intellegens

APPLIED MACHINE LEARNING

Towards net zero with machine learning: battery and materials development

Dr Gareth Conduit

Introducing Intellegens

Unique **deep learning** software and expertise

- Get value from **sparse, noisy data** to solve complex **high-dimensional** problems

Easily deploy models to deliver **immediate ROI**

- Integrate with existing systems and/or applied through a web based platform

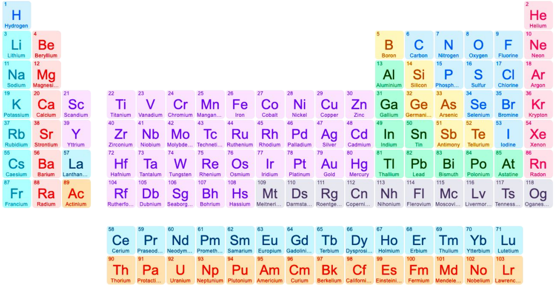
Can be applied to any **numerical dataset**

- Key focus areas: materials, chemicals, manufacturing, batteries, drug discovery

Two ways machine learning could help to achieve net zero

Machine learning materials and formulations

Formulation



Black box

Properties

Cells

Modules

Packs

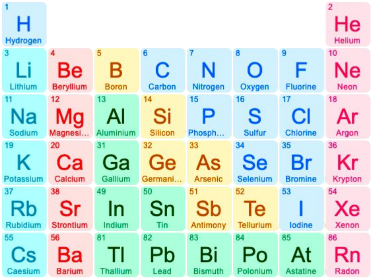
In service

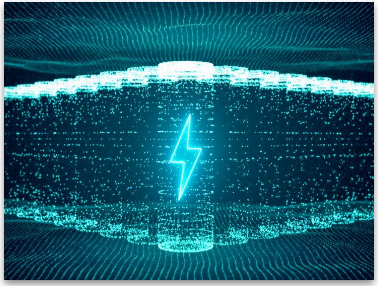
With machine learning you could…

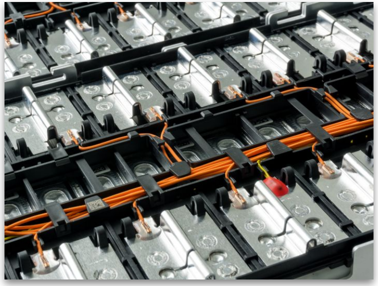
Materials and formulation

Management software

Cell & pack design







Materials → Cells → Modules → Packs → In service

But it’s not so easy in real-word R&D!

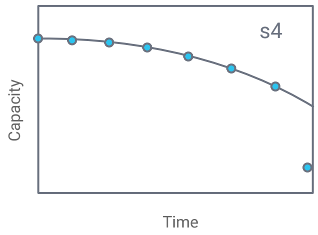
Challenge 1: Working with real-world data

Sparse
Data is missing

High-dimensional
Many independent inputs & outputs

Cell 1	5.5	149	0.6	1	1.4±0.2		7,4	15.1	8.
Cell 2	0.2		0.9	0	2.3±0.3	s2	3.8		8.3
Cell 3	22.4	170		1	4.5±1.1	s3	6.4	-2.3	
Cell 4	12.3	179	0.4	1	3.7±0..6	s4		12.1	0.
Cell 5		160	0.3			s5	6.1		6.
Cell 6	8.9	154	0.6	0	6.1±1.2	s6	4.2	22.1	
Cell 7	16.4		0.5	1	2.6±0.2	s7	5.7	13.2	
Cell 8	[illegible]				[illegible]				

Series data
e.g., time series



Noisy
Errors or inherent variability

Challenge 2: Making ML work in practice

Data scientists

Sparse data problems require time-consuming workarounds

You build valuable models but colleagues don't use them

Scientists, engineers, analysts…

Too much setup/training required

Fails for your (sparse) data

Difficult to interpret the results

The Alchemite™ solution

Introducing Alchemite™

Unique, proprietary algorithm from the University of Cambridge

Deep, iterative **imputation** method

- Novel implementation of a neural network, where all inputs are also outputs

Quantifies **uncertainty** through advanced, non-parametric probability distributions

Design **optimal** materials

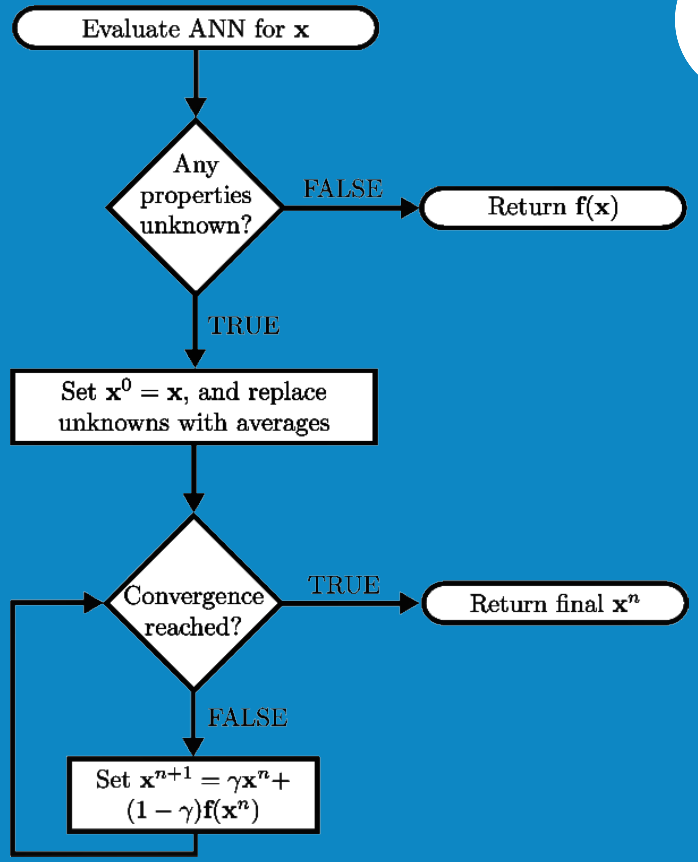
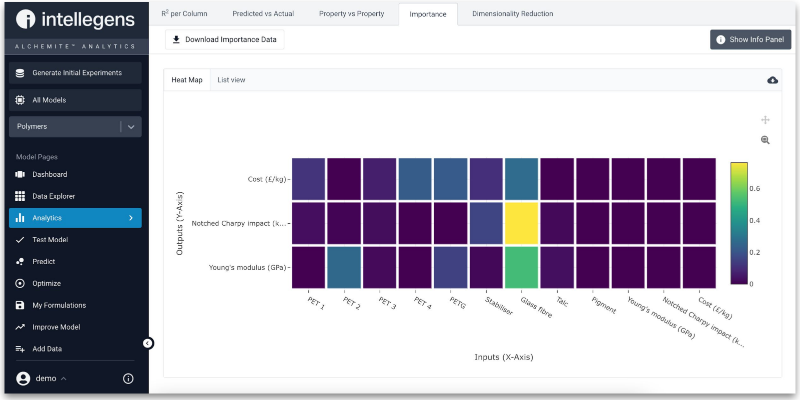
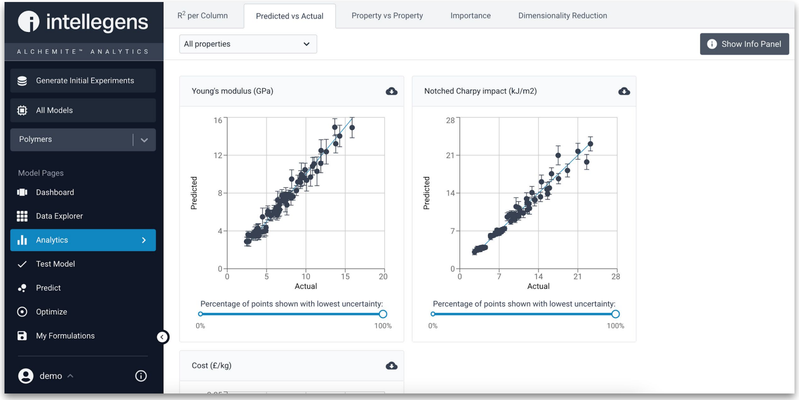
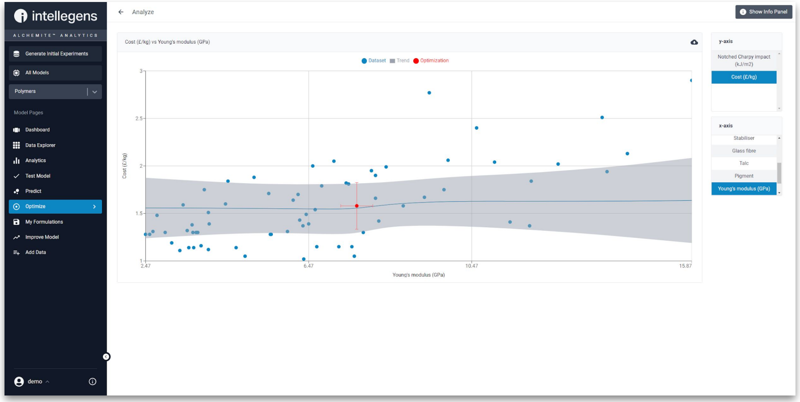


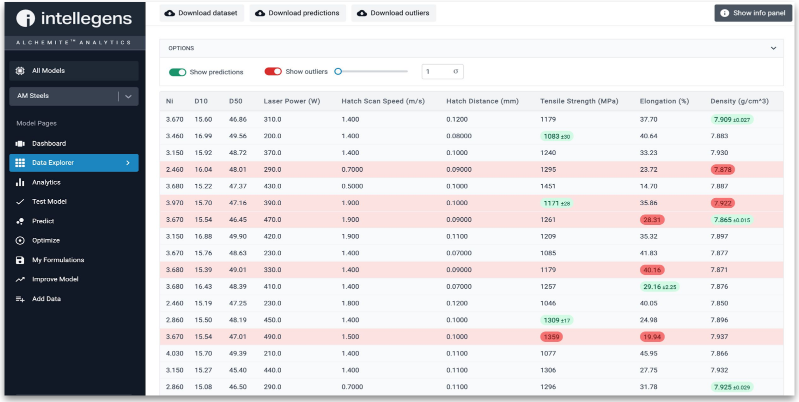
Figure 2 from Computational Materials Science ***147****, 176 (2018)*

‘Explainable AI’ with an easy-to-use interface



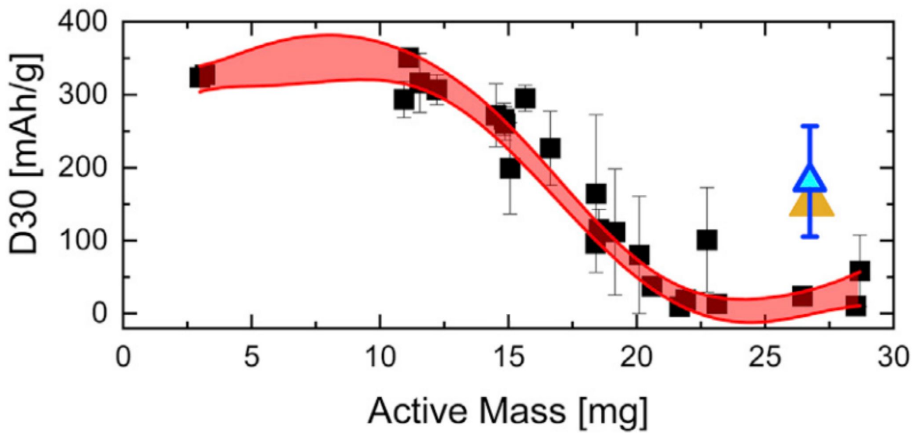






Case studies

Electrode materials



Cell Reports Physical Science
2, 100683 (2021)

New electrode designed using Alchemite™ (▲) to deliver high discharge specific capacity (D30) and high active mass

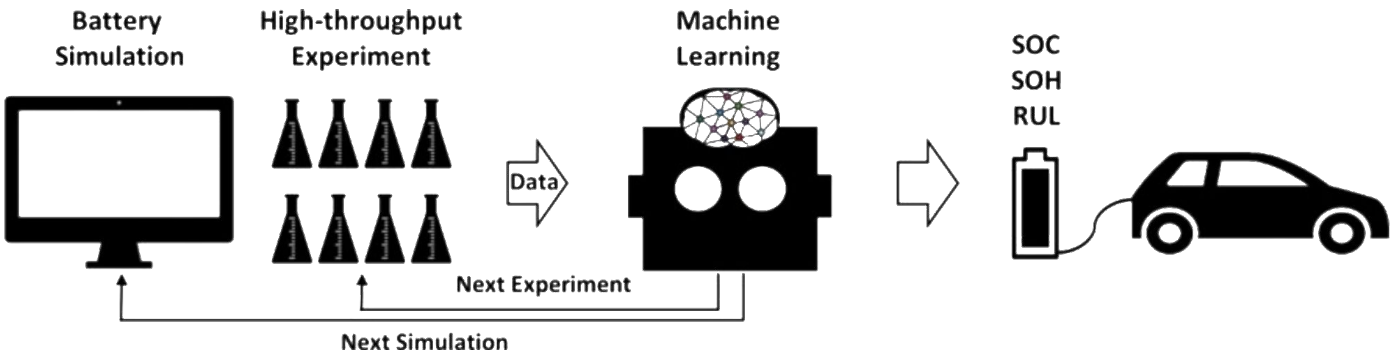
Experimentally verified (▲) to outperform existing cells (■)

UNIVERSITY OF BIRMINGHAM

Ansys

THE FARADAY INSTITUTION

Management software



Nature Machine Intelligence **2** 161-170 (2020)

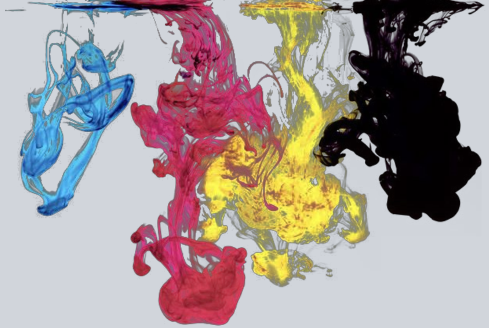
Predict the State of Charge / Health & Remaining Useful Life using ML

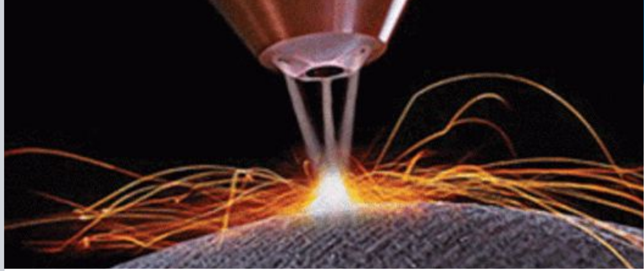
Result: accurate predictions for EV batteries at low computational cost

Agency for Science, Technology and Research SINGAPORE

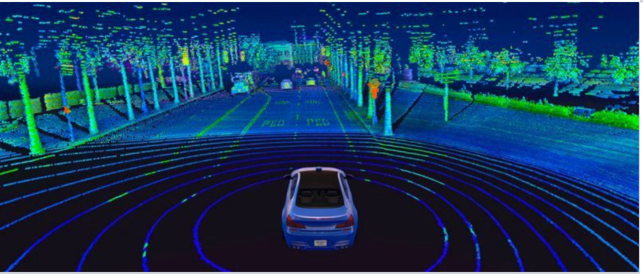
NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

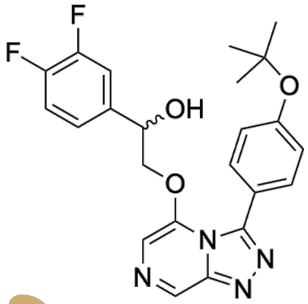
UNIVERSITY OF CAMBRIDGE

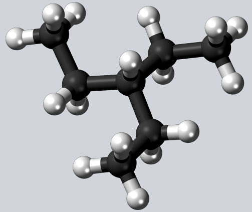




Heat exchanger
& shape memory
alloy applications





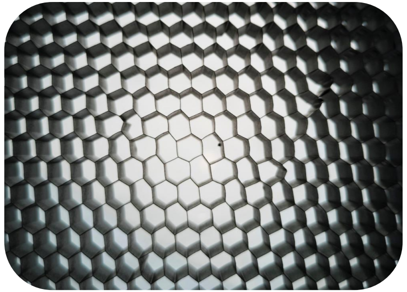


Fluid Phase Equilibria
501, 112259 (2019)

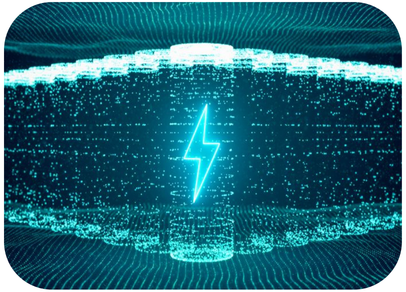
Journal of Chemical Physics
153, 014102 (2020)

Summary

Applied machine learning for energy storage



Solve materials and formulation challenges with fewer experiments, saving time & cost



Optimise battery cells and packs, reducing the number of tests and prototypes

Understand and predict key battery metrics for improved performance

Next steps

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Website https://intellegens.ai

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

Demo https://app.intellegens.ai

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