



# 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

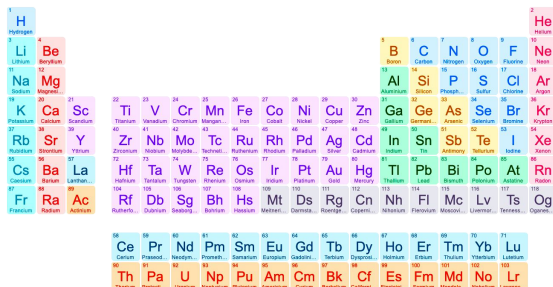
# Machine learning materials and formulations



Formulation

Black box

Properties



A standard periodic table of elements, color-coded by groups. The elements are arranged in rows and columns, with their symbols and names visible.



Cells

Modules

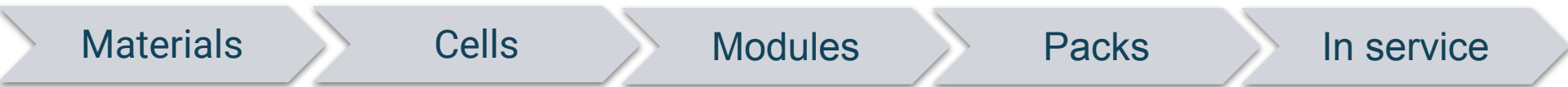
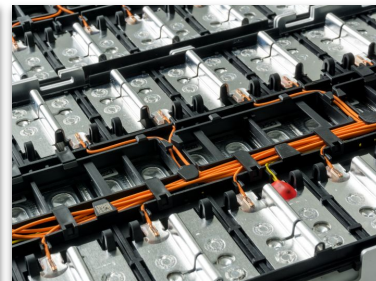
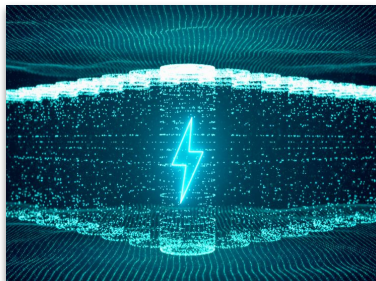
Packs

In service

# With machine learning you could...



1 H Hydrogen	2 He Helium																														
3 Li Lithium	4 Be Beryllium	5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon																								
11 Na Sodium	12 Mg Magnesium	13 Al Aluminum	14 Si Silicon	15 P Phosph...	16 S Sulfur	17 Cl Chlorine	18 Ar Argon																								
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germani...	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton														
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon														
55 Cs Caesium	56 Ba Barium	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodym...	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon





But it's not so easy in real-world R&D!

# Challenge 1: Working with real-world data



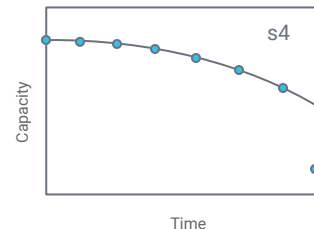
**Sparse**  
Data is missing

**High-dimensional**  
Many independent inputs & outputs

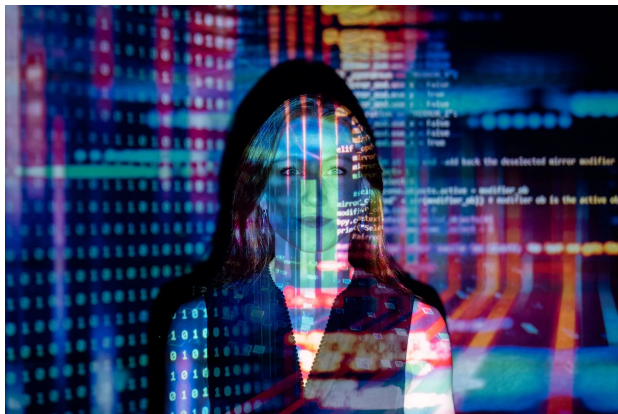
Cell 1	5.5	149	0.6	1	1.4±0.2		7.4	15.1	8.5
Cell 2	0.2		0.9	0	2.3±0.3	s2	3.8		8.3
Cell 3	22.4	170		1	4.5±1.1	s3	6.4	-2.3	
Cell 4	12.3	179	0.4	1	3.7±0.6	s4		12.1	0.4
Cell 5		160	0.3			s5	6.1		
Cell 6	8.9	154	0.6	0	6.1±1.2	s6	4.2	22.1	
Cell 7	16.4		0.5	1	2.6±0.2	s7	5.7	13.2	
Cell 8									

**Noisy**  
Errors or inherent variability

**Series data**  
e.g., time series



# 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

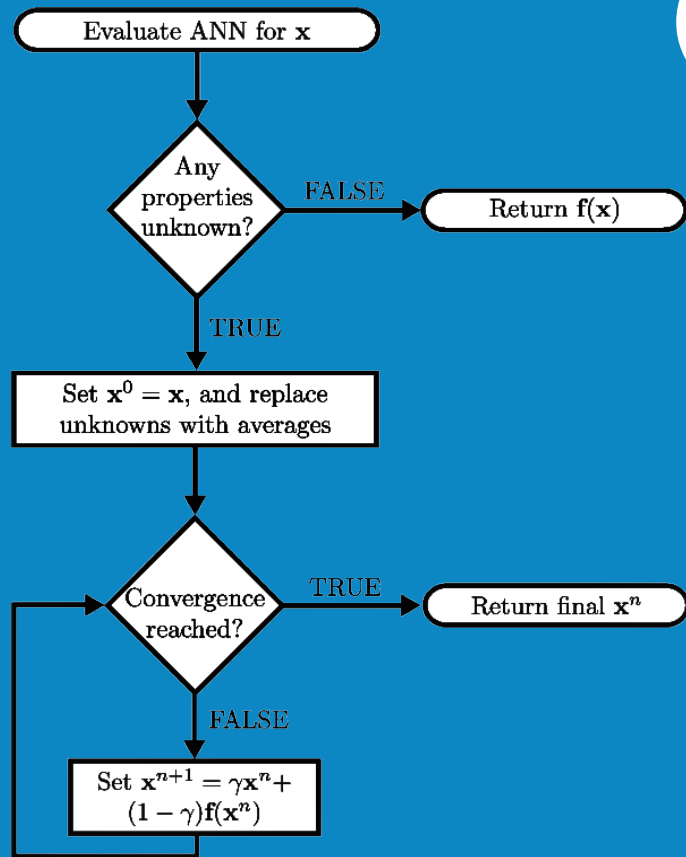


Figure 2 from *Computational Materials Science* **147**, 176 (2018)



# 'Explainable AI' with an easy-to-use interface

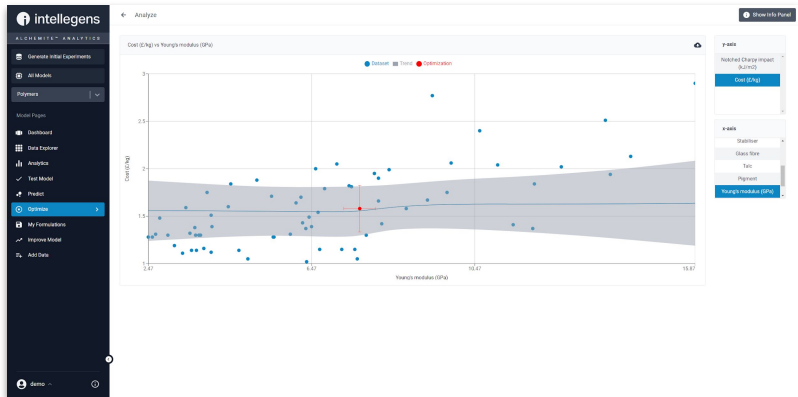
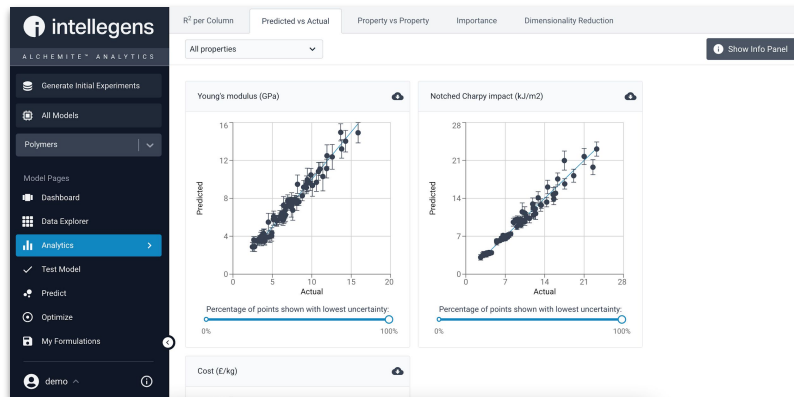
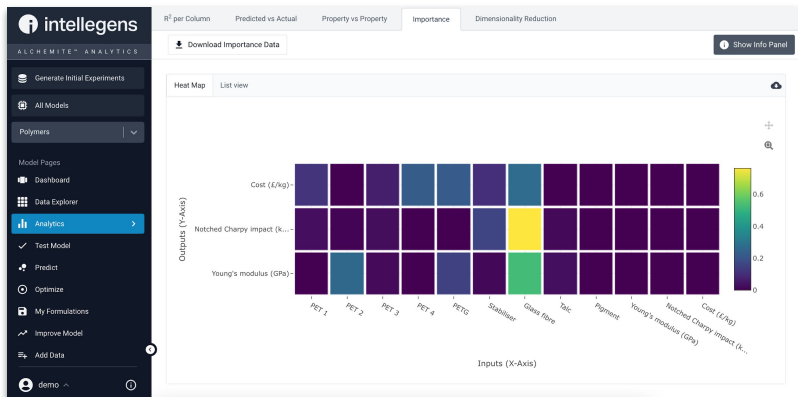


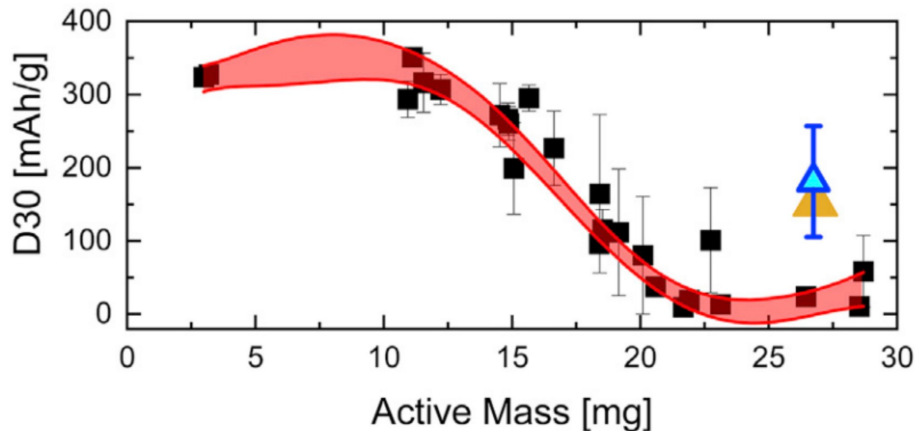
Table showing model predictions and outliers for various material properties. The table includes columns for Ni, D10, D50, Laser Power (W), Hatch Scan Speed (m/s), Hatch Distance (mm), Tensile Strength (MPa), Elongation (%), and Density (g/cm<sup>3</sup>).

Ni	D10	D50	Laser Power (W)	Hatch Scan Speed (m/s)	Hatch Distance (mm)	Tensile Strength (MPa)	Elongation (%)	Density (g/cm <sup>3</sup> )
3.670	15.60	46.86	310.0	1.400	0.1200	1179	37.70	7.909 ±0.027
3.460	16.99	49.56	200.0	1.400	0.08000	1063 xvi	40.64	7.883
3.150	15.92	48.72	370.0	1.400	0.1000	1240	33.23	7.930
2.460	16.04	48.01	290.0	0.7000	0.09000	1295	23.72	7.878
3.680	15.22	47.37	430.0	0.5000	0.1000	1451	14.70	7.887
3.970	15.70	47.16	390.0	1.900	0.1000	1177 xxi	35.06	7.922
3.670	15.54	46.45	470.0	1.900	0.09000	1261	26.31	7.865 ±0.015
3.150	16.88	49.96	420.0	1.900	0.1100	1209	35.32	7.897
3.670	15.76	48.63	230.0	1.400	0.07000	1085	41.83	7.877
3.680	15.39	49.01	330.0	1.400	0.09000	1179	45.16	7.871
3.680	16.43	48.39	410.0	1.400	0.07000	1257	29.16 ±0.15	7.876
2.460	15.19	47.25	230.0	1.800	0.1200	1046	40.05	7.850
2.860	15.90	48.19	490.0	1.400	0.1000	1309 xiv	24.98	7.896
3.670	15.54	47.01	490.0	1.500	0.1000	1350	19.34	7.937
4.030	15.70	49.39	210.0	1.400	0.1100	1077	45.95	7.866
3.150	15.27	45.40	440.0	1.400	0.1100	1066	27.75	7.932
2.860	15.08	46.50	290.0	0.7000	0.1100	1296	31.78	7.925 ±0.021



# Case studies

# Electrode materials



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

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

Cell Reports Physical Science  
2, 100683 (2021)

Confidential



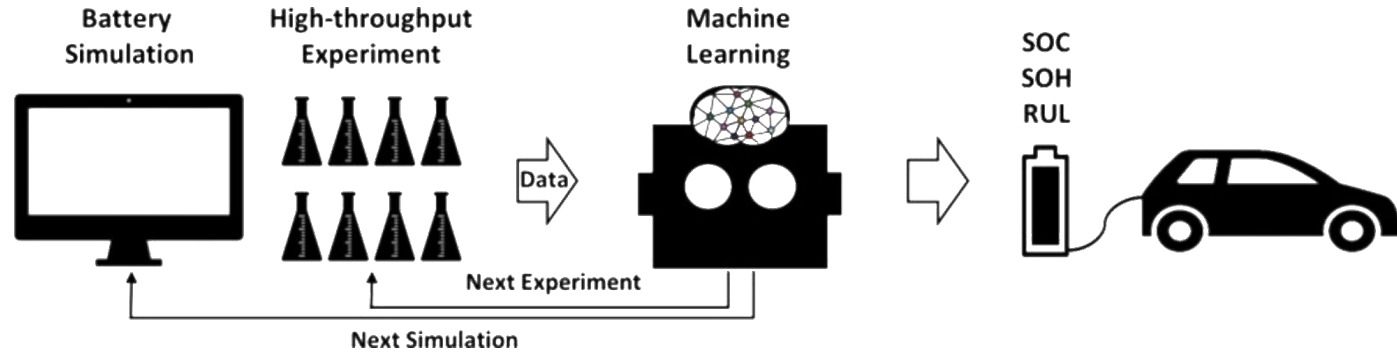
UNIVERSITY OF  
BIRMINGHAM

Ansys



THE FARADAY  
INSTITUTION

# Management software



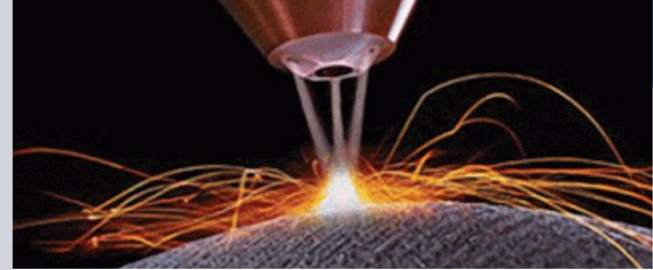
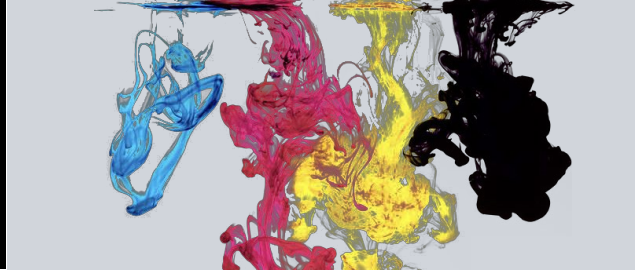
Nature Machine Intelligence 2 161-170 (2020)

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

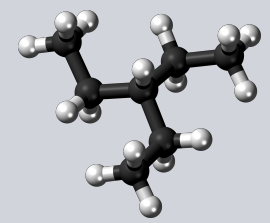
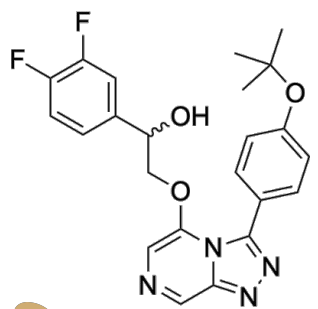
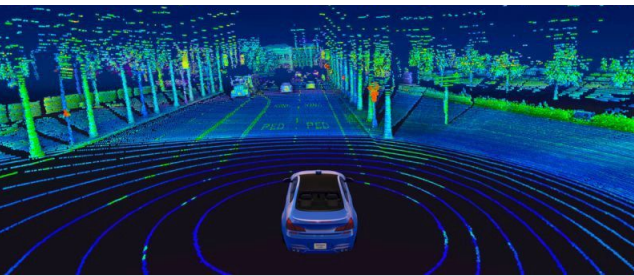
Result: accurate predictions for EV  
batteries at low computational cost



UNIVERSITY OF  
CAMBRIDGE



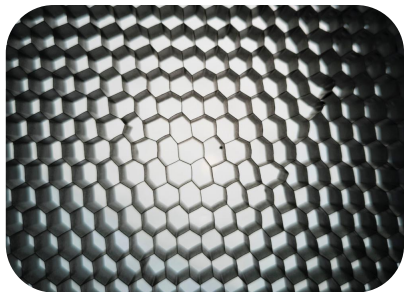
Heat exchanger  
& shape memory  
alloy applications



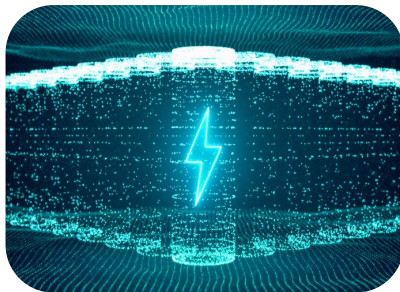
Fluid Phase Equilibria  
501, 112259 (2019)  
Journal of Chemical Physics  
153, 014102 (2020)



## 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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