intellegens

Applied machine learning

Sustainable formulation and battery development using machine learning

Dr Tom Whitehead

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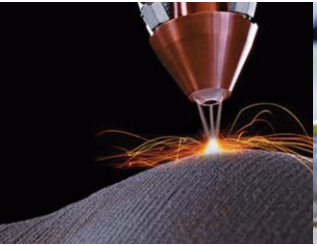
Introducing Intellegens






Applied machine learning

- Key use cases: Chemicals, Materials, Life Sciences, Manufacturing Processes
- Innovative method extracts value from sparse, noisy data to solve complex, high-dimensional problems
- Strong focus on ease-of-deployment for immediate ROI

Optimise products and processes

Save time and cost in experiment

Outline

- The sustainability challenge for formulation chemistry
- ML for formulation development
- Case study: machine learning-driven battery development

The sustainability challenge for chemistry

Driver	Technical objectives and constraints
Consumption	Minimise energy required for processing Minimise raw materials
Sustainability	Minimise carbon footprint of ingredients and processing Maximise use of recycled feedstock
Supply chains	Identify alternative materials

The sustainability challenge for chemistry

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Competitiveness	Maximise ‘performance’ Meet market requirements Minimise time-to-market

Keystone chemistry

“[T]he chemical industry is possibly the most integrated one. As much as 96 percent of everything that is produced needs chemicals”

Jan Secher, CEO of Perstorp, in *Politico*

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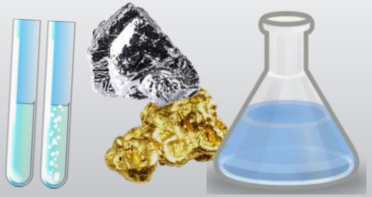
"[T]he chemical industry is possibly the most integrated one. As much as 96 percent of everything that is produced needs chemicals, ***which means that, when chemical products become more sustainable, there is a huge multiplier effect.****"*

Jan Secher, CEO of Perstorp, in *Politico*

The trillion $ formulation problem

High-dimensional, sparse, noisy data

Ingredients



Processes

Properties

Mechanical properties
Cost
Density
Environmental impact
Rheology
Stability ...

Polymers, chemicals, pharmaceuticals, alloys, foods, paints, cosmetics...

High reliance on costly, time-consuming experiment

How do you solve a problem like formulation design?

Try every possible formulation

Guaranteed to find the best formulation

- May be infinitely many possibilities
- Budgets / timescales are finite

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Uses knowledge from past projects

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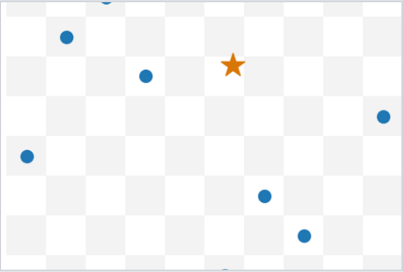
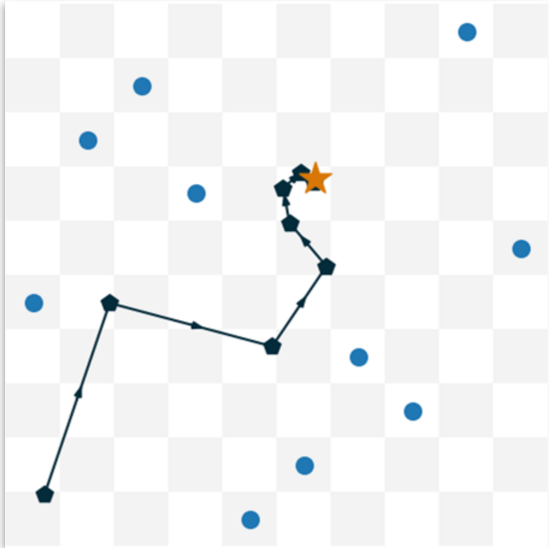


Structured design / DoE

Efficiently covers design space

- May require a large number of experiments
- Requires statistical knowledge

Adaptive Experimental Design



Machine learning-driven
Adaptive Experimental Design

- Target-driven: actively search for successful materials
- Natively handle 100s or 1000s of variables
- No statistical or ML knowledge needed

Alchemite™ technology offers a unique combination

Handle sparse, noisy, complex data

Get value from sparse, noisy data

Unique self-consistent, iterative algorithm imputes sparse data

Optimise against multiple targets

Solves high-dimensional problems that were intractable

Quantify uncertainty to enable rational decisions

Accurate method (nonparametric probability distributions)

A ready-to-use solution

Make a fast start

Auto-generates models, requiring minimal assumptions

Speed and scalability

Light CPU / memory footprint: fast and works for huge datasets

A global view

E.g., ingredients *and* processing parameters in a combined study

How can machine learning help me?

Alchemite™ feature

Data analysis

Understand your data & your formulations

Analytics

How can machine learning help me?

Alchemite™ feature

	**Data analysis**	Understand your data & your formulations	Analytics
	**Screen experiments**	Virtual experiments - 'Which of my many ideas should I prioritize and why?'	Predict

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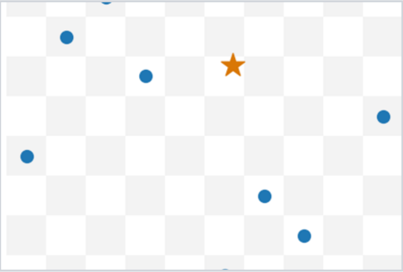
Predict

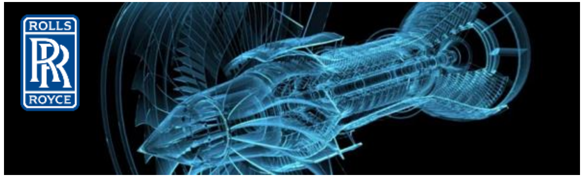


Suggest experiments

'What new formulation space could I explore?' List of potential experiments

Improve Model

Successful applications



Design of an aero alloy

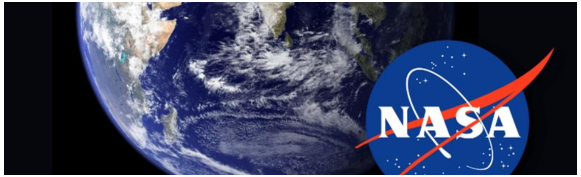
Multi-million $ savings in discovery of new alloy

Ink reformulation

Cut experimental timescales from months to minutes

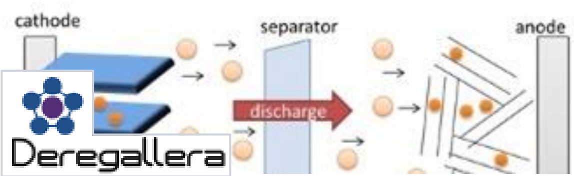
Drug discovery

Predict pharmacokinetics to improve compound selection



Component design

Validating Alchemite™ for advanced engineering at NASA



Sodium-ion batteries

Focus experiment to explore a daunting parameter space

Flavours and fragrances

Predict the sensory properties of compounds

Battery formulation and manufacturing optimization

- Optimization of lithium-ion graphite-based electrodes
- Formulation and manufacturing protocols both have large impact on eventual performance
    - Difficult to uncouple

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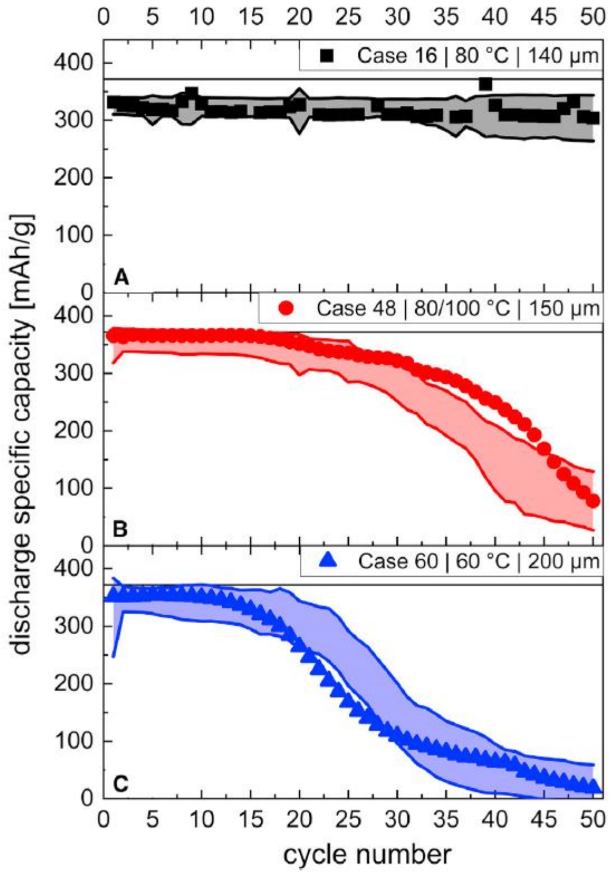
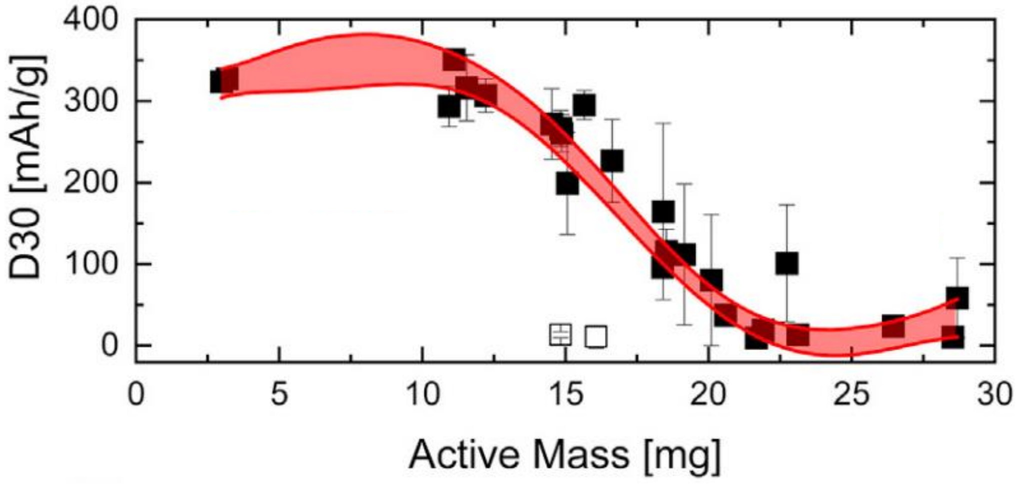
Predicting discharge performance



- Alchemite™ model trained on 85 cells
- Tested against cells generated after training data collected, with different manufacturing processes
- Good qualitative and quantitative agreement between model and predictions

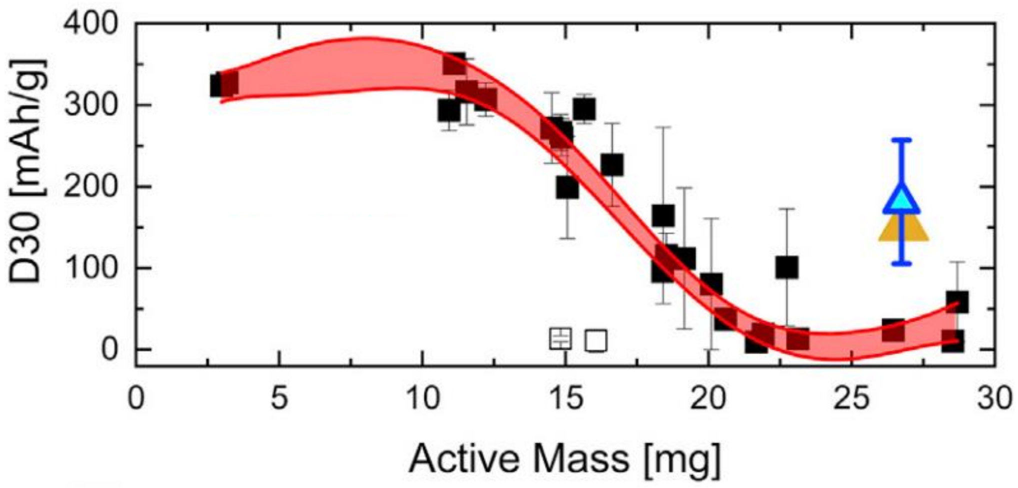
Electrode optimization

- High specific capacity (D30>150 mA.h/g) only achieved for cells with low active mass (<20 mg) and thickness (<100 μm) in existing cells
    - Faster lithiation and delithiation
- For high-energy-density applications we need improved areal capacity



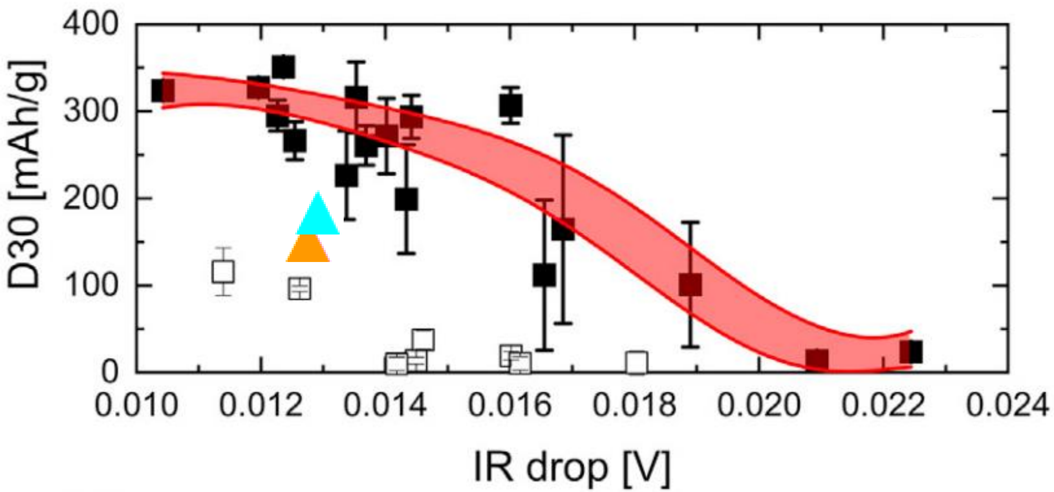
Electrode optimization

- Alchemite™ proposed cell with lower carbon black, reducing binder requirement and increasing graphite content
- Alchemite™ predictions (▲) confirmed by experiment (▲)
- **2.5x** higher D30 (152 mA.h/g) than cells with similar active mass



Other properties

- Internal resistance of cell gives clues to mechanism
- Alchemite™ able to predict all experimental properties simultaneously: analyse mechanism without running all experiments



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Any questions?

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