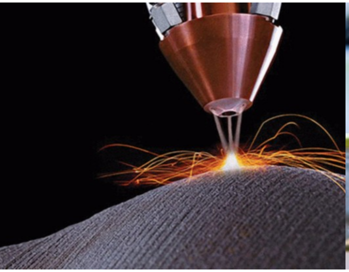
intellegens

Applied machine learning

Unveil the unseen: uncover hidden information with machine learning

Dr Gareth Conduit

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

Exploit property-property correlations to overcome sparse data for probabalistic design of concrete

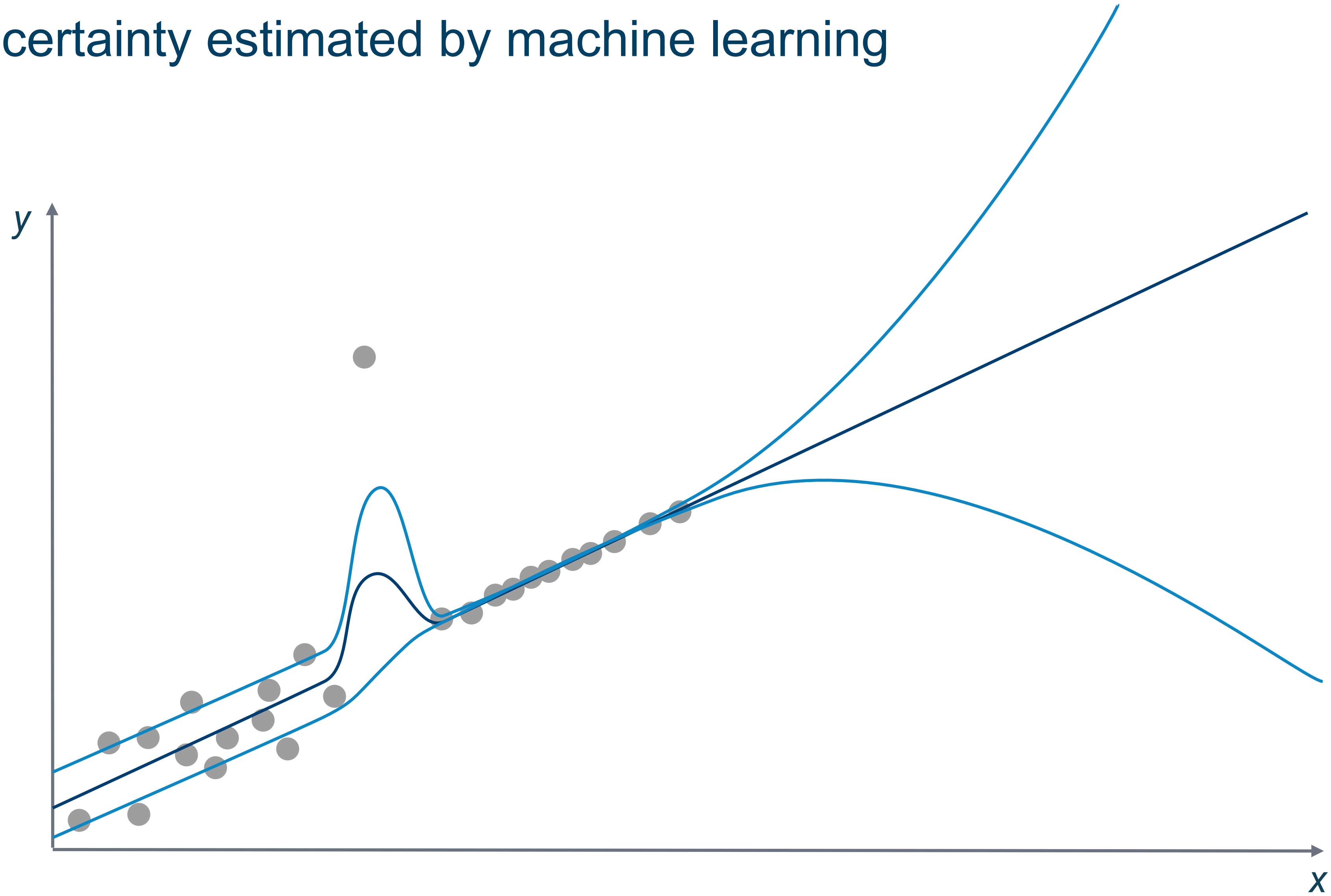
Use case of machine learning to extract information from noise to design concrete

Applications of generic Alchemite™ to materials design

Machine learning architecture that understands uncertainty

Bogdan Zviazhynski

Uncertainty estimated by machine learning



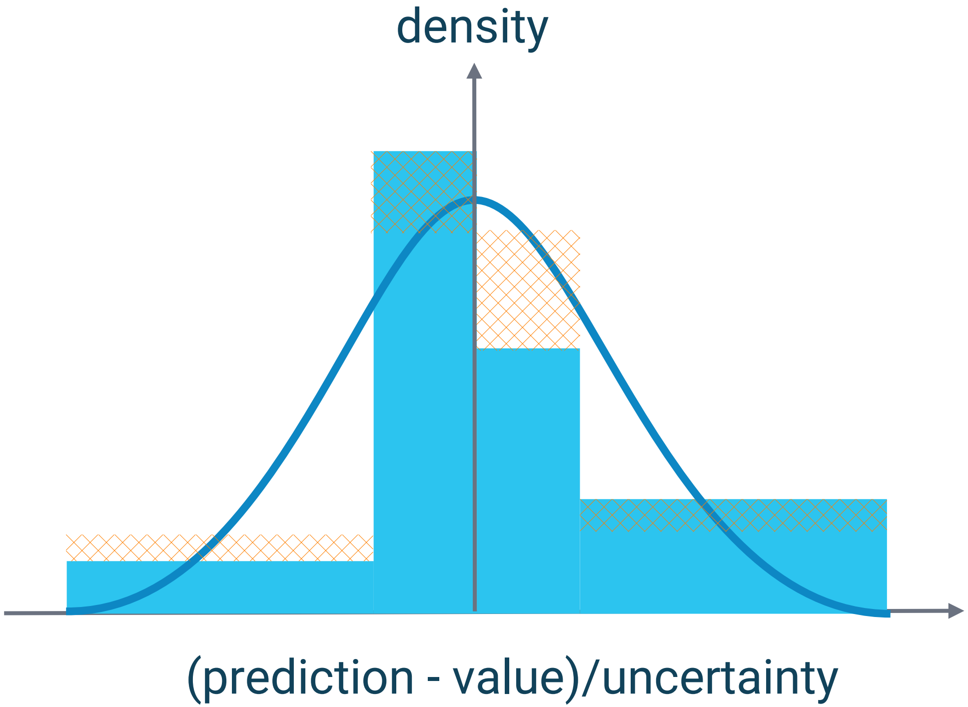
Improved uncertainty predictions

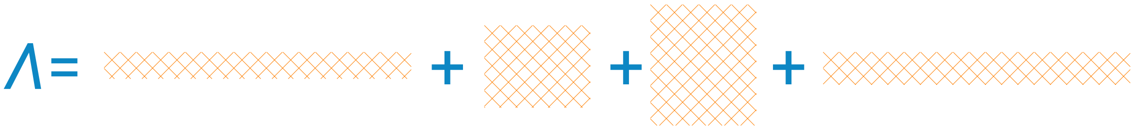
$$R^2 - \frac{2\sqrt{2}}{\sqrt{1-2/\pi}}\left(1-R^2\right)\Lambda$$

R^2 is coefficient of determination

Λ is error in uncertainties

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





Exemplar information extracted from noise

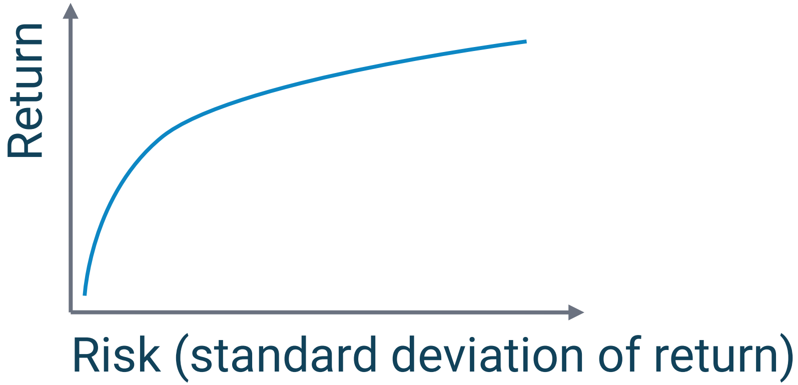
Renormalization group theory

applied to phase transitions

1982 Nobel Prize in Physics

Markowitz model

1990 Nobel Memorial Prize



Handling uncertainty

Discover property-property correlations

Design robust formulations

Outlier detection

Design of experiments

Information from noise

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

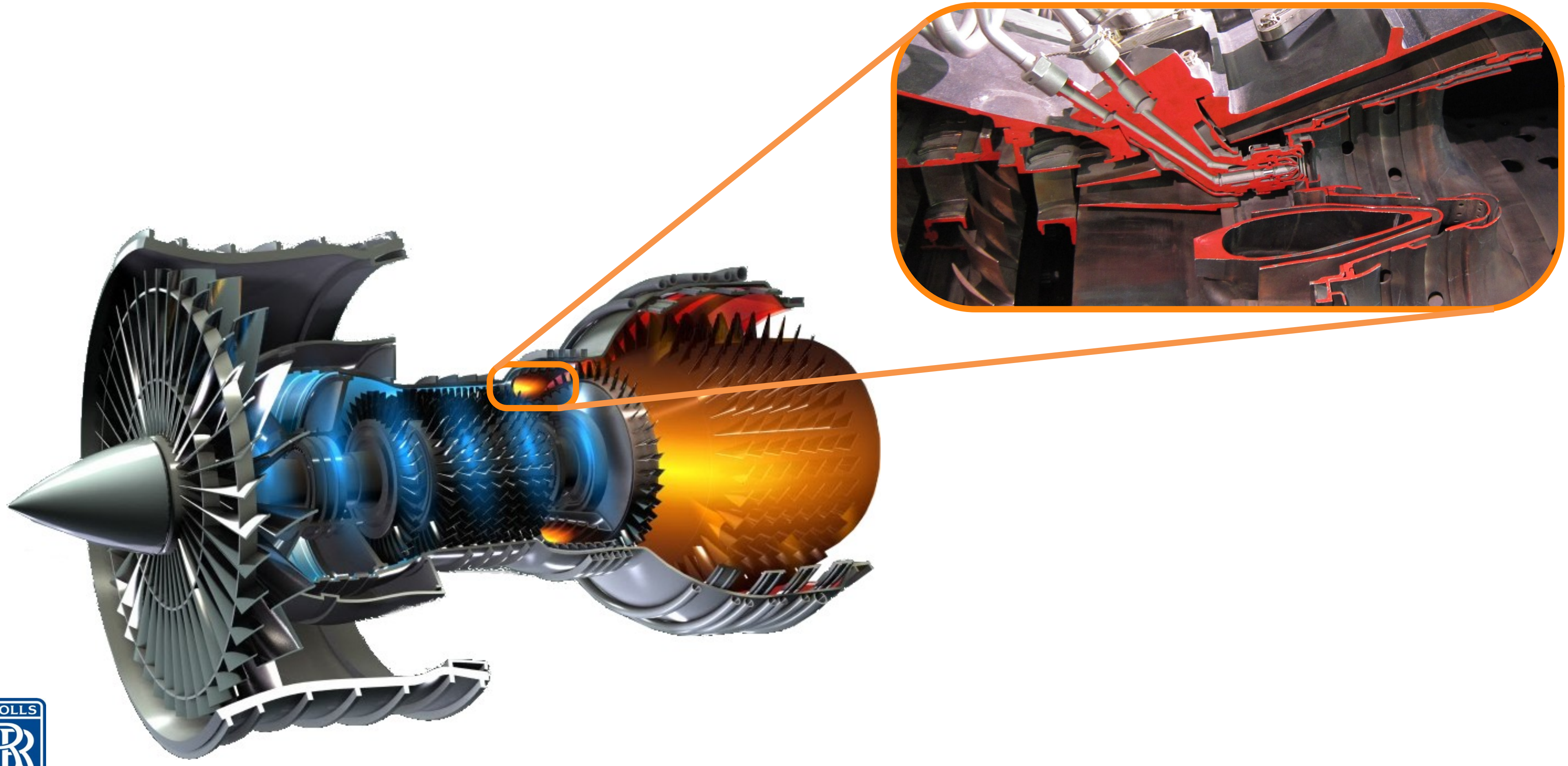
Nickel superalloys with Rolls Royce

Vadegadde Duggappa

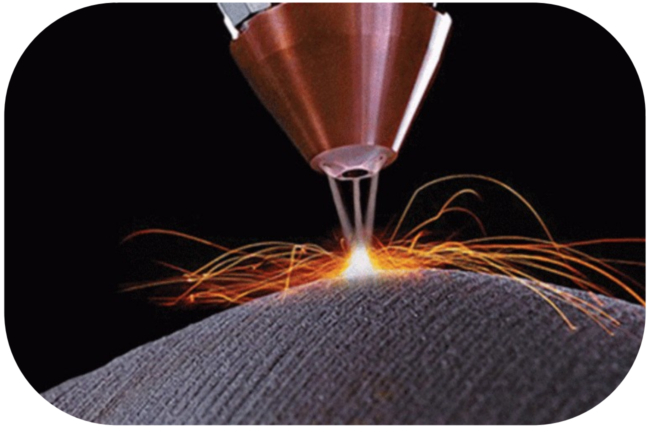
Bryce Conduit

Professor Howard Stone

Combustor in a jet engine

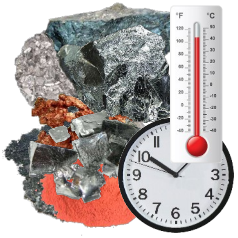


Defects form during printing



Laser

Data available to model defect density

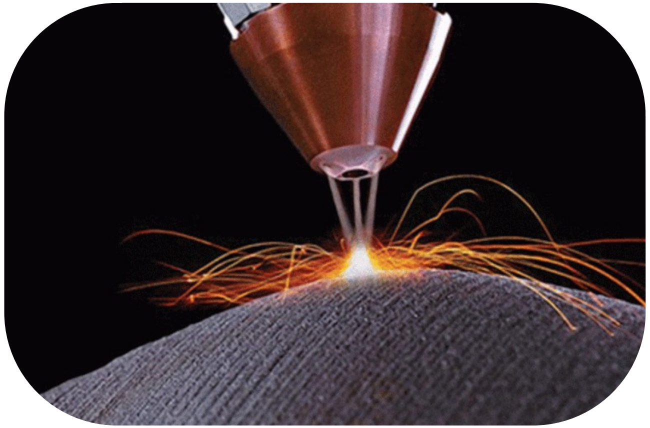


Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

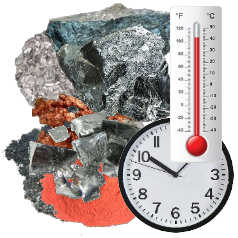
Ability for printing and welding are strongly correlated



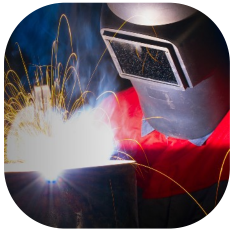
Laser

Electricity

First predict weldability

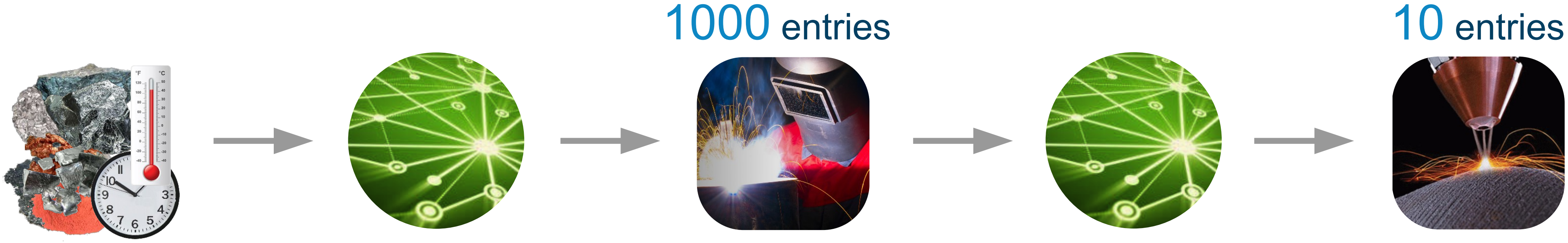


1000 entries



Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed



Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation

Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Defects	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Probability of fulfiling each target

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
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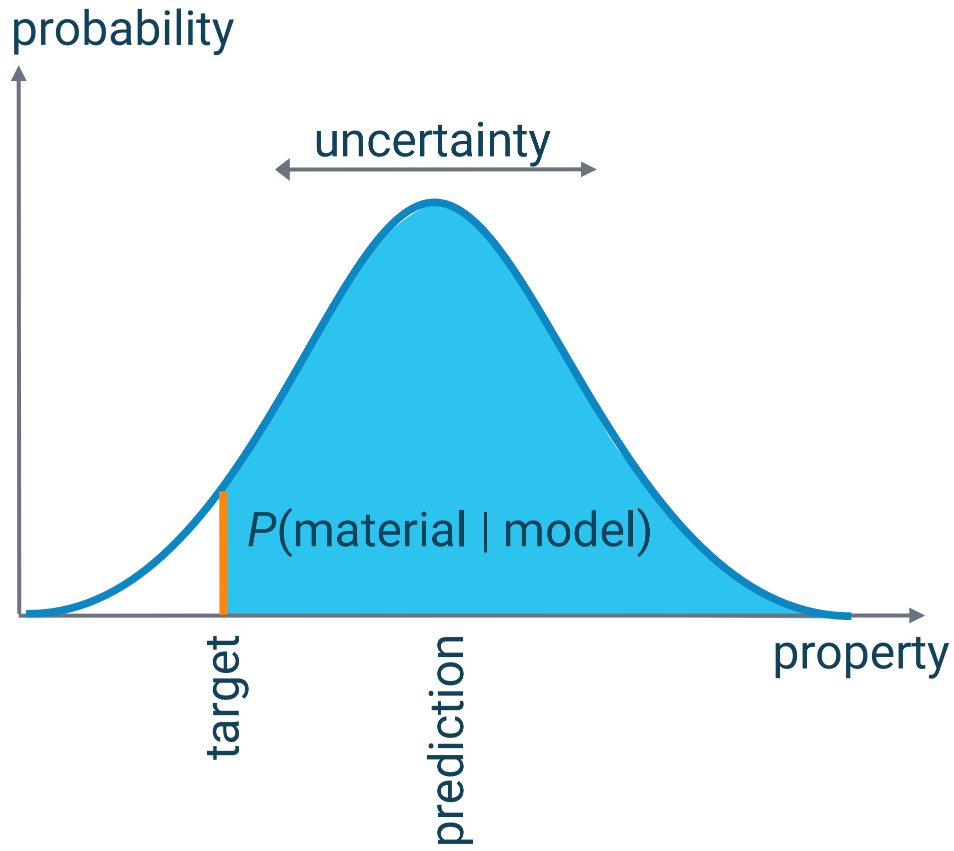
$P(\text{material} \mid \text{model})P(\text{model})$



Composition and processing variables

Cr 19%

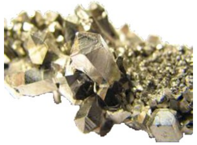
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



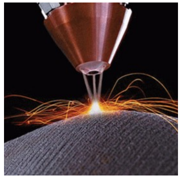
Al 2.9%

C 0.04%

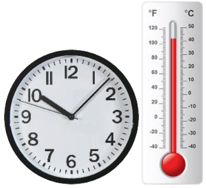
B 0.01%

Ni

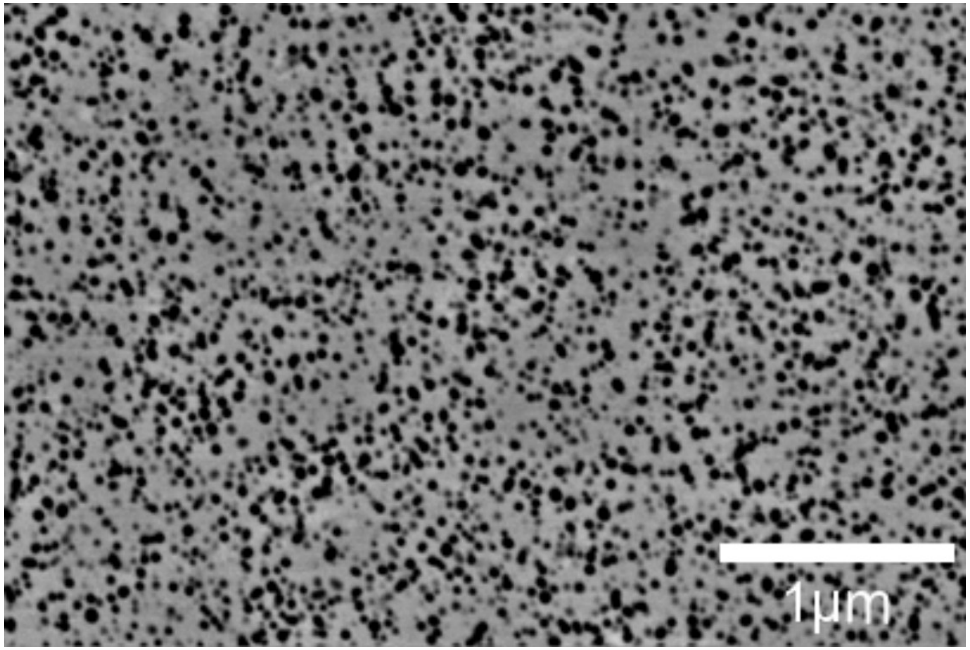
Expose 0.8



T_{HT} 1300ºC

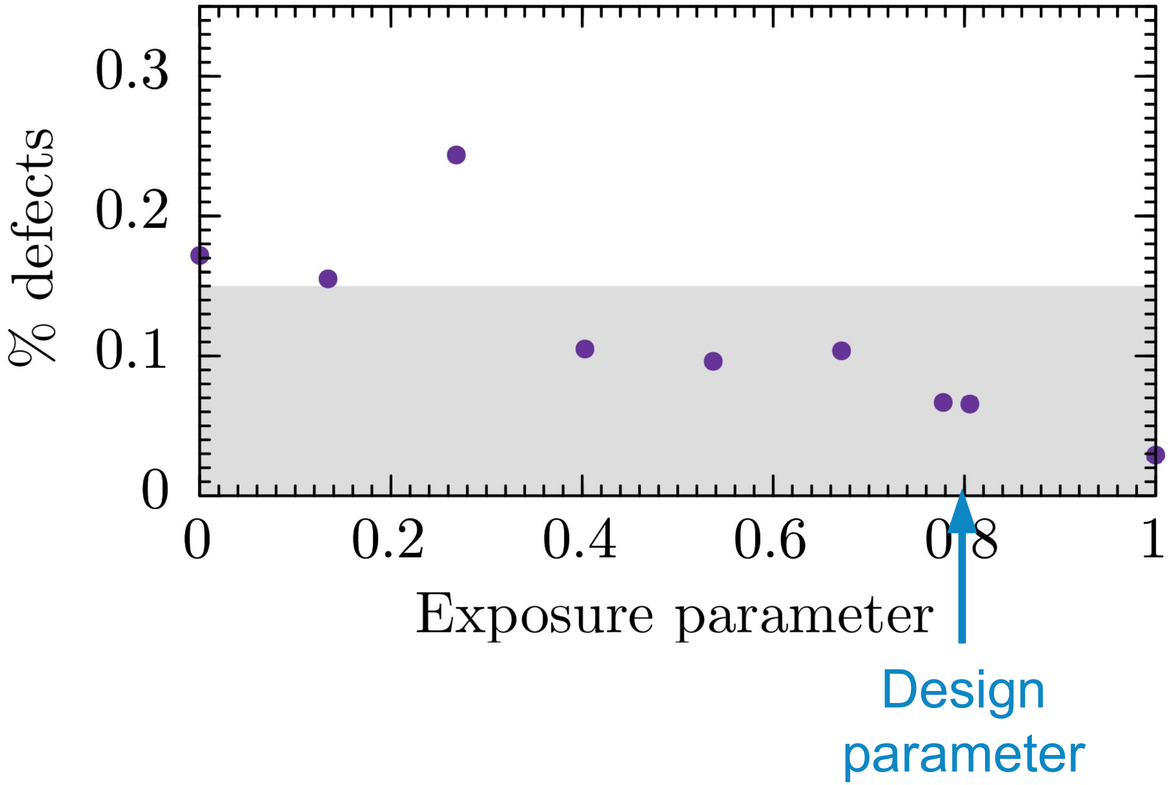


Microstructure



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

Test the defect density



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

Exploit uncertainty to design concrete

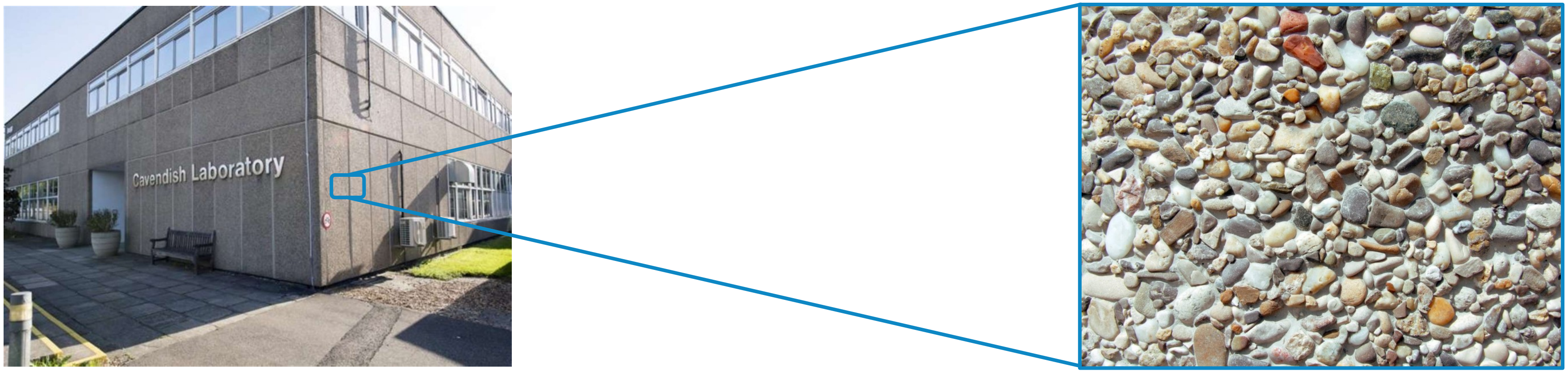
Jess Forsdyke

Bogdan Zviazhynski

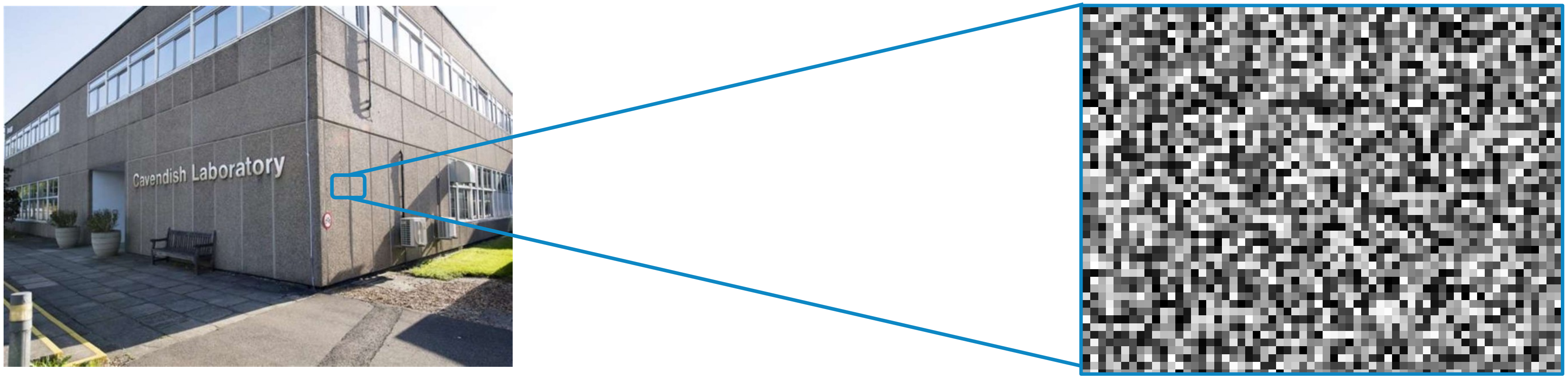
Professor Janet Lees

Concrete in construction

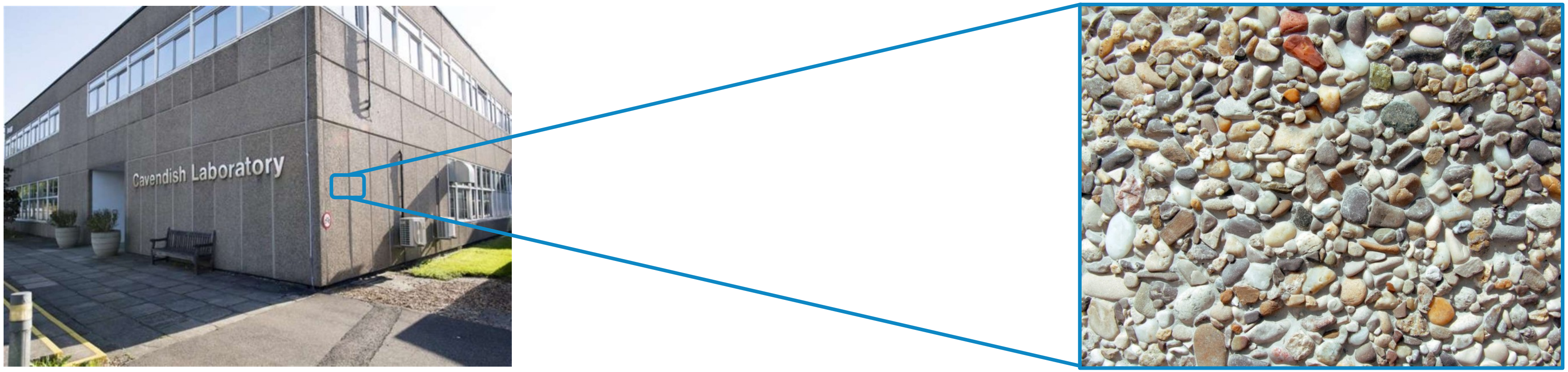
Cement & aggregate



Cement & aggregate look like noise

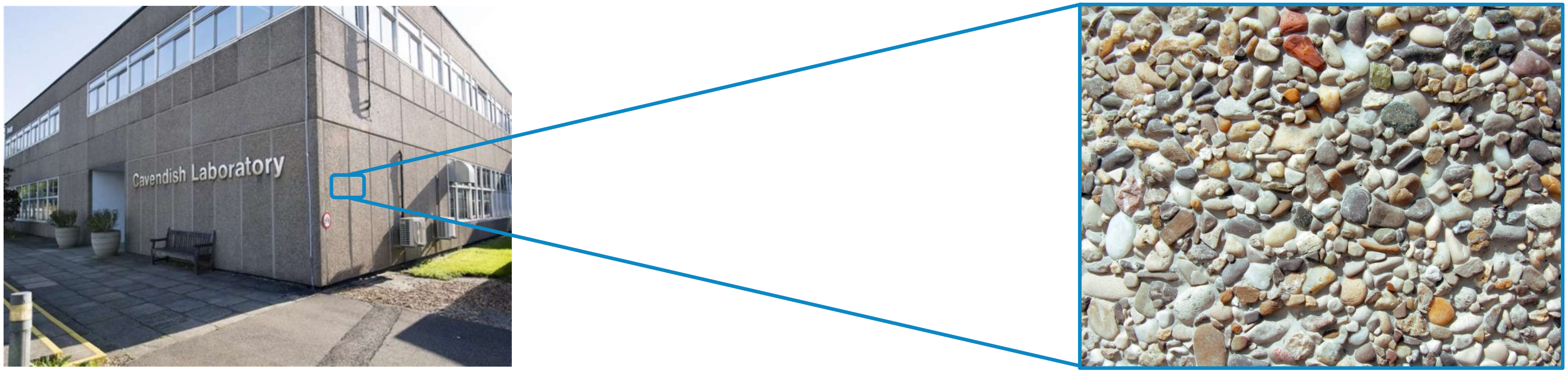


Mission



Design a concrete that is robust and environmentally friendly

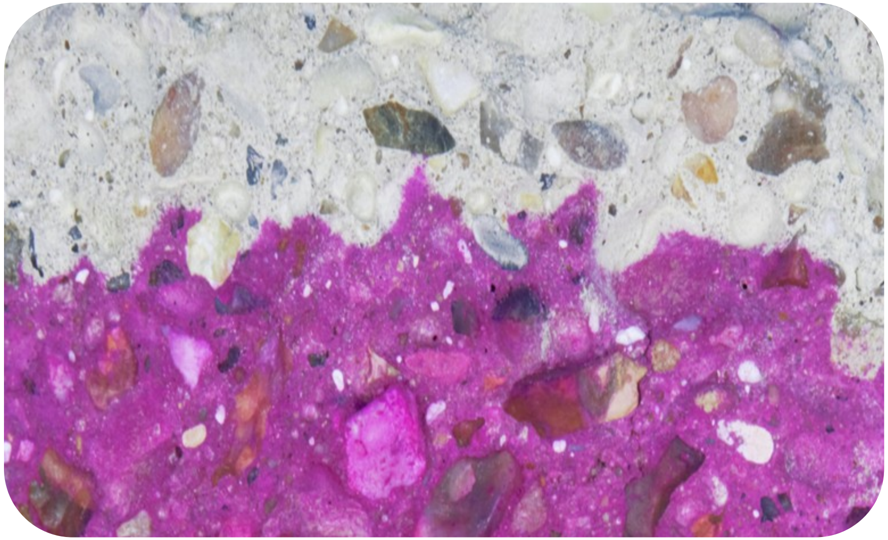
Mission



Design a concrete that is robust and environmentally friendly

Experimentally validate the concrete

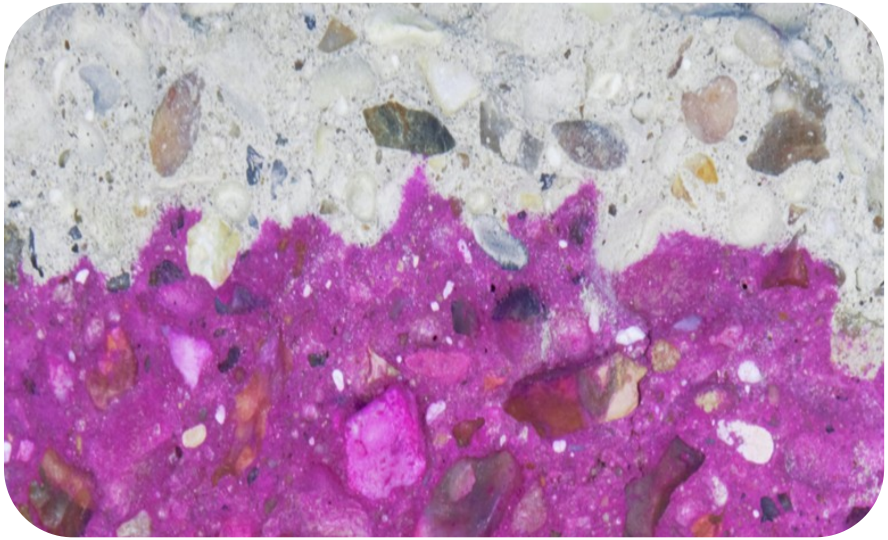
Carbonation is the probe of noise



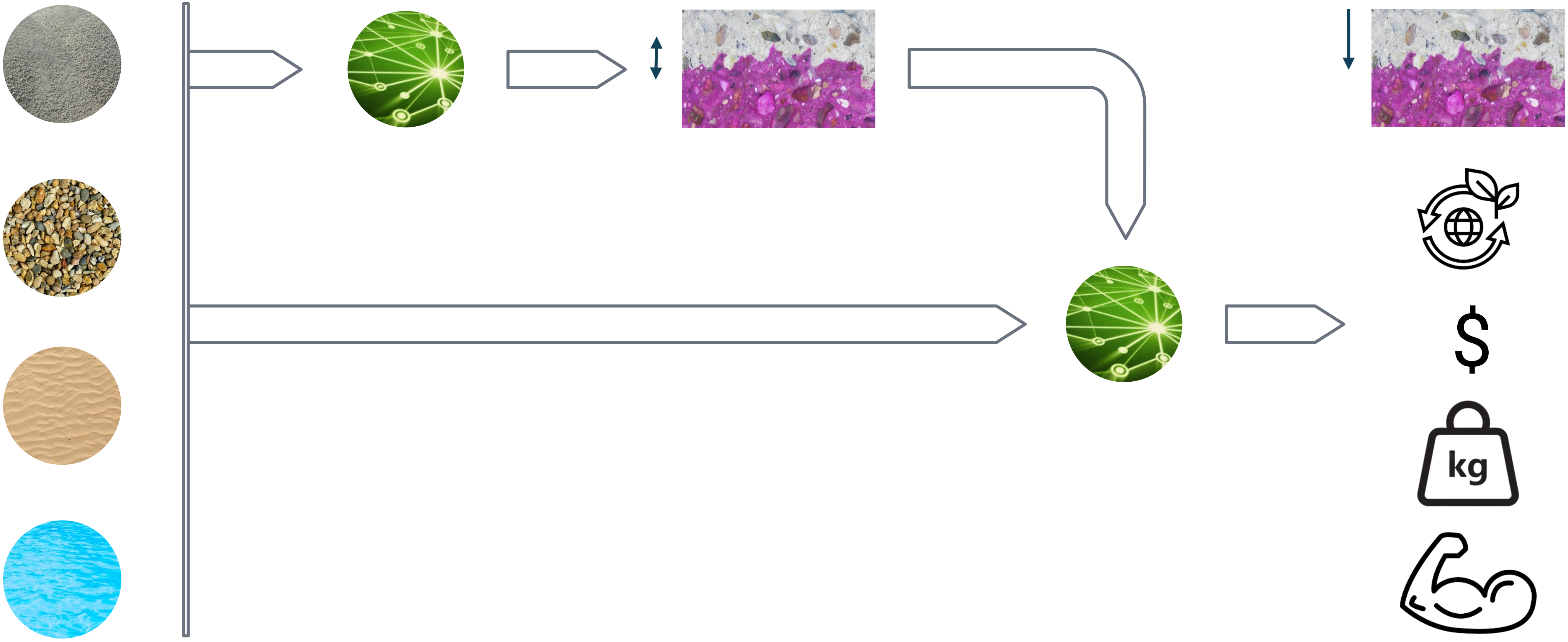
Depth and uncertainty in carbonation

Depth

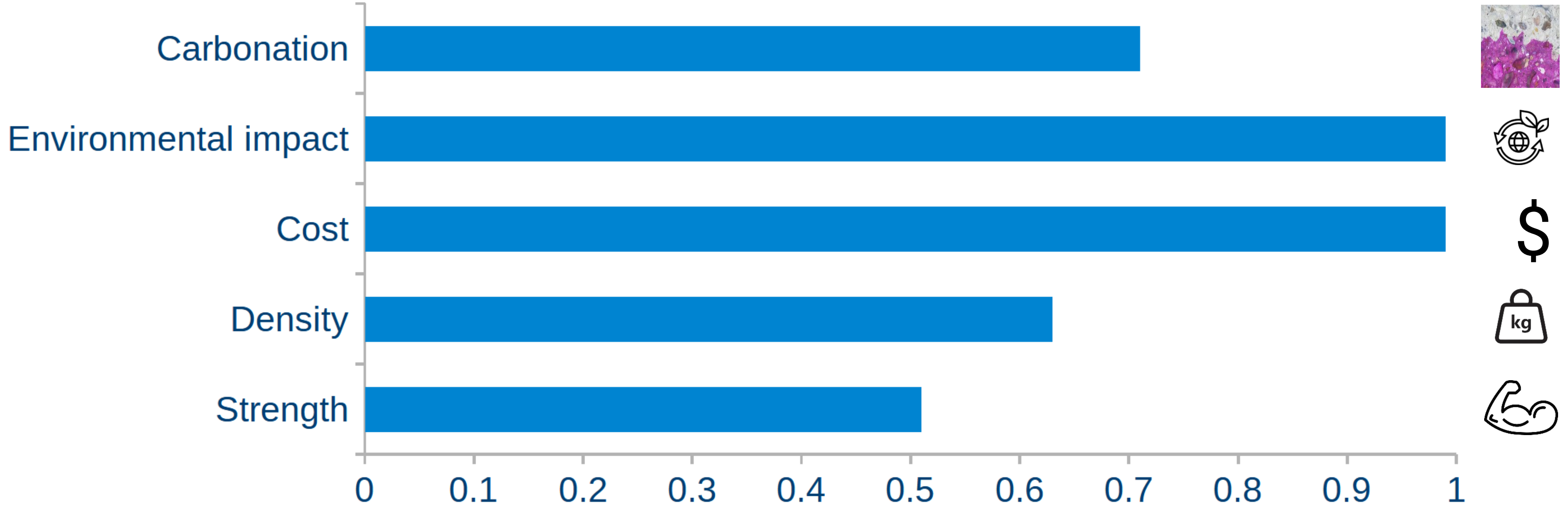
Uncertainty



Machine learning exploits uncertainty



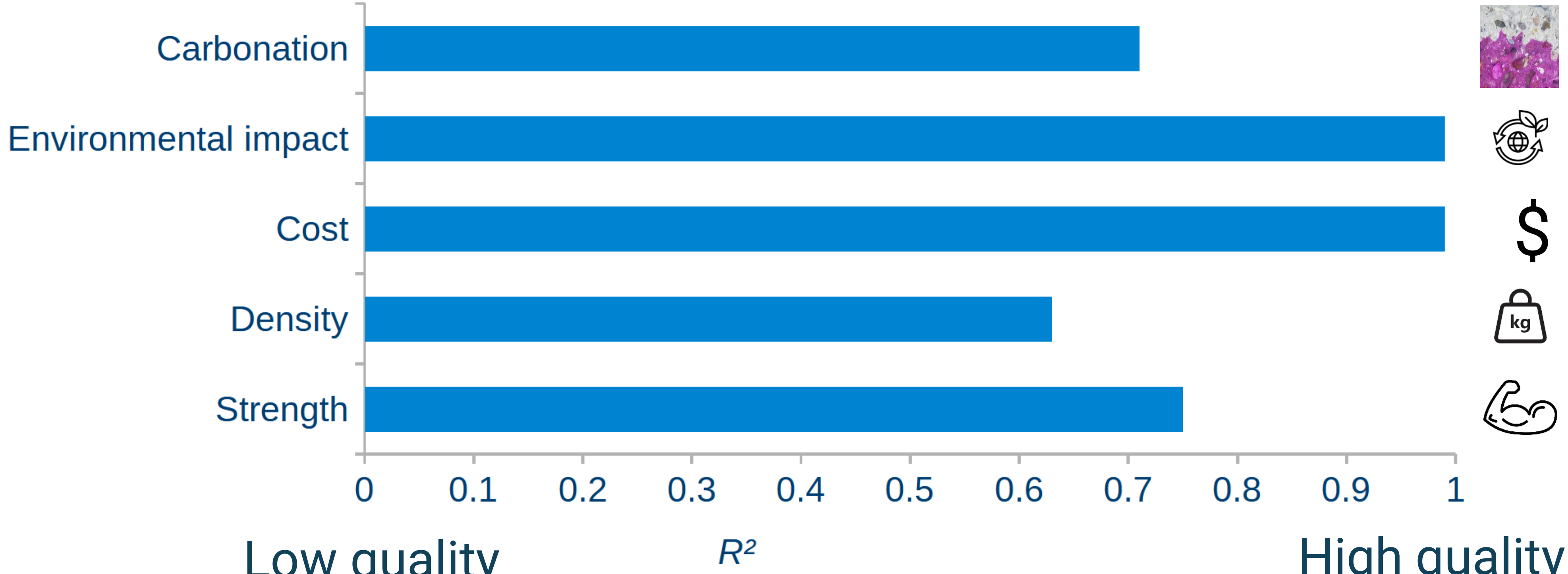
Original model accuracy



Low quality

High quality

Uncertainty improves the model accuracy



Low quality

High quality

Concrete specification

First mix		Second mix
⬇ carbonation		✔ carbonation
✔ environmental impact		⬇ environmental impact
✔ cost	$	✔ cost
✔ density		✔ density
✔ strength		✔ strength

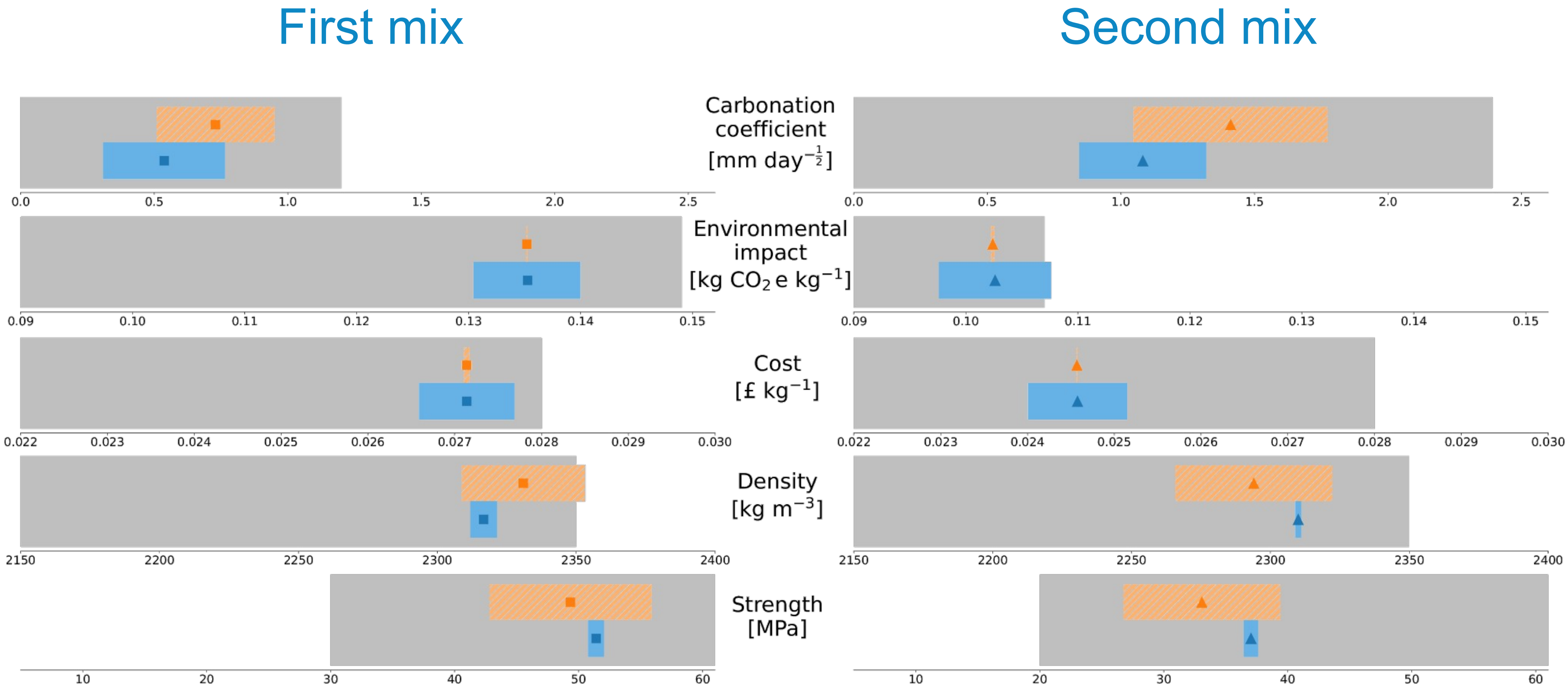
Phase behavior targets

First mix		Second mix
14.2% cement		10.5% cement
48.9% gravel		48.4% gravel
28.4% sand		32.6% sand
8.5% water		8.5% water

Concrete manufacture

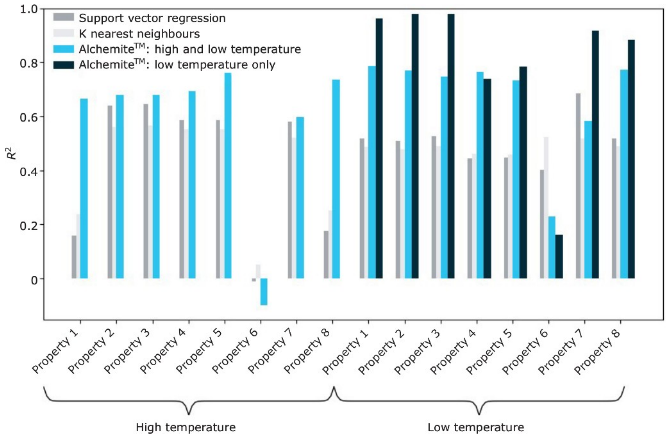
Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

Experimental validation of the proposed mixes

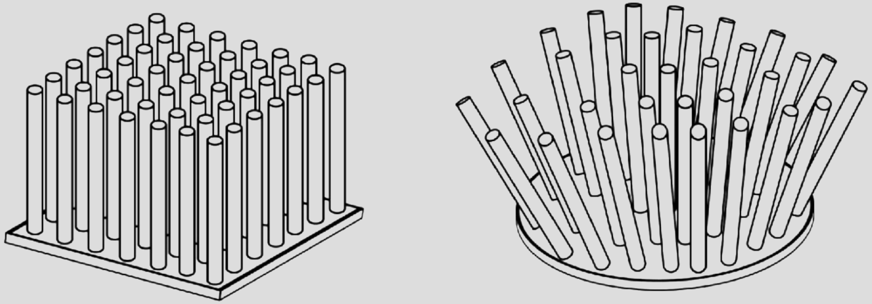


Experiment Model Target

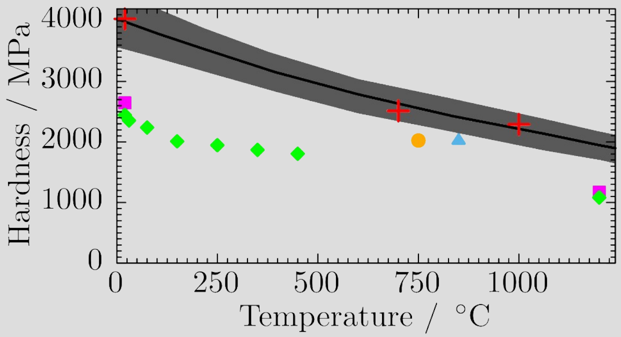
Real-life use of Alchemite™



Johnson Matthey Technology Review
66, 130 (2022)



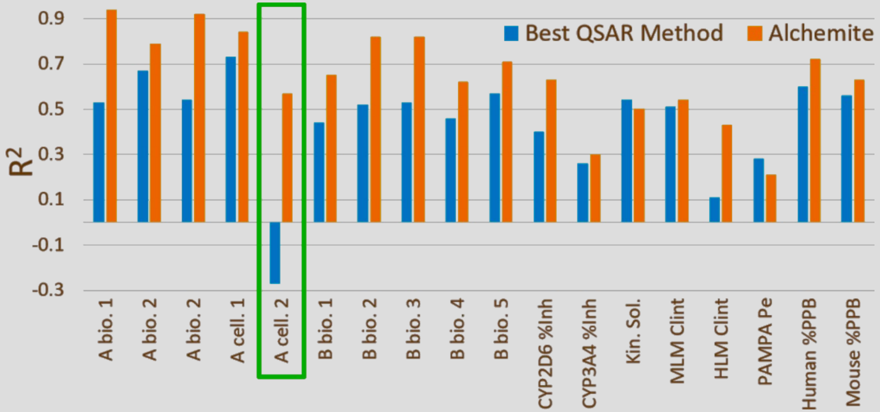
NASA Technical Memorandum
20220008637



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	≥550[23]

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

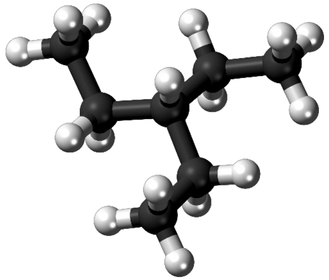


J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

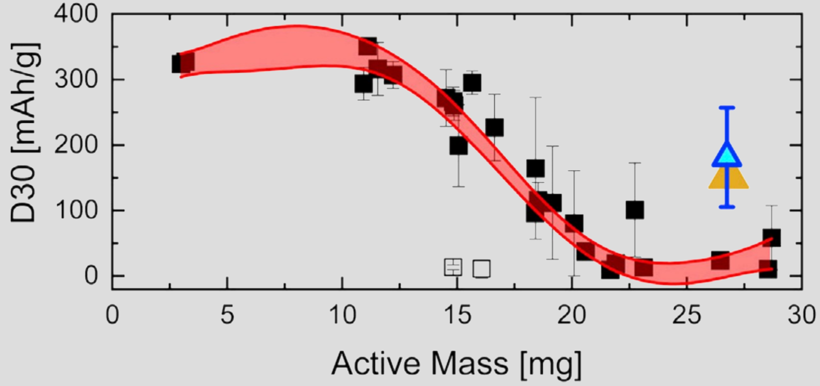
optibrium
iff

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



bp

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

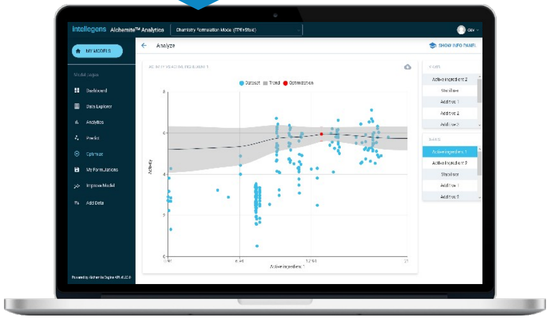


UNIVERSITY OF BIRMINGHAM
Ansys GRANTA

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

Data scientists
Add to your ML toolkit

Optional connectors

Lab systems

Software & scripts

Sharing & collaboration

Alchemite™ Analytics

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

Alchemite™ Engine

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

Academia

Alchemite™ academic licenses available for non-comercial research

Alchemite™ enables machine learning beyond data

Exploit property-property correlations to design alloy for 3D printing

Extract information from noise to design concrete

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

Webinar *Design of Experiments made easy with machine learning*, 8 May

OPTIMADE, API to access leading electronic structure databases