intellegens

Applied machine learning

Apply Alchemite™ machine learning to academic research

14 June 2023

Today's live, interactive session

Host
Stephen Warde
Intellegens Marketing

Presentation
Dr Gareth Conduit
Intellegens CSO

Please ask **questions** at any time

- Use the "Questions" box on the control panel
- Questions will be answered at the end of the webinar

Look out for a follow-up email with links to the **presentation slides** and a **recording** of the webinar

Introducing Intellegens

Applied machine learning

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

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

Strong focus on ease-of-deployment for immediate return on investment

Agenda

Gareth Conduit
Alchemite™ use in academic research

Stephen Warde
Alchemite™ Academic Programme

Q&A

Genesis of Alchemite™

Early development of the methodology

2013

Multiple properties for Rolls Royce engines

Further development of the methodology

2013	2014
Multiple properties for Rolls Royce engines	Property- property correlations with Rolls Royce and BP

Nickel superalloys with
Rolls Royce University Technology Centre

Dr Vadegadde Duggappa

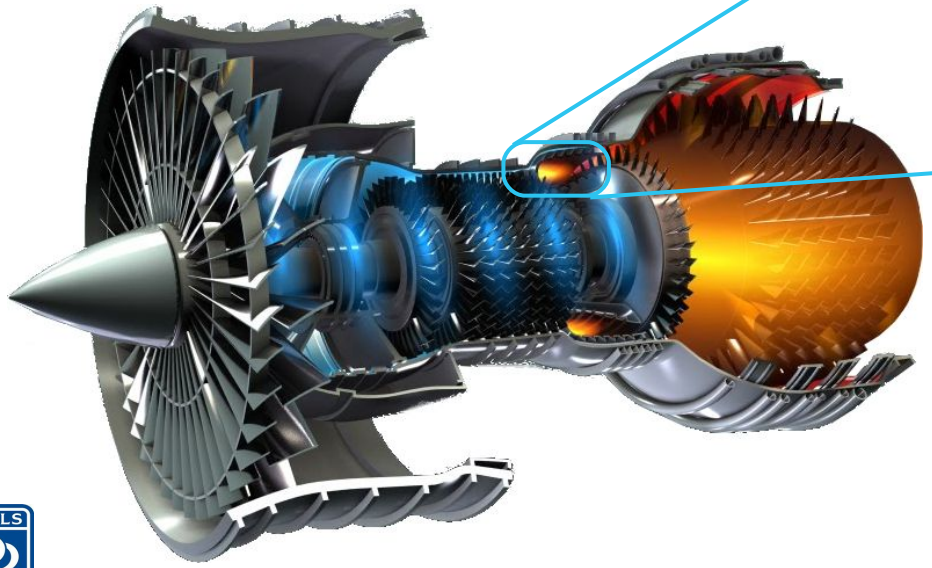
Dr Bryce Conduit

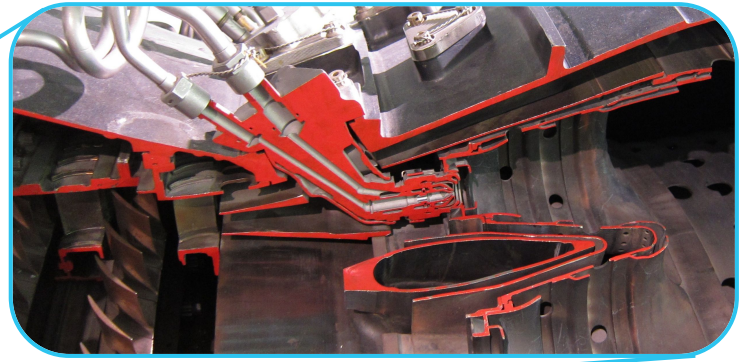
Professor Howard Stone

Dr Gareth Conduit

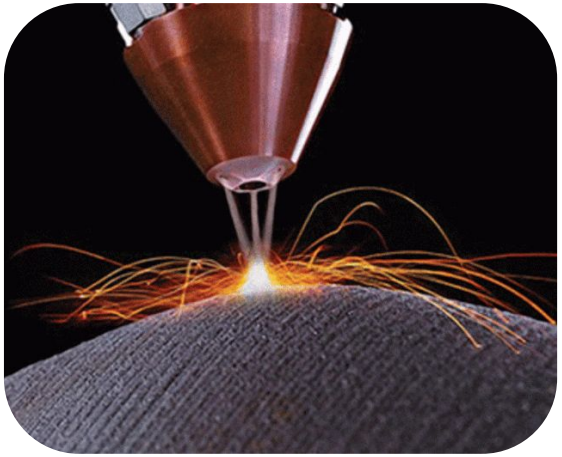
Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)

Jet engine schematic



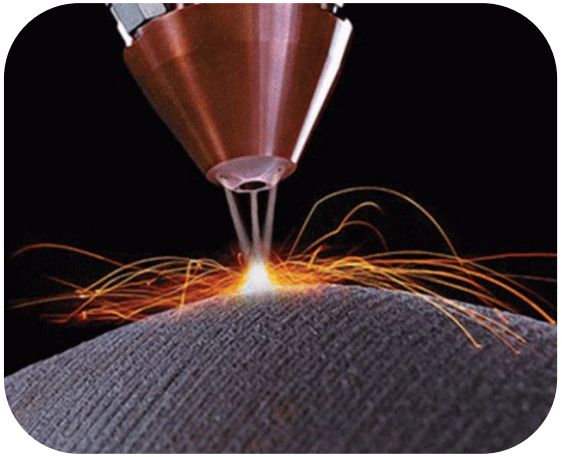


Little data for 3D printing



3D printing

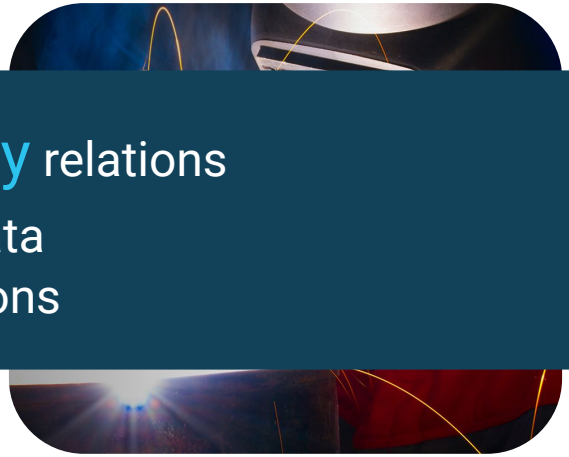
Ability for printing and welding are strongly correlated



3D printing

Welding

Ability for printing and welding are strongly correlated

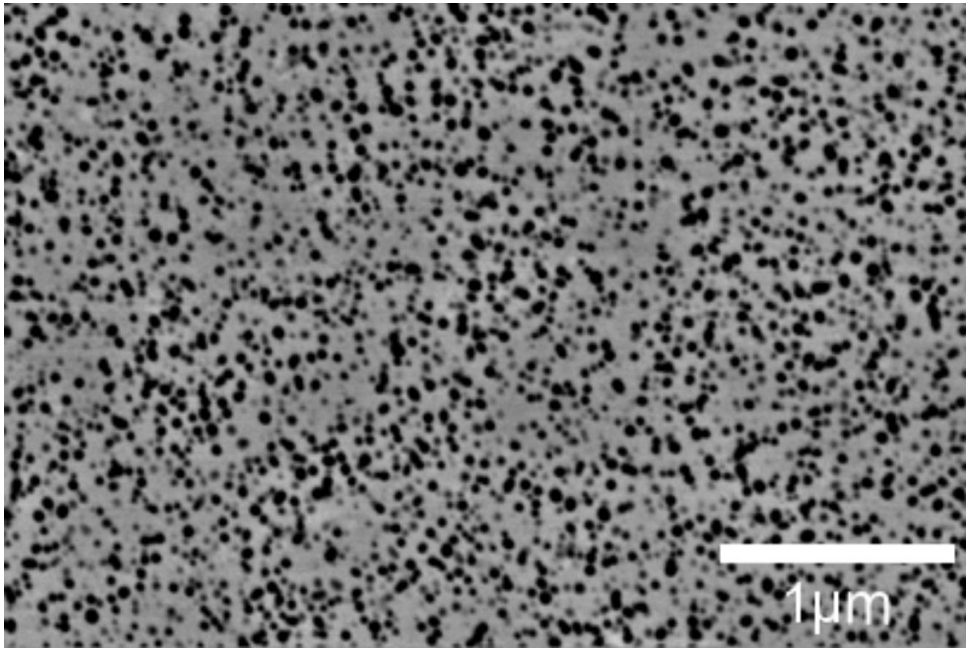


Exploit property-property relations
to impute spare data
and improve predictions

3D printing

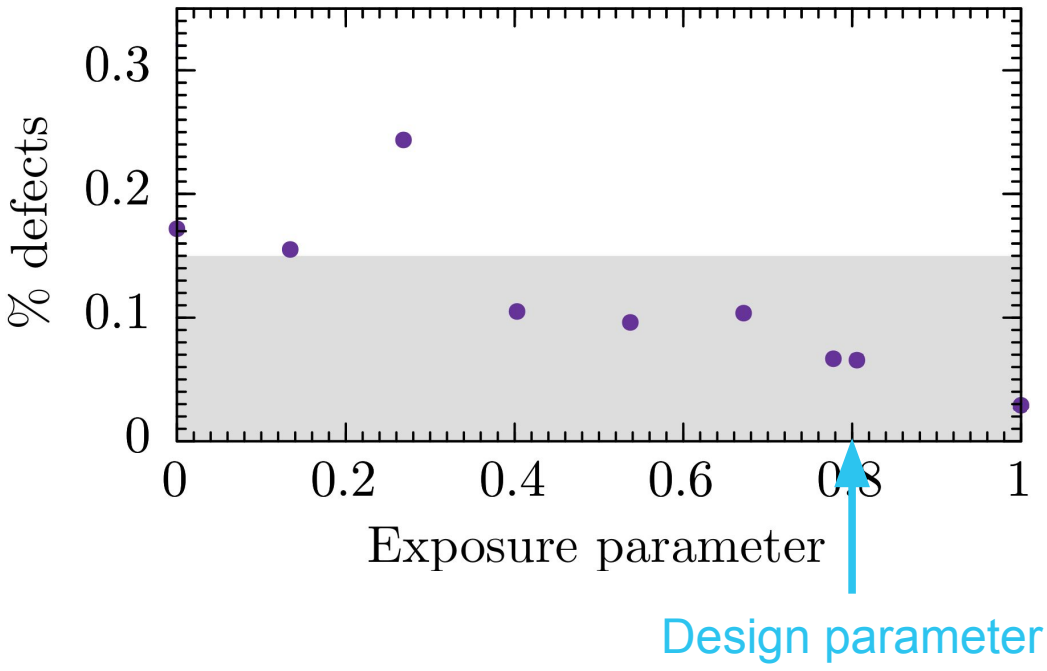
Welding

Microstructure



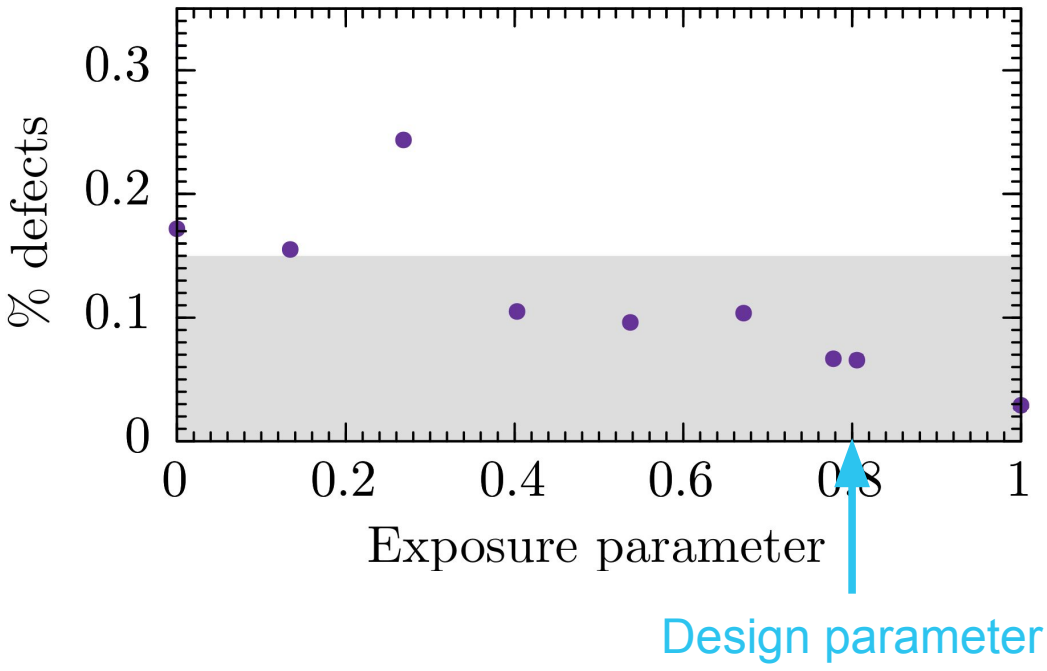
Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design **168**, 107644 (2019)

Testing the defect density



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

Testing the defect density



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

Focus on machine learning

Concurrent materials design

2013

Multiple properties for Rolls Royce engines

2014

Property- property correlations with Rolls Royce and BP

2015

Royal Society University Research Fellowship

Apply and refine approach to other areas

Concurrent materials design

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

First study in drug discovery

Concurrent materials design

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

Founding of Intellegens

Ben Pellegrini

Dr Gareth Conduit

Case studies with customers

2019

Develop approach and publish case studies

Drug design with Optibrium
for the Open Source Malaria contest

Dr Ben Irwin

Dr Mario Öeren

Dr Tom Whitehead

Dr Gareth Conduit

An Open Drug Discovery Competition: Experimental Validation of Predictive Models in a Series of Novel Antimalarials
Journal of Medicinal Chemistry 64, 16450 (2021)

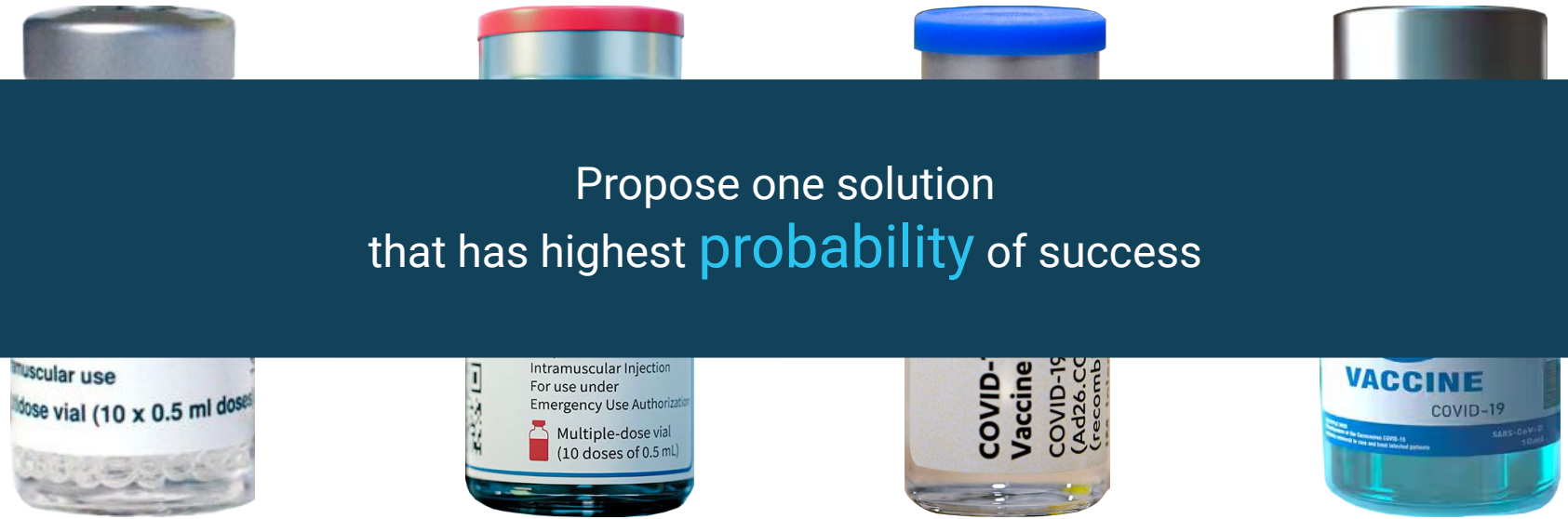
Open Source Malaria contest

OPEN SOURCE MALARIA

Looking for New Medicines

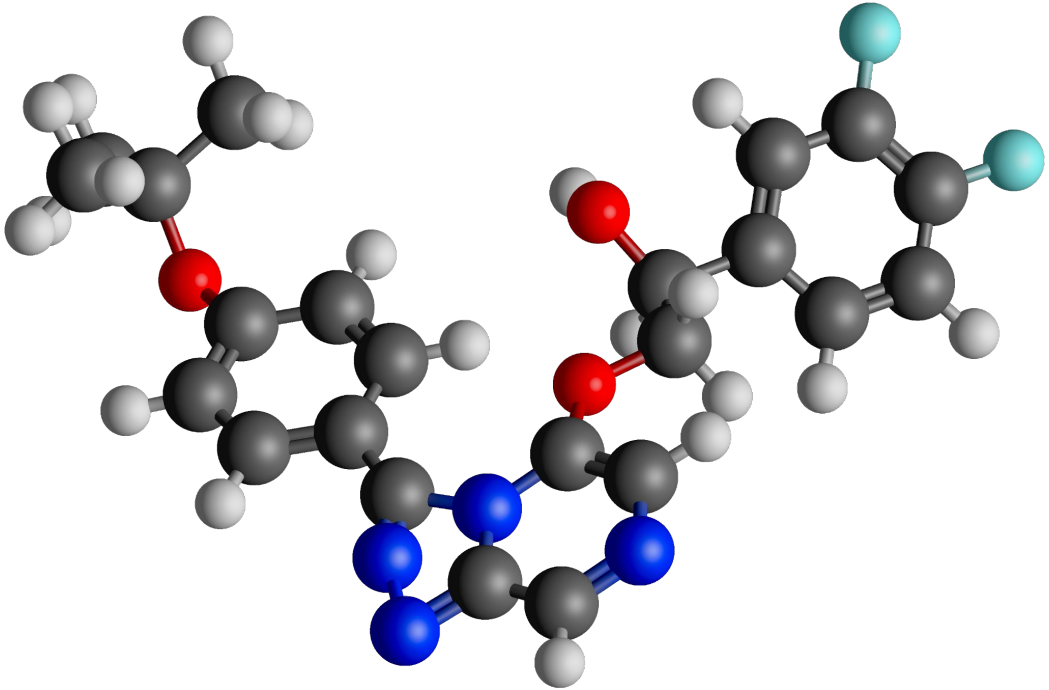
Different drugs can treat the same ailment

Different drugs can treat the same ailment



Propose one solution
that has highest probability of success

Open Source Malaria experimental validation



Activity 0.647 µM

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

Launch of Alchemite™ product

2019	2020
Develop approach and publish case studies	Launch Alchemite Analytics™ product

Focused product for drug discovery

optibrium

2019	2020	2021
Develop approach and publish case studies	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium

Algorithms to extract further information

optibrium

Cerella

2019	2020	2021	2022
Develop approach and publish case studies	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Extract additional information from noise

Exploit uncertainty to design concrete with

Department of Civil Engineering

Bogdan Zviazhynski

Jess Forsdyke

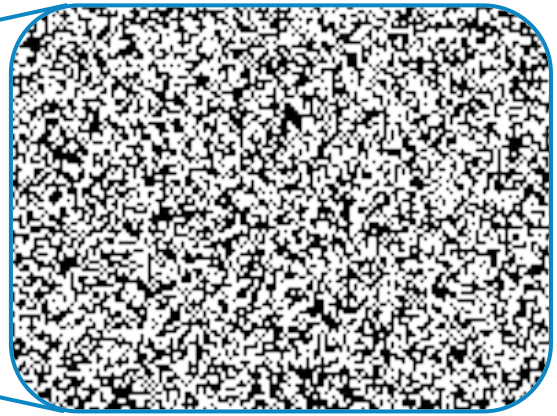
Professor Janet Lees

Dr Gareth Conduit

Unveil the unseen: exploit information hidden in noise
Applied Intelligence **53**, 11966 (2023)
Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

Cement & aggregate comprise concrete

Cement & aggregate look like noise

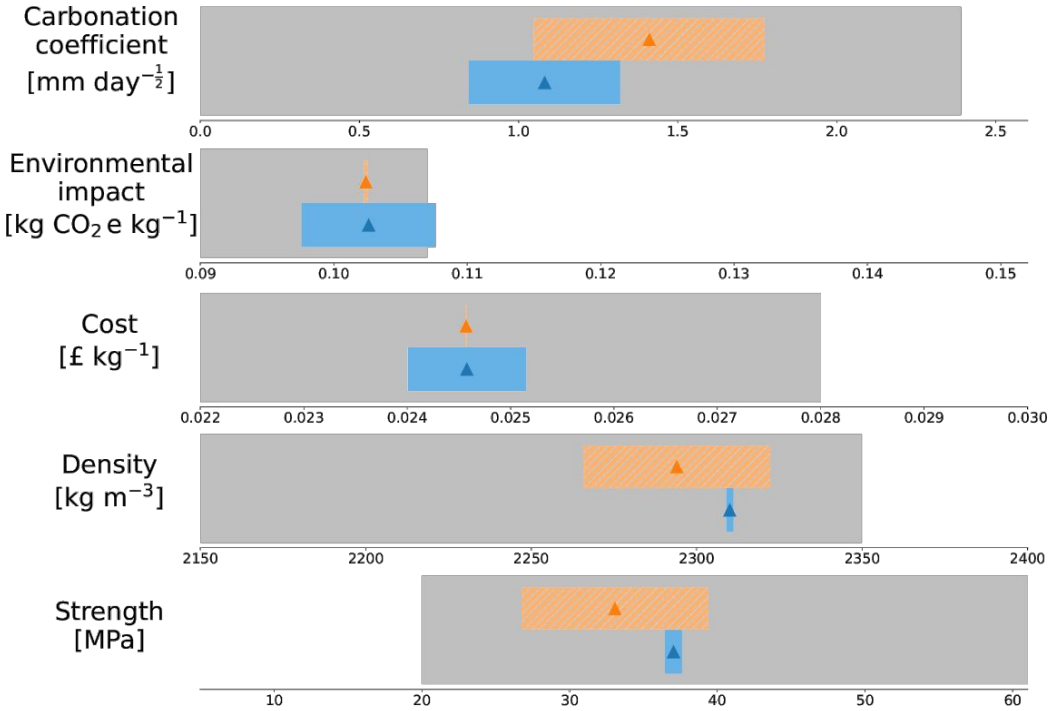


Cement & aggregate look like noise

Extract information from
amplitude of noise

Concrete manufacture

Experimental validation



Target

Prediction

Experiment

Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

Further academic work

THE FARADAY INSTITUTION

Agency for Science, Technology and Research
SINGAPORE

The University Of Sheffield.

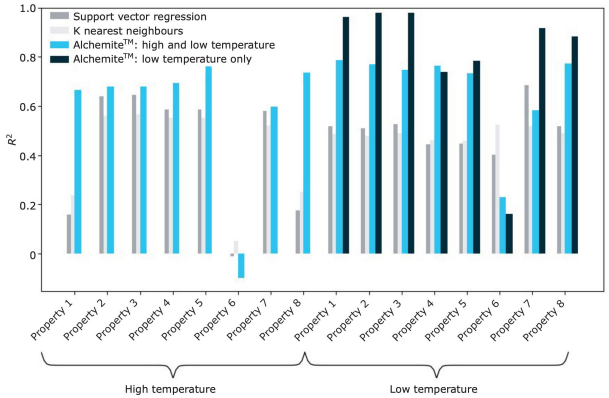
COLORADO SCHOOL OF MINES

UNIVERSITY OF BIRMINGHAM

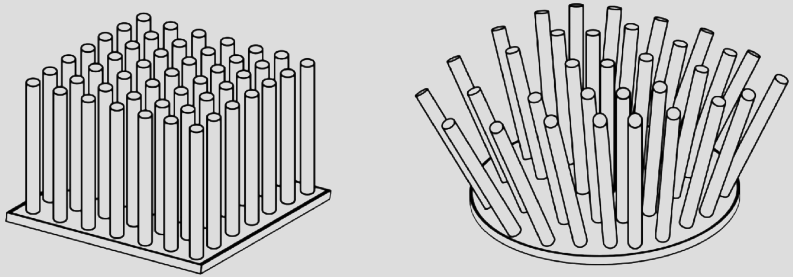
CBPF

UNIVERSITEIT GENT

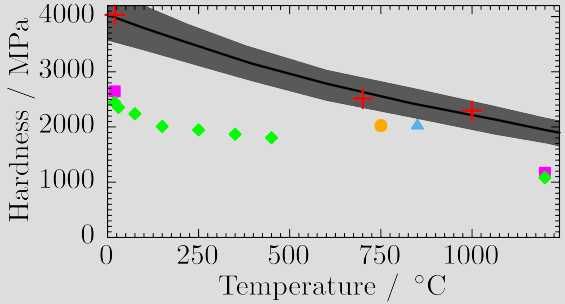
UNIVERSITY OF CAMBRIDGE

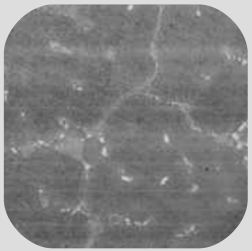


Johnson Matthey Technology Review **66**, 130 (2022)



NASA Technical Memorandum 20220008637

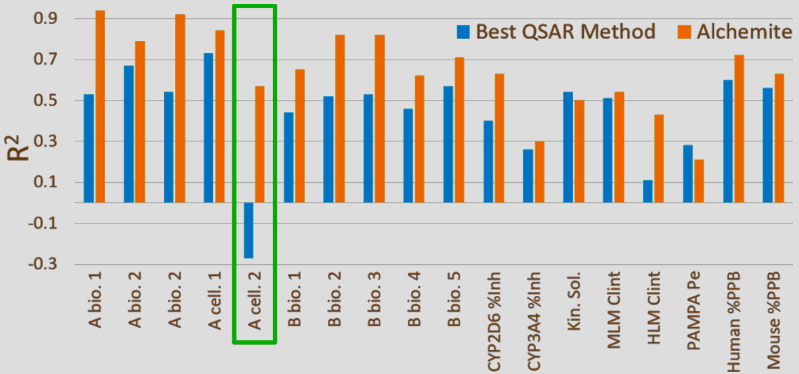




Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

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]

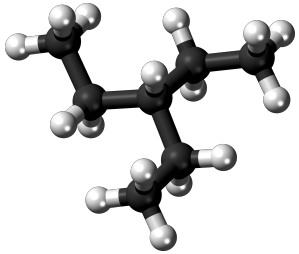
Computational Materials Science **147**, 176 (2018)



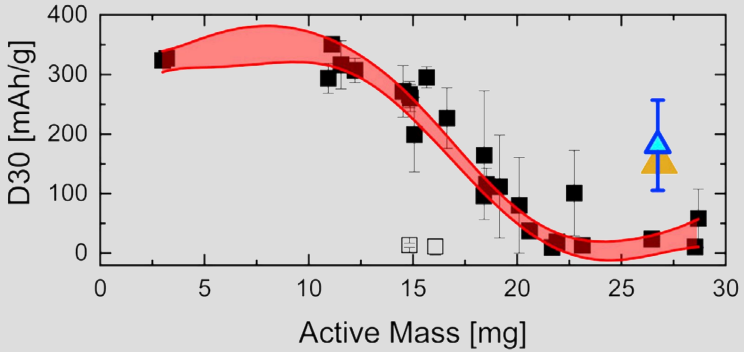
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

optibrium™

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



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

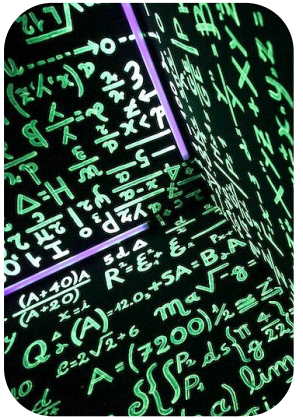


Nature Machine Intelligence **2**, 161 (2020)
Cell Reports Physical Science **2**, 100683 (2021)

Alchemite™ for academics

optibrium

Cerella



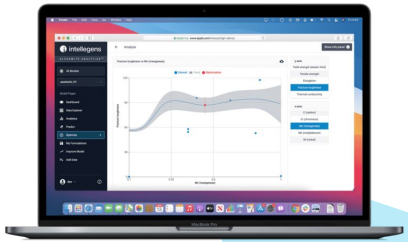
2019	2020	2021	2022	2023
Develop approach and publish case studies	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Extract additional information from noise	Alchemite™ academic program

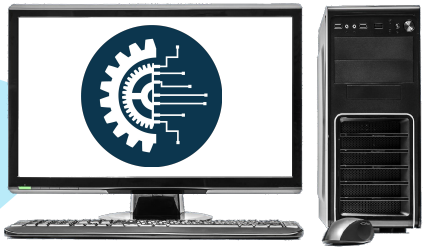
Alchemite™ Academic Programme

The Alchemite™ Products

Alchemite™ Analytics

- Web UI – insights on your desktop
- Optimise products, extract value from data, guide experiment





Alchemite™ Engine

- Integrate into your workflows (API, Python)
- Advanced configuration, deploy models

Lab systems

Software & scripts

Sharing & collaboration

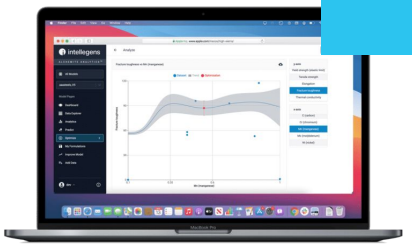
Alchemite™ Success

- Use our expertise in applying ML
- Ranging from ‘getting started’ advice to full project management

The Alchemite™ Academic Programme

Alchemite™ Analytics

- Web UI – insights on your desktop
- Optimise products, extract value from data, guide experiment



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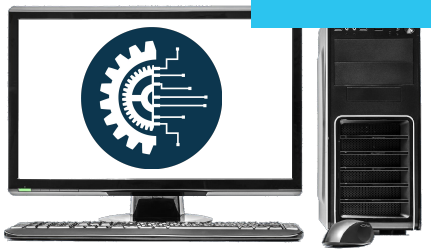

Alchemite™ Engine

- Integrate into your workflows (API, Python)
- Advanced configuration, deploy models

Lab systems

Software & scripts

Sharing & collaboration

80%+ discount on commercial pricing of Alchemite™

1 year or 3 year options

Members have full access to documentation but scientific support services are not included.

To qualify for the Programme you must…

Be engaged in **academic research** at a university

Not use the software to support any commercial collaboration or for-profit activity

Reference use **Alchemite™** in any **presentation** or **publication** describing work that included processing or analysis of data using the software

Summary

Applied machine learning

Research insights for materials, chemicals, life sciences, and beyond...

What?

Apply a proven, leading edge ML method

Key features

Handles sparsity, Accurate uncertainty calcs, Computationally efficient

So what?

Free up research time otherwise spent on method R&D, coding, analytics, etc…

What's next?

gareth@intellegens.com

/company/intellegensai

Academic Programme
intellegens.com/academic

Scientific papers
intellegens.com/article-type/papers/

Next webinar (6 July)
Combining ML with physics and chemistry modelling
intellegens.com/webinars

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