intellegens

Applied machine learning

The modern-day blacksmith

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

Nickel superalloys with Rolls Royce

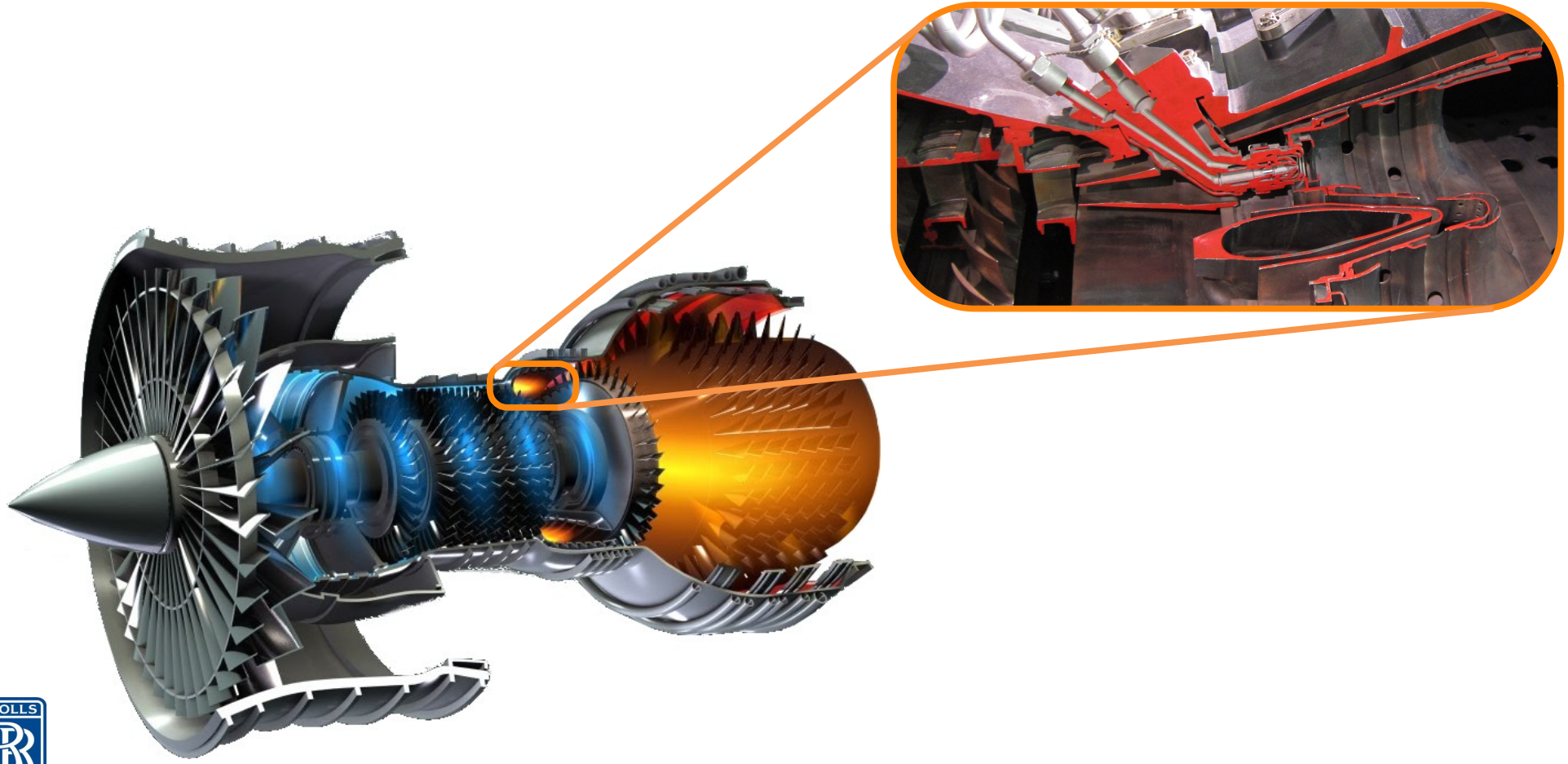
Rolls Royce University Technology Centre, Cambridge

Vadegadde Duggappa

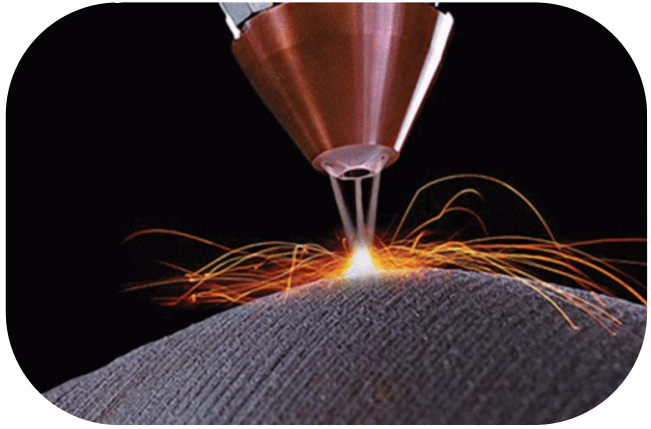
Bryce Conduit

Professor Howard Stone

Combustor in a jet engine

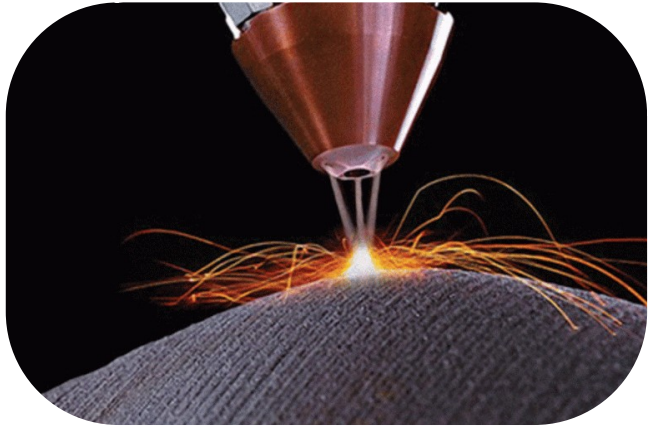


Defects form during printing



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%

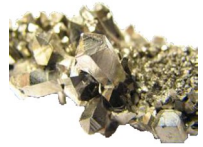
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



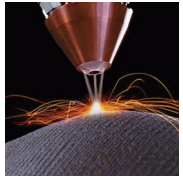
Al 2.9%

C 0.04%

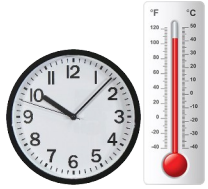
B 0.01%

Ni

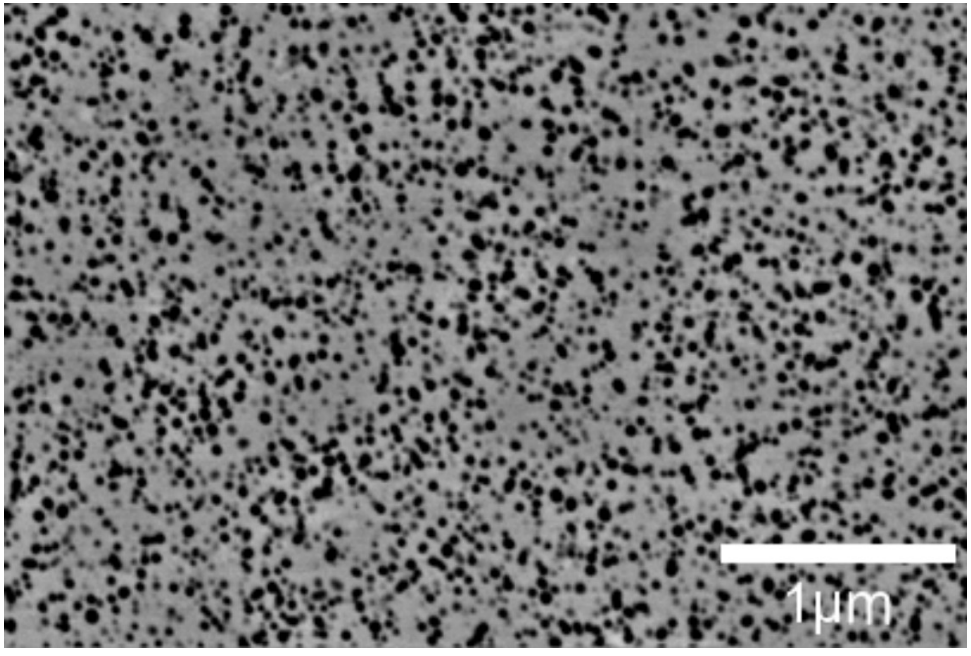
Expose 0.8



T_{HT} 1300ºC

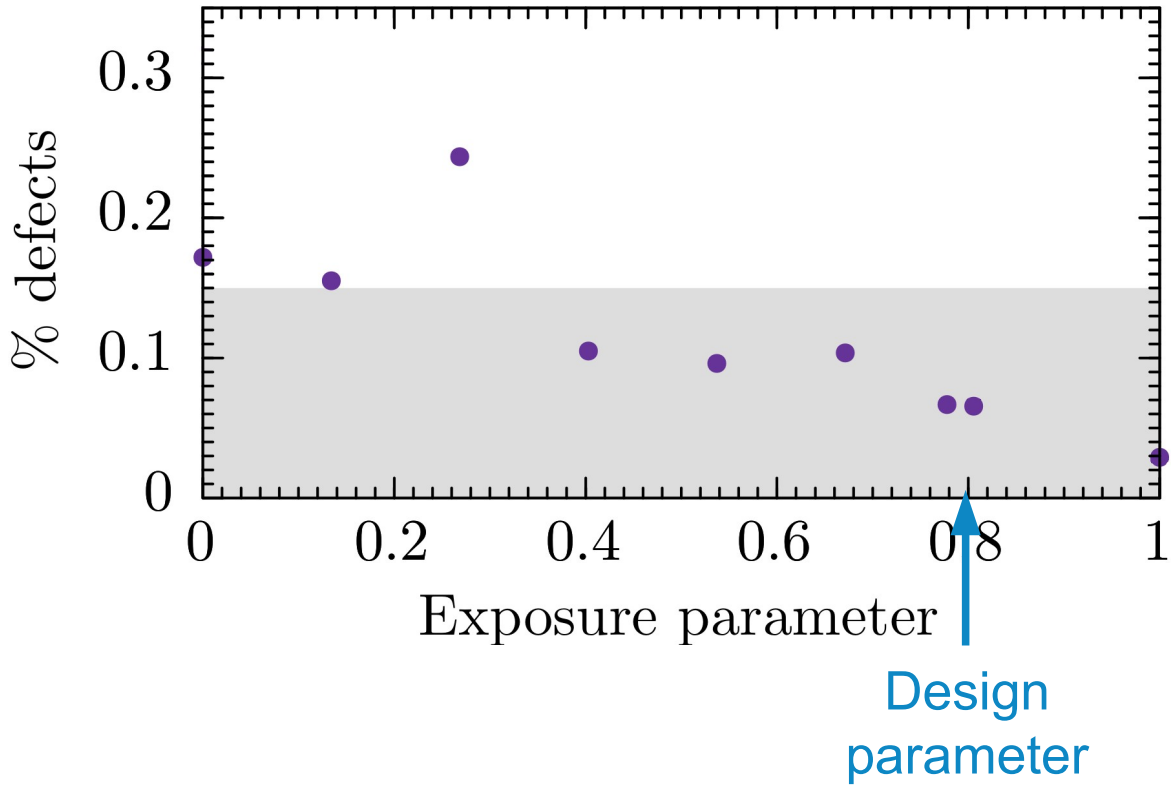


Microstructure



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
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From University to industry

Transition from University to industry

2013

Multiple properties for Rolls Royce engines

Transition from University to industry

Concurrent materials design

2013

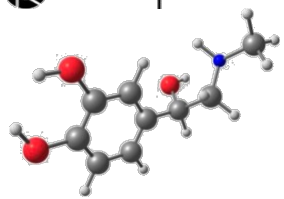
Multiple properties for Rolls Royce engines

2015

Royal Society University Research Fellowship

Transition from University to industry

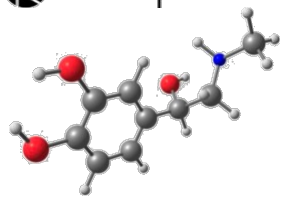
Concurrent materials design



2013	2015	2016
Multiple properties for Rolls Royce engines	Royal Society University Research Fellowship	Projects with Samsung and etherapeutics

Transition from University to industry

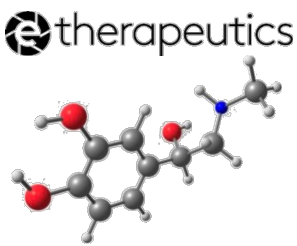
Concurrent materials design



2013	2015	2016	2018
Multiple properties for Rolls Royce engines	Royal Society University Research Fellowship	Projects with Samsung and etherapeutics	Founding of Intellegens

Transition from University to industry

Concurrent materials design

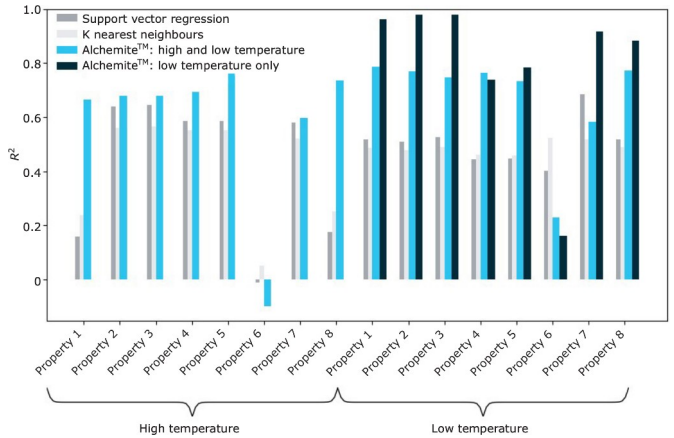


2013	2015	2016	2018	2020
Multiple properties for Rolls Royce engines	Royal Society University Research Fellowship	Projects with Samsung and etherapeutics	Founding of Intellegens	Launch Alchemite Analytics™ product

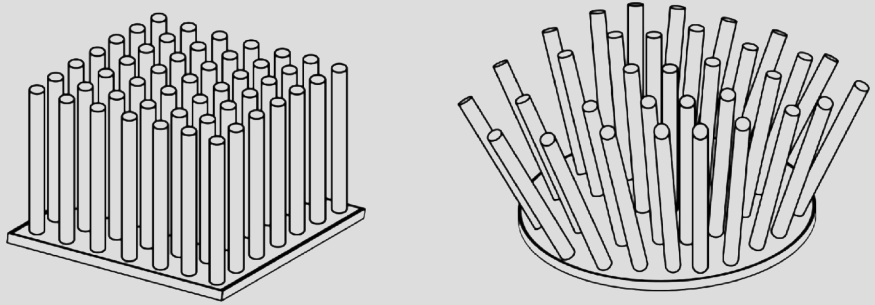
Transition from University to industry

Concurrent materials design

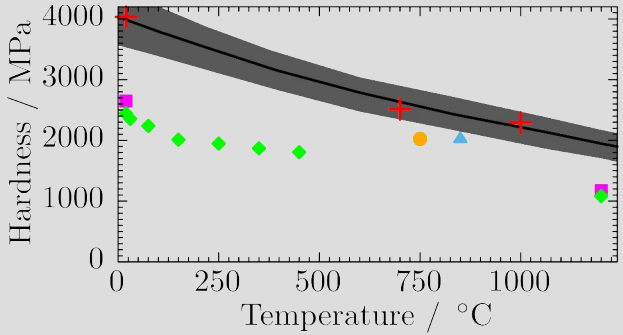
2013	2015	2016	2018	2020	2023
Multiple properties for Rolls Royce engines	Royal Society University Research Fellowship	Projects with Samsung and etherapeutics	Founding of Intellegens	Launch Alchemite Analytics™ product	Enterprise licenses

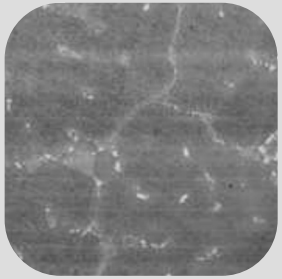


Johnson Matthey Technology Review
66, 130 (2022)



NASA Technical Memorandum
20220008637

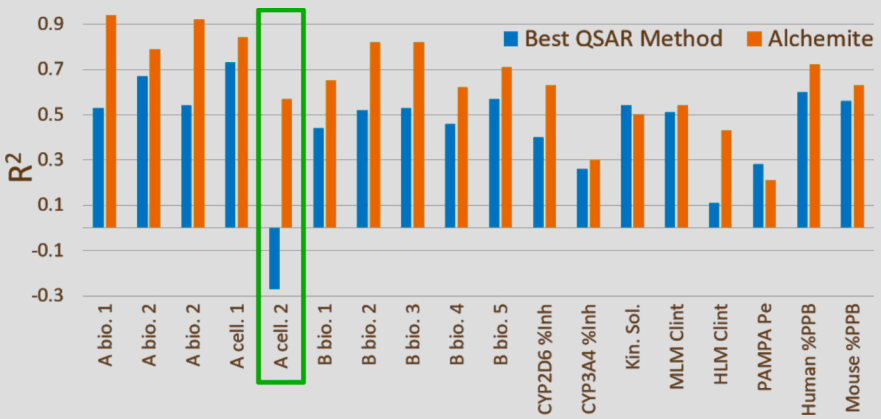




Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

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	$\geq$550[23]

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



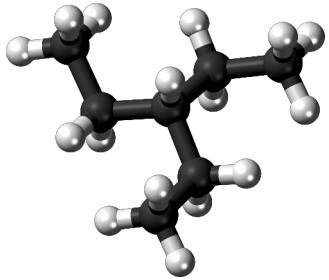
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

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)

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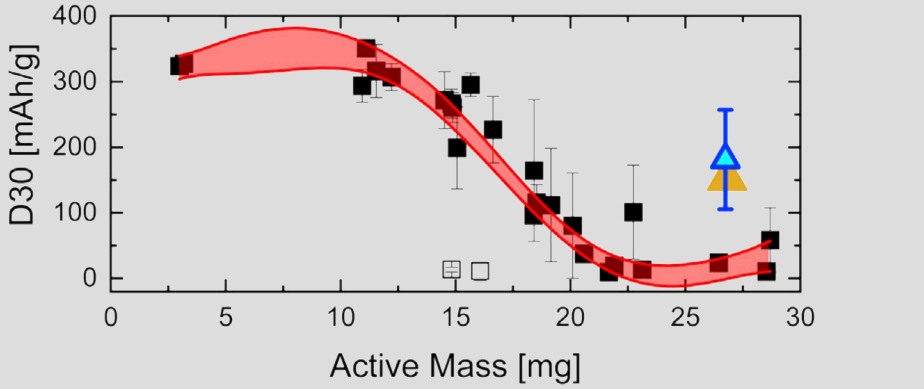
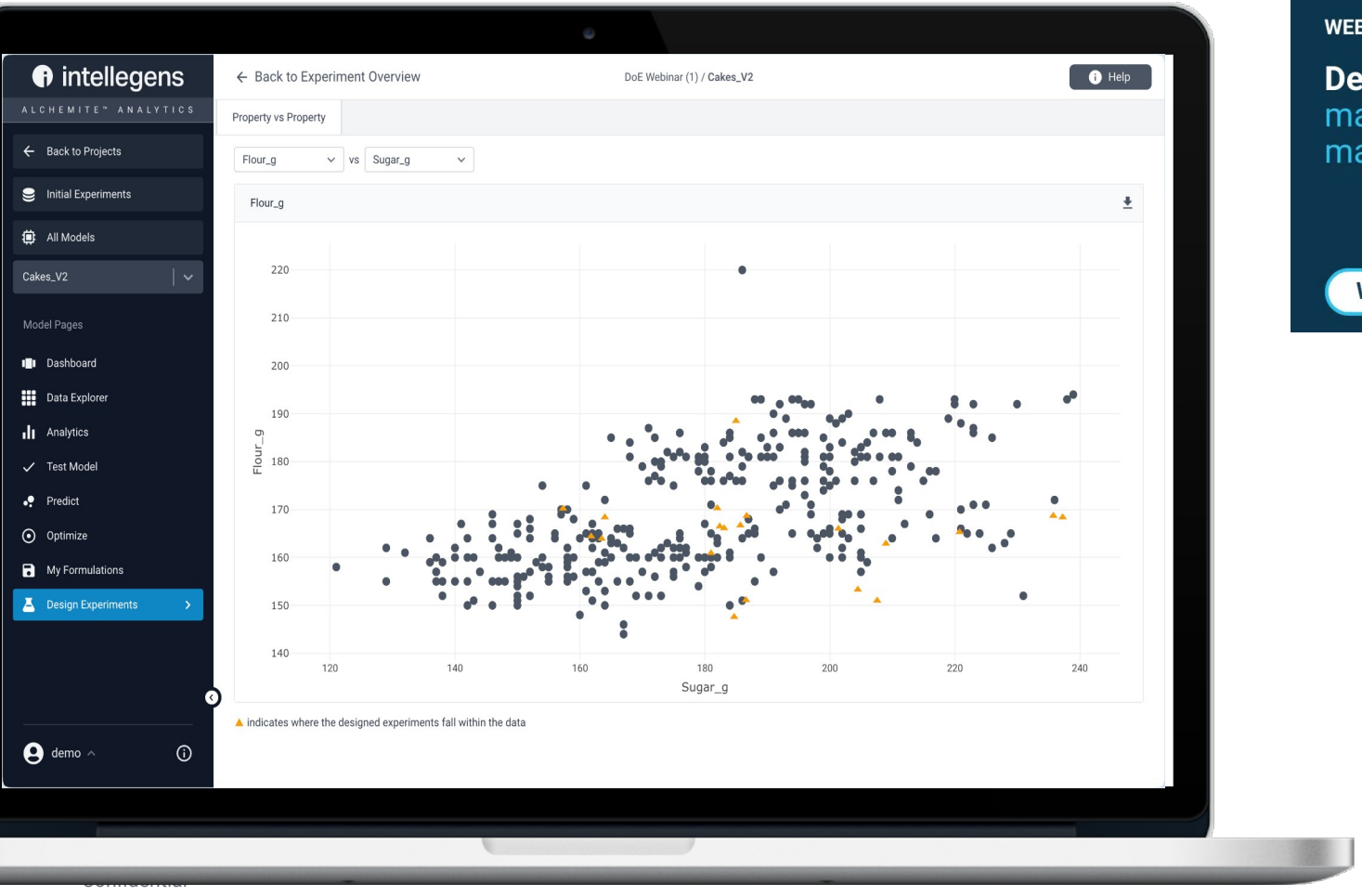


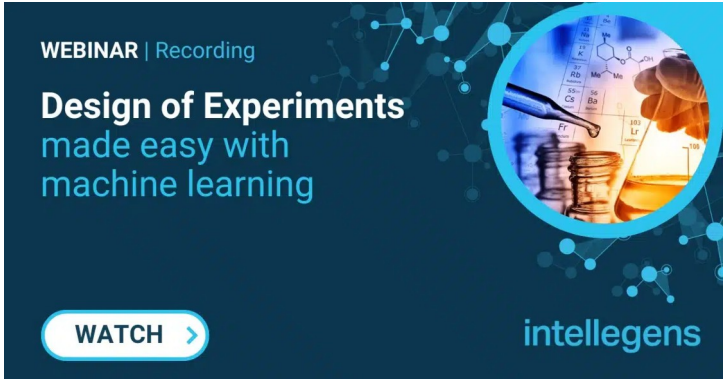
Nature Machine Intelligence **2**, 161 (2020)
Cell Reports Physical Science **2**, 100683 (2021)

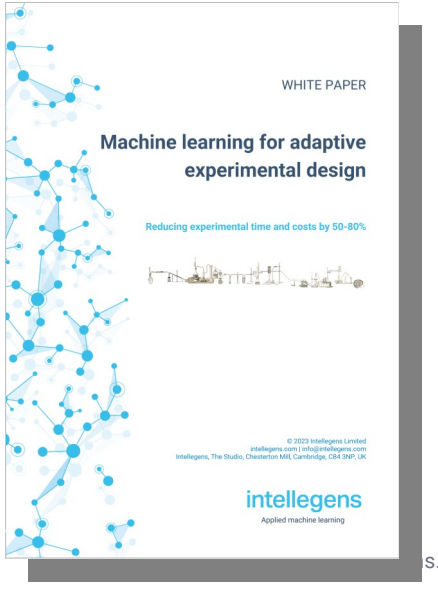
UNIVERSITY OF BIRMINGHAM

Ansys GRANTA

Alchemite™ module for adaptive experimental design







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