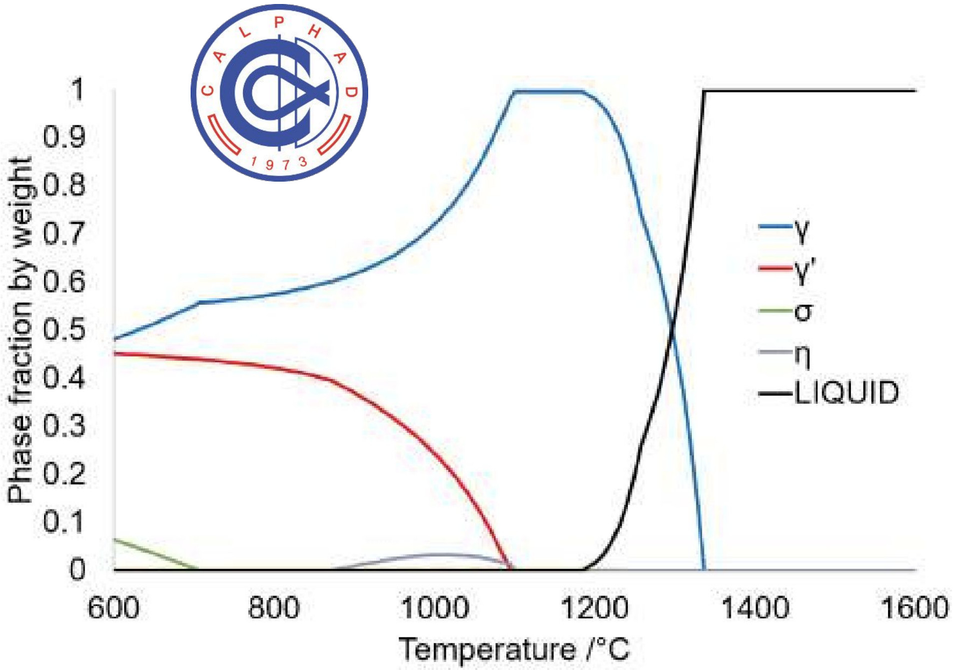
Expose 0.8



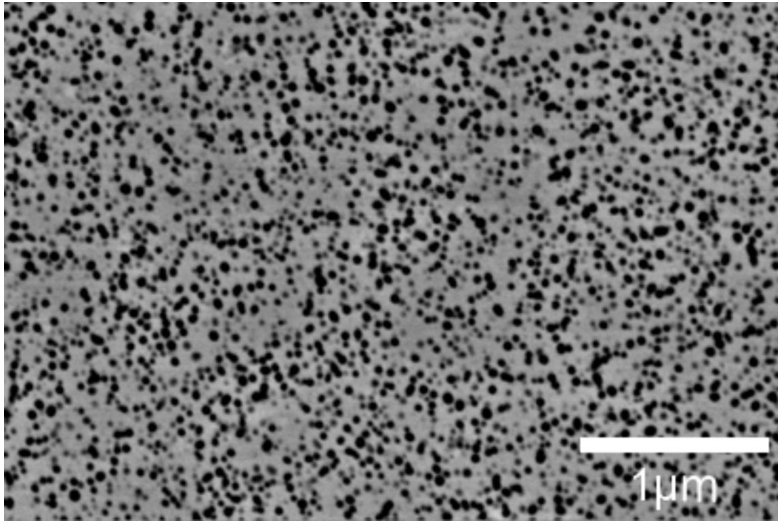
T_{HT} 1230ºC



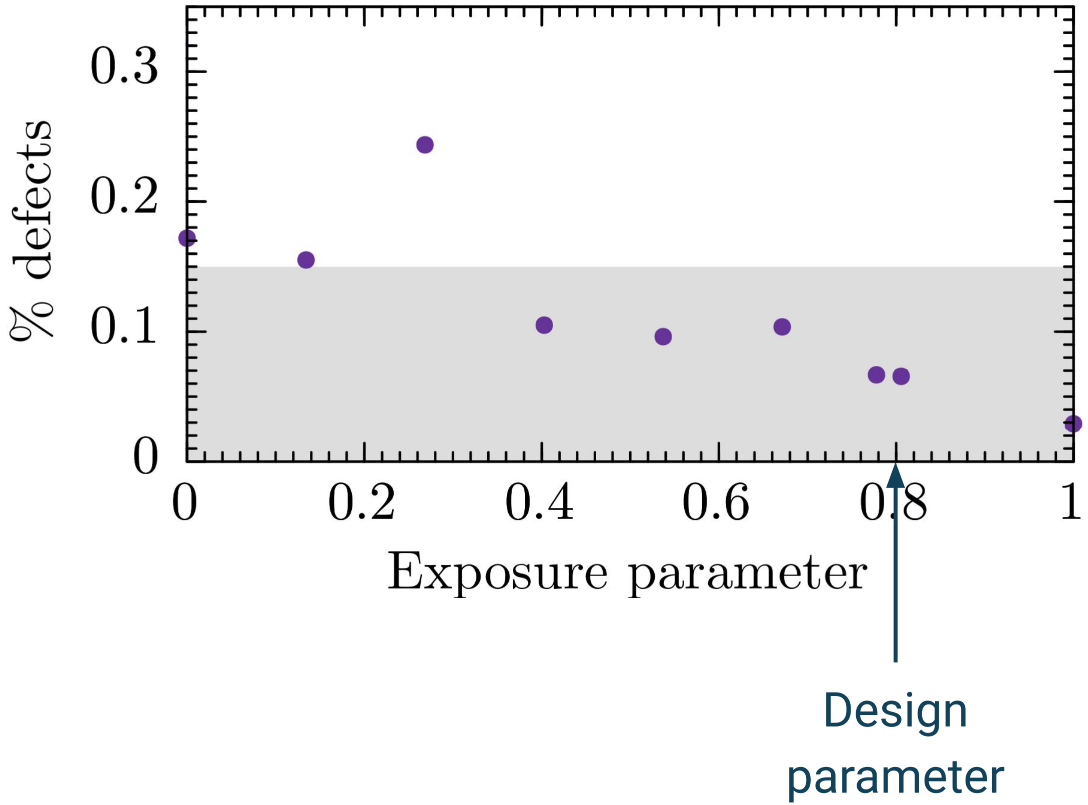
Phase behavior



Microstructure

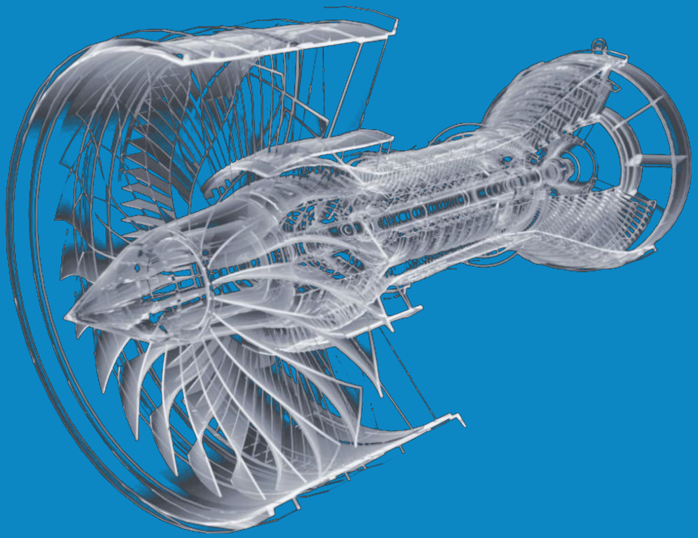


Defects



0.3
0.2
0.1
0
% defects
0
0.2
0.4
0.6
0.8
1
Exposure parameter
Design
parameter

ROLLS ROYCE



Materials & Design ***168***, *107644 (2019)*

AM Powered by ASME
INNOVATION AWARD
Intellegens Startup
2021

AM Powered by ASME
INNOVATION AWARD
Intellegens Software
2021

High temperature alloy

Validated a new alloy for 20+ composition/process parameters to satisfy 11 physical criteria

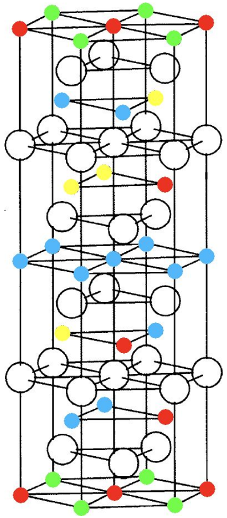
Just 8 printability experimental values

90% fewer costly experiments

Reduced costs by $10 million

Accelerated typical discovery and validation time from 20 to 2 years

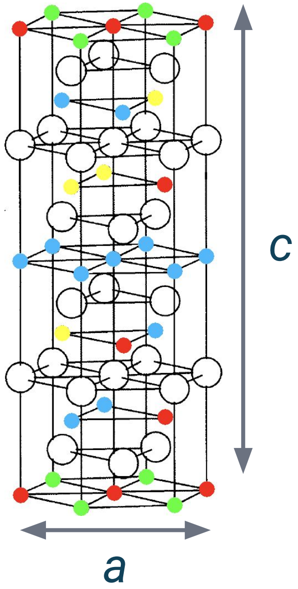
Battery cathode NCM material



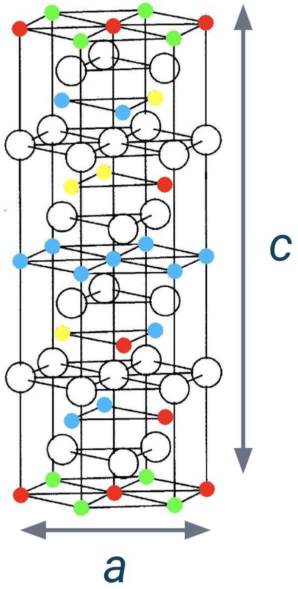
- Nickel
- Cadmium
- Manganese
- Oxygen
- Lithium

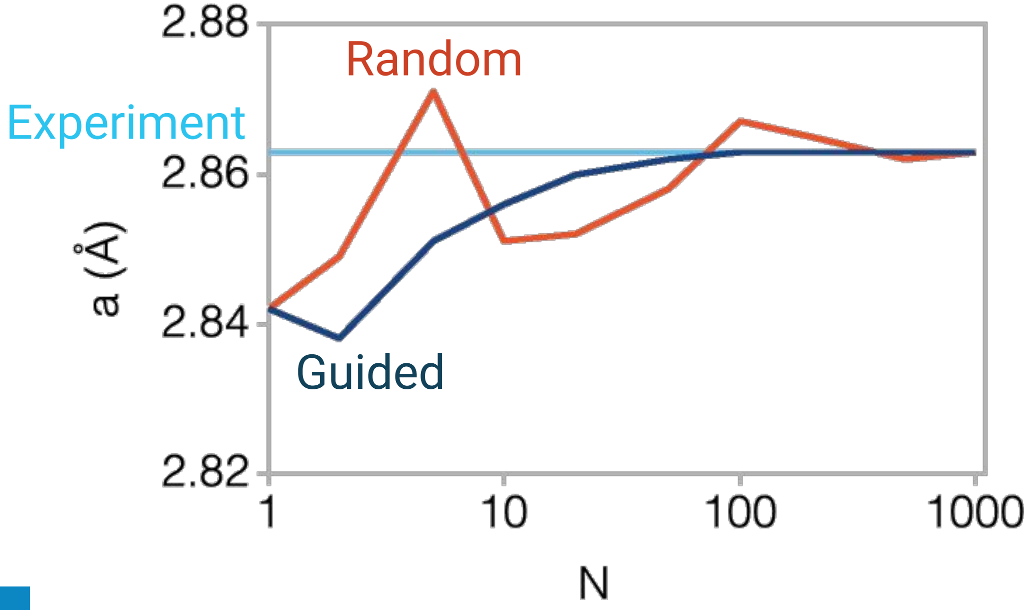
Design a NCM cathode that is more **robust** against **Li migration** and maintains other properties

Lattice constants



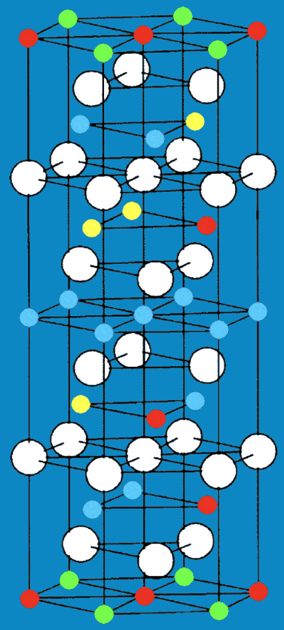
How many simulations are required?



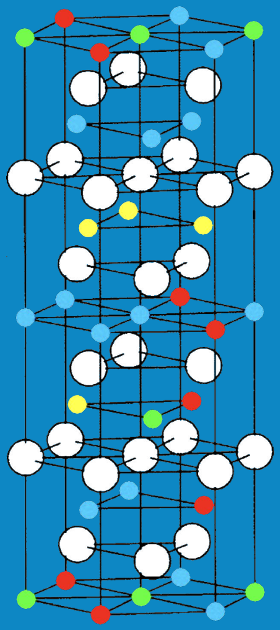


Structure	a (Å)	c (Å)
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ predict	2.863	14.257
$LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ exp.	2.866	14.254

Battery cathodes



Original
82% robust



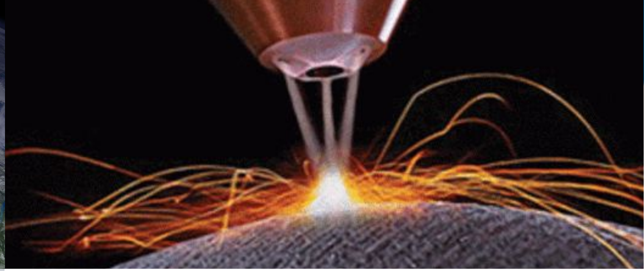
Proposed
100% robust

Machine learning required 20x fewer density functional theory calculations

Reduce Li migration to improve battery life

Maintain voltage, charge stored, density, and cost

Bespoke battery design for each customer



DOMINO

NASA

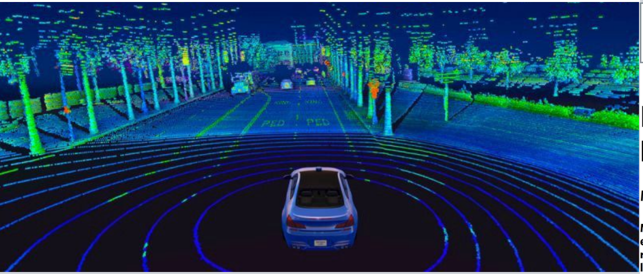
Heat exchanger
& shape memory
alloy applications

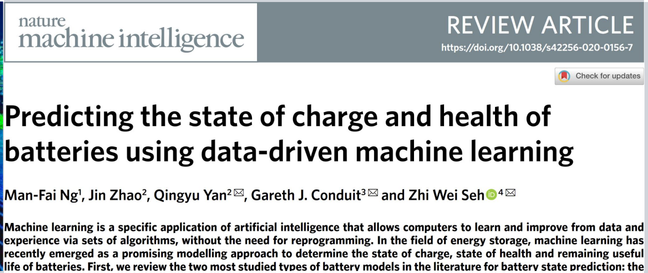
GKN

BOEING

The University Of Sheffield. AMRC Advanced Manufacturing Research Centre

Welding Alloys Group





nature machine intelligence

REVIEW ARTICLE

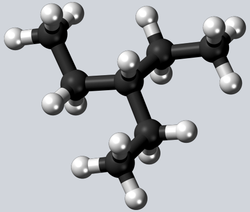
https://doi.org/10.1038/s42256-020-0156-7

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2], Gareth J. Conduit[3] and Zhi Wei Seh[4]

Machine learning is a specific application of artificial intelligence that allows computers to learn and improve from data and experience via sets of algorithms, without the need for reprogramming. In the field of energy storage, machine learning has recently emerged as a promising modelling approach to determine the state of charge, state of health and remaining useful life of batteries. First, we review the two most studied types of battery models in the literature for battery state prediction: the



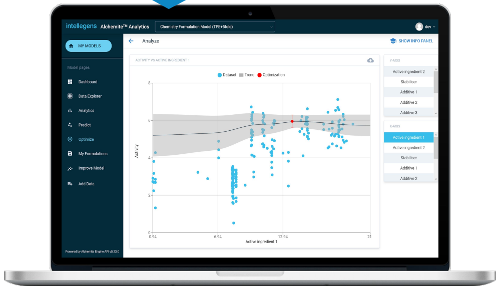
Ordnance Survey

Battery management software
Nature Machine Intelligence 2, 161 (2020)

bp

Alchemite™ product family

Scientists & engineers
Fast start, easy-to-use, visual



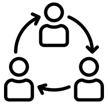
Option to deploy models

Data scientists
Add to your ML toolkit

Optional connectors

Lab systems

Software & scripts



Sharing & collaboration

Alchemite™ Analytics

Deep data insights on your desktop

Guide experiments, predict, design, optimise

Alchemite™ Engine

Integrate into your workflow (API, Python)

Advanced configuration, enterprise deployment

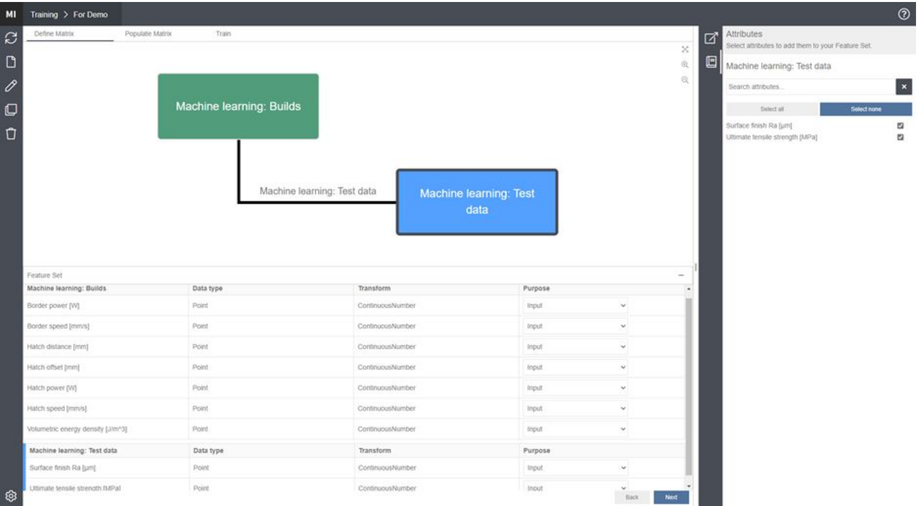
Alchemite™ Success

Access Intellegens deep learning expertise

Advice to your data science team or full project management

Intellegens and Ansys

Granta MI™ plus Alchemite™



Sparse data, uncertainty & simulations

Alchemite™ uses property-property correlations, uncertainty estimates, and first principles simulations to overcome sparse data

Designed experimentally verified materials with impossibly small data

Connect with first principles simulations including:

- CALPHAD
- Density functional theory
- Finite element
- Computational fluid dynamics
- Molecular dynamics

Next steps

Contact gareth@intellegens.ai

Website https://intellegens.ai

Papers https://intellegens.ai/article-type/papers/

Demo https://app.intellegens.ai

@intellegensai

/company/intellegensai