intellegens

Applied machine learning

Research commercialization in Cambridge

Dr Gareth Conduit

Introducing Alchemite™ applied machine learning

Developed at University of Cambridge

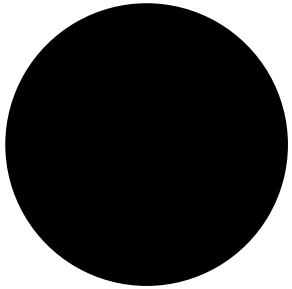
Innovative method extracts value from sparse, noisy data to solve complex, high-dimensional problems

Key use cases: chemicals, materials, life sciences, and manufacturing

Focus on ease-of-deployment for immediate return on investment

Black box machine learning for materials design

Composition



Properties

Defects

Fatigue

Strength

Train the machine learning

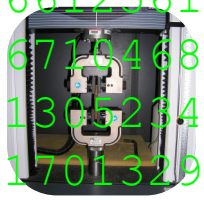
Composition

Properties

Defects

Fatigue

Strength



Machine learning predicts material properties

Composition

Properties

Defects

Fatigue

Strength

Nickel superalloys with Rolls Royce

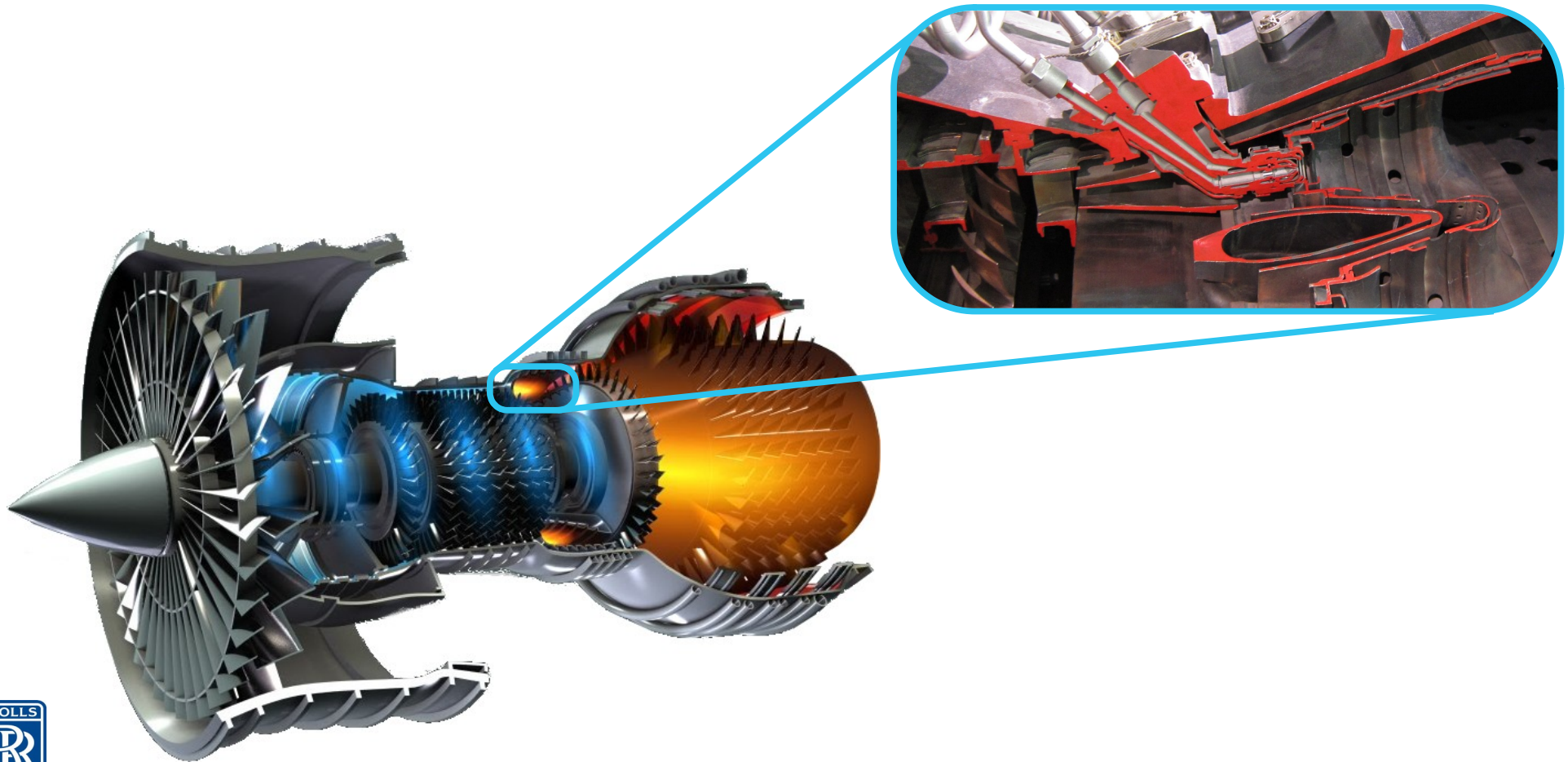
Rolls Royce University Technology Centre, Cambridge

Dr Vadegadde Duggappa

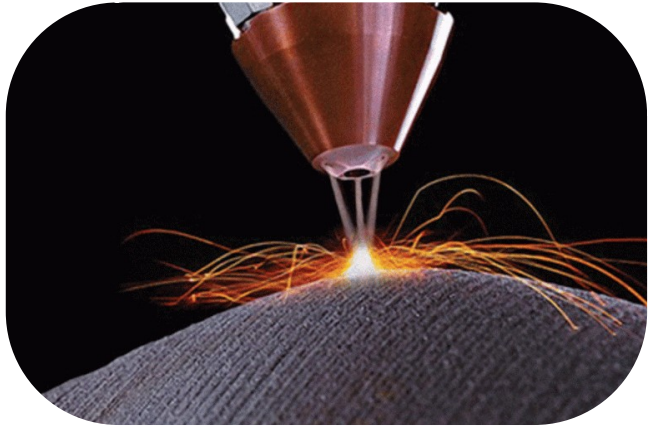
Dr Bryce Conduit

Professor Howard Stone

Combustor in a jet engine

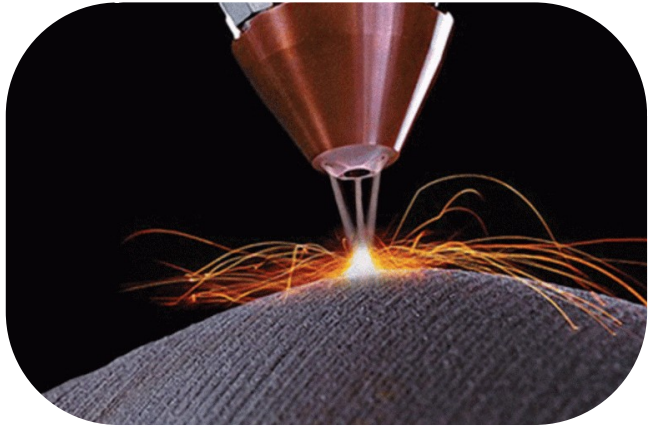


Defects form during printing



Laser

Ability for printing and welding are strongly correlated



Laser

Electricity

Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Defects	< 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%

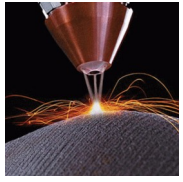
Al 2.9%

C 0.04%

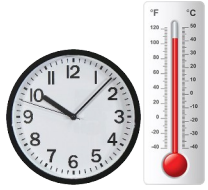
B 0.01%

Ni

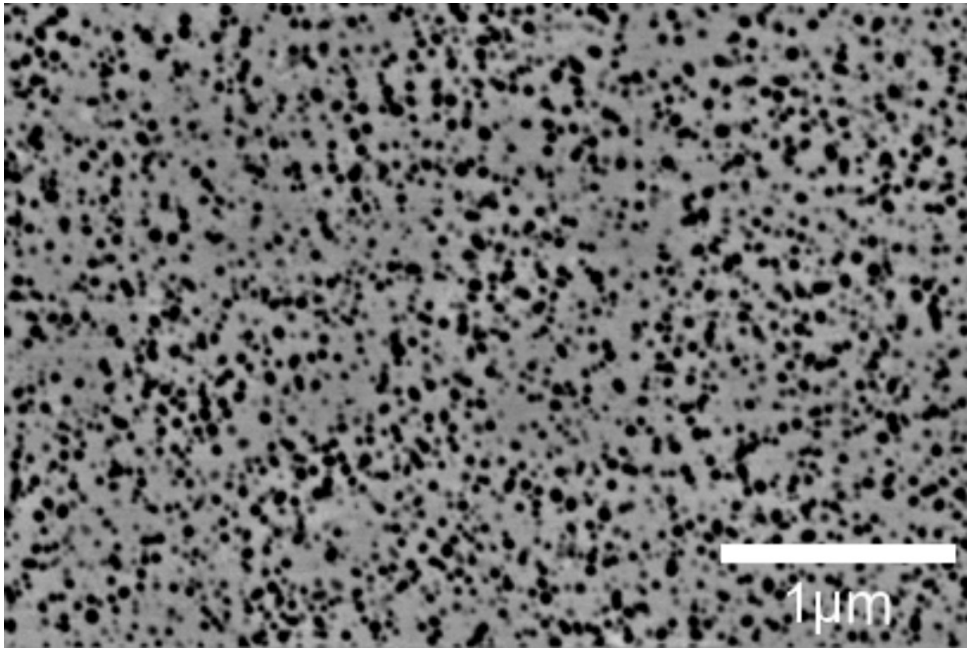
Expose 0.8



T_{HT} 1300ºC

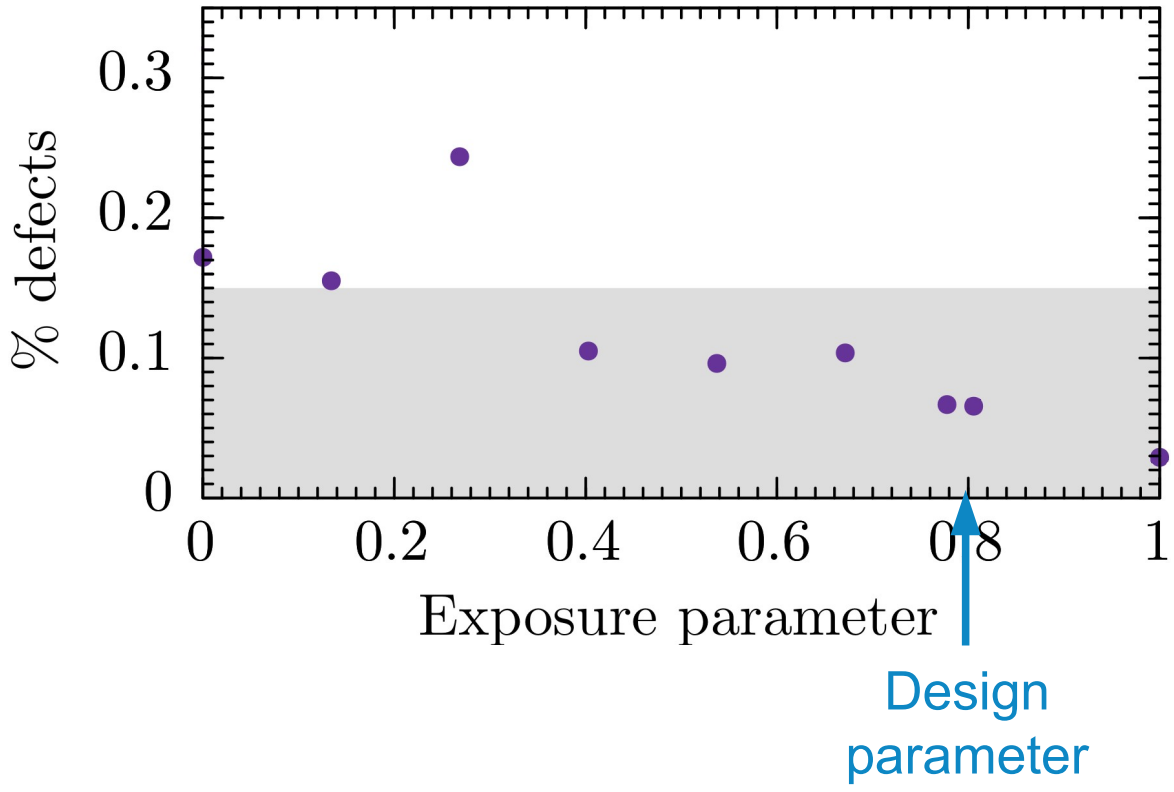


Microstructure



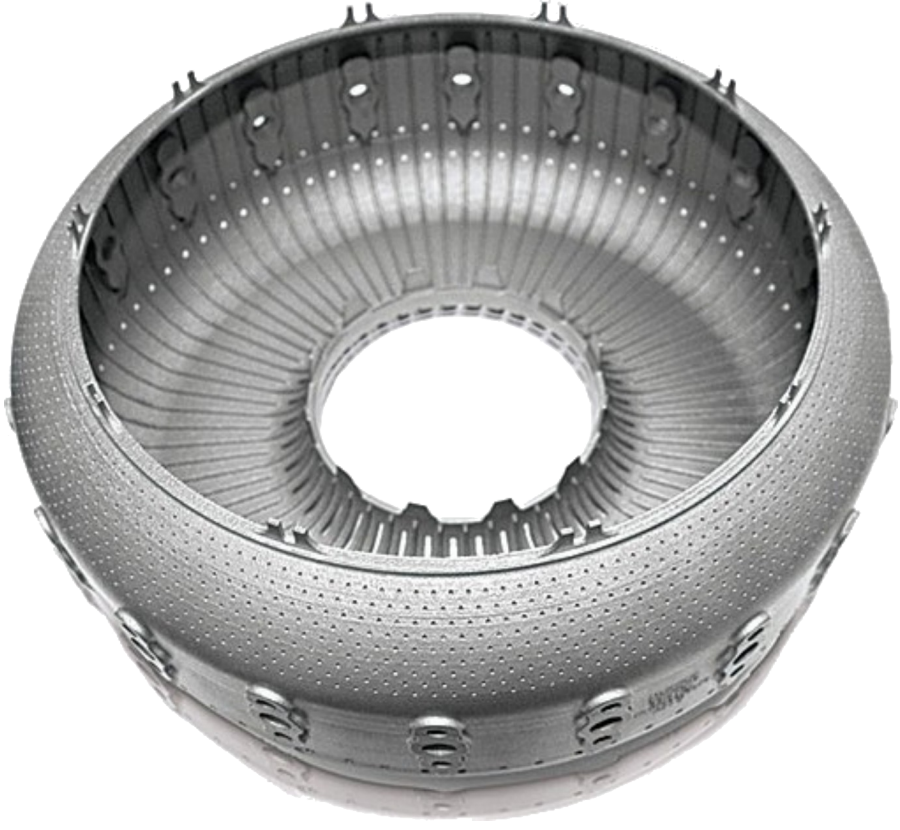
Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)

Test the defect density



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)

Printing a combustor



AM Powered by ASME
INNOVATION AWARD
Intellegens
Startup
2021

AM Powered by ASME
INNOVATION AWARD
Intellegens
Software
2021

Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)

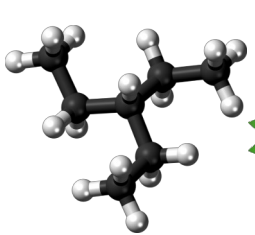
From University to industry

Transition from University to industry

2013

Multiple properties for Rolls Royce engines

Transition from University to industry



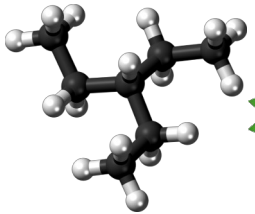
2013

2014

Multiple properties for Rolls Royce engines

Property-property correlations with BP and Rolls Royce

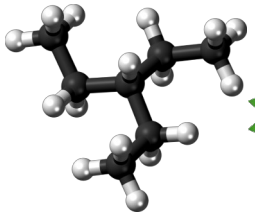
Transition from University to industry



Concurrent materials design

2013	2014	2015
Multiple properties for Rolls Royce engines	Property-property correlations with BP and Rolls Royce	Royal Society University Research Fellowship

Transition from University to industry



bp

THE ROYAL SOCIETY

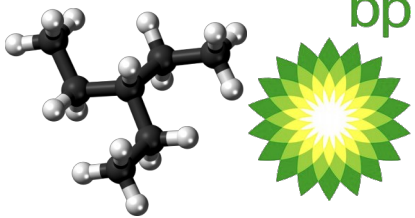
Concurrent materials design

UNIVERSITY OF CAMBRIDGE

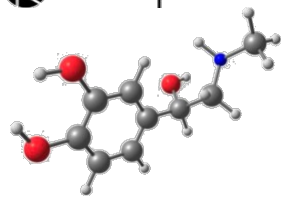
SAMSUNG

2013	2014	2015	2016
Multiple properties for Rolls Royce engines	Property-property correlations with BP and Rolls Royce	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics

Transition from University to industry

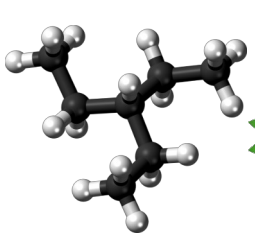


Concurrent materials design

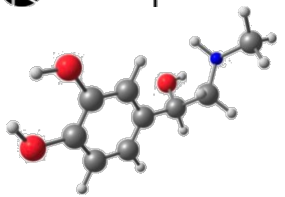


2013	2014	2015	2016	2017
Multiple properties for Rolls Royce engines	Property-property correlations with BP and Rolls Royce	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics	Drug discovery with etherapeutics

Transition from University to industry

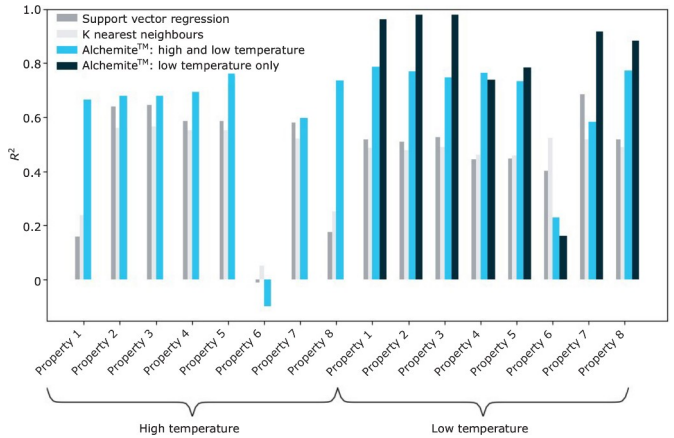


Concurrent materials design

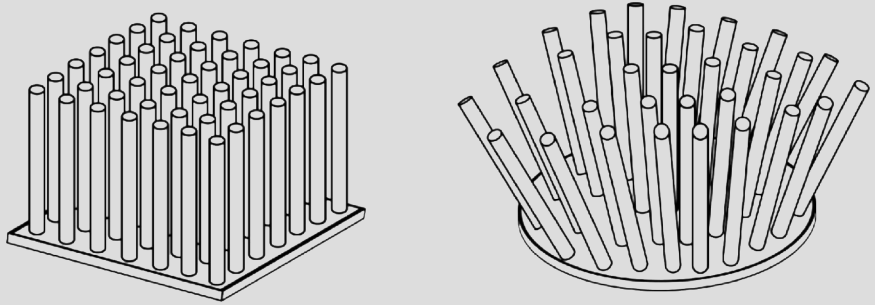


2013	2014	2015	2016	2017	2018
Multiple properties for Rolls Royce engines	Property-property correlations with BP and Rolls Royce	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung Electronics	Drug discovery with etherapeutics	Founding of Intellegens

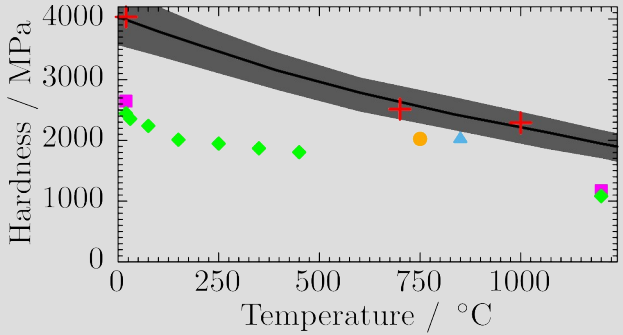
Formulations developed

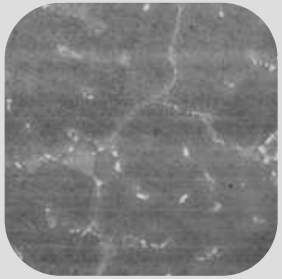


Johnson Matthey Technology Review
66, 130 (2022)



NASA Technical Memorandum
20220008637

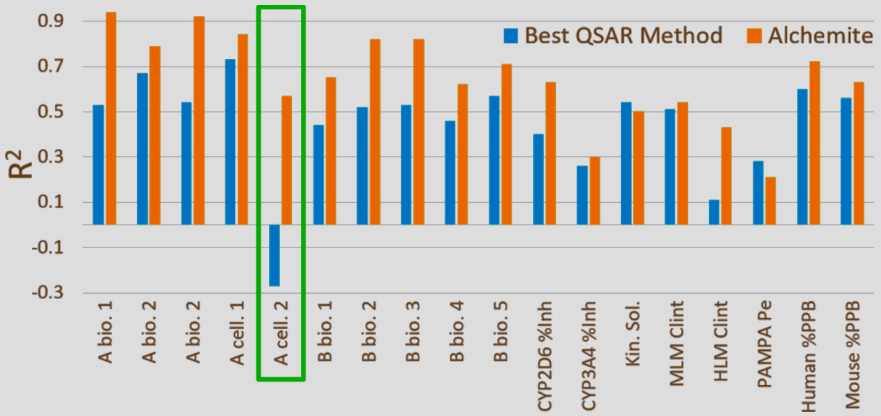




Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

Alloy	Source	ANN	Δ_σ	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	≥550[23]

Computational Materials
Science **147**, 176 (2018)



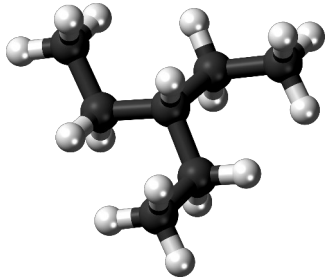
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

optibrium

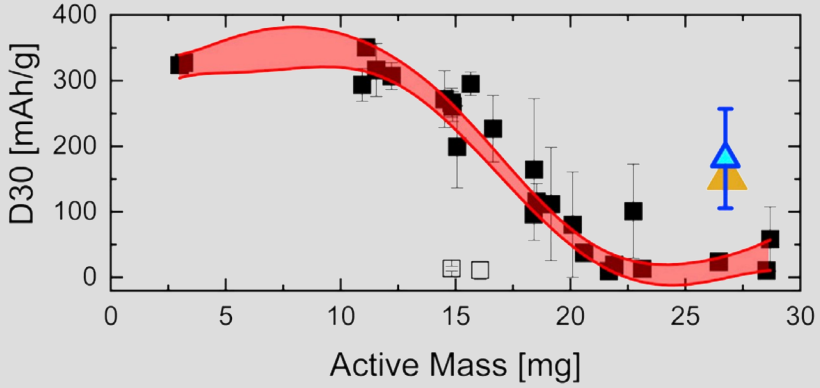
iff

Journal of Computer-Aided
Molecular Design **35**, 112501140 (2021)



Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)

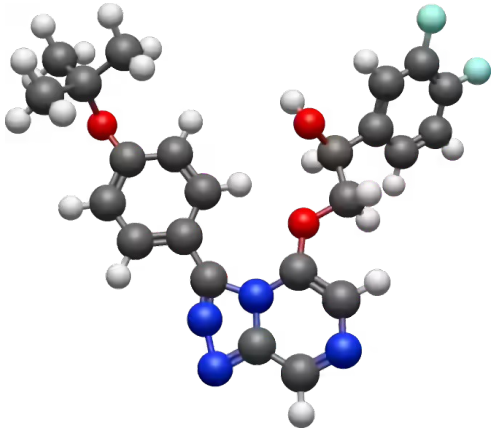
bp



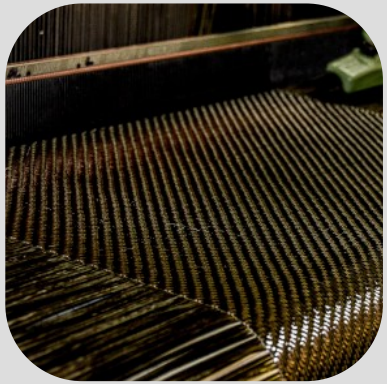
Nature Machine Intelligence **2**, 161 (2020)
Cell Reports Physical Science **2**, 100683 (2021)

UNIVERSITY OF BIRMINGHAM

Ansys GRANTA



Journal of Medicinal Chemistry **64**, 16450 (2021)



Computer-Aided Design **167**, 103637 (2023)

Webinar and white paper (2023)

BioData Mining **17**, 24 (2024)

Commerical developments of Intellegens

Commerical drive to product

2018

Optibrium reseller leads to Cerella™ product

Commerical drive to product

2018 | 2019

Optibrium reseller leads to Cerella™ product

Consultancy work and product development

Commerical drive to product

2018 | 2019 | 2020

Optibrium reseller leads to Cerella™ product

Consultancy work and product development

Release Alchemite Analytics™ product

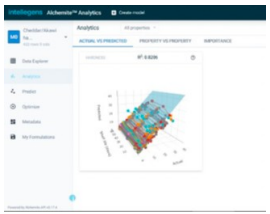
Commerical drive to product

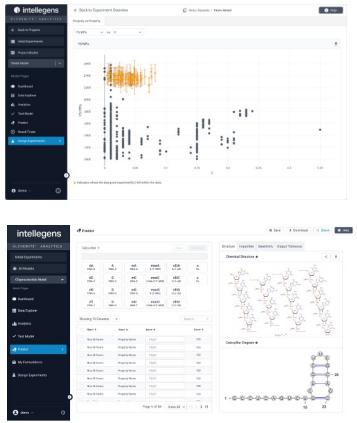
2018	2019	2020	2021
Optibrium reseller leads to Cerella™ product	Consultancy work and product development	Release Alchemite Analytics™ product	Reseller agreement with Ansys

Commerical drive to product

2018	2019	2020	2021	2022
Optibrium reseller leads to Cerella™ product	Consultancy work and product development	Release Alchemite Analytics™ product	Reseller agreement with Ansys	Enterprise licenses & healthcare market

Commerical drive to product



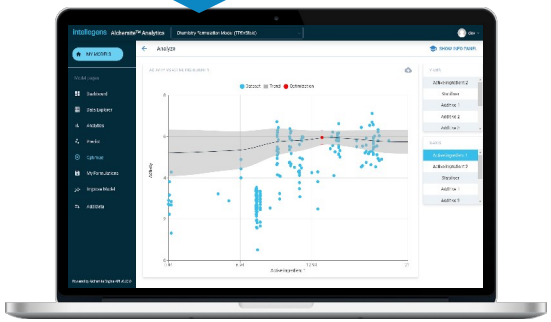


2018	2019	2020	2021	2022	2023
Optibrium reseller leads to Cerella™ product	Consultancy work and product development	Release Alchemite Analytics™ product	Reseller agreement with Ansys	Enterprise licenses & healthcare market	Additional products

Product offering

Intellegens offers the 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, optimize

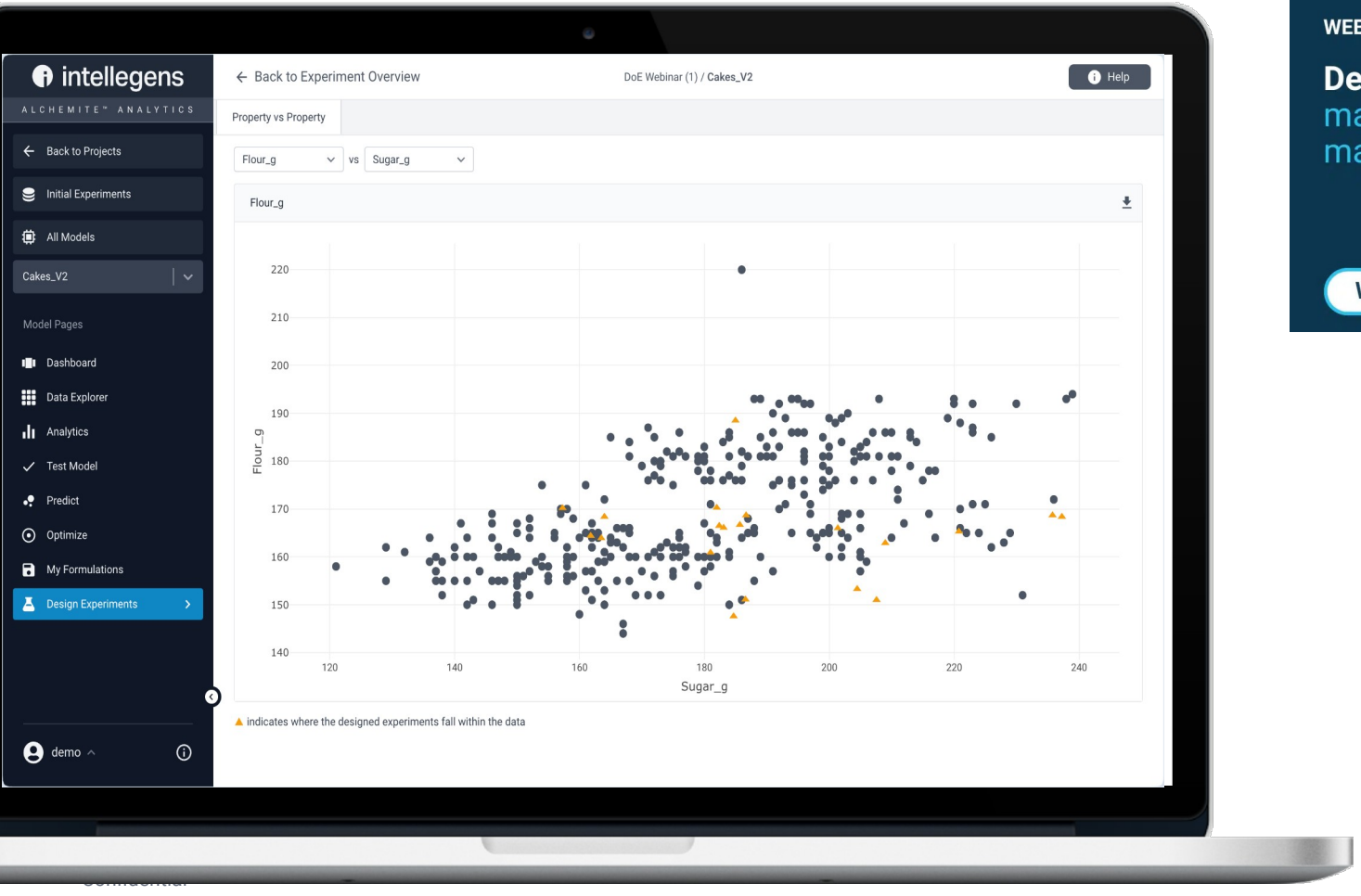
Alchemite™ Engine

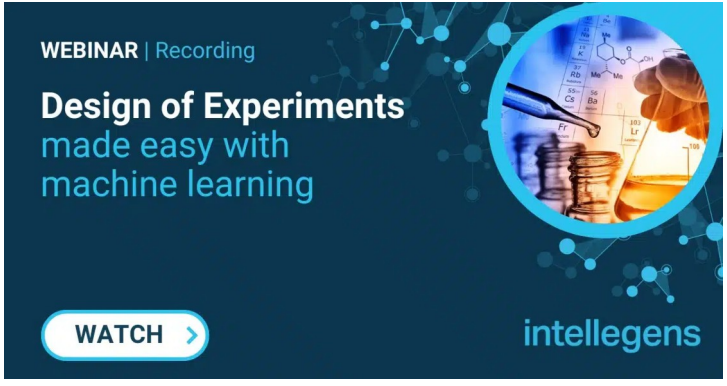
Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

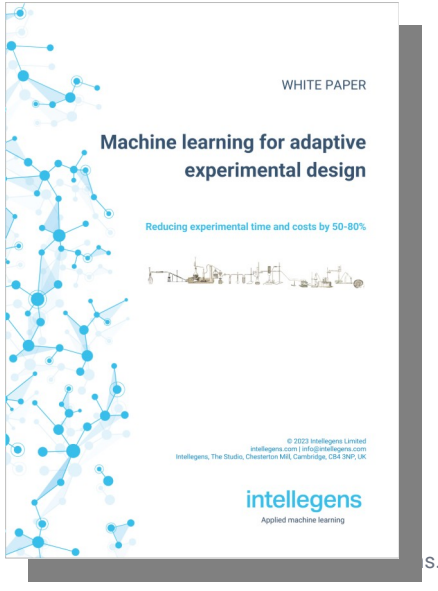
Academia

Alchemite™ academic licenses available for non-comercial research

Alchemite™ module for adaptive experimental design







Demo

Alchemite™ developed at University of Cambridge
applies machine learning to real-life data

Exploit property-property correlations to design alloy for 3D printing

Developed into software package by Intellegens

Generic tool applied to many physical, chemical, and biological sciences

Learn more

gareth@intellegens.com

/company/intellegensai

Subscribe for newsletter and webinar alerts

intellegens.com/subscribe

Website intellegens.com

Case studies intellegens.com/article-type/case-studies/

Next webinar (17 September)

The fast track to better formulations with machine learning

intellegens.com/webinars