



# intellegens

Applied machine learning

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Unveil the unseen:  
uncover hidden information with machine learning

Dr Gareth Conduit

# Alchemite™ machine learning

Use case of machine learning to extract information from **noise**

Applications of **generic** Alchemite™ to **materials** design



# 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**

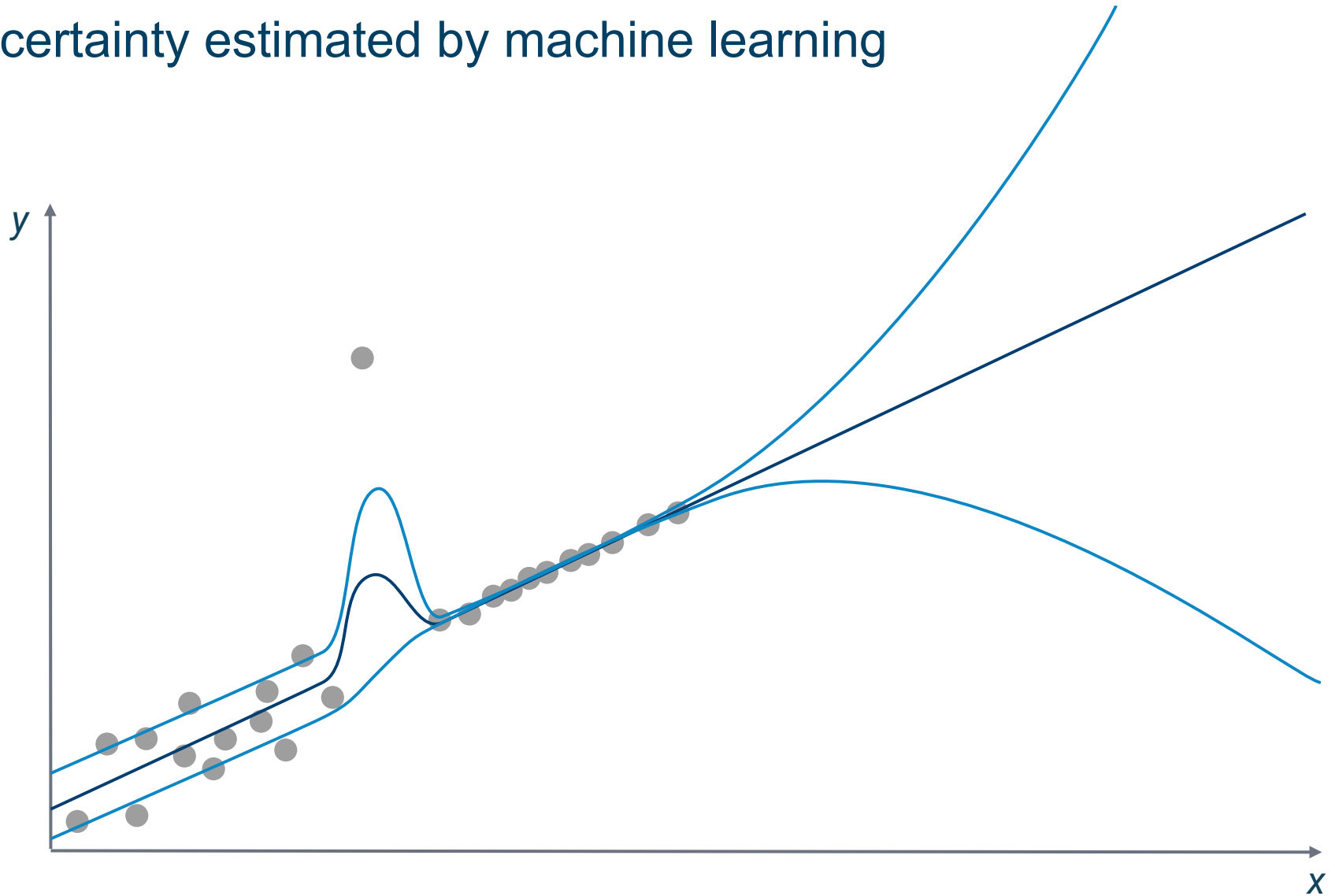
# Machine learning architecture that can exploit uncertainty



Bogdan Zviazhynski



# Uncertainty estimated by machine learning



# Improved uncertainty predictions

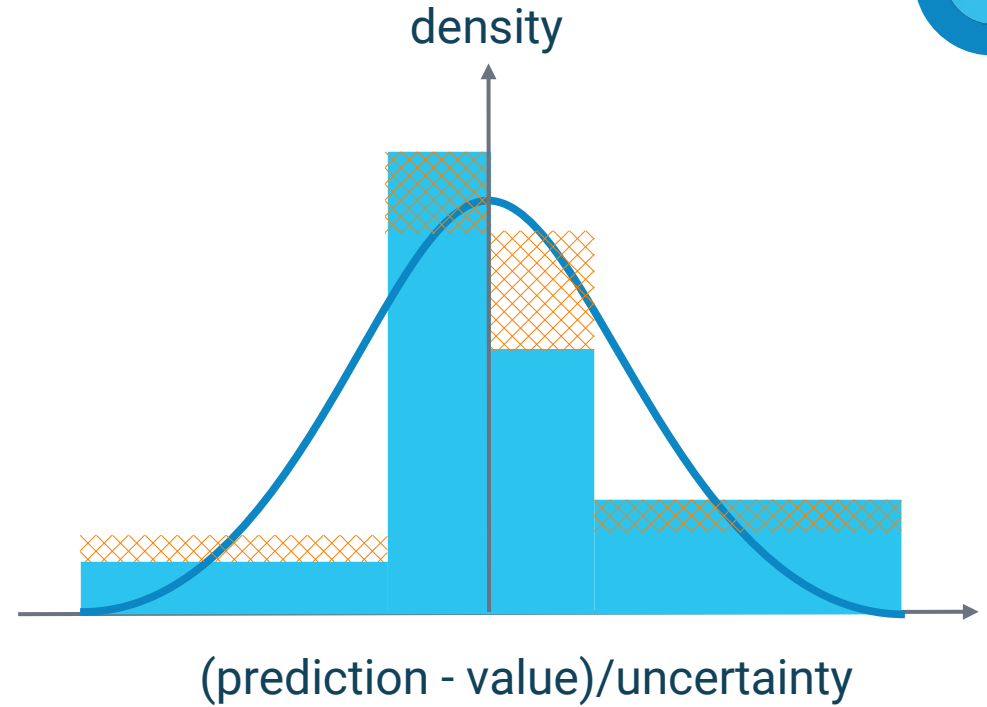


$$R^2 - \frac{2\sqrt{2}}{\sqrt{1-2/\pi}}(1-R^2)\Lambda$$

$R^2$  is coefficient of determination

$\Lambda$  is error in uncertainties

Focus on  $R^2$  for accurate models,  
emphasis on uncertainties when  
accuracy falls



# Exemplar information extracted from noise



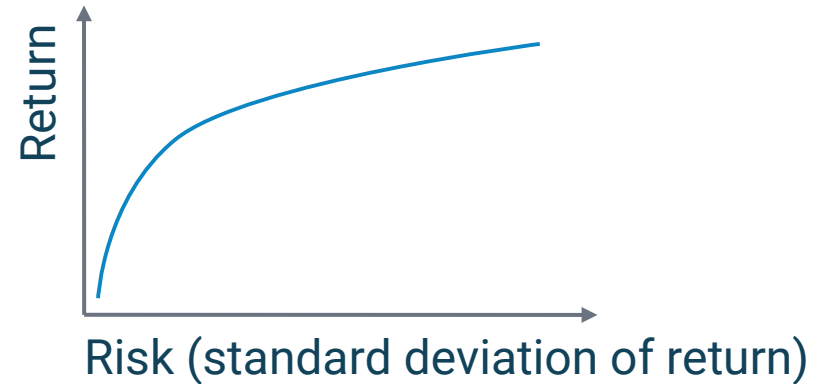
## Renormalization group theory

applied to phase transitions  
1982 Nobel Prize in Physics



## Markowitz model

1990 Nobel Memorial Prize



# Handling uncertainty

Design robust formulations

Outlier detection

Design of experiments

# Information from noise

*Unveil the unseen:  
exploit information hidden in noise*  
B. Zviashynski & GJC  
Applied Intelligence **53**, 11966 (2023)



# Exploit uncertainty to design concrete



Jess Forsdyke



Bogdan Zviazhynski



Professor Janet Lees



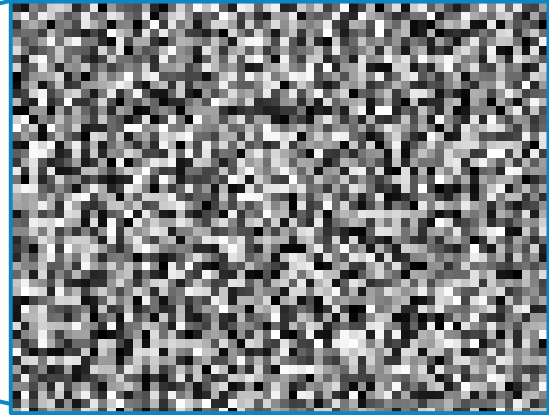
# Concrete in construction



# Cement & aggregate



# Cement & aggregate look like noise



# Mission



Design a concrete that is **robust** and **environmentally friendly**

# Mission



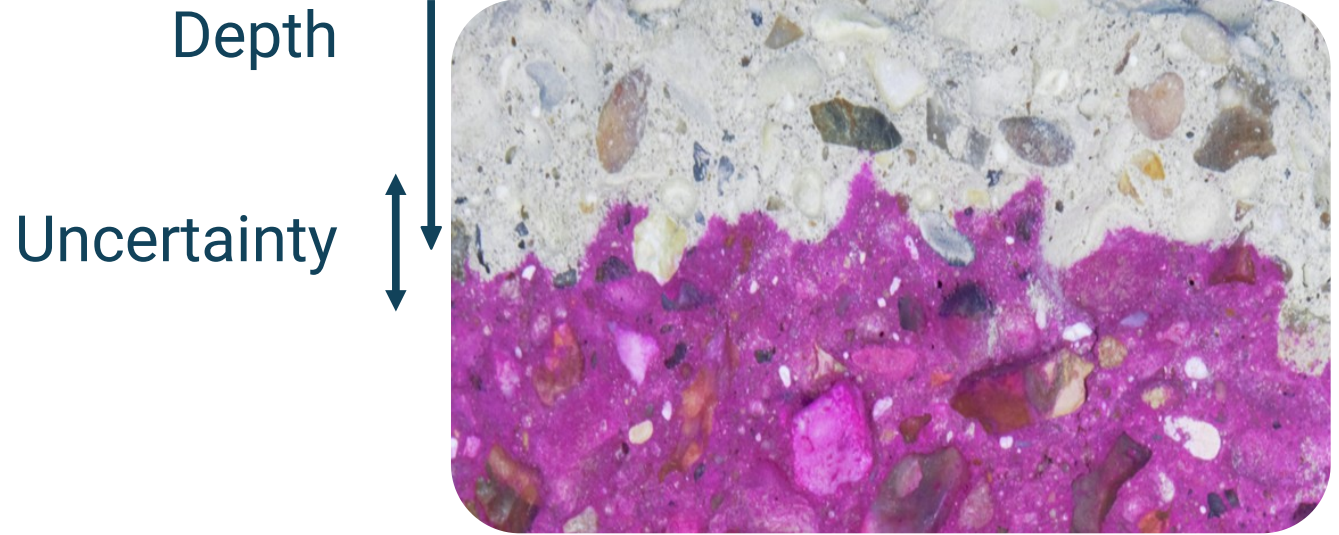
Design a concrete that is **robust** and **environmentally friendly**

**Experimentally validate** the concrete

# Carbonation is the probe of noise

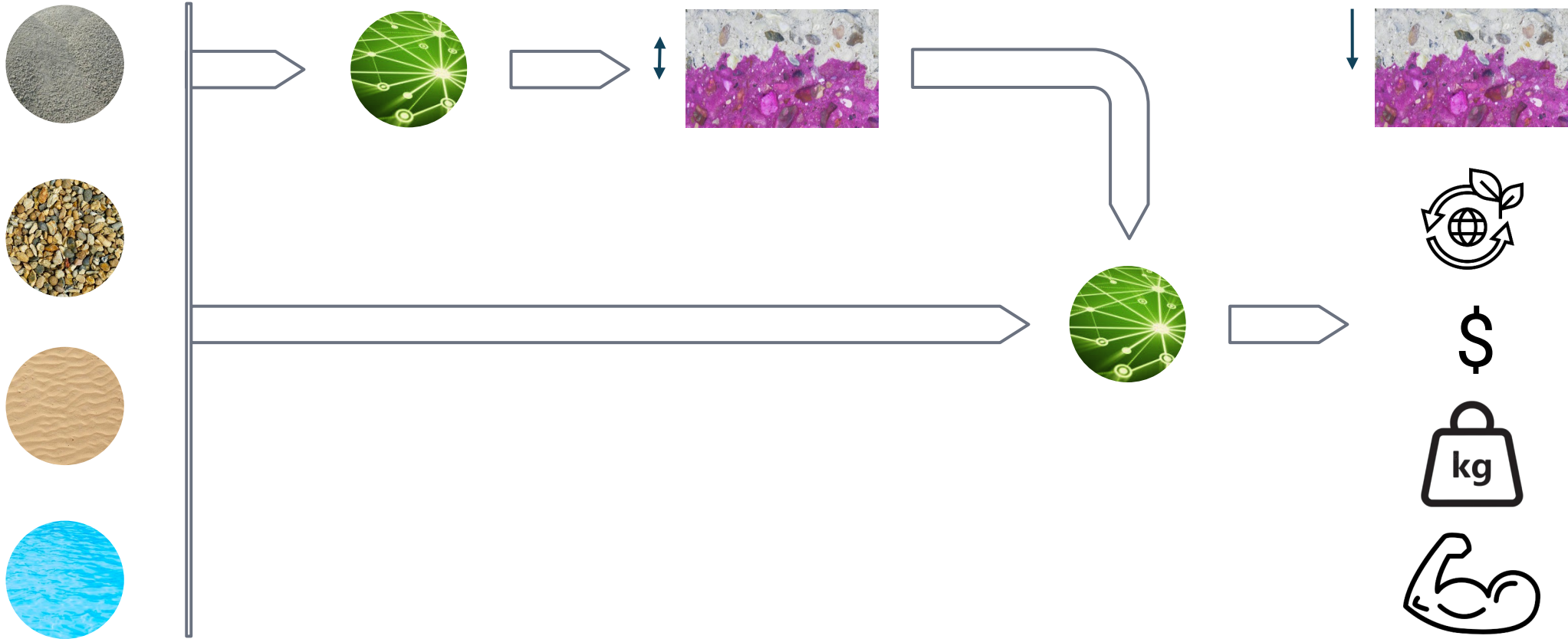


# Depth and uncertainty in carbonation

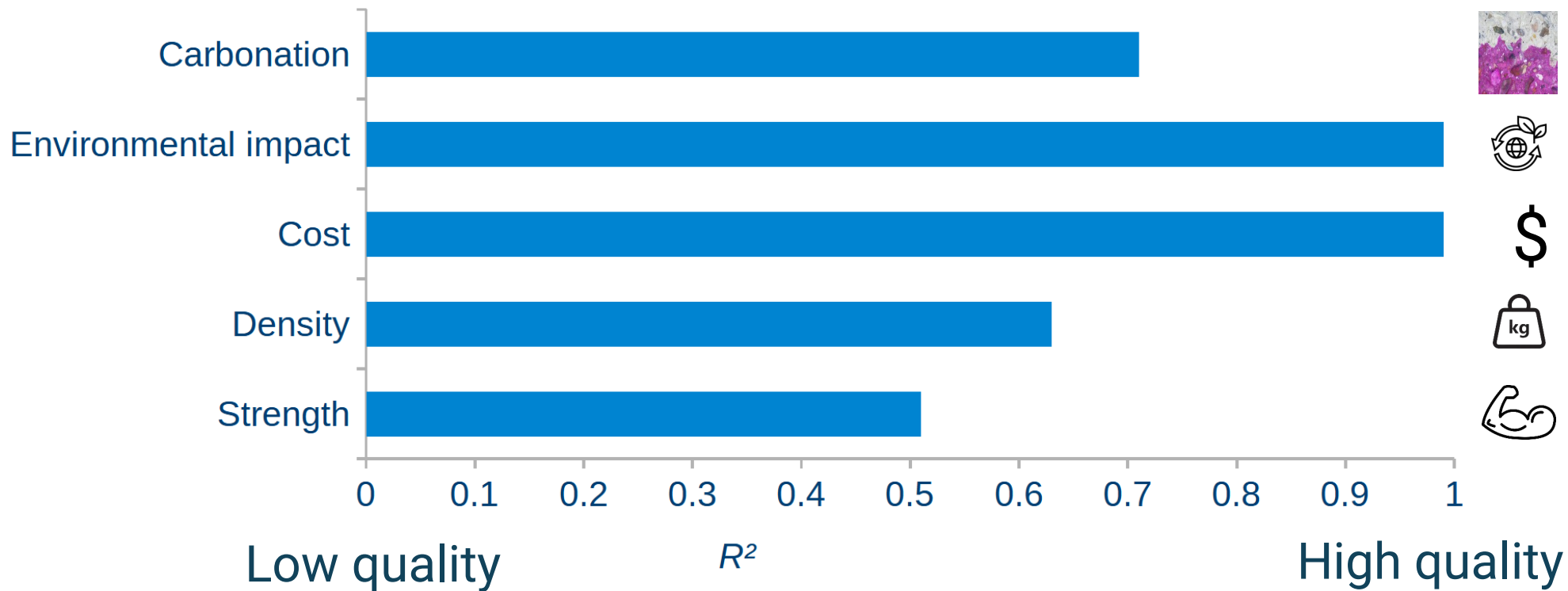




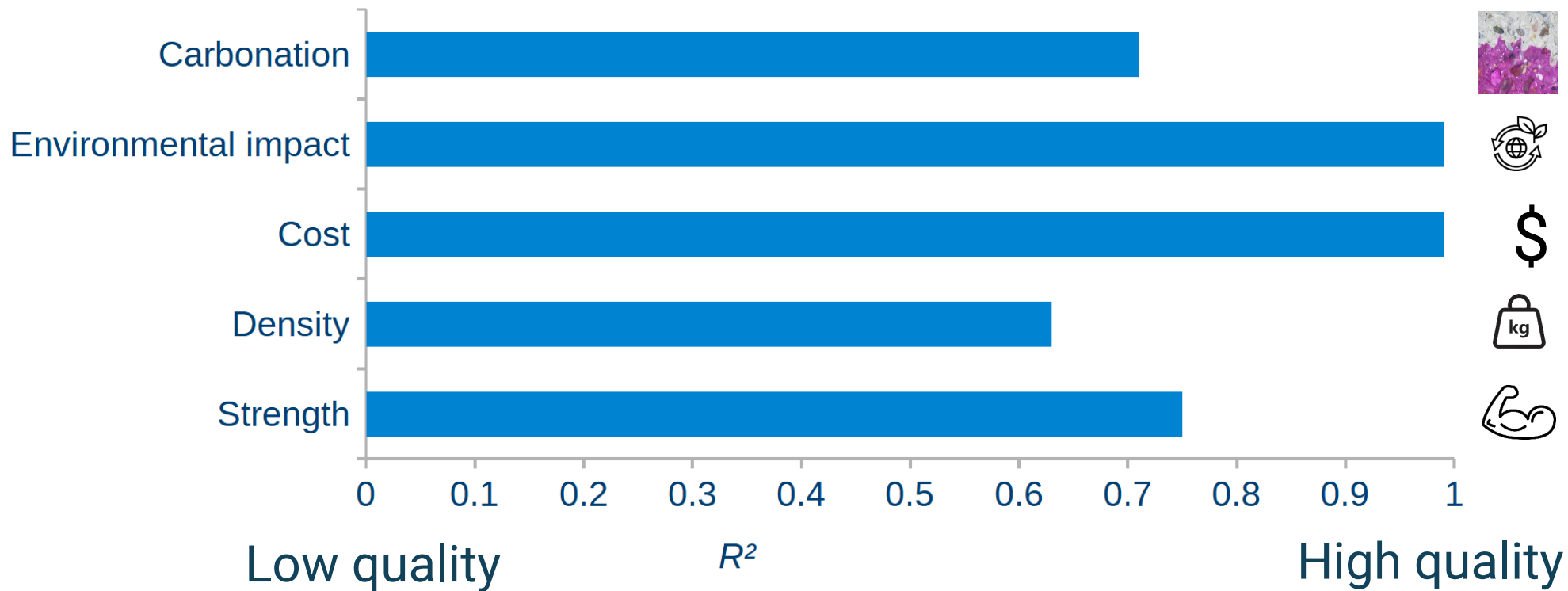
# Machine learning exploits uncertainty



# Original model accuracy



# Uncertainty improves the model accuracy



# Concrete specification



## First mix

↓ carbonation

✓ environmental impact

✓ cost

✓ density

✓ strength



## Second mix

✓ carbonation

↓ environmental impact

✓ cost

✓ density

✓ strength

# Phase behavior targets



## First mix

14.2% cement



48.9% gravel



28.4% sand



8.5% water



## Second mix

10.5% cement

48.4% gravel

32.6% sand

8.5% water

# Concrete manufacture

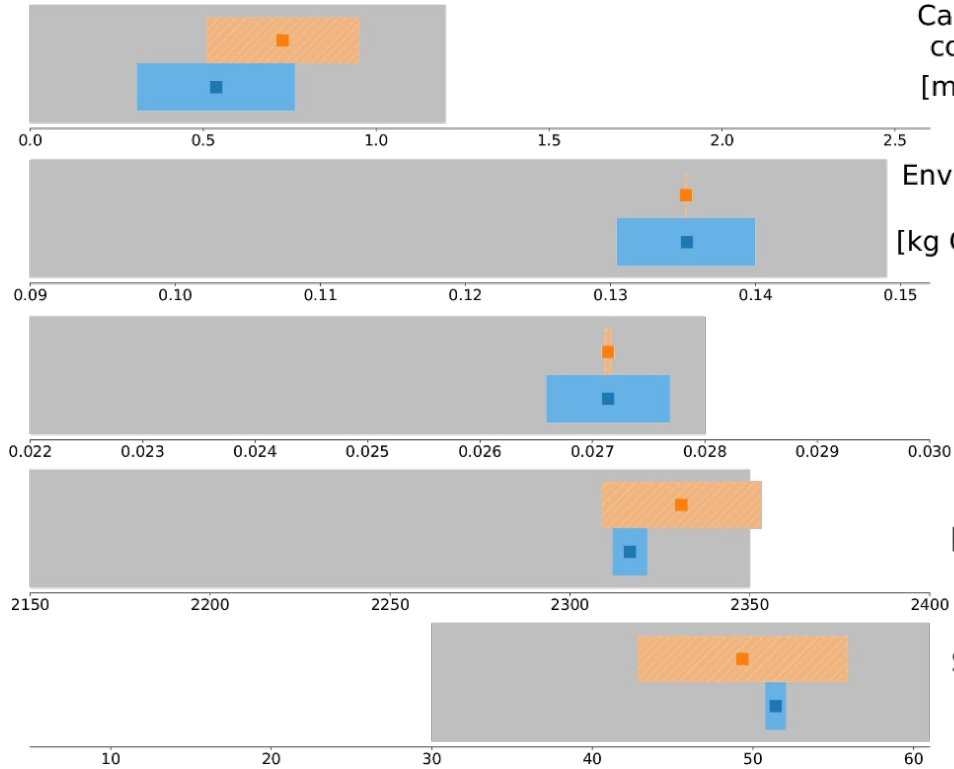


*Probabilistic selection and design of concrete using machine learning*  
Data-Centric Engineering 4, e9 (2023)

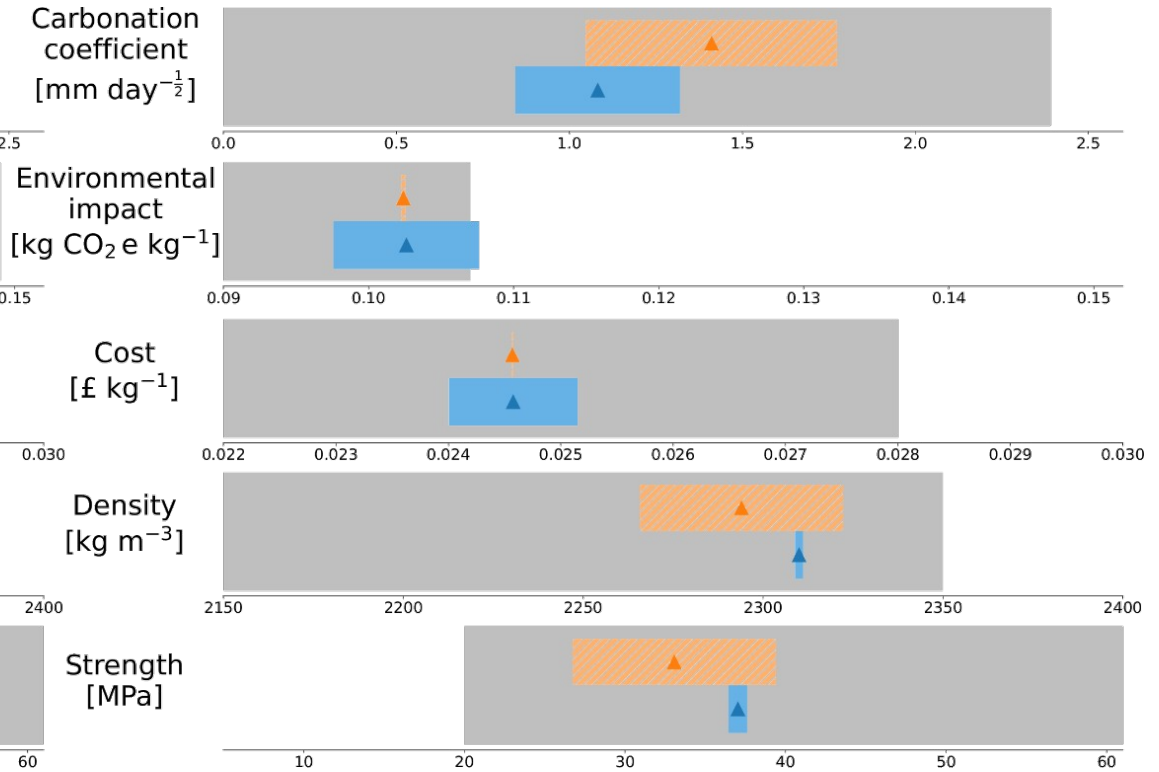
# Experimental validation of the proposed mixes



## First mix



## Second mix



Experiment

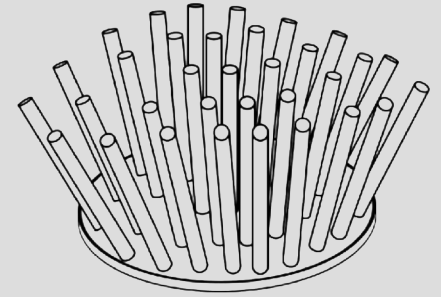
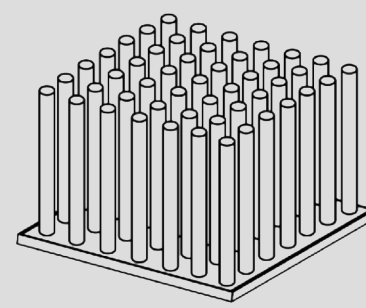
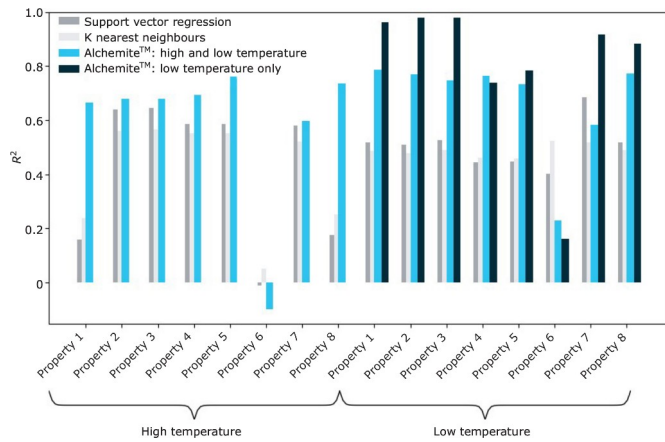
Model

Target

# Real-life use of Alchemite™



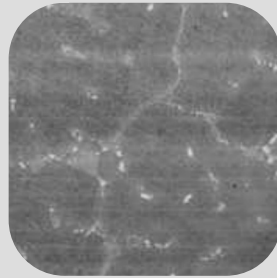
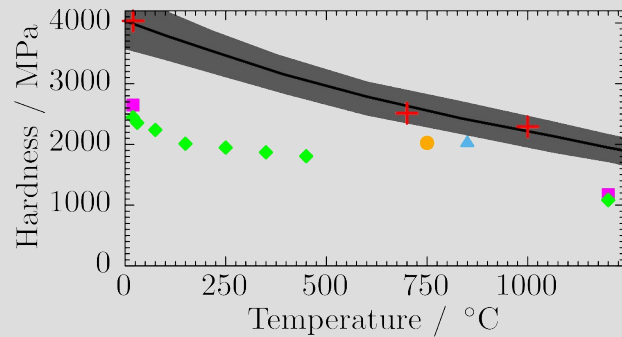




## Johnson Matthey Technology Review 66, 130 (2022)



## NASA Technical Memorandum 20220008637



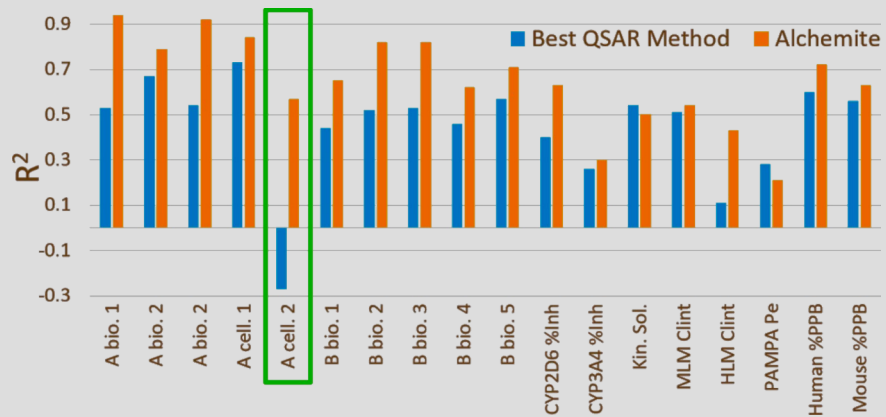
Alloy	Source	ANN	$\Delta\sigma$	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	$\geq 550$ [23]

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



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

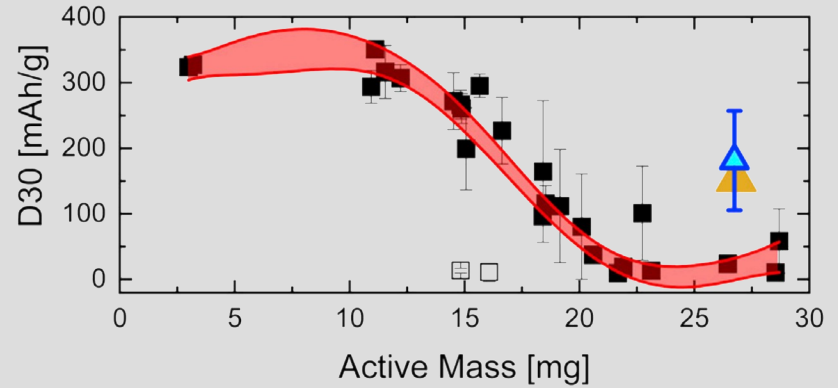
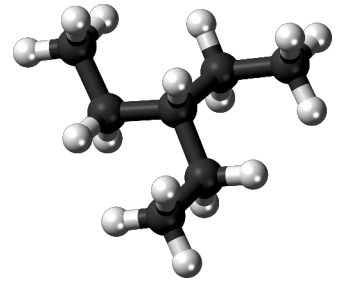




J. of Chem. Info. & Model. **60**, 2848 (2020)  
 Applied AI Letters **2**, e31 (2021)  
 Molecular Pharmaceutics **19**, 1488 (2022)



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)

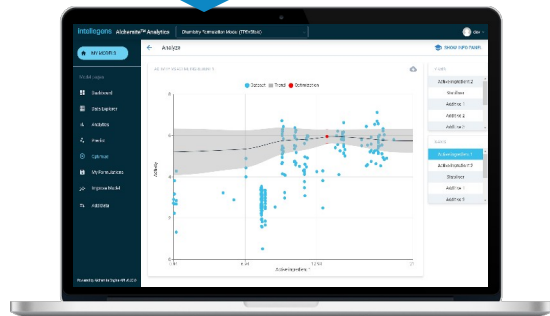


# Intellegens offers the Alchemite™ product family



**Scientists & engineers**

Fast start, easy-to-use, visual



←  
*Option to  
deploy models*

## Alchemite™ Analytics

Deep data insights on your desktop  
Guide experiments, predict, design, optimize

**Data scientists**

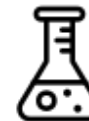
Add to your ML toolkit



## Alchemite™ Engine

Integrate into your workflow (API, Python)  
Advanced configuration, enterprise deployment

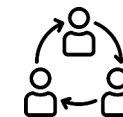
*Optional  
connectors*



*Lab systems*



*Software &  
scripts*



*Sharing &  
collaboration*

**Alchemite™  
Success**

Apply Intellegens deep learning expertise  
Advice to your data science team or full project management

Alchemite™ enables machine learning **beyond data**

Extract information from **noise** to design **concrete**

**Generic** approach applied to many physical, chemical, and biological sciences

Webinar  
Book

*Design of Experiments made easy with machine learning*, 8 May  
The Digital Transformation of Product Formulation,  
Concepts, Challenges, and Applications for Accelerated Innovation

